Weierstraß–Institut
für Angewandte Analysis und Stochastik

im Forschungsverbund Berlin e.V.

Preprint ISSN 0946 – 8633

Existence of bounded steady state solutions to spin-polarized drift-diffusion systems

Annegret Glitzky, Klaus Gärtner

submitted: 2nd September 2008

Weierstrass Institute for
Applied Analysis and Stochastics
Mohrenstraße 39
D – 10117 Berlin, Germany
E-Mail: glitzky@wias-berlin.de
gaertner@wias-berlin.de

Preprint No. 1357

Berlin 2008

2000 *Mathematics Subject Classification.* 35J55, 65N12, 35B45, 35R05.

Key words and phrases. Reaction–diffusion systems, spin-polarized drift–diffusion processes, motion of charged particles, steady states, existence, a priori estimates, uniqueness, Scharfetter-Gummel scheme, boundary conforming Delaunay grid.

Edited by
Weierstraß–Institut für Angewandte Analysis und Stochastik (WIAS)
Mohrenstraße 39
D — 10117 Berlin
Germany

Fax: + 49 30 2044975
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We study a stationary spin-polarized drift-diffusion model for semiconductor spintronic devices. This coupled system of continuity equations and a Poisson equation with mixed boundary conditions in all equations has to be considered in heterostructures. In 3D we prove the existence and boundedness of steady states. If the Dirichlet conditions are compatible or nearly compatible with thermodynamic equilibrium the solution is unique. The same properties are obtained for a space discretized version of the problem: Using a Scharfetter-Gummel scheme on 3D boundary conforming Delaunay grids we show existence, boundedness and, for small applied voltages, the uniqueness of the discrete solution.

1 Introduction and model equations

Spin-polarized drift-diffusion models as proposed in [20, 21, 22, 23] are a generalization of the classical van Roosbroeck equations [16, 17]. Spin-resolved densities are introduced for electrons $n_\uparrow$ and $n_\downarrow$ and holes $p_\uparrow$ and $p_\downarrow$. For electrons as well as for holes there occurs spin relaxation, moreover a spin dependent generation/recombination of electrons and holes has to be taken into account. Such spin-polarized drift-diffusion model consist of four continuity equations for $n_\uparrow$, $n_\downarrow$, $p_\uparrow$ and $p_\downarrow$ which are coupled with a Poisson equation for the electrostatic potential.

In the following, we label the spin-resolved quantities (densities, current densities, quasi Fermi energies, band-edges) by $\uparrow$ for spin-up and $\downarrow$ for spin-down along a chosen quantization axis for the spin angular momentum.

We use a scaling such that potentials and energies are considered in units of k_BT/q and k_BT, respectively. For the derivation of the in sequel used scaled spin-polarized drift-diffusion system from the papers [20, 21, 22, 23] see [7].

We count the four different species in the following order: electrons with spin up, electrons with spin down, holes with spin up and holes with spin down. We introduce the four component vectors $\lambda = (-1, -1, 1, 1)$ of specific charge numbers, $D = (D_{n\uparrow}, D_{n\downarrow}, D_{p\uparrow}, D_{p\downarrow})$ of diffusion coefficients, and

$$\overline{u} = \Big(\frac{N_c}{2}\exp\big[\frac{-E_{c0}+qg_c}{k_BT}\big], \frac{N_c}{2}\exp\big[\frac{-E_{c0}-qg_c}{k_BT}\big], \frac{N_v}{2}\exp\big[\frac{E_{v0}-qg_v}{k_BT}\big], \frac{N_v}{2}\exp\big[\frac{E_{v0}+qg_v}{k_BT}\big]\Big)$$

of reference densities involving the spin-split band edges. Here N_c and N_v are the corresponding band-edge densities, E_{c0} and E_{v0} denote the variation of the bulk conduction and valence band-edge energies of the semiconductor material, respectively. The spin-splitting of the conduction and the valence bands (see [21]) is expressed by qg_c and qg_v, where q is the elementary charge, T is the temperature and k_B is Boltzmann's constant.

The particle densities are collected in the vector

$$u = (u_1, \dots, u_4) = (n_\uparrow, n_\downarrow, p_\uparrow, p_\downarrow).$$

Scaling the electrostatic potential ψ by q/k_BT and the Quasi-Fermi energies $\varphi_{n\uparrow}$, $\varphi_{n\downarrow}$, $\varphi_{p\uparrow}$ and $\varphi_{p\downarrow}$ by $1/k_BT$, we obtain the (scaled) electrostatic potential v_0 and chemical potentials, v_i, $i=1,\dots,4$,

$$v_0 = \frac{q\psi}{k_BT}, \quad (v_1,\dots,v_4) = \frac{1}{k_BT}\big(\varphi_{n\uparrow}+q\psi, \varphi_{n\downarrow}+q\psi, -\varphi_{p\uparrow}-q\psi, -\varphi_{p\downarrow}-q\psi\big).$$

Denoting by ζ_i the (scaled) electrochemical potential and by a_i the electrochemical activity of the ith species we have $\zeta_i = v_i + \lambda_i v_0$, $a_i = \mathrm{e}^{\zeta_i}$. The statistic relations reflecting Boltzmann statistics have the form

$$u_i = \overline{u}_i \mathrm{e}^{v_i} = \overline{u}_i \mathrm{e}^{\zeta_i - \lambda_i v_0} = \overline{u}_i \mathrm{e}^{-\lambda_i v_0} a_i, \quad i=1,\dots,4. \tag{1.1}$$

The particle flux densities J_i read as

$$J_i = -D_i u_i \nabla\zeta_i = -D_i \overline{u}_i \mathrm{e}^{-\lambda_i v_0}\nabla a_i = -D_i\big(\overline{u}_i\nabla\frac{u_i}{\overline{u}_i} + u_i\lambda_i\nabla v_0\big), \quad i=1,\dots,4. \tag{1.2}$$

In this notation the spin polarized drift-diffusion model can be written in the form

$$\begin{aligned} &-\nabla\cdot(\varepsilon\nabla v_0) = f + \sum_{i=1}^4 \lambda_i u_i, \\ &\frac{\partial u_i}{\partial t} + \nabla\cdot J_i = -R_i, \quad i=1,\dots,4, \quad \text{on } (0,\infty)\times\Omega, \end{aligned} \tag{1.3}$$

where in the Poisson equation, f is a fixed charge density produced by densities of ionized acceptors and donors and $\varepsilon = \epsilon k_BT/q^2$ is the scaled dielectric permittivity. Moreover, in the continuity equations

$$\begin{aligned} R_1 &= r_{13}(a_1a_3-1) + r_{14}(a_1a_4-1) + r_{12}\,\mathrm{e}^{v_0}(a_1-a_2), \\ R_2 &= r_{23}(a_2a_3-1) + r_{24}(a_2a_4-1) - r_{12}\,\mathrm{e}^{v_0}(a_1-a_2), \\ R_3 &= r_{13}(a_1a_3-1) + r_{23}(a_2a_3-1) + r_{34}\,\mathrm{e}^{-v_0}(a_3-a_4), \\ R_4 &= r_{14}(a_1a_4-1) + r_{24}(a_2a_4-1) - r_{34}\,\mathrm{e}^{-v_0}(a_3-a_4) \end{aligned}$$

with

$$r_{ii'} = r\overline{u}_i\overline{u}_{i'},\ ii' = 13,14,23,24,$$
$$r_{12} = \frac{1-\tanh h_c}{2\tau_{sn}}\overline{u}_1, \quad r_{34} = \frac{1-\tanh h_v}{2\tau_{sp}}\overline{u}_3$$

and $r = r(x,u) > 0$. Here τ_{sn} and τ_{sp} are the spin relaxation times for electrons and holes, respectively, and

$$h_c = \frac{qg_c}{k_BT}, \quad h_v = -\frac{qg_v}{k_BT}.$$

Ω denotes the domain which is occupied by the spintronic device. We split $\partial\Omega$ into the disjoint subsets of insulating parts Γ_N and Ohmic contacts Γ_D, $\partial\Omega = \Gamma_D\cup\Gamma_N$, $\Gamma_D = \cup_{k=1}^{n_D}\Gamma_{Dk}$. On insulating parts of the boundary of the device the normal derivatives of the electrostatic potential and of the electrochemical potentials vanish,

$$\frac{\partial v_0}{\partial\nu} = 0, \quad \frac{\partial\zeta_i}{\partial\nu} = 0, \quad i=1,\dots,4, \quad \text{on } \Gamma_N.$$

At the kth Ohmic contact Γ_{D_k} charge neutrality, infinite velocity of electronic reactions and infinite conductivity of the metallic contact lead to

$$v_0|_{\Gamma_{D_k}} = v_{0k} + v_{0k}^{bi}, \quad f|_{\Gamma_{D_k}} - (\overline{u}_1 + \overline{u}_2)\mathrm{e}^{v_{0k}^{bi}} + (\overline{u}_3 + \overline{u}_4)\mathrm{e}^{-v_{0k}^{bi}} = 0,$$
$$\zeta_i|_{\Gamma_{D_k}} = -\lambda_i v_{0k}, \quad i = 1, \ldots, 4,$$

where $v_{0k} = \zeta_{1k} = \zeta_{2k} = -\zeta_{3k} = -\zeta_{4k}$ is the applied potential which is zero in thermodynamic equilibrium. And the built-in-potential v_{0k}^{bi} is chosen such that the device is in thermal equilibrium if all externally applied potentials are zero,

$$v_{0k}^{bi} = \ln \frac{f|_{\Gamma_{D_k}} + \sqrt{f|_{\Gamma_{D_k}}^2 + 4(\overline{u}_1 + \overline{u}_2)(\overline{u}_3 + \overline{u}_4)}}{2(\overline{u}_1 + \overline{u}_2)}.$$

In this paper Gate and Schottky contacts prescribed by third kind boundary conditions are omitted for reasons of simplicity. We complete the system (1.3) by boundary and initial conditions

$$\begin{aligned} v_0 = v_0^D, \quad \zeta_i = \zeta_i^D, \quad i = 1, \ldots, 4, \quad &\text{on } (0, \infty) \times \Gamma_D, \\ \varepsilon \nabla v_0 \cdot \nu = 0, \quad J_i \cdot \nu = 0, \quad i = 1, \ldots, 4, \quad &\text{on } (0, \infty) \times \Gamma_N, \\ u_i(0) = U_i, \quad i = 1, \ldots, 4, \quad \text{on } \Omega & \end{aligned} \tag{1.4}$$

where the Dirichlet data is assumed to be traces of functions v_0^D, ζ_i^D, $i = 1, \ldots, 4$, defined on $\overline{\Omega}$ for analytical convenience.

Remark 1.1 *For two space dimensions, in [7] we proved an existence and uniqueness result for the instationary problem* (1.3), (1.4) *as well as the existence of stationary states of the system. For boundary data compatible with thermodynamic equilibrium the stationary solution is unique and it is a thermodynamic equilibrium. Moreover we obtained the following results concerning the instationary problem: If the boundary data is compatible with thermodynamic equilibrium then the free energy along the solution decays monotonously and exponentially to its equilibrium value. In other cases it may be increasing but we estimated its growth. Moreover we gave upper and lower estimates for the solution.*

The present paper is devoted to the investigation of the stationary problem

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla v_0) &= f + \sum_{i=1}^{4} \lambda_i \overline{u}_i \mathrm{e}^{\zeta_i - \lambda_i v_0} \quad \text{on } \Omega, \\ \nabla \cdot (D_i u_i \nabla \zeta_i) &= R_i, \quad i = 1, \ldots, 4, \quad \text{on } \Omega, \\ v_0 &= v_0^D, \ \zeta_i = \zeta_i^D, \quad i = 1, \ldots, 4, \quad \text{on } \Gamma_D, \\ \frac{\partial v_0}{\partial \nu} &= 0, \quad \frac{\partial \zeta_i}{\partial \nu} = 0, \quad i = 1, \ldots, 4, \quad \text{on } \Gamma_N \end{aligned} \tag{1.5}$$

(with(1.1), (1.2)) in three space dimensions. In Section 2 we show upper and lower a priori bounds for solutions to the continuous problem (cf. Theorem 2.1) and prove solvability (cf. Theorem 2.2). Additionally, we verify uniqueness for Dirichlet data compatible or nearly compatible with thermodynamic equilibrium (cf. Theorem 2.3). In Section 3 we study a discretized stationary spin-polarized drift-diffusion system. We establish an existence result and show that bounds for the solutions can be carried over from the continuous problem (cf. Theorem 3.1). Moreover, we prove that the stationary spin-polarized drift-diffusion model has exactly one solution if the applied voltage is sufficiently small (cf. Theorem 3.2).

2 The continuous stationary spin-polarized drift-diffusion system

2.1 Assumptions

At first we collect general assumptions our analytical investigations are based on.

(A1) $\Omega \subset \mathbb{R}^N$ bounded Lipschitzian domain, $N \leq 3$,
Γ_N relative open subset of $\partial\Omega$, $\Gamma_D := \partial\Omega \setminus \Gamma_N$, $\operatorname{mes}\Gamma_D > 0$.

(A1*) For all $x \in \partial\Omega$ there exists an open neighborhood U of x in $\mathbb{R}^N$ and a Lipschitz transformation $\Phi : U \to \mathbb{R}^N$ such that $\Phi(U \cap (\Omega \cup \Gamma_N)) \in \{E_1, E_2, E_3\}$ where
$E_1 = \{x \in \mathbb{R}^N : \|x\| < 1,\, x_N < 0\}$, $E_2 = \{x \in \mathbb{R}^N : \|x\| < 1,\, x_N \leq 0\}$,
$E_3 = \{x \in E_2 : x_1 > 0 \text{ or } x_N < 0\}$.

(A2) $D_i \in L^\infty(\Omega)$, $D_i \geq c > 0$ a.e. on Ω, $i = 1, \dots, 4$.

(A3) $r_{ii'} \in L^\infty_+(\Omega)$, $ii' = 12, 34$.
$r_{ii'} : \Omega \times (0,\infty)^4 \to \mathbb{R}_+$, $r_{ii'}(x,\cdot) \in C^1((0,\infty)^4)$ for a.a. $x \in \Omega$.
$r_{ii'}(\cdot,u)$, $\frac{\partial r_{ii'}}{\partial u}(\cdot,u)$ are measurable for all $u \in (0,\infty)^4$.

(A3*) For every compact subset $\mathcal{K} \subset (0,\infty)^4$ there exists a $\Delta > 0$ such that
$|r_{ii'}(x,u)|$, $\|\frac{\partial r_{ii'}}{\partial u}(x,u)\| \leq \Delta$ for all $u \in \mathcal{K}$ and a.a. $x \in \Omega$.
For every compact subset $\mathcal{K} \subset (0,\infty)^4$ and $\epsilon > 0$ there exists a $\delta > 0$ such that
$|r_{ii'}(x,u) - r_{ii'}(x,\widehat{u})| < \epsilon$, $\|\frac{\partial r_{ii'}}{\partial u}(x,u) - \frac{\partial r_{ii'}}{\partial u}(x,\widehat{u})\| < \epsilon$ for all u, $\widehat{u} \in \mathcal{K}$ with
$\|u - \widehat{u}\| \leq \delta$ and a.a. $x \in \Omega$, $ii' = 13, 14, 23, 24$.

(A4) ε, f, $\overline{u}_i \in L^\infty(\Omega)$, $\varepsilon \geq c > 0$, $0 < c_f \leq f \leq C_f$, $c_u \leq \overline{u}_i \leq C_u$, $i = 1, 2, 3, 4$,
a.e. on Ω, $v_0^D, \zeta_i^D \in W^{1,2}(\Omega) \cap L^\infty(\Omega)$, $i = 1, \dots, 4$.
There exists $M > 0$ such that $\operatorname{ess\,sup}_{\Gamma_D} v_0^D - \operatorname{ess\,inf}_{\Gamma_D} v_0^D \leq M$ and
$-M \leq \zeta_i^D \leq M$ a.e. on Γ_D.

Here and in the following we denote by c (possibly different) positive constants. Using the bounds from (A4) we define the following quantities

$$\begin{aligned}
&\underline{K} := \ln \frac{c_f+\sqrt{c_f^2+16C_u c_u}}{4C_u} - M, && \overline{K} := \ln \frac{C_f+\sqrt{C_f^2+16C_u c_u}}{4c_u} + M, \\
&\underline{L} := \min(\operatorname{ess\,inf}_{\Gamma_D} v_0^D, \underline{K}), && \overline{L} := \max(\operatorname{ess\,sup}_{\Gamma_D} v_0^D, \overline{K}), \\
&\kappa := \max\{|\underline{L}|, |\overline{L}|\}.
\end{aligned} \tag{2.1}$$

Remark 2.1 *The assumptions in* (A3) *concerning the coefficients $r_{ii'}$, $ii' = 13, 14, 23, 24$, are formulated in this weak form to include Shockley-Read-Hall as well as Auger generation/recombination processes.*

(A1*), *meaning that $\Omega \cup \Gamma_N$ is regular in the sense of Gröger, and* (A3*) *concerning the coefficients $r_{ii'}$, $ii' = 13, 14, 23, 24$, are only used to obtain the uniqueness of steady states for Dirichlet data ζ_i^D nearly compatible with thermodynamic equilibrium* (*see Theorem 2.3 and its proof*).

2.2 A priori bounds for the steady state solutions

Theorem 2.1 *Let* (A1) – (A4) *be fulfilled. Then all steady state solutions* $(v_0, \zeta_1, \ldots, \zeta_4) \in (W^{1,2}(\Omega) \cap L^\infty(\Omega))^5$ *to* (1.5) *fulfill the estimates*

$$v_0 \in [\underline{L}, \overline{L}], \quad \zeta_i \in [-M, M], \quad a_i \in [e^{-M}, e^{M}], \quad i = 1, \ldots, 4, \ \textit{a.e. in } \Omega. \tag{2.2}$$

Proof. 1. Due to the choice of M in (A4) the positive and negative parts $(\zeta_i - M)^+$, $(\zeta_i + M)^-$, $i = 1, \ldots, 4$, belong to $W_0^{1,2}(\Omega \cup \Gamma_N)$. Testing the first, second, third and last continuity equation by $(\zeta_1 - M)^+$, $(\zeta_2 - M)^+$, $-(\zeta_3 + M)^-$, $-(\zeta_4 + M)^-$, respectively, and adding them we obtain

$$\begin{aligned}
0 = &\int_\Omega \Big\{ \sum_{i=1,2} D_i u_i |\nabla(\zeta_i - M)^+|^2 + \sum_{i=3,4} D_i u_i |\nabla(\zeta_i + M)^-|^2 \Big\}\, dx \\
&+ \int_\Omega r_{12}\, e^{v_0} (e^{\zeta_1} - e^{\zeta_2}) \big((\zeta_1 - M)^+ - (\zeta_2 - M)^+\big)\, dx \\
&+ \int_\Omega r_{34}\, e^{-v_0} (e^{\zeta_3} - e^{\zeta_4}) \big((\zeta_4 + M)^- - (\zeta_3 + M)^-\big)\, dx \\
&+ \int_\Omega \sum_{ii'=13,14,23,24} r_{ii'} (e^{\zeta_i + \zeta_{i'}} - 1) \big((\zeta_i - M)^+ - (\zeta_{i'} + M)^-\big)\, dx.
\end{aligned}$$

Since the terms in the last three lines are nonnegative for all values of ζ_i, $i = 1, \ldots, 4$, this implies ζ_1, $\zeta_2 \le M$ and ζ_3, $\zeta_4 \ge -M$. On the other hand, testing by $-(\zeta_1 + M)^-$, $-(\zeta_2 + M)^-$, $(\zeta_3 - M)^+$, $(\zeta_4 - M)^+$, respectively, ensures ζ_1, $\zeta_2 \ge -M$ and ζ_3, $\zeta_4 \le M$.

2. For $a_i > 0$, $i = 1, \ldots, 4$, the mapping $y \mapsto \sum_{i=1}^4 \lambda_i \overline{u}_i a_i e^{-\lambda_i y}$ is strictly monotone decreasing. For $a_i \in [e^{-M}, e^{M}]$ the uniquely determined solution y of the equation $f + \sum_{i=1}^4 \lambda_i \overline{u}_i a_i e^{-\lambda_i y} = 0$ fulfills

$$(e^y)^2 - \frac{f}{\overline{u}_1 a_1 + \overline{u}_2 a_2} e^y - \frac{\overline{u}_3 a_3 + \overline{u}_4 a_4}{\overline{u}_1 a_1 + \overline{u}_2 a_2} = 0$$

and

$$\mathrm{e}^y = \frac{f}{2(\overline{u}_1 a_1 + \overline{u}_2 a_2)} + \sqrt{\frac{f^2}{4(\overline{u}_1 a_1 + \overline{u}_2 a_2)^2} + \frac{\overline{u}_3 a_3 + \overline{u}_4 a_4}{\overline{u}_1 a_1 + \overline{u}_2 a_2}}.$$

Using the bounds for f and u_i, the estimation

$$\begin{aligned}\frac{c_f^2 + 16 C_u c_u}{4(2C_u \mathrm{e}^M)^2} = \frac{c_f^2}{4(2C_u \mathrm{e}^M)^2} + \frac{2c_u \mathrm{e}^{-M}}{2C_u \mathrm{e}^M} &\le \frac{f^2}{4(\overline{u}_1 a_1 + \overline{u}_2 a_2)^2} + \frac{\overline{u}_3 a_3 + \overline{u}_4 a_4}{\overline{u}_1 a_1 + \overline{u}_2 a_2} \\ &\le \frac{C_f^2}{4(2c_u \mathrm{e}^{-M})^2} + \frac{2C_u \mathrm{e}^M}{2c_u \mathrm{e}^{-M}} = \frac{C_f^2 + 16 C_u c_u}{4(2c_u \mathrm{e}^{-M})^2}\end{aligned}$$

and the definition of $\underline{K}$, $\overline{K}$ in (2.1) we find that $y \in [\underline{K}, \overline{K}]$.

3. For $\overline{L}$ from (2.1) we have $(v_0 - \overline{L})^+ \in W_0^{1,2}(\Omega \cup \Gamma_N)$ and we can use it as test function for the Poisson equation in (1.5) to obtain

$$\int_\Omega \varepsilon |\nabla (v_0 - \overline{L})^+|^2 \,\mathrm{d}x = \int_\Omega \big(f + \sum_{i=1}^4 \lambda_i \overline{u}_i a_i \mathrm{e}^{-\lambda_i v_0}\big)(v_0 - \overline{L})^+ \,\mathrm{d}x.$$

Due to (1.1) and step 2 the integral on the right hand side is nonpositive, since according to the choice of $\overline{L}$ in (2.1) we have $f + \sum_{i=1}^4 \lambda_i \overline{u}_i a_i \mathrm{e}^{-\lambda_i v_0} < 0$ if $(v_0 - \overline{L})^+ \neq 0$. Therefore, $v_0 \le \overline{L}$ a.e. in Ω. Analogously, the test function $-(v_0 + \underline{L})^-$, $\underline{L}$ from (2.1), yields $v_0 \ge \underline{L}$ a.e. in Ω. $\square$

2.3 Existence result

As approved for the van Roosbroeck system using Slotboom variables (see e.g. [14, 3, 5]), we formulate our equations in the electrostatic potential v_0 and the electrochemical activities a_i, $i = 1, \dots, 4$, by taking into account that $u_i = \overline{u}_i \mathrm{e}^{-\lambda_i v_0} a_i$ and $\nabla \zeta_i = \nabla a_i / a_i$:

$$\begin{aligned} -\nabla \cdot (\varepsilon \nabla v_0) &= f + \sum_{i=1}^4 \lambda_i \overline{u}_i a_i \mathrm{e}^{-\lambda_i v_0} \quad \text{on } \Omega, \\ \nabla \cdot (D_i \overline{u}_i \mathrm{e}^{-\lambda_i v_0} \nabla a_i) &= R_i, \quad i = 1, \dots, 4, \quad \text{on } \Omega, \\ v_0 = v_0^D, \quad a_i &= a_i^D = \mathrm{e}^{\zeta_i^D}, \quad i = 1, \dots, 4, \quad \text{on } \Gamma_D, \\ \frac{\partial v_0}{\partial \nu} = 0, \quad \frac{\partial a_i}{\partial \nu} &= 0, \quad i = 1, \dots, 4, \quad \text{on } \Gamma_N. \end{aligned} \tag{2.3}$$

Theorem 2.2 *We assume* (A1) – (A4). *There exists a least one steady state solution* $(v_0, a) \in (W^{1,2}(\Omega) \cap L^\infty(\Omega))^5$ *to* (1.5). *It fulfills the bounds stated in Theorem 2.1.*

The proof is based on an iteration procedure and an application of Schauders fixed point theorem in $L^2(\Omega)^4$. Starting from functions a_i^o, $i = 1, \dots, 4$, we evaluate functions a_i^n, $i = 1, \dots, 4$, as follows. First we determine v_0^n as the unique solution to

$$-\nabla \cdot (\varepsilon \nabla v_0^n) = f + \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{-\lambda_i v_0^n} a_i^o \text{ on } \Omega, \quad v_0^n|_{\Gamma_D} = v_0^D \text{ on } \Gamma_D, \quad \frac{\partial v_0^n}{\partial \nu} = 0 \text{ on } \Gamma_N \tag{2.4}$$

(see Lemma 2.1). Next, using this v_0^n we solve the four decoupled continuity equations

$$
\begin{aligned}
-\nabla\cdot(D_1\overline{u}_1 \mathrm{e}^{v_0^n}\nabla a_1^n) &= \sum_{i=3,4} r_{1i}(x,\widehat{u})(1-a_i^o a_1^n) + r_{12}\,\mathrm{e}^{v_0^n}(a_2^o - a_1^n),\\
-\nabla\cdot(D_2\overline{u}_2 \mathrm{e}^{v_0^n}\nabla a_2^n) &= \sum_{i=3,4} r_{2i}(x,\widehat{u})(1-a_i^o a_2^n) - r_{12}\,\mathrm{e}^{v_0^n}(a_2^n - a_1^o),\\
-\nabla\cdot(D_3\overline{u}_3 \mathrm{e}^{-v_0^n}\nabla a_3^n) &= \sum_{i=1,2} r_{i3}(x,\widehat{u})(1-a_i^o a_3^n) + r_{34}\,\mathrm{e}^{-v_0^n}(a_4^o - a_3^n),\\
-\nabla\cdot(D_4\overline{u}_4 \mathrm{e}^{-v_0^n}\nabla a_4^n) &= \sum_{i=1,2} r_{i4}(x,\widehat{u})(1-a_i^o a_4^n) - r_{34}\,\mathrm{e}^{-v_0^n}(a_4^n - a_3^o),\\
a_i^n|_{\Gamma_D} = a_i^D \text{ on } \Gamma_D, &\quad \frac{\partial a_i^n}{\partial \nu} = 0 \text{ on } \Gamma_N, \quad i=1,\dots,4,
\end{aligned}
\tag{2.5}
$$

with $\widehat{u}_i = \overline{u}_i \mathrm{e}^{-\lambda_i v_0^n} a_i^o$, $i=1,\dots,4$, to evaluate $a^n = (a_1^n,\dots,a_4^n)$. We show that the four decoupled problems in (2.5) are uniquely solvable if a^o lies in

$$
\mathcal{M}_c = \{a \in L^2(\Omega)^4 : a_i \in [\mathrm{e}^{-M}, \mathrm{e}^{M}] \text{ a.e. in } \Omega,\ i=1,\dots,4\} \tag{2.6}
$$

(see Lemma 2.2). We define the solution operator $Q_c : \mathcal{M}_c \to L^2(\Omega)^4$ by $Q_c(a^o) = a^n$. Then each fixed point $a^\bullet$ of the operator Q_c gives a solution $(v_0^\bullet, a^\bullet)$ to the stationary spin-polarized drift-diffusion model (2.3) where $v_0^\bullet$ is obtained as solution to (2.4) for $a^\bullet$ instead of a^o.

Lemma 2.1 *We assume* (A1) *and* (A4). *Let $a^o \in \mathcal{M}_c$. Then there is a unique solution v_0^n to* (2.4). *It fulfills $v_0^n \in [\underline{L}, \overline{L}]$ a.e. in Ω. The solution depends continuously on a^o.*

Proof. 1. Let

$$
P_\kappa(y) = \begin{cases} \kappa & y \ge \kappa \\ y & y \in [-\kappa,\kappa] \\ -\kappa & y \le -\kappa \end{cases} \qquad \text{for } \kappa \text{ from (2.1).}
$$

The operator $E_\kappa : v_0^D + W_0^{1,2}(\Omega\cup\Gamma_N) \to W^{-1,2}(\Omega\cup\Gamma_N)$,

$$
\langle E_\kappa v_0, \overline{v}_0\rangle := \int_\Omega \Big\{\varepsilon \nabla v_0\cdot\nabla\overline{v}_0 - \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{-\lambda_i P_\kappa v_0^n} a_i^o \overline{v}_0\Big\}\,\mathrm{d}x \quad \forall \overline{v}_0 \in W_0^{1,2}(\Omega\cup\Gamma_N),
$$

is strongly monotone and Lipschitz continuous. Thus, for each given $a^o \in \mathcal{M}_c$ the regularized nonlinear Poisson equation

$$
-\nabla\cdot(\varepsilon\nabla v_0^n) = f + \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{-\lambda_i P_\kappa v_0^n} a_i^o \text{ on } \Omega, \quad v_0^n|_{\Gamma_D} = v_0^D \text{ on } \Gamma_D, \quad \frac{\partial v_0^n}{\partial\nu} = 0 \text{ on } \Gamma_N \tag{2.7}
$$

has exactly one weak solution $v_0^n \in W^{1,2}(\Omega)$. Testing (2.7) by $(v_0^n - \overline{L})^+$ and $-(v_0^n + \underline{L})^-$, respectively, and taking into account that

$$
f + \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{-\lambda_i P_\kappa v_0^n} a_i^o \le f + \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{-\lambda_i \overline{L}} a_i^o \le 0 \quad \text{if } (v_0^n - \overline{L})^+ \ne 0,
$$

$$-f-\sum_{i=1}^{4}\lambda_i\overline{u}_i\mathrm{e}^{-\lambda_i P_\kappa v_0^n}a_i^o \le -f-\sum_{i=1}^{4}\lambda_i\overline{u}_i\mathrm{e}^{-\lambda_i\underline{L}}a_i^o\le 0 \quad \text{if } (v_0^n+\underline{L})^-\neq 0$$

we prove that $v_0^n\in[\underline{L},\overline{L}]$ a.e. in Ω. Thus, v_0^n is a solution to (2.4), too.

2. If there would be two solutions v_0^{n1}, v_0^{n2} to (2.4), the test with $v_0^{n1}-v_0^{n2}$ yields

$$\int_\Omega \varepsilon|\nabla(v_0^{n1}-v_0^{n2})|^2\,\mathrm{d}x=\int_\Omega\sum_{i=1}^4\lambda_i\overline{u}_i a_i^o(\mathrm{e}^{-\lambda_i v_0^{n1}}-\mathrm{e}^{-\lambda_i v_0^{n2}})(v_0^{n1}-v_0^{n2})\,\mathrm{d}x.$$

Due to the monotonicity of the functions $y\mapsto\lambda_i\mathrm{e}^{-\lambda_i y}$ the right hand side is nonpositive and we obtain that $v_0^{n1}=v_0^{n2}$.

3. To prove the continuous dependency of v_0^n on a^o we consider $a^{om}\to a^o$ in $L^2(\Omega)^4$, $a^{om}\in\mathcal{M}_c$ and the corresponding solutions v_0^{nm} to (2.4). We test the corresponding problems (2.4) by $\overline{v}_0^m:=v_0^n-v_0^{nm}$,

$$\begin{aligned}c\|\overline{v}_0^m\|_{W^{1,2}}^2 &\le \int_\Omega\varepsilon|\nabla\overline{v}_0^m|^2\,\mathrm{d}x=\int_\Omega\sum_{i=1}^4\lambda_i\overline{u}_i\big\{a_i^o\mathrm{e}^{-\lambda_i v_0^n}-a_i^{om}\mathrm{e}^{-\lambda_i v_0^{nm}}\big\}\overline{v}_0^m\,\mathrm{d}x\\ &\le\sum_{i=1}^4\int_\Omega\lambda_i\overline{u}_i\big\{a_i^o(\mathrm{e}^{-\lambda_i v_0^n}-\mathrm{e}^{-\lambda_i v_0^{nm}})+(a_i^o-a_i^{om})\mathrm{e}^{-\lambda_i v_0^{nm}}\big\}\overline{v}_0^m\,\mathrm{d}x\\ &\le c\mathrm{e}^\kappa\sum_{i=1}^4\|a_i^o-a_i^{om}\|_{L^2}\|\overline{v}_0^m\|_{W^{1,2}}.\end{aligned}$$

Thus the continuity follows. □

Lemma 2.2 *We assume* (A1) – (A4). *Let* $a^o\in\mathcal{M}_c$ *and let* v_0^n *be the solution to* (2.4). *Then there exist unique solutions* $a_i^n\in W^{1,2}(\Omega)$, $i=1,\dots,4$, *to the four decoupled equations* (2.5). *They fulfil* $a^n=(a_1^n,a_2^n,a_3^n,a_4^n)\in\mathcal{M}_c$. *Moreover,* a^n *depends continuously on* v_0^n *and* a^o.

Proof. 1. Since $v_0^n\in[\underline{L},\overline{L}]$, $a_{i'}^o\in[\mathrm{e}^{-M},\mathrm{e}^M]$ a.e. on Ω, $r_{ii'}(\cdot,\widehat{u})\ge 0$, $ii'=13,14,23,24$, $r_{12}\mathrm{e}^{v_0^n}\ge 0$, $r_{34}\mathrm{e}^{-v_0^n}\ge 0$ a.e. on Ω there exist unique solutions in $W^{1,2}(\Omega)$ to the four decoupled linear elliptic equations for a_i^n in (2.5).

2. Testing the ith equation in (2.5) by $(a_i^n-\mathrm{e}^M)^+$ and taking into account that $r_{ii'}(\cdot,\widehat{u})\ge 0$, $ii'=13,14,23,24$, $r_{12}\mathrm{e}^{v_0^n}\ge 0$, $r_{34}\mathrm{e}^{-v_0^n}\ge 0$ a.e. on Ω and

$$(a_{i'}^o-a_i^n)(a_i^n-\mathrm{e}^M)^+\le 0,\quad (1-a_{i'}a_i^n)(a_i^n-\mathrm{e}^M)^+\le 0$$

we obtain $a_i^n\le\mathrm{e}^M$ a.e. in Ω. Moreover, the test function $-(a_i^n+\mathrm{e}^{-M})^-$ and having in mind

$$-(a_{i'}^o-a_i^n)(a_i^n+\mathrm{e}^{-M})^-\le 0,\quad -(1-a_{i'}a_i^n)(a_i^n+\mathrm{e}^{-M})^-\le 0$$

yields $a_i^n\ge\mathrm{e}^{-M}$ a.e. in Ω.

3. According to our assumptions on the coefficients and on the bounds of v_0^n and a_i^o we find that the coefficients and right hand sides of the four decoupled linear equations depend

continuously on v_0^n and a_i^o. Therefore the solution of the four decoupled linear equations depend continuously on v_0^n and a_i^o. $\square$

Proof of Theorem 2.2. Lemma 2.1 and Lemma 2.2 guarantee that the mapping $Q_c : \mathcal{M}_c \to L^2(\Omega)^4$, $Q_c(a^0) = a^n$, is continuous and maps the bounded, closed, convex and nonempty set $\mathcal{M}_c$ into itself. We show that Q_c maps $\mathcal{M}_c$ into a precompact subset of $L^2(\Omega)^4$, then the assertion of Theorem 2.2 follows by Schauders fixed point theorem. (By Lemma 2.2 the fixed point then lies in $(W^{1,2}(\Omega) \cap L^\infty(\Omega))^4$.)

Let $a^0 \in \mathcal{M}_c$, $a^n = Q_c(a^0)$. Testing the equation for a_i^n from (2.5) by $a_i^n - a_i^D$, using that $a^0 \in [\mathrm{e}^{-M}, \mathrm{e}^M]^4$, $v_0^n \in [\underline{L}, \overline{L}]$, that $r_{ii'}$ are bounded for bounded arguments (cf. (A3)) and $\|a_i^D\|_{W^{1,2}}$ is bounded (cf. (A4)) we obtain a bound for $\|a_i^n - a_i^D\|_{W^{1,2}}$ which implies $\|a_i\|_{W^{1,2}} \le c$, $i = 1, \ldots, 4$. Due to the compact embedding of $W^{1,2}(\Omega)$ into $L^2(\Omega)$ then $Q_c[\mathcal{M}_c]$ is a precompact subset of $L^2(\Omega)^4$. $\square$

2.4 Uniqueness for Dirichlet data compatible or nearly compatible with thermodynamic equilibrium

Lemma 2.3 *We assume* (A1) – (A4)*. Let the Dirichlet data be compatible with thermodynamic equilibrium,*

$$a_i^{D*} = e^{\zeta_i^{D*}} = const, \quad i = 1, \ldots, 4, \quad \zeta_1^{D*} = \zeta_2^{D*} = -\zeta_3^{D*} = -\zeta_4^{D*}. \tag{2.8}$$

Then the thermodynamic equilibrium $(v_0^*, a^*) = (v_0^*, a_1^{D*}, \ldots, a_4^{D*})$ *where* v_0^* *solves*

$$-\nabla \cdot (\varepsilon \nabla v_0^*) = f + \sum_{i=1}^{4} \lambda_i \overline{u}_i e^{-\lambda_i v_0^*} a_i^{D*} \ \text{on } \Omega, \quad v_0^*|_{\Gamma_D} = v_0^{D*} \ \text{on } \Gamma_D, \quad \frac{\partial v_0^*}{\partial \nu} = 0 \ \text{on } \Gamma_N$$

is the unique solution to (2.3)*.*

Proof. Clearly, the thermodynamic equilibrium (v_0^*, a^*) is a solution to (2.3). Suppose there would be another solution $(\widehat{v}_0, \widehat{a})$ to (2.3). Using the test function $\ln \widehat{a}_i - \zeta_i^{D*} \in W_0^{1,2}(\Omega \cup \Gamma_N)$ for the ith continuity equation in (2.3), add for $i = 1, \ldots, 4$ and taking into account the boundedness of solutions to (2.3), that $\zeta_i^{D*} = \text{const}$ and that $\nabla \widehat{a}_i = \widehat{a}_i \nabla(\ln \widehat{a}_i - \zeta_i^{D*})$ we obtain

$$\begin{aligned} c \sum_{i=1}^{4} \|\ln \widehat{a}_i - \zeta_i^{D*}\|_{W^{1,2}}^2 \le \int_\Omega \Big\{ & r_{12} \mathrm{e}^{\widehat{v}_0} (\widehat{a}_1 - \widehat{a}_2) \ln \frac{\widehat{a}_2}{\widehat{a}_1} + r_{34} \mathrm{e}^{-\widehat{v}_0} (\widehat{a}_3 - \widehat{a}_4) \ln \frac{\widehat{a}_4}{\widehat{a}_3} \\ & + \sum_{ii'=13,14,23,24} r_{ii'}(\cdot, \widehat{u})(1 - \widehat{a}_i \widehat{a}_{i'}) \ln \widehat{a}_i \widehat{a}_{i'} \Big\} \, \mathrm{d}x \le 0 \end{aligned}$$

such that $\widehat{a} = a^*$ and therefore due to the unique solvability of the nonlinear Poisson equation $\widehat{v}_0 = v_0^*$. $\square$

Remark 2.2 *Especially, for the equilibrium boundary conditions motivated in Section 1*

$$v_0^D = v^{bi}, \quad \zeta_i^D = 0, \ i = 1, \ldots, 4,$$

the unique solution to (2.3) *is the thermodynamic equilibrium* $(v_0^*, 1, 1, 1, 1)$ *where* v_0^* *solves*

$$-\nabla \cdot (\varepsilon \nabla v_0^*) = f + \sum_{i=1}^{4} \lambda_i \overline{u}_i e^{-\lambda_i v_0^*} \text{ on } \Omega, \quad v_0^*|_{\Gamma_D} = v_0^{bi} \text{ on } \Gamma_D, \quad \frac{\partial v_0^*}{\partial \nu} = 0 \text{ on } \Gamma_N.$$

To prove a uniqueness result for Dirichlet values nearly compatible with thermodynamic equilibrium we work with a formulation of the stationary spin-polarized drift-diffusion system (1.5) in Sobolev-Campanato spaces. Here we use techniques provided in [10, 11, 12]. We introduce the needed notation. For $p \in [1, \infty)$ and $0 \le \omega \le 2 + N$ we denote by

$$\mathfrak{L}^{p,\omega}(\Omega) := \{w \in L^p(\Omega) : \|w\|_{\mathfrak{L}^{p,\omega}(\Omega)} < \infty\}$$

the Campanato space with its norm

$$\|w\|_{\mathfrak{L}^{p,\omega}(\Omega)} := \Big(\|w\|_{L^p}^p + \sup_{x\in\Omega, \rho>0} \Big\{\rho^{-\omega} \int_{B(x,\rho)} |w(y) - w_{B(x,\rho)}|^p \,\mathrm{d}y \Big\}\Big)^{1/p},$$

where

$$B(x,\rho) := \{y \in \Omega : \|y - x\| < \rho\}, \quad w_{B(x,\rho)} := \frac{1}{|B(x,\rho)|} \int_{B(x,\rho)} w(y) \,\mathrm{d}y.$$

Then $\mathfrak{L}^{p,0}(\Omega) = L^p(\Omega)$. We work with Sobolev-Campanato spaces

$$W^{1,2,\omega}(\Omega) := \big\{w \in W^{1,2}(\Omega) : \frac{\partial w}{\partial x_j} \in \mathfrak{L}^{2,\omega}(\Omega), \ j = 1, \dots, N\big\}$$

and their norms

$$\|w\|_{W^{1,2,\omega}(\Omega)}^2 := \|w\|_{L^2}^2 + \sum_{j=1}^{N} \|\frac{\partial w}{\partial x_j}\|_{\mathfrak{L}^{2,\omega}(\Omega)}^2.$$

According to [6] the continuous embeddings $W^{1,2,\omega}(\Omega) \hookrightarrow C^{0,\gamma}(\overline{\Omega})$ for $N - 2 < \omega \le N$ and $\gamma = 1 - \frac{N-\omega}{2}$ are valid. Moreover we introduce the space of functions vanishing on $\partial\Omega \setminus \Gamma_N$

$$W_0^{1,2,\omega}(\Omega \cup \Gamma_N) := W_0^{1,2}(\Omega \cup \Gamma_N) \cap W^{1,2,\omega}(\Omega)$$

and use the Sobolev-Campanato spaces of functionals

$$W^{-1,2,\omega}(\Omega \cup \Gamma_N) := \{F \in W^{-1,2}(\Omega \cup \Gamma_N) : \|F\|_{W^{-1,2,\omega}(\Omega\cup\Gamma_N)} < \infty\}.$$

$\|F\|_{W^{-1,2,\omega}(\Omega\cup\Gamma_N)}$ for $F \in W^{-1,2,\omega}(\Omega \cup \Gamma_N)$ is defined as the supremum of the set of all $\rho^{-\omega/2}|\langle F, w\rangle|$, where $w \in W_0^{1,2}(\Omega \cup \Gamma_N)$, $\|w\|_{W^{1,2}(\Omega)} \le 1$, $\operatorname{supp}(w) \subset B(x, \rho)$, $x \in \Omega$ and $\rho > 0$. Here $\langle \cdot, \cdot \rangle : W^{-1,2}(\Omega \cup \Gamma_N) \times W_0^{1,2}(\Omega \cup \Gamma_N) \to \mathbb{R}$ is the dual pairing. We use the abbreviations

$$\mathcal{W}^{1,2} := W^{1,2}(\Omega)^5, \quad \mathcal{W}_0^{1,2} := W_0^{1,2}(\Omega \cup \Gamma_N)^5,$$

$$\mathcal{W}^{1,2,\omega} := W^{1,2,\omega}(\Omega)^5, \quad \mathcal{W}_0^{1,2,\omega} := W_0^{1,2,\omega}(\Omega \cup \Gamma_N)^5, \quad \mathcal{W}^{-1,2,\omega} := W^{-1,2,\omega}(\Omega \cup \Gamma_N)^5,$$

and write $\langle \cdot, \cdot \rangle$ for the duality pairing. For convenience, in this subsection we use the vector $z = (z_0, \dots, z_4)$, where $z_0 = v_0$ and $z_i = \zeta_i$, $i = 1, \dots, 4$. We split up z in $z = Z + z^D$, where $z^D = (v_0^D, \zeta_1^D, \dots, \zeta_4^D)$.

Let z^{D*} with $z_0^{D*} = v_0^{D*} \in W^{1,2,\omega_D}(\Omega)$ for some $\omega_D \in (N-2, N)$ and (2.8). Then $z^{D*} \in \mathcal{W}^{1,2,\omega_D}$. Let $z^* = Z^* + z^{D*} = (v_0^*, \zeta_i^*, \dots, \zeta_4^*)$ be the corresponding thermodynamic equilibrium (see Lemma 2.3). We look for a weak formulation of the spin-polarized drift-diffusion system (1.5) in a neighbourhood of this equilibrium solution. Let $\mathcal{U}$ be an open subset of $[L^\infty(\Omega)]^5 \cap \mathcal{W}_0^{1,2}$, $\mathcal{V}$ an open subset in $\mathcal{W}^{1,2,\omega_D}$ with $Z^* \in \mathcal{U}$ and $z^{D*} \in \mathcal{V}$. We consider the variational equation for $Z \in \mathcal{U}$ and $z^D \in \mathcal{V}$:

$$\int_\Omega \Big\{ \varepsilon \nabla Z_0 \cdot \nabla \psi_0 + \sum_{i=1}^4 D_i \overline{u}_i \mathrm{e}^{z_i - \lambda_i z_0} \nabla Z_i \cdot \nabla \psi_i \Big\} \,\mathrm{d}x = \langle \mathcal{F}(Z, z^D), \psi \rangle \quad \forall \psi \in \mathcal{W}_0^{1,2}, \tag{2.9}$$

where

$$\begin{aligned} \langle \mathcal{F}(Z, z^D), \psi \rangle = \int_\Omega \Big\{ & -\varepsilon \nabla z_0^D \cdot \nabla \psi_0 - \sum_{i=1}^4 D_i \overline{u}_i \mathrm{e}^{z_i - \lambda_i z_0} \nabla z_i^D \cdot \nabla \psi_i + h(\cdot, Z, z^D)\psi_0 \\ & + r_{12} \mathrm{e}^{z_0}(\mathrm{e}^{z_1} - \mathrm{e}^{z_2})(\psi_2 - \psi_1) + r_{34}\mathrm{e}^{-z_0}(\mathrm{e}^{z_3} - \mathrm{e}^{z_4})(\psi_4 - \psi_3) \\ & + \sum_{ii'=13,14,23,24} r_{ii'}(\cdot, u)(1 - \mathrm{e}^{z_i + z_{i'}})(\psi_i + \psi_{i'}) \Big\} \,\mathrm{d}x \end{aligned}$$

and $z = Z + z^D$, $u = (u_1, \dots, u_4)$, $u_i = \overline{u}_i \mathrm{e}^{z_i - \lambda_i z_0}$, $h(\cdot, Z, z^D) := f + \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{z_i - \lambda_i z_0}$.

Theorem 2.3 *We assume* (A1) – (A4), (A1*) *and* (A3*). *Let z^{D*} with $z_0^{D*} = v_0^{D*} \in W^{1,2,\omega_D}(\Omega)$ for some $\omega_D \in (N-2, N)$ and* (2.8). *Let $z^* = Z^* + z^{D*} = (v_0^*, \zeta_i^*, \dots, \zeta_4^*)$ be the corresponding thermodynamic equilibrium* (*see Lemma 2.3*). *Then there exists an $\widehat{\omega} \in (N-2, \omega_D]$ and neighborhood $\mathcal{U}_0 \subset \mathcal{U}$ of Z^* in $L^\infty(\Omega)^5 \cap \mathcal{W}_0^{1,2}$ such that there exists a neighbourhood of Dirichlet values $\mathcal{V}_0 \subset \mathcal{V}$ of z^{D*} in $\mathcal{W}^{1,2,\omega_D}$ and a map $\Phi \in C^1(\mathcal{V}_0, \mathcal{W}_0^{1,2,\widehat{\omega}})$ such that $(Z, z^D) \in \mathcal{U}_0 \times \mathcal{V}_0$ is a solution to* (2.9) *if and only if $Z = \Phi(z^D)$. In particular, for each solution $(Z, z^D) \in \mathcal{U}_0 \times \mathcal{V}_0$ to* (2.9) *we have $Z \in \mathcal{W}_0^{1,2,\widehat{\omega}}$, $z = Z + z^D \in \mathcal{W}^{1,2,\widehat{\omega}}$. For Dirichlet values $z^D = (v_0^D, \zeta_i^D, \dots, \zeta_4^D) \in \mathcal{V}_0$ the corresponding solution to* (2.9), *i.e. the weak solution to* (1.5) *is unique.*

Proof. 1. The main part in the variational problem (2.9) is diagonal and the mappings $(Z, z^D) \mapsto D_i \overline{u}_i \mathrm{e}^{Z_i + z_i^D - \lambda_i(Z_0 + z_0^D)}$ belong to $C^1(\mathcal{U} \times \mathcal{V}, L^\infty(\Omega))$. Moreover, the maps $(Z, z^D) \mapsto \varepsilon \nabla z_0^D$, $(Z, z^D) \mapsto D_i \overline{u}_i \mathrm{e}^{Z_i + z_i^D - \lambda_i(Z_0 + z_0^D)} \nabla z_i^D$ belong to $C^1(\mathcal{U} \times \mathcal{V}, \mathfrak{L}^{2,\omega_D}(\Omega)^N)$ since $\nabla z_i^D \in \mathfrak{L}^{2,\omega_D}(\Omega)^N$ and $L^\infty(\Omega)$ is a multiplier of $\mathfrak{L}^{2,\omega_D}(\Omega)$. Due to our assumptions (A3*) for $r_{ii'}$ and the definition of h we obtain that $h(\cdot, Z, z^D)$, $r_{12}\mathrm{e}^{Z_0 + z_0^D}(\mathrm{e}^{Z_1 + z_1^D} - \mathrm{e}^{Z_2 + z_2^D})$, $r_{34}\mathrm{e}^{-(Z_0 + z_0^D)}(\mathrm{e}^{Z_3 + z_3^D} - \mathrm{e}^{Z_4 + z_4^D})$ and

$$r_{ii'}(\cdot, \overline{u}_1 \mathrm{e}^{Z_1 + z_1^D - \lambda_1(Z_0 + z_0^D)}, \dots, \overline{u}_4 \mathrm{e}^{Z_4 + z_4^D - \lambda_4(Z_0 + z_0^D)})(\mathrm{e}^{Z_i + z_i^D + Z_{i'} + z_{i'}^D} - 1), \ ii' = 13, 14, 23, 24,$$

are in $C^1(\mathcal{U} \times \mathcal{V}, L^\infty(\Omega))$ and thus belong to $C^1(\mathcal{U} \times \mathcal{V}, \mathfrak{L}^{2N/(N+2), \omega_D N/(N+2)}(\Omega))$. According to [12, Proposition 6.1 (i), (ii)] for the composed right hand side $\mathcal{F}$ in (2.9) we find that $\mathcal{F} \in C^1(\mathcal{U} \times \mathcal{V}, \mathcal{W}^{-1,2,\omega_D})$ and that $\frac{\partial \mathcal{F}}{\partial Z}(Z, z^D)$ is completely continuous from $L^\infty(\Omega)^5 \cap \mathcal{W}_0^{1,2}$ into $\mathcal{W}^{-1,2,\omega_D}$. This guarantees the assumptions (3.1) and (3.3) in [12, Theorem 3.1].

2. By Lemma 2.3, $(Z^*, z^{D*}) = \big((v_0^* - v_0^{D*}, 0, 0, 0, 0), (v_0^{D*}, \zeta_1^{D*}, \dots, \zeta_4^{D*})\big)$ is a solution to the variational problem (2.9). From Theorem 2.1 we obtain $\frac{1}{c} \le D_i \overline{u}_i \mathrm{e}^{Z_i^* + z_i^{D*} - \lambda_i(Z_0^* + z_0^{D*})} \le c$

a.e. on Ω such that the assumption (3.4) in [12, Theorem 3.1] is fulfilled, too. Finally, we prove that the linearization of (2.9) with respect to Z in (Z^*, z^{D*}) is injective. Since z^{D*} fulfills (2.8) we have to show that the equation for $\overline{Z} \in \mathcal{W}_0^{1,2}$

$$\int_\Omega \Big\{\varepsilon \nabla \overline{Z}_0 \cdot \nabla \psi_0 + \sum_{i=1}^4 D_i \overline{u}_i \mathrm{e}^{z_i^* - \lambda_i z_0^*} \nabla \overline{Z}_i \cdot \nabla \psi_i \Big\}\,\mathrm{d}x$$
$$= \int_\Omega \Big\{ r_{12} \mathrm{e}^{z_0^* + z_1^*} (\overline{Z}_1 - \overline{Z}_2)(\psi_2 - \psi_1) + r_{34} \mathrm{e}^{-z_0^* + z_3^*} (\overline{Z}_3 - \overline{Z}_4)(\psi_4 - \psi_3)$$
$$- \sum_{ii'=13,14,23,24} r_{ii'}(\cdot, u^*)(\overline{Z}_i + \overline{Z}_{i'})(\psi_i + \psi_{i'}) + \frac{\partial h}{\partial Z}(\cdot, Z^*, z^{D*}) \cdot \overline{Z} \psi_0 \Big\}\,\mathrm{d}x \quad \forall \psi \in \mathcal{W}_0^{1,2}$$

possesses only the zero solution. Testing this equation by $\psi = (0, \overline{Z}_1, \ldots, \overline{Z}_4)$ the right hand side becomes non-positive. And since $\operatorname{mes} \Gamma_D > 0$ we obtain $\overline{Z}_i = 0$, $i = 1, \ldots, 4$. Next, we use the test function $(\overline{Z}_0, 0, 0, 0, 0)$ and get

$$\int_\Omega \Big\{ \varepsilon |\nabla \overline{Z}_0|^2 - \frac{\partial h}{\partial Z_0}(\cdot, Z^*, z^{D*})\, \overline{Z}_0^2 \Big\}\,\mathrm{d}x = 0.$$

Since $\frac{\partial h}{\partial Z_0}(\cdot, Z^*, z^{D*}) < 0$, $\varepsilon > c$ a.e. on Ω this leads to $\overline{Z}_0 = 0$ and finally to the desired injectivity result needed for [12, Theorem 3.1].

3. Therefore all assumptions of [12, Theorem 3.1] are verified and we can apply [12, Theorem 3.1] which guarantees an $\widehat{\omega} \in (N-2, \omega_D]$ and a neighborhood $\mathcal{U}_0 \subset \mathcal{U}$ of Z^* in $L^\infty(\Omega)^5 \cap \mathcal{W}_0^{1,2}$ such that there exists a neighborhood $\mathcal{V}_0 \subset \mathcal{V}$ of z^{D*} in $\mathcal{W}^{1,2,\omega_D}$ and a map $\Phi \in C^1(\mathcal{V}_0, \mathcal{W}_0^{1,2,\widehat{\omega}})$ such that $(Z, z^D) \in \mathcal{U}_0 \times \mathcal{V}_0$ is a solution to (2.9) if and only if $Z = \Phi(z^D)$. In particular, for each solution $(Z, z^D) \in \mathcal{U}_0 \times \mathcal{V}_0$ to (2.9) we have $Z \in \mathcal{W}_0^{1,2,\widehat{\omega}}$, $z = Z + z^D \in \mathcal{W}^{1,2,\widehat{\omega}}$. This proves Theorem 2.3. $\square$

Remark 2.3 *The proof of [12, Theorem 3.1] mainly uses that the linearization of* (2.9) *in thermodynamic equilibrium* (Z^*, z^{D*}) *is an injective Fredholm operator of index zero from* $\mathcal{W}_0^{1,2,\widehat{\omega}}$ *into* $\mathcal{W}^{-1,2,\widehat{\omega}}$ *and applies the implicit function theorem in these scales of spaces.*

Remark 2.4 *In [8, 9] we investigated stationary energy models for semiconductor devices which correspond to strongly coupled elliptic systems. To obtain in two space dimensions a local existence and uniqueness result for data nearly compatible with thermodynamic equilibrium we used there regularity and surjectivity results in* $W^{1,p}(\Omega)$, $p > 2$ *and applied the implicit function theorem in that scale of spaces.*

3 The discrete stationary spin-polarized drift-diffusion system

3.1 Voronoi diagrams and finite volume discretization

The notation for the space discretized problem is closely related to that used in [3, 4, 5]. In this section we additionally suppose that

(A5) $\Omega \subset \mathbb{R}^N$ is a polyhedral domain, $N \leq 3$, with a finite polyhedral partition $\Omega = \cup_I \Omega^I$. On each Ω^I the functions ε, $\overline{u}_i$, D_i, $i = 1, \dots, 4, r_{12}$, r_{34}, $r_{ii'}(\cdot, u)$, $ii' = 13, 14, 23, 24$, are constants. The discretization is boundary conforming Delaunay (see Definition 3.1) with r grid points.

(A5) implies that Ω is supposed to be composed by subdomains Ω^I, each Ω^I is associated with a homogeneous material. Let us remark that $C^0 \cap L^\infty$ coefficient functions can be handled by properly chosen averaging schemes, but they are omitted for reasons of notational simplicity. For the space discretization we use N-dimensional simplices (elements) $\mathbf{E}_l^N$ such that

$$\Omega^I = \cup_l \mathbf{E}_l^N.$$

The orientation is taken positive with respect to a right handed coordinate system and the outer normal. N-dimensional simplices can be prescribed by their $N+1$ vertices. We denote by $\mathbf{x}_j^T = (x_{1,j}, \dots, x_{N,j})$ the vector of space coordinates of the vertex j. Edges of simplices are denoted by $\mathbf{e}_{jk} = \mathbf{x}_k - \mathbf{x}_j$, indexed by their starting and ending vertex. The simplex $\mathbf{E}_j^{N-1}$ is the 'surface' opposite to vertex j of the simplex $\mathbf{E}_l^N$.

Definition 3.1 A discretization by simplices $\mathbf{E}_l^N$ is called a Delaunay grid if the balls defined by the $N+1$ vertices of $\mathbf{E}_l^N$ $\forall l$ do not contain any vertex $\mathbf{x}_k$, $\mathbf{x}_k \in \mathbf{E}_m^N$, $\mathbf{x}_k \notin \mathbf{E}_l^N$ (see [1]). Let the Delaunay criterion be fulfilled and let all smallest circum balls of all simplices $\mathbf{E}_l^d \subset \partial\Omega^I$, $d = 1, \dots, N-1$, contain not any vertex $\mathbf{x}_k \in \Omega^I$, $\mathbf{x}_k \notin \mathbf{E}_l^d$, this mesh is called boundary conforming Delaunay (see [2]).

Definition 3.2 Let $V_j = \{\mathbf{x} \in \mathbb{R}^N : \|\mathbf{x} - \mathbf{x}_j\| < \|\mathbf{x} - \mathbf{x}_k\| \ \forall \text{ vertices } \mathbf{x}_k \in \Omega\}$ denote the Voronoi box of vertex $\mathbf{x}_j$ and $\partial V_j = \overline{V}_j \backslash V_j$ the corresponding Voronoi surface. The Voronoi volume element V_{jl} of the vertex j with respect to the simplex $\mathbf{E}_l^N$ is the intersection of the simplex $\mathbf{E}_l^N$ and the Voronoi volume V_j of vertex j.

Moreover, $\partial V_{jl} = \partial(V_j \cap \mathbf{E}_l^N)$ denotes the Voronoi surface of vertex j in simplex $\mathbf{E}_l^N$. Each planar part of ∂V_{jl} is either a part of the Voronoi surface, hence orthogonal to an edge $\mathbf{e}_{jk(j,l)}$ (from vertex $\mathbf{x}^j$ to vertex $\mathbf{x}^k$ in simplex $\mathbf{E}_l^N$, in short $\partial V_{j,k(j,l)}$) or it is a part of $\partial\mathbf{E}_l^N$. Fluxes through these last surfaces are compensated by neighbor simplices or are prescribed by boundary conditions of third kind

$$\alpha_1 w + \alpha_2 \frac{\partial w}{\partial \nu} + \alpha_3 = 0, \quad \alpha_1 \geq 0, \ \alpha_2 > 0.$$

We explain the discretization scheme for the equation $-\nabla \cdot \varepsilon \nabla w = g$. Functions g defined on $\mathbf{E}_l^N$ are replaced by vectors $\mathbf{g} = (g(\mathbf{x}_1), \dots, g(\mathbf{x}_{N+1}))^T$ and

$$\int_{V_{jl}} g(x)\,\mathrm{d}x \approx |V_{jl}| g(\mathbf{x}_j), \quad [V]_j = \sum_l |V_{jl}|, \quad \sum_{j,l} |V_{jl}| = |\Omega|$$

where $[\cdot]$ denotes a diagonal matrix, $[\cdot]_j$ its jth diagonal element. Moreover, functions and relations like $\sqrt{[x]}$, $\ln(\mathbf{g})$, $(\mathbf{g} - L)^+$,..., $\mathbf{x} < \mathbf{y}$ should be understood in a per element meaning.

Differential operators of the form $-\nabla\cdot\varepsilon\nabla w$ (ε constant on each simplex) are discretized using Gauss Theorem

$$\begin{aligned}\int_{V_{jl}} -\nabla\cdot\varepsilon\nabla w\,\mathrm{d}x &= -\varepsilon \sum_{k\neq j:\,\mathbf{x}_k\in\mathbf{E}_l^N} \int_{\partial V_{j,k(j,l)}} \nu\cdot\nabla w\,\mathrm{d}\Gamma + BI_{V_{jl}} \\ &\approx -\varepsilon \sum_{k\neq j:\,\mathbf{x}_k\in\mathbf{E}_l^N} \frac{|\partial V_{j,k(j,l)}|}{|\mathbf{e}_{jk(j,l)}|}(w_k-w_j) + BI_{V_{jl}} \\ &= \varepsilon[\gamma_{k(j,l)}]\widetilde{G}_N\mathbf{w}|_{\mathbf{E}_l^N} + BI_{V_{jl}}\end{aligned} \tag{3.1}$$

where

$$\gamma_{k(j,l)} = \frac{|\partial V_{j,k(j,l)}|}{|\mathbf{e}_{jk(j,l)}|}$$

denotes the elements of a diagonal matrix of geometric weights per simplex. The explicit form of the boundary integrals $BI_{V_{jl}}$ is given by

$$\begin{aligned}BI_{V_{jl}} &= -\sum_{j'\neq j:\,\mathbf{x}_{j'},\mathbf{x}_j\in\mathbf{E}_l^N,\,\mathbf{E}_{j'}^{N-1}\subset\partial\Omega} \int_{\mathbf{E}_{j'}^{N-1}\cap\partial V_{jl}} \nu\cdot(\varepsilon\nabla w)\,\mathrm{d}\Gamma \\ &\approx \sum_{j'\neq j:\,\mathbf{x}_{j'},\mathbf{x}_j\in\mathbf{E}_l^N,\,\mathbf{E}_{j'}^{N-1}\subset\partial\Omega} \frac{\varepsilon}{\alpha_{2j'}}(\alpha_{1j'}w_j+\alpha_{3j'})|\mathbf{E}_{j'}^{N-1}\cap\partial V_{jl}|,\end{aligned}$$

where $\mathbf{E}_{j'}^{N-1}$ denotes the $N-1$ dimensional simplex opposite to $\mathbf{x}_{j'}\in\mathbf{E}_l^N$, $\mathbf{E}_{j'}^{N-1}\subset\partial\Omega$. $\widetilde{G}_N$ is a number of edges $\times$ number of vertices matrix which maps from nodes to edges of a triangle or tetrahedron. Possible representations are

$$\widetilde{G}_2 = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \end{pmatrix}, \quad \widetilde{G}_3 = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix}.$$

From now on we neglect the lower index N. $\widetilde{G}$ fulfills

$$(\widetilde{G}^T\widetilde{G})_{jj} > 0, \quad (\widetilde{G}^T\widetilde{G})_{j>k} < 0, \quad \mathbf{1}^T\widetilde{G}^T = \mathbf{0}^T. \tag{3.2}$$

Summation of (3.1) over the vertices of the simplex yields

$$\sum_{j:\,V_{jl}\subset\mathbf{E}_l^N} \int_{V_{jl}} -\nabla\cdot\varepsilon\nabla w\,\mathrm{d}x \approx \varepsilon\widetilde{G}^T[\gamma]\widetilde{G}\mathbf{w}|_{\mathbf{E}_l^N} + BI \tag{3.3}$$

with $BI = \sum_{j:\, V_{jl}\subset \mathbf{E}_l^N} BI_{V_{jl}}$. Boundary conditions modify the right hand side and lead to nonnegative contributions to diagonal entries. To simplify the notation $G = \sqrt{[\gamma]}\widetilde{G}$ is used as 'discrete gradient matrix'. Moreover, the notation $G^T[\cdot]G\mathbf{w}$ is used to indicate the global function including boundary conditions, too. The summation over all simplices and its reordering over edges, nodes, etc. is not indicated explicitly as long as the global or local meaning follows from the context.

Remark 3.1 *The boundary conforming Delaunay property yields*

$$[\gamma]_m \geq 0, \quad [\gamma]_m = \Big[\sum_{\mathbf{E}_l^N \ni \mathbf{e}_{ij}} [\gamma]\Big]_m, \quad \mathbf{e}_{ij} = \mathbf{e}_m, \quad \mathbf{E}_l^N \subset \Omega^I.$$

Let the grid be connected and let $\alpha_1\alpha_2 > 0$ for at least one $\mathbf{E}_l^{N-1}$. Summing (3.3) over all simplices results an irreducible, weakly diagonally dominant matrix. This matrix has a bounded, non negative inverse – due to maximum principle or Perron-Frobenius theory (see [18]).

3.2 Scharfetter-Gummel scheme

Having in mind the definitions of $\widetilde{G}$ and G in Subsection 3.1 we define

$$A_i^S(\mathbf{v_0}) := G^T[D_i\overline{u}_i\mathrm{e}^{-\lambda_i \underline{v_0}}/\mathrm{sh}(\widetilde{G}\frac{\mathbf{v_0}}{2})]G, \quad i = 1, \dots 4, \tag{3.4}$$

where

$$\mathrm{sh}(t) = \frac{\sinh t}{t}, \quad \underline{v_0} = \frac{v_{0,j} + v_{0,k(j,l)}}{2}.$$

This 'average' $D_i\overline{u}_i\mathrm{e}^{-\lambda_i \underline{v_0}}/\mathrm{sh}(\widetilde{G}\frac{\mathbf{v_0}}{2})$ is called Scharfetter-Gummel scheme and results from solving a two-point boundary value problem along each edge, $(\mathrm{e}^{-\lambda_i v_0} a_i{}')' = 0$, compare e.g. [17]. Then the discrete stationary spin-polarized drift-diffusion model reads as

$$\begin{aligned}
G^T\varepsilon G\mathbf{v_0} &= [V]\mathbf{g}(\mathbf{f},\mathbf{u}), \quad \mathbf{g} = \mathbf{f} + \sum_{i=1}^{4}\lambda_i\mathbf{u_i}, \quad \mathbf{u_i} = [\overline{u}_i\mathrm{e}^{-\lambda_i v_0}]\mathbf{a_i}, \\
A_1^S(\mathbf{v_0})\mathbf{a_1} &= \sum_{i=3,4}[V][r_{1i}(\mathbf{x},\mathbf{u})](\mathbf{1} - [a_i]\mathbf{a_1}) + [V][r_{12}(\mathbf{x})\,\mathrm{e}^{v_0}](\mathbf{a_2} - \mathbf{a_1}), \\
A_2^S(\mathbf{v_0})\mathbf{a_2} &= \sum_{i=3,4}[V][r_{2i}(\mathbf{x},\mathbf{u})](\mathbf{1} - [a_i]\mathbf{a_2}) - [V][r_{12}(\mathbf{x})\,\mathrm{e}^{v_0}](\mathbf{a_2} - \mathbf{a_1}), \\
A_3^S(\mathbf{v_0})\mathbf{a_3} &= \sum_{i=1,2}[V][r_{i3}(\mathbf{x},\mathbf{u})](\mathbf{1} - [a_i]\mathbf{a_3}) + [V][r_{34}(\mathbf{x})\,\mathrm{e}^{-v_0}](\mathbf{a_4} - \mathbf{a_3}), \\
A_4^S(\mathbf{v_0})\mathbf{a_4} &= \sum_{i=1,2}[V][r_{i4}(\mathbf{x},\mathbf{u})](\mathbf{1} - [a_i]\mathbf{a_4}) - [V][r_{34}(\mathbf{x})\,\mathrm{e}^{-v_0}](\mathbf{a_4} - \mathbf{a_3}),
\end{aligned} \tag{3.5}$$

shortly $F_i(\mathbf{x},\mathbf{y}) = 0$, $\mathbf{y} = (\mathbf{v_0},\mathbf{a})$, $i = 0,\dots,4$.

3.3 Existence

In analogy to the proof of Theorem 2.2 for the continuous situation we use for the proof of the existence of a solution to the discrete stationary spin-polarized drift-diffusion system the following iteration procedure. Starting from vectors $\mathbf{a_i}^o$, $i = 1, \ldots, 4$, we evaluate vectors $\mathbf{a_i}^n$, $i = 1, \ldots, 4$, as follows. First we determine $\mathbf{v_0}^n$ as the unique solution to

$$G^T \varepsilon G \mathbf{v_0}^n = [V](\mathbf{f} + \sum_{i=1}^{4} \lambda_i [\overline{u}_i \mathrm{e}^{-\lambda_i v_0^n}] \mathbf{a_i}^o). \tag{3.6}$$

Next, using this $\mathbf{v_0}^n$ we solve the four decoupled discretized continuity equations

$$\begin{aligned}
A_1^S(\mathbf{v_0}^n)\mathbf{a_1}^n &= \sum_{i=3,4} [V][r_{1i}(\mathbf{x}, \widehat{\mathbf{u}})](\mathbf{1} - [a_i^o]\mathbf{a_1}^n) + [V][r_{12}(\mathbf{x})\, \mathrm{e}^{v_0^n}](\mathbf{a_2}^o - \mathbf{a_1}^n),\\
A_2^S(\mathbf{v_0}^n)\mathbf{a_2}^n &= \sum_{i=3,4} [V][r_{2i}(\mathbf{x}, \widehat{\mathbf{u}})](\mathbf{1} - [a_i^o]\mathbf{a_2}^n) - [V][r_{12}(\mathbf{x})\, \mathrm{e}^{v_0^n}](\mathbf{a_2}^n - \mathbf{a_1}^o),\\
A_3^S(\mathbf{v_0}^n)\mathbf{a_3}^n &= \sum_{i=1,2} [V][r_{i3}(\mathbf{x}, \widehat{\mathbf{u}})](\mathbf{1} - [a_i^o]\mathbf{a_3}^n) + [V][r_{34}(\mathbf{x})\, \mathrm{e}^{-v_0^n}](\mathbf{a_4}^o - \mathbf{a_3}^n),\\
A_4^S(\mathbf{v_0}^n)\mathbf{a_4}^n &= \sum_{i=1,2} [V][r_{i4}(\mathbf{x}, \widehat{\mathbf{u}})](\mathbf{1} - [a_i^o]\mathbf{a_4}^n) - [V][r_{34}(\mathbf{x})\, \mathrm{e}^{-v_0^n}](\mathbf{a_4}^n - \mathbf{a_3}^o)
\end{aligned} \tag{3.7}$$

with $\widehat{\mathbf{u}}_i = [\overline{u}_i \mathrm{e}^{-\lambda_i v_0^n}]\mathbf{a_i}^o$, $i = 1, \ldots, 4$, to evaluate $\mathbf{a}^n = (\mathbf{a_1}^n, \ldots, \mathbf{a_4}^n)$. We show that the four problems in (3.7) are uniquely solvable if $\mathbf{a}^o$ is in

$$\mathcal{M} := \{\mathbf{a} \in \mathbb{R}^{4r} : a_{ij} \in [\mathrm{e}^{-M}, \mathrm{e}^{M}], \quad j = 1, \ldots, r, \quad i = 1, \ldots, 4\}. \tag{3.8}$$

For these $\mathbf{a}^o$ we define the solution operator $Q : \mathcal{M} \to \mathbb{R}^{4r}$ by $Q(\mathbf{a}^o) = \mathbf{a}^n$. Then each fixed point $\mathbf{a}^\bullet$ of Q gives a solution $(\mathbf{v_0}^\bullet, \mathbf{a}^\bullet)$ to the discrete stationary spin-polarized drift-diffusion model (3.5) where $\mathbf{v_0}^\bullet$ is obtained as solution to (3.6) for $\mathbf{a}^\bullet$ instead of $\mathbf{a}^o$.

Using the constants from (A4) and (2.1) and assume that $\mathbf{a}^o \in \mathcal{M}$ we find analogously to step 2 of the proof of Theorem 2.1 that at any vertex $\mathbf{x}_j$ the unique solution y_j to

$$f_j + \sum_{i=1}^{4} \lambda_i \overline{u}_i a_{ij}^o \mathrm{e}^{-\lambda_i y_j} = 0$$

fulfills $y_j \in [\underline{K}, \overline{K}]$.

Lemma 3.1 *We assume* (A1), (A4) *and* (A5). *Let be* $\mathbf{a}^o \in \mathcal{M}$. *Then there exists a unique solution* $\mathbf{v_0}^n$ *to* (3.6). *It fulfills* $v_{0j}^n \in [\underline{L}, \overline{L}]$, $j = 1, \ldots, r$. *The solution depends continuously on* $\mathbf{a}^o$.

Proof. 1. We suppose that $\mathbf{v_0}^n$ is a solution to (3.6) and that there would be a vertex $\mathbf{x}_j$ with $v_{0j}^n > \overline{L}$ and lead this to a contradiction. Testing (3.6) by $(\mathbf{v_0}^n - \overline{L})^{+T}$ we find

$$(\mathbf{v_0}^n - \overline{L})^{+T} G^T \varepsilon G \mathbf{v_0}^n - (\mathbf{v_0}^n - \overline{L})^{+T}[V](\mathbf{f} + \sum_{i=1}^{4} \lambda_i [\overline{u}_i \mathrm{e}^{-\lambda_i v_0^n}]\mathbf{a_i}^o) = 0. \tag{3.9}$$

The inequality $v_{0j}^n > \overline{L}$ implies $f_j + \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{-\lambda_i v_{0j}^n} a_{ij}^o < 0$ and

$$-(\mathbf{v_0}^n - \overline{L})^{+T}[V](\mathbf{f} + \sum_{i=1}^4 \lambda_i [\overline{u}_i \mathrm{e}^{-\lambda_i v_0^n}]\mathbf{a_i}^o) > 0.$$

Moreover, generally $(\mathbf{v_0}^n - \overline{L})^{+T} G^T \varepsilon G \mathbf{v_0}^n \geq 0$, and this expression is positive if $v_{0j}^n > \overline{L}$ for at least one j. This yields a contradiction to (3.9). The lower bound is obtained similarly by testing with $-(\mathbf{v_0}^n + \underline{L})^{-T}$.

2. Solving

$$G^T \varepsilon G \mathbf{v_0}^n = [V]\Big(\mathbf{f} + \sum_{i=1}^4 \lambda_i [\overline{u}_i \mathrm{e}^{-\lambda_i v_0^n}]\mathbf{a_i}^o\Big)$$

is equivalent to finding the minimizer $\mathbf{v_0}^n$ of $h : \mathbb{R}^r \to \mathbb{R}$,

$$h(\mathbf{w}) = \frac{1}{2}\mathbf{w}^T G^T \varepsilon G \mathbf{w} - \mathbf{w}^T [V]\Big(\mathbf{f} + \sum_{i=1}^4 [\overline{u}_i \mathrm{e}^{-\lambda_i w}]\mathbf{a_i}^o\Big).$$

Since h is continuously differentiable and

$$\tau h(\mathbf{w}) + (1-\tau) h(\mathbf{z}) - h(\tau \mathbf{w} + (1-\tau)\mathbf{z}) \geq \frac{1}{2}(\mathbf{w}-\mathbf{z})^T G^T \varepsilon G (\mathbf{w}-\mathbf{z}) \quad \forall \mathbf{w}, \mathbf{z} \in \mathbb{R}^r, \forall \tau \in (0,1)$$

there exists a unique minimizer for h (see [15, Chap. 7]) which gives the solution $\mathbf{v_0}^n$ to (3.6). The solution to (3.6) depends continuously on $\mathbf{a}^o$.

3. For uniqueness we argue as follows: If there would be two solutions $\mathbf{v_0}^n$ and $\widetilde{\mathbf{v_0}}^n$ to (3.6) with $v_{0j}^n > \widetilde{v}_{0j}^n$ for at least one j, we use the test function $(\mathbf{v_0}^n - \widetilde{\mathbf{v_0}}^n)^+$,

$$(\mathbf{v_0}^n - \widetilde{\mathbf{v_0}}^n)^{+T} G^T \varepsilon G (\mathbf{v_0}^n - \widetilde{\mathbf{v_0}}^n) - (\mathbf{v_0}^n - \widetilde{\mathbf{v_0}}^n)^{+T}[V] \sum_{i=1}^4 \lambda_i [\overline{u}_i (\mathrm{e}^{-\lambda_i v_0^n} - \mathrm{e}^{-\lambda_i \widetilde{v}_0^n})]\mathbf{a_i}^o = 0$$

and obtain $(\mathbf{v_0}^n - \widetilde{\mathbf{v_0}}^n)^{+T} G^T \varepsilon G (\mathbf{v_0}^n - \widetilde{\mathbf{v_0}}^n) > 0$. Due to the monotonicity of the functions $y \mapsto \sum_{i=1}^4 \lambda_i \overline{u}_i \mathrm{e}^{-\lambda_i y} a_{ij}^o$, $j = 1, \ldots, r$, this leads to a contradiction. □

Lemma 3.2 *We assume* (A1) – (A3) *and* (A5). *Suppose* $-c \leq v_{0j} \leq c$ *for some constant* $c > 0$. *Then* $A_i^S(\mathbf{v_0})$ *are weakly diagonally dominant matrices,* $i = 1, \ldots, 4$. *And they have bounded positive inverses for homogeneous Dirichlet data.*

Proof. Since $0 < \big[\, D_i \overline{u}_i \mathrm{e}^{-\lambda_i \underline{v_0}} / \mathrm{sh}(\widetilde{G}\frac{\mathbf{v_0}}{2})\big] < \infty$ we obtain for the matrices

$$\widetilde{H}_i := \sqrt{\big[\, D_i \overline{u}_i \mathrm{e}^{-\lambda_i \underline{v_0}} / \mathrm{sh}(\widetilde{G}\frac{\mathbf{v_0}}{2})\big]}\, G, \quad i = 1, \ldots, 4,$$

the same properties (sign pattern and sum rules) as formulated for $\widetilde{G}$ in (3.2). Therefore $A_i^S(\mathbf{v_0}) = \widetilde{H}_i^T \widetilde{H}_i$ have bounded positive inverses for homogeneous Dirichlet data, $i = 1, \ldots, 4$. □

Lemma 3.3 *We assume* (A1) – (A5)*. Let* $\mathbf{v_0}^n$ *be the solution to* (3.6) *with* $\mathbf{a}^o$ *fulfilling* (3.8)*. Then there exist unique solutions* $\mathbf{a_i}^n$*,* $i = 1, \ldots, 4$*, to the four decoupled equations* (3.7)*. They fulfill*

$$a_{ij}^n \in [e^{-M}, e^M], \quad j = 1, \ldots, r, \quad i = 1, \ldots, 4.$$

The solutions $\mathbf{a_i}^n$ *to* (3.7) *depend continuously on* $\mathbf{v_0}^n$ *and* $\mathbf{a_i}^o$*,* $i = 1, \ldots, 4$*.*

Proof. 1. We show the result for the first equation in (3.7)

$$A_1^S(\mathbf{v_0}^n)\mathbf{a_1}^n = \sum_{i=3,4} [V][r_{1i}(\mathbf{x}, \widehat{\mathbf{u}})](\mathbf{1} - [a_i^o]\mathbf{a_1}^n) + [V][r_{12}(\mathbf{x})\,\mathrm{e}^{v_0^n}](\mathbf{a_2}^o - \mathbf{a_1}^n).$$

Since $\sum_{i=3,4}[V][r_{1i}(\mathbf{x}, \widetilde{\mathbf{u}})][a_i^o] + [V][r_{12}(\mathbf{x})\,\mathrm{e}^{v_0^n}]$ is a diagonal matrix with nonnegative entries, Lemma 3.2 guarantees that the matrix

$$C(\mathbf{v_0}^n, \mathbf{a}^o) := A_1^S(\mathbf{v_0}^n) + \sum_{i=3,4} [V][r_{1i}(\mathbf{x}, \widetilde{\mathbf{u}})][a_i^o] + [V][r_{12}(\mathbf{x})\,\mathrm{e}^{v_0^n}]$$

has a bounded inverse such that the problem is uniquely solvable.

2. Assuming that $a_{ij}^n > e^M$ for at least one $\mathbf{x}_j \in \Omega$ and $i = 1$. We test the first equation in (3.7) by $(\mathbf{a_1}^n - \mathrm{e}^M)^{+T}$,

$$\begin{aligned}
&(\mathbf{a_1}^n - \mathrm{e}^M)^{+T} A_i^S(\mathbf{v_o}^n)\mathbf{a_1}^n \\
&\quad = (\mathbf{a_1}^n - \mathrm{e}^M)^{+T}[V]\Big(\sum_{i=3,4}[V][r_{1i}(\mathbf{x}, \widehat{\mathbf{u}})](\mathbf{1} - [a_i^o]\mathbf{a_1}^n) + [r_{12}(\mathbf{x})\,\mathrm{e}^{v_0^n}](\mathbf{a_2}^o - \mathbf{a_1}^n)\Big).
\end{aligned}$$

Under our assumption then $(\mathbf{a_1}^n - \mathrm{e}^M)^{+T} A_i^S(\mathbf{v_o}^n)\mathbf{a_1}^n > 0$. Additionally $(\mathbf{1} - [a_i^o]\mathrm{e}^M) \le 0$, $\mathbf{a_2}^o - \mathrm{e}^M \le 0$, $[r_{1i}(\mathbf{x}, \widehat{\mathbf{u}})] \ge 0$, $[r_{12}(\mathbf{x})\,\mathrm{e}^{v_0^n}] \ge 0$. This gives a contradiction. The lower bound is obtained by testing with $-(\mathbf{a_1}^n + \mathrm{e}^{-M})^{-T}$.

3. The matrix $C(\mathbf{v_0}^n, \mathbf{a}^o)$ depends continuously on $\mathbf{v_0}^n$, $\mathbf{a}^o$. Due to the perturbation lemma we have for matrices C_1, C_2 where C_1 is a regular matrix with $\|C_1^{-1}\| \le \beta$, $\|C_1 - C_2\| \le \beta_1$, $\beta\beta_1 < 1$ that C_2 is regular and

$$\|C_2^{-1}\| \le \frac{\beta}{1 - \beta\beta_1}, \quad \|C_1^{-1} - C_2^{-1}\| \le \frac{\beta^2\beta_1}{1 - \beta\beta_1}.$$

Additionally, our right hand side in $C(\mathbf{v_0}^n, \mathbf{a}^o) = \sum_{i=3,4}[V][r_{1i}(\mathbf{x}, \widehat{\mathbf{u}})]\mathbf{1} + [V][r_{12}(\mathbf{x})\,\mathrm{e}^{v_0^n}]\mathbf{a_2}^o$ depends continuously on $\mathbf{v_0}^n$, $\mathbf{a}^o$. Thus in summary $\mathbf{a}^n$ depends continuously on $\mathbf{v_0}^n$, $\mathbf{a}^o$.
□

Theorem 3.1 *We assume* (A1) – (A5)*. Then there exists at least one solution* $(\mathbf{v_0}^\bullet, \mathbf{a}^\bullet)$ *to the discrete stationary spin-polarized drift-diffusion model* (3.5)*. Solutions to* (3.5) *fulfill the bounds*

$$a_{ij}^\bullet \in [e^{-M}, e^M], \quad i = 1, \ldots, 4, \quad v_{0j}^\bullet \in [\underline{L}, \overline{L}], \quad j = 1, \ldots, r.$$

Proof. According to Lemma 3.1, Lemma 3.3 the mapping $Q : \mathcal{M} \to \mathbb{R}^{4r}$, $Q(\mathbf{a}^o) = \mathbf{a}^n$, is continuous and maps the convex, bounded, closed and non empty set $\mathcal{M}$ (see (3.8)) into itself. Therefore Brouwer's fixed point theorem (see [19]) guarantees at least one fixed point $\mathbf{a}^\bullet$ of Q. Solving (3.6) for $\mathbf{a}^\bullet$ instead of $\mathbf{a}^o$ leads to $\mathbf{v_0}^\bullet$. And $\mathbf{u}^\bullet$ is obtained by $\mathbf{u_i}^\bullet = [\overline{u}_i \mathrm{e}^{-\lambda_i v_0^\bullet}]\mathbf{a_i}^\bullet$, $i = 1, \ldots, 4$. The bounds are guaranteed by Lemma 3.1, Lemma 3.3. □

Remark 3.2 *Theorem 3.1 ensures for the solutions to the discretized problem exactly the same upper and lower bounds as proved for the continuous problem in Theorem 2.1. An analogous result for the van Roosbroeck system is obtained in [5] where also the Scharfetter-Gummel scheme is used. In [13] this question is discussed for non-monotone elliptic equations and a finite element approximation. There the lower bounds of the continuous problem can not be saved since the necessary truncated functions can not be used as test functions for the discretized problem.*

3.4 Uniqueness for small applied voltages

Lemma 3.4 *We assume* (A1) – (A5). *If no voltage is applied to the device* (*hence, the boundary conditions*

$$v_0|_{\Gamma_D} = v_0^{bi}, \quad a_i|_{\Gamma_D} = 1, \quad i = 1, \ldots, 4,$$

which are compatible with thermodynamic equilibrium) *then there exists a unique solution* $(\mathbf{v_0}^*, \mathbf{a}^*)$ *to* (3.5). *This solution is a thermodynamic equilibrium with* $\mathbf{a_i}^* = \mathbf{1}$ *and* $\mathbf{v_0}^*$ *is the unique solution to the Poisson equation in* (3.5) *where* $\mathbf{a}$ *is substituted by* $\mathbf{a}^*$.

Proof. Clearly $(\mathbf{v_0}^*, \mathbf{a}^*)$ is a solution to (3.5). It remains to show its uniqueness. Let $(\mathbf{v_0}, \mathbf{a})$ be a solution to (3.5). The $\mathbf{a_i}$ fulfill the bounds and the boundary conditions, hence each boundary integral expression in the discrete continuity equations vanishes. Testing the continuity equation for $\mathbf{a_i}$ in (3.5) with $\ln(\mathbf{a_i}^T)$ is possible due to the bounds. Summing them yields the dissipation expression

$$\begin{aligned}\sum_{i=1}^{4} \ln(\mathbf{a_i}^T) A_i^S(\mathbf{v_0})\mathbf{a_i} = [V] &\sum_{ii'=13,14,23,24} \ln(\mathbf{a_i}^T[a_{i'}])[r_{ii'}]([a_{i'}]\mathbf{a_i} - \mathbf{1}) \\ &+ [V] \sum_{ii'=12,34} \ln(\mathbf{a_i}^T[a_{i'}]^{-1})[a_{i'}][r_{ii'}](\mathbf{a_i}[a_{i'}]^{-1} - \mathbf{1}).\end{aligned} \tag{3.10}$$

The monotonicity of the logarithm and the positivity of diagonal weights (see (3.4)) summed over all contributions to one edge yields per edge and hence for $\ln(\mathbf{a_i}^T)A_i^S(\mathbf{v_0})\mathbf{a_i} \geq 0$ for all i. Because $[V] > 0$, $[r_{ii'}] > 0$ each expression on the right hand side of (3.10) is non positive. Hence all expressions have to be zero to fulfill (3.10). This implies $\mathbf{a_i} = \mathbf{1}$, due to the boundary conditions. For these thermodynamic equilibrium activities the Poisson equation yields the unique thermodynamic equilibrium solution $(\mathbf{v_0^*}, \mathbf{a}^*)$ (compare Lemma 3.1). □

Theorem 3.2 *We assume* (A1) – (A5). *If the applied voltage is sufficiently small, then the discrete stationary spin-polarized drift-diffusion model* (3.5) *possesses exactly one solution.*

Proof. 1. We show that the linearization of (3.5) in the unique thermodynamic equilibrium $(\mathbf{v_0}^*, \mathbf{a}^*)$ (corresponding to no applied voltage) has a bounded inverse. Due to the continuous dependence of the mapping (3.5) of $(\mathbf{v_0}, \mathbf{a})$ the implicit function theorem gives the desired uniqueness result for small voltages.

2. We discuss the linearization of (3.5) in the Form $F_i(\mathbf{x}, \mathbf{y}) = 0$ at approximated solutions $\mathbf{Y}$, $\mathbf{y} = \mathbf{Y} + \delta\mathbf{y}$ of (3.5). Denoting

$$T_i := [G\mathbf{a_i}] \frac{\partial}{\partial v_0} [D_i \overline{u}_i \mathrm{e}^{-\underline{v_0}} / \operatorname{sh}(\widetilde{G}(\mathbf{v_0}/2)], \quad i = 1, \ldots, 4,$$

$$[\frac{\partial r_{ii'}}{\partial v_0}] = [-\sum_{l=1}^{4} \lambda_l \overline{u}_l \mathrm{e}^{-\lambda_l v_0} \frac{\partial r_{ii'}}{\partial u_l}], \quad [\frac{\partial r_{ii'}}{\partial a_l}] = [\overline{u}_l \mathrm{e}^{-\lambda_l v_0} \frac{\partial r_{ii'}}{\partial u_l}], \quad ii' = 13, 14, 23, 24,$$

and omitting the arguments in $r_{ii'}$ the linearization applied to $(\delta\mathbf{v_0}, \delta\mathbf{a})$ has the form

$$\Big\{G^T \varepsilon G + [V][\sum_{i=1}^{4} u_i]\Big\}\delta\mathbf{v_0} - \sum_{i=1}^{4} \lambda_i [V \overline{u}_i \mathrm{e}^{-\lambda_i \widetilde{v}_0}]\delta\mathbf{a_i} + F_0 = 0, \tag{3.11}$$

$$\begin{aligned}
&\Big\{G^T T_1 - \sum_{i=3,4} [V](I - [a_1 a_i])[\frac{\partial r_{1i}}{\partial v_0}] - [V][a_2 - a_1][r_{12}\mathrm{e}^{v_0}]\Big\}\delta\mathbf{v_0} \\
&\quad + \Big\{A_1^S(v_0) - \sum_{i=3,4} [V](I - [a_1 a_i])[\frac{\partial r_{1i}}{\partial a_1}] + \sum_{i=3,4} [V][r_{1i} a_i] + [V][r_{12}\mathrm{e}^{v_0}]\Big\}\delta\mathbf{a_1} \\
&\quad + \Big\{-\sum_{i=3,4} [V](I - [a_1 a_i])[\frac{\partial r_{1i}}{\partial a_2}] - [V][r_{12}\mathrm{e}^{v_0}]\Big\}\delta\mathbf{a_2} \\
&\quad + \Big\{-\sum_{i=3,4} [V](I - [a_1 a_i])[\frac{\partial r_{1i}}{\partial a_3}] + [V][r_{13} a_1]\Big\}\delta\mathbf{a_3} \\
&\quad + \Big\{-\sum_{i=3,4} [V](I - [a_1 a_i])[\frac{\partial r_{1i}}{\partial a_4}] + [V][r_{14} a_1]\Big\}\delta\mathbf{a_4} + F_1 = 0,
\end{aligned}$$

$$\begin{aligned}
&\Big\{G^T T_2 - \sum_{i=3,4} [V](I - [a_2 a_i])[\frac{\partial r_{2i}}{\partial v_0}] + [V][a_2 - a_1][r_{12}\mathrm{e}^{v_0}]\Big\}\delta\mathbf{v_0} \\
&\quad + \Big\{-\sum_{i=3,4} [V](I - [a_2 a_i])[\frac{\partial r_{2i}}{\partial a_1}] - [V][r_{12}\mathrm{e}^{v_0}]\Big\}\delta\mathbf{a_1} \\
&\quad + \Big\{A_2^S(v_0) - \sum_{i=3,4} [V](I - [a_2 a_i])[\frac{\partial r_{2i}}{\partial a_2}] + \sum_{i=3,4} [V][r_{2i} a_i] + [V][r_{12}\mathrm{e}^{v_0}]\Big\}\delta\mathbf{a_2} \\
&\quad + \Big\{-\sum_{i=3,4} [V](I - [a_2 a_i])[\frac{\partial r_{2i}}{\partial a_3}] + [V][r_{23} a_2]\Big\}\delta\mathbf{a_3} \\
&\quad + \Big\{-\sum_{i=3,4} [V](I - [a_2 a_i])[\frac{\partial r_{2i}}{\partial a_4}] + [V][r_{24} a_2]\Big\}\delta\mathbf{a_4} + F_2 = 0,
\end{aligned}$$

$$
\begin{aligned}
&\Big\{G^T T_3 - \sum_{i=1,2}[V](I-[a_i a_3])\big[\frac{\partial r_{i3}}{\partial v_0}\big] + [V][a_4 - a_3][r_{34}\mathrm{e}^{-v_0}]\Big\}\delta\mathbf{v_0}\\
&\quad + \Big\{-\sum_{i=1,2}[V](I-[a_i a_3])\big[\frac{\partial r_{i3}}{\partial a_1}\big] + [V][r_{13}a_3]\Big\}\delta\mathbf{a_1}\\
&\quad + \Big\{-\sum_{i=1,2}[V](I-[a_i a_3])\big[\frac{\partial r_{i3}}{\partial a_2}\big] + [V][r_{23}a_3]\Big\}\delta\mathbf{a_2}\\
&\quad + \Big\{A_3^S(v_0) - \sum_{i=1,2}[V](I-[a_i a_3])\big[\frac{\partial r_{i3}}{\partial a_3}\big] + \sum_{i=1,2}[V][r_{i3}a_i] + [V][r_{34}\mathrm{e}^{-v_0}]\Big\}\delta\mathbf{a_3}\\
&\quad + \Big\{-\sum_{i=1,2}[V](I-[a_i a_3])\big[\frac{\partial r_{i3}}{\partial a_4}\big] - [V][r_{34}\mathrm{e}^{-v_0}]\Big\}\delta\mathbf{a_4} + F_3 = 0,
\end{aligned}
$$

$$
\begin{aligned}
&\Big\{G^T T_4 - \sum_{i=1,2}[V](I-[a_i a_4])\big[\frac{\partial r_{i4}}{\partial v_0}\big] + [V][a_4 - a_3][r_{34}\mathrm{e}^{-v_0}]\Big\}\delta\mathbf{v_0}\\
&\quad + \Big\{-\sum_{i=1,2}[V](I-[a_i a_4])\big[\frac{\partial r_{i4}}{\partial a_1}\big] + [V][r_{14}a_4]\Big\}\delta\mathbf{a_1}\\
&\quad + \Big\{-\sum_{i=1,2}[V](I-[a_i a_4])\big[\frac{\partial r_{i4}}{\partial a_2}\big] + [V][r_{24}a_4]\Big\}\delta\mathbf{a_2}\\
&\quad + \Big\{-\sum_{i=1,2}[V](I-[a_i a_4])\big[\frac{\partial r_{i4}}{\partial a_3}\big] - [V][r_{34}\mathrm{e}^{-v_0}]\Big\}\delta\mathbf{a_3}\\
&\quad + \Big\{A_4^S(v_0) - \sum_{i=1,2}[V](I-[a_i a_4])\big[\frac{\partial r_{i4}}{\partial a_4}\big] + \sum_{i=1,2}[V][r_{i4}a_i] + [V][r_{34}\mathrm{e}^{-v_0}]\Big\}\delta\mathbf{a_4} + F_4 = 0.
\end{aligned}
$$

3. For the thermodynamic equilibrium solution $(\mathbf{v_0}^*, \mathbf{a}^*)$ we have

$$
G\mathbf{a_i}^* = \mathbf{0}, \quad [a_i - a_{i'}] = [0], \quad ii' = 12, 34, \quad I - [a_i a_{i'}] = [0], \quad ii' = 13, 14, 23, 24.
$$

According to the form of the linearization of (3.5) obtained in step 2, therefore it is sufficient to show the existence of a bounded inverse for the linearized continuity equations. We use the following abbreviations

$$
A = \operatorname{diag}\big(A_i^S(\mathbf{v_0}^*)\big)_{i=1,\dots,4},
$$

with diag indicating a block matrix in the 4×4 block system,

$$
S_{ii'} = [V][r_{ii'}(\mathbf{x}, \mathbf{u}^*)], \quad ii' = 13, 14, 23, 24, \quad S_{12} = [V][r_{12}\mathrm{e}^{v_0^*}], \quad S_{34} = [V][r_{34}\mathrm{e}^{-v_0^*}].
$$

Then the linearization of the continuity equations in thermodynamic equilibrium $\mathcal{L}(\mathbf{v_0}^*, \mathbf{a}^*)$ has the form $\mathcal{L}(\mathbf{v_0}^*, \mathbf{a}^*) = A + B$ where

$$
B = \begin{pmatrix}
S_{13}+S_{14}+S_{12} & -S_{12} & S_{13} & S_{14}\\
-S_{12} & S_{23}+S_{24}+S_{12} & S_{23} & S_{24}\\
S_{13} & S_{23} & S_{13}+S_{23}+S_{34} & -S_{34}\\
S_{14} & S_{24} & -S_{34} & S_{14}+S_{24}+S_{34}
\end{pmatrix}.
$$

The linearizations $A_i^S(\mathbf{v_0}^*)$ in thermodynamic equilibrium in Slotboom variables are symmetric and positive definite. Thus the same for A is true. The matrix B is symmetric, too. Due to the Gershgorins circle theorem all eigenvalues of B lie in the closed interval

$$[0, \max_{i=1,\dots,4} \max_{j=1,\dots,r} 2 \sum_{i' \neq i} [S_{ii'}]_j]$$

where $[S_{ii'}]_j \geq 0$ denotes the jth diagonal element of the $r \times r$ diagonal matrix $S_{ii'}$. Therefore B is positive semidefinite, and the linearization of the continuity equations in thermodynamic equilibrium $\mathcal{L}(\mathbf{v_0}^*, \mathbf{a}^*)$ is symmetric and positive definite. Thus the in thermodynamic equilibrium linearized discrete continuity equations can uniquely be solved for $\delta\mathbf{a}$. Inserting this in (3.11) taken at thermodynamic equilibrium we obtain unique solvability of this equation w.r.t. $\delta\mathbf{v}_0$. □

Summary: The static spin-polarized drift-diffusion system possesses very similar analytical and numerical properties compared to the stationary classical van Roosbroeck system (see [14, 5]).

References

1. B. Delaunay, *Sur la sphére*, Izvestia Akademii Nauk SSSR. Otd. Matem. Estestv. Nauk **7** (1034), 793–800.

2. P. Fleischmann, *Mesh generation for technology CAD in three dimensions*, Dissertation, Technische Universität Wien, 1999.

3. H. Gajewski and K. Gärtner, *On the discretization of van Roosbroeck's equations with magnetic field*, Z. Angew. Math. Mech. **76** (1996), 247–264.

4. H. Gajewski and K. Gärtner, *A dissipative discretization scheme for a nonlocal phase segregation model*, Z. Angew. Math. Mech. **85** (2005), 815–822.

5. K. Gärtner, *Existence of bounded discrete steady state solutions of the van Roosbroeck system on boundary conforming Delaunay grids*, Preprint 1258, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, 2007.

6. E. Giusti, *Metodi diretti nel calcolo delle variazioni*, Unione Matematica Italiana, Bologna, 1994.

7. A. Glitzky, *Analysis of a spin-polarized drift-diffusion model*, Preprint 1300, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, 2008, to appear in Adv. Math. Sci. Appl.

8. A. Glitzky and R. Hünlich, *Stationary energy models for semiconductor devices with incompletely ionized impurities*, Z. Angew. Math. Mech. **85** (2005), 778–792.

9. A. Glitzky and R. Hünlich, *Stationary solutions to an energy model for semiconductor devices where the equations are defined on different domains*, Preprint 1173, Weierstraß-Institut für Angewandte Analysis und Stochastik, Berlin, 2006, to appear in Math. Nach.

10. J. A. Griepentrog, *Linear elliptic boundary value problems with non-smooth data: Campanato spaces of functionals*, Math. Nach. **243** (2002), 19–42.

11. J. A. Griepentrog and L. Recke, *Linear elliptic boundary value problems with non-smooth data: Normal solvability on sobolev-campanato spaces*, Math. Nach. **225** (2001), 39–74.

12. K. Gröger and L. Recke, *Applications of differential calculus to quasilinear elliptic boundary value problems with non-smooth data*, NoDEA Nonlinear Differential Equations Appl. **13** (2006), 263–285.

13. A. Jüngel and A. Unterreiter, *Discrete minimum and maximum principles for finite element approximations of non-monotone elliptic equations*, Numerische Mathematik **99** (2005), 485–508.

14. P. A. Markowich, *The stationary semiconductor device equations*, Springer, Wien, New York, 1986.

15. A. Quarteroni, R. Sacco, and F. Saleri, *Numerical mathematics*, Springer, Berlin, Heidelberg, 2007.

16. W. V. van Roosbroeck, *Theory of flow of electrons and holes in germanium and other semiconductors*, Bell Syst. Techn. J. **29** (1950), 560–607.

17. S. Selberherr, *Analysis and simulation of semiconductor devices*, Springer, Wien, 1984.

18. R. S. Varga, *Matrix iterative analysis*, Prentice-Hall, Englewood Cliffs N. J., 1962.

19. E. Zeidler, *Vorlesungen über nichtlineare Funktionalanalysis I - Fixpunktsätze*, Teubner-Texte zur Mathematik, Teubner, Leipzig, 1976.

20. I. Zutic and J. Fabian, *Bipolar spintronics*, Concepts in Spin Electronics (S. Maekawa, ed.), Oxford, 2006.

21. I. Zutic, J. Fabian, and S. C. Erwin, *Bipolar spintronics: Fundamentals and applications*, IBM J. Res. & Dev. **50** (2006), 121–139.

22. I. Zutic, J. Fabian, and S. Das Sarma, *Spin-polarized transport in inhomogeneous magnetic semiconductors: Theory of magnetic/nonmagnetic p-n junctions*, Phys. Rev. Lett. **88** (2002), 066603.

23. ______, *Spintronics: Fundamentals and applications*, Rev. Mod. Phys. **76** (2004), 323–410.