THE STATIONARY CURRENT–VOLTAGE CHARACTERISTICS OF THE QUANTUM DRIFT DIFFUSION MODEL *

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Abstract. This paper is concerned with numerical algorithms for the bipolar quantum drift diffusion model. For the thermal equilibrium case a quasi-gradient method minimizing the energy functional is introduced and strong convergence is proven. The computation of current–voltage characteristics is performed by means of an extended *Gummel–iteration.* It is shown that the involved fixed point mapping is a contraction for small applied voltages. In this case the model equations are uniquely solvable and convergence of the proposed iteration scheme follows. Numerical simulations of a one dimensional resonant tunneling diode are presented. The computed current–voltage characteristics are in good qualitative agreement with experimental measurements. The appearance of negative differential resistances is verified for the first time in a Quantum Drift Diffusion model.

Key words. Resonant tunneling diode, bipolar quantum drift diffusion model, projected quasi–gradient method, internal approximation, generalized Gummel iteration, convergence.

AMS subject classifications. 35J55, 35J60, 49M07, 49M37, 65J15, 76Y05.

1. Introduction. The performance of increasingly many ultra–small semiconductor devices relies on quantum mechanical phenomena. The incorporation of these quantum effects is one of the major tasks of modern semiconductor device modeling. Especially the numerical verification of negative differential resistance effects (NDR) exhibited by resonant tunneling diodes (RTD) has gained considerable attention in the literature, see e.g. [8, 10, 16, 20, 26, 11].

The approaches range from *microscopic* to *macroscopic* models. At the most fundamental level there are *microscopic* quantum models such as Schrödinger–Poisson or (kinetic) Wigner–Poisson systems [25]. It is meanwhile well-known that these models give a fairly accurate account to quantum-dominated device behaviour [26, 28, 32, 33].

From an applicational point of view these approaches are not completely satisfactory. Firstly, the computation of *macroscopic* current–voltage characteristics is settled on the computation on *microscopic quantities* such as Schrödinger functions or Wigner functions. Hence, the simulation of realistic devices requires high computational costs. Secondly, the identification of the system's parameters and the incorporation of relaxation terms is difficult to perform. (Up to now it is not clear how to add relaxation terms to Schrödinger's equation.) Thirdly, quantum effects play an important role only in small parts of the device (e.g. across heterojunctions), i.e. there is some redundancy in the microscopic approach. Finally, the appropriate choice of boundary data is an open problem [30].

The *macroscopic* quantum models are settled on the density-functional theory (DFT). Based on the electron density rather than the density matrix as fundamental variable the DFT has been successfully employed in atomic, nuclear, molecular and solid state physics, see [13] for a review. The core of DFT is the attempt to build a "classical" picture of quantum mechanics in terms of macroscopic variables. DFTs are essentially based on Madelung's transformation (published in 1926) of the Schrödinger equation into quantum fluid-dynamical equations (c.f. [21]).

The corresponding models for semiconductors are usually referred to as quantum hydrodynamic models (QHD). QHDs consist in a hierarchy of coupled moment

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equations [10, 12, 16] which are supplemented with closure conditions [23]. Naturally, the more moment equations are considered the closer the model is to the microscopic approach. The price one has to pay is an increasingly cumbersome implementation and the specification of the moment's boundary conditions.

In this paper we shall be concerned with a first-moment version of the QHD. Neglecting — as in the classical case — velocity's convection term one gets the quantum drift-diffusion model (QDD) [3, 4]. The advantage of this approach is threefold. Firstly, the model equations equal up to a quantum correction term the classical drift diffusion model. Hence the computation of current–voltage characteristics can be carried out with comparably little effort. A reduction of redundancy in regions where the device behaves "almost" classical can be expected. Secondly, there is a natural way to prescribe boundary conditions — at least in situations where the device's state is not "far away" from thermal equilibrium. Thirdly, for the QDD investigated here unipolar *and* bipolar versions are available. The bipolar version extends available QHDs and allows to incorporate generation–recombination effects.

The scaled, stationary QDD stated on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or $d = 3$ reads [1]

$$\left\{\begin{aligned} -\varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V + B_n &= F, \\ -\xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}} + \log(p) - V + B_p &= G, \\ \operatorname{div}(\mu_n\, n \nabla F) &= R(n,p)\,\left(\exp(F+G) - \delta^2\right), \\ \operatorname{div}(\mu_p\, p \nabla G) &= R(n,p)\,\left(\exp(F+G) - \delta^2\right), \\ -\lambda^2 \Delta V &= n - p - C_{dot}. \end{aligned}\right. \tag{1.1}$$

The *scaled* physical parameters are the Planck constant ε, the ratio ξ of the effective masses of electrons and holes and the mobilities μ_n, μ_p of electrons and holes, respectively, and the Debye length λ. All these quantities are assumed to be positive constants, excluding especially field dependent mobilities. The doping profile $C_{dot} = C_{dot}(x)$ (where x is the spatial variable ranging in Ω) representing a fixed charge distribution and the non-negative quantum well potentials $B_{n,p} = B_{n,p}(x)$ are assumed to be fixed. Equation (1.1) includes generation-recombination processes of the form $R(n,p)\left(\exp(F+G) - \delta^2\right)$, where $R : \mathbb{R}^2 \to \mathbb{R}$ and $\delta > 0$. In thermal equilibrium there is no generation-recombination process. Hence, $\delta^2 = \exp(F_{eq} + G_{eq})$, where F_{eq}, G_{eq} are the (constant!) equilibrium values of the Quantum Quasi Fermi Levels, see [1]. The model includes Shockley–Read–Hall and Auger generation-recombination processes but excludes generation through impact ionization [24].

In (1.1) the electron density $n = n(x) \geq 0$, the hole density $p = p(x) \geq 0$, the Quantum Quasi Fermi levels $F = F(x), G = G(x)$ and the electrostatic potential $V = V(x)$ are unknown. The current densities of electrons and holes are determined by the charge densities, the quantum quasi Fermi levels F, G and the mobilities:

$$J_n = \mu_n\, n \nabla F, \quad J_p = -\mu_p\, p \nabla G. \tag{1.2}$$

The model equations (1.1) are supplemented with mixed Dirichlet-Neumann boundary conditions

$$n = n_D, \quad p = p_D, \quad V = V_{eq} + V_{ext} \text{ on } \Gamma_D, \tag{1.3a}$$

$$F = F_{eq} + V_{ext}, \quad G = G_{eq} - V_{ext} \text{ on } \Gamma_D, \tag{1.3b}$$

$$\nabla n \cdot \nu = \nabla p \cdot \nu = \nabla V \cdot \nu = 0 \text{ on } \Gamma_N, \tag{1.3c}$$

$$\nabla F \cdot \nu = \nabla G \cdot \nu = 0 \text{ on } \Gamma_N, \tag{1.3d}$$

where Γ_D and Γ_N are disjoint parts of the boundary of Ω with $\Gamma_D \cup \Gamma_N = \partial\,\Omega$ and ν is the unit outward normal vector along Γ_N. Along Γ_D Dirichlet boundary conditions are prescribed. The thermal equilibrium densities n_{eq} and p_{eq} are possible candidates for n_D and p_D. V_{eq} is the thermal equilibrium potential. V_{ext} is an external voltage.

Let us briefly recall available analytical results. The thermal equilibrium version of (1.1) has been analyzed in [29, 37]. The core of these investigations is the introduction of an energy functional $\mathcal{E}$ minimized in an appropriately chosen set of comparison functions. The minimizer of $\mathcal{E}$ constitutes the unique thermal equilibrium solution of (1.1). The full model equations (1.1),(1.3) were analyzed in [1] (under mild assumptions on the data) where the existence of solutions was established. The proofs rely on a combination of approximations and fixed point and minimization arguments.

The paper is organized as follows. Section 2 is devoted to the computation of the thermal equilibrium solution of (1.1). In Section 2.1 the model equations are re-formulated as a variational problem, i.e. $\mathcal{E}$ has to be minimized in a closed, convex subset C of a Hilbert space X. We prove a general Poincaré–type inequality which ensures that $\mathcal{E}$ is locally uniformly convex at its minimizer. This suggests the employment of a projected gradient method to generate minimizing sequences. However, $\mathcal{E}$ is not Fréchet–differentiable but only Gateâux differentiable in directions ranging in a dense subset D, $D \neq X$, of X. Hence, it is a priori not possible to define a gradient method. This topic is discussed in Section 2.2 for a general class of variational problems. The concept of a quasi–gradient is introduced and a *projected quasi–gradient method* is defined. We show — under mild additional assumptions — the strong convergence of minimizing sequences generated by this algorithm. In Section 2.3 the projected quasi-gradient method is discretized by means of a Galerkin-like internal approximation. Based on the general results derived so far we prove convergence for a large class of approximations.

The thermal equilibrium quantities computed by the (discretized) projected quasi-gradient method of Subsection 2.4 are employed in Section 3 where the full model equations (1.1), (1.3) are investigated. In Subsection 3.1 various (mild) assumptions on the data are collected. In Subsection 3.2 a fixed point map (modifying the argumentation of [1]) is constructed. The equations are decoupled and become numerically more tractable. Their numerical treatment is performed by an extended *Gummel–iteration* [17], which has been intensively studied in connection with the classical drift diffusion equations [19, 24] and is still successfully used in simulation codes for semiconductor devices. It is shown that the suggested fixed point mapping is actually a contraction. Thus, the convergence of the iteration scheme essentially follows from Banach's fixed point theorem. In Subsection 3.3 convergence properties of this method are investigated. We distinguish the cases of vanishing and non vanishing generation–recombination terms. In the former we prove contractivity of the fixed point mapping for sufficiently small values of the applied bias potential. This settles global convergence of the iteration scheme. In the latter we derive additional conditions (the Quantum Quasi Fermi Levels F, G have to be "close" to their equilibrium values F_{eq}, G_{eq}) to ensure that the mapping is still a contraction. In Subsection 3.4 numerical simulations of a one dimensional RTD are presented. The computed current–voltage characteristics (IVCs) show NDR for the first time in a QDD model and are in good qualitative agreement with experimental measurements.

2. Computation of the Thermal Equilibrium State. The boundary conditions (1.3) involve the thermal equilibrium solution of (1.1) which is the minimizer of an energy functional $\mathcal{E}$ in a subset C of a Hilbert space X. Such minimizers are frequently computed by descent gradient algorithms, see e.g. [22], for which various convergence results are available. The assumptions on $\mathcal{E}$ vary from mild ones (which ensure convergence in a weak sense [34]) to stringent ones (which allow to estimate the rate of convergence [9]).

The functional $\mathcal{E}$ investigated here fails to be Gateâux–differentiable. $\mathcal{E}$ is only "quasi–differentiable". Roughly speaking the domain of $\mathcal{E}$ is "too small" to take directional derivatives in *all* directions of X. Hence $\mathcal{E}$ has no gradient. On the other hand $\mathcal{E}$ need not have a gradient to define a descent–gradient–like algorithm: If the linear Taylor expansion of $\mathcal{E}$ is available on C for "sufficiently many" directions, then it will be possible to define the "quasi–gradient" of $\mathcal{E}$. For energy functionals with quasi–gradients a "projected quasi–gradient method" can be defined. By this method approximative minimizers are generated which converge (under additional assumptions not mentioned here) strongly to the minimizer of $\mathcal{E}$ in C.

2.1. The Variational Problem. The investigations of this subsection are based on the following assumptions:

A.1 $\Omega \subset \mathbb{R}^d, d = 1, 2$ or $d = 3$ is a non-void, convex, bounded domain.

A.2 There exists a constant $K = K(\Omega) \in (0, \infty)$ such that for all $f \in L^2(\Omega)$,

$$\|V[f]\|_{L^\infty(\Omega)} \le K \|f\|_{L^2(\Omega)},$$

where $\Delta V[f] = f$.

A.3 $B_n, B_p, C_{dot} \in L^\infty(\Omega)$ and $B_{n,p} \ge 0$.

Remark 1. *Assumption* **A**.*2 is essentially a requirement on the smoothness of $\partial\Omega$. For instance it is well known, see e.g. [7], that for $\partial\Omega \in C^\infty$ and $f \in L^2(\Omega)$ the estimate*

$$\|V[f]\|_{H^2(\Omega)} \le K \|f\|_{L^2(\Omega)}$$

holds. This estimate implies in dimensions $d \le 3$ assumption **A**.*2, because due to $\partial\Omega \in C^{0,1}$ (Ω is convex by* **A**.*1) the embedding $H^2(\Omega) \to C_B(\Omega)$ is continuous [2].*

The thermal equilibrium state is the state of minimal total energy [29, 37]

$$\begin{aligned} \mathcal{E}(n,p) = \varepsilon^2 \int_\Omega \left|\nabla\sqrt{n}\right|^2 \, dx + \xi\varepsilon^2 \int_\Omega \left|\nabla\sqrt{p}\right|^2 \, dx + \int_\Omega H(n) \, dx + \int_\Omega H(p) \, dx \\ + \frac{\lambda^2}{2} \int_\Omega \left|\nabla V\left[n - p - C_{dot}\right]\right|^2 \, dx + \int_\Omega B_n \, n \, dx + \int_\Omega B_p \, p \, dx. \end{aligned}$$

in the set

$$\begin{aligned} \mathcal{C} := \Big\{(n,p) \in L^1(\Omega) \times L^1(\Omega) : \quad n, p \ge 0, \quad \sqrt{n}, \sqrt{p} \in H^1(\Omega)\,, \\ \int_\Omega n \, dx = N, \quad \int_\Omega p \, dx = P\Big\}, \end{aligned}$$

where $H(t) = t\log(t) - t + 1$ is a primitive of $h(t) = \log t$, $N := \int_\Omega C_{dot}^+ \, dx$, $P := \int_\Omega C_{dot}^- \, dx$ and $V = V[n-p-C_{dot}]$ is the self consistent electrostatic potential defined via $-\lambda^2 \Delta V = n - p - C_{dot}$ with $\int_\Omega V(x) \, dx = \int_\Omega (n - p - C_{dot}) \, dx$. (We note that $\int_\Omega (n - p - C_{dot}) \, dx = 0$ for all $(n,p) \in \mathcal{C}$.)

Let us recall [37] that

Theorem 2. *Assume* **A**.*1*–**A**.*3. Then* $\mathcal{E}$ *has a unique minimizer* (n_{eq}, p_{eq}) *in* $\mathcal{C}$ *and* n_{eq}, p_{eq} *and* $V_{eq} := V[n_{eq} - p_{eq} - C_{dot}]$ *have the following properties:*
a) $n_{eq}, p_{eq}, V_{eq} \in C_B(\Omega) \cap H^1(\Omega)$.
b) There exists a constant $\theta_{eq} \in (0,1)$ *such that* $\theta_{eq} \leq n_{eq}, p_{eq} \leq 1/\theta_{eq}$.
c) There exist constants $F_{eq}, G_{eq} \in \mathbb{R}$ *such that*

$$-\varepsilon^2 \frac{\Delta\sqrt{n_{eq}}}{\sqrt{n_{eq}}} + \log(n_{eq}) + V_{eq} + B_n = F_{eq}$$

$$-\xi\varepsilon^2 \frac{\Delta\sqrt{p_{eq}}}{\sqrt{p_{eq}}} + \log(p_{eq}) - V_{eq} + B_p = G_{eq}$$

We want to construct an algorithm which generates minimizing sequences of $\mathcal{E}$ converging in some strong sense to (n_{eq}, p_{eq}). It is adviseful to exploit the fact that (n_{eq}, p_{eq}) not only belongs to $L^1(\Omega) \times L^1(\Omega)$ but also to the Hilbert space $X := H^1(\Omega) \times H^1(\Omega)$. We therefore consider $\mathcal{E}$ as a mapping from the convex set

$$M := \left\{(n,p) \in X : \quad n, p \geq 0, \quad \sqrt{n}, \sqrt{p} \in H^1(\Omega)\right\}$$

to $\mathbb{R}^+ \cup \{0\}$. The reader may wish to verify

Proposition 3. *Assume* **A**.*1*–**A**.*3. Then* $\mathcal{E}$ *is sequentially lower semi continuous, strictly convex and coercive on* M.

We furthermore observe that n_{eq}, p_{eq} belong to $H^2(\Omega)$: By Theorem 2 we have $\Delta\sqrt{n_{eq}}, \Delta\sqrt{p_{eq}} \in L^\infty(\Omega)$ and both $\sqrt{n_{eq}}$ and $\sqrt{p_{eq}}$ satisfy homogeneous Neumann boundary conditions. Thus, we have $\sqrt{n_{eq}}, \sqrt{p_{eq}} \in H^2(\Omega)$, see [15], and therefore due to the uniform bounds on n_{eq}, p_{eq} it follows that $n_{eq}, p_{eq} \in H^2(\Omega)$. This observation makes it possible to replace $\mathcal{C}$ by a set C of smoother functions without changing the minimizer of $\mathcal{E}$:
Since $\partial\Omega$ belongs to $C^{0,1}$ we can find $r, s \in (2, \infty]$ with $r^{-1} + s^{-1} = 2^{-1}$ such that [2]

$$H^1(\Omega) \hookrightarrow L^s(\Omega) \quad \text{and} \quad H^2(\Omega) \hookrightarrow W^{1,r}(\Omega).$$

In fact, we can choose if $d = 1$: $r = 2, s = \infty$, and if $d = 2$: $s \in (2, \infty)$ and if $d = 3$: $r = 3, s = 6$. We define

$$C := \left\{(n,p) \in X : \quad \underline{K} \leq n, p \leq \overline{K}, \quad \int_\Omega n\, dx = N, \int_\Omega p\, dx = P, \right.$$
$$\left. \|n\|_{W^{1,r}(\Omega)}, \|p\|_{W^{1,r}(\Omega)} \leq \overline{K} \right\},$$

where we take $\underline{K}, \overline{K} \in (0, \infty)$ such that $(n_{eq}, p_{eq}) \in C$. One easily verifies that

Proposition 4. *Assume* **A**.*1*–**A**.*3. Then* C *is a closed and convex subset of* X, $C \subseteq M$ *and* (n_{eq}, p_{eq}) *is the unique minimizer of* $\mathcal{E}$ *in* C.

Our next observation concerns the local behaviour of $\mathcal{E}$ at (n_{eq}, p_{eq}). We need a technical Poincaré-type lemma whose proof can be found in the appendix.

Lemma 5. *Assume* **A**.*1 and let* $u \in W^{1,r}(\Omega)$ *with* $m \leq u \leq M$ *a.e. for some* $0 < m < M < \infty$. *Then there exists for all* $\beta \in \mathbb{R}$ *a constant* $K = K(\Omega, u, \beta) \in (0, \infty)$ *such that for all* $\phi \in H^1(\Omega)$ *with* $\int_\Omega \phi\, dx = 0$*:*

$$\int_\Omega u^\beta \left|\nabla\left(\frac{\phi}{u}\right)\right|^2 dx \geq K \|\nabla\phi\|^2_{L^2(\Omega)}. \tag{2.1}$$

With the aid of lemma 5 we can prove

Lemma 6. *Assume* **A**.*1*–**A**.*3. Then* $\mathcal{E}$ *is uniformly convex at* (n_{eq}, p_{eq}), *i.e.*

$$\exists\, m > 0 \quad \forall\, (n,p) \in C: \quad \mathcal{E}(n,p) - \mathcal{E}(n_{eq}, p_{eq}) \geq m \, \|(n,p) - (n_{eq}, p_{eq})\|_X^2 .$$

The proof of lemma 6 is deferred to the appendix.

This uniform convexity of $\mathcal{E}$ at its minimizer makes it adviseful to choose a projected gradient method to generate minimizing sequences. However, $\mathcal{E}$ is defined on a set with empty interior. Hence, $\mathcal{E}$ cannot be Fréchet differentiable on X and it is not possible to define the projected gradient method. On the other hand $\mathcal{E}$ is Gateâux differentiable in directions ranging in a dense subset of X.

Lemma 7. *Assume* **A**.*1*–**A**.*3. Let* $D = \left(H^1(\Omega) \cap L^\infty(\Omega)\right)^2$. *Then:*

a) D *is a dense subset of* X.

b) $C - C \subseteq D$.

c) For all $(\varphi_1, \varphi_2) \in D$ *there is* $t_\circ = t_\circ(\varphi_1, \varphi_2) \in (0, \infty)$ *such that* $(n,p) + t(\varphi_1, \varphi_2) \in M$ *for all* $(n,p) \in C$ *and all* $t \in [0, t_\circ]$.

d) The Gateâux derivative $\mathcal{E}'(n,p)[\varphi_1, \varphi_2]$ *exists for all* $(n,p) \in C$ *and all directions* $(\varphi_1, \varphi_2) \in D$:

$$\begin{aligned}
\mathcal{E}'(n,p)[\varphi_1, \varphi_2] = \; & \frac{\varepsilon^2}{4} \int_\Omega \frac{2\, n\, \nabla n \nabla \varphi_1 - |\nabla n|^2 \varphi_1}{n^2} \, dx \\
& + \frac{\varepsilon^2}{4} \int_\Omega \frac{2\, p\, \nabla p \nabla \varphi_2 - |\nabla p|^2 \varphi_2}{p^2} \, dx \\
& + \int_\Omega \log(n) \varphi_1 \, dx + \int_\Omega \log(p) \varphi_2 \, dx \\
& + \int_\Omega V[n - p - C_{dot}] \, (\varphi_1 - \varphi_2) \, dx \\
& + \int_\Omega B_n \, \varphi_1 \, dx + \int_\Omega B_p \, \varphi_2 \, dx.
\end{aligned}$$

e) For all $(n,p) \in C$ *the mapping* $(\varphi_1, \varphi_2) \mapsto \mathcal{E}'(n,p)[\varphi_1, \varphi_2]$ *is linear and bounded on* D.

The proof of Lemma 7 can be found in the appendix.

Due to e) of Lemma 7 there is for all $(n,p) \in C$ a unique linear and bounded extension $\delta\mathcal{E}(n,p) \in X'$ of $\mathcal{E}'(n,p)$. We shall call this extension the "quasi–gradient of $\mathcal{E}$ at (n,p)". Concerning the mapping $\delta\mathcal{E} : C \to X'$ we have the following regularity result whose proof is deferred to the appendix.

Lemma 8. *Assume* **A**.*1*–**A**.*3. Then* $\delta\mathcal{E}$ *is Lipschitz continuous on* C.

As we shall immediately see, the properties of $\mathcal{E}$ derived so far are sufficient to define a projected quasi–gradient method. The definition of this method and its analysis is the content of the following subsection. We will prove the strong convergence of minimizing sequences generated by this algorithm and establish the respective convergence of a discretized version for a large class of approximations.

2.2. The Projected Quasi–Gradient Method. Let X be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. Let C, M, D be subsets of X. We assume

V.1 D is dense in X.

V.2 C and M are convex sets with $\emptyset \neq C \subseteq M$.

V.3 C is closed and $C - C \subset D$.

V.4 For all $\varphi \in D$ there is $t_\circ = t_\circ(\varphi) \in (0, \infty)$ such that $c + t\varphi \in M$ for all $c \in C$ and all $t \in [0, t_\circ]$.

We consider a functional $\mathcal{E} : M \to \mathbb{R}^+ \cup \{0, \infty\}$ where we assume that

V.5 $\mathcal{E} \not\equiv \infty$ is sequentially lower semi continuous, strictly convex and coercive.

V.6 The Gateâux derivative $\mathcal{E}'(c)[\varphi]$ exists for all $c \in C$ and all directions $\varphi \in D$.

V.7 $\mathcal{E}'(c) : D \to \mathbb{R}$ is linear and bounded for all $c \in C$.

Since D is dense in X we can define the "quasi-gradient" of $\mathcal{E}$:

Definition 9. *Assume* **V**.*1*–**V**.*7 and let $c \in C$. The uniquely determined linear and bounded extension $\delta\mathcal{E}(c) \in X'$ of $\mathcal{E}'(c)$ is called the* quasi–gradient *of $\mathcal{E}$ at c.*

Remark 10.

a) If $\mathcal{E}$ is Gateâux-differentiable at $c \in C$ then the quasi-gradient of $\mathcal{E}$ at c coincides with the gradient of $\mathcal{E}$ at c.

b) Since we are working in a Hilbert space we identify $\delta\mathcal{E}$ with its Riesz–representative, again denoted by $\delta\mathcal{E}$.

We furthermore assume

V.8 The mapping $c \mapsto \delta\mathcal{E}(c)$ is Lipschitz continuous on C, i.e. there is a constant $L > 0$ such that for all $c_1, c_2 \in C$

$$\|\delta\mathcal{E}(c_1) - \delta\mathcal{E}(c_2)\|_X \leq L \|c_1 - c_2\|_X$$

In the sequel we shall be concerned with the constrained minimization problem

$$\min_{c \in C} \mathcal{E}(c).$$

Due to the assumptions imposed so far it follows from standard results (see, e.g. [35]) that $\mathcal{E}$ has a unique minimizer $\tilde{c}$ in C. We additionally require

V.9 $\mathcal{E}$ is uniformly convex at $\tilde{c}$, i.e. there exists an $m > 0$ such that for all $c \in C$

$$\mathcal{E}(c) - \mathcal{E}(\tilde{c}) \geq m \|c - \tilde{c}\|_X^2 . \tag{2.2}$$

Since C is closed and convex the projection

$$\begin{array}{cccc} P & : & X & \to & C \\ & & u & \mapsto & P(u) \end{array}$$

is well defined. (We recall that $P(u)$ is the unique minimizer of the mapping $\|. - u\|_X : C \to [0,\infty), c \mapsto \|c - u\|_X$.) We are now in the position to define the projected quasi–gradient method.

Algorithm 1.

1. *Choose $c^0 \in C$, $\gamma \in (0,1)$ and $\bar{a} > 0$.*
2. *For $k \in \mathbb{N}_0$ compute the step length*

$$\alpha^k = \sup \left\{ \alpha \in [0, \bar{a}] : \mathcal{E}\left(c^k\right) - \mathcal{E}\left(P\left(c^k - \alpha\, \delta\mathcal{E}(c^k)\right)\right) \geq \gamma \left\langle \delta\mathcal{E}\left(c^k\right), c^k - P\left(c^k - \alpha\, \delta\mathcal{E}(c^k)\right)\right\rangle \right\} \tag{2.3}$$

and set $c^{k+1} = P\left(c^k - \alpha^k\, \delta\mathcal{E}(c^k)\right)$.

Remark 11. *Equation* (2.3) *is known as Armijo's rule (see [22]).*

The main result of this subsection is

Theorem 12. *Assume* **V**.*1* - **V**.*9. Then the sequence $\left(c^k\right)_{k \in \mathbb{N}_0}$ of Algorithm 1 converges to $\tilde{c}$ strongly in X as $k \to \infty$.*

The proof of Theorem 12 is deferred to the appendix.

2.3. Internal Approximation. As in Subsection 2.2. let X be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. Let C, M be subsets of X where we assume

D.0 C, M are convex subsets of X. C is closed. $\emptyset \neq C \subseteq M$.

Assumption **D**.0 ensures that the projection P of X onto C is well defined.

To compute the minimizer $\tilde{c}$ of $\mathcal{E}$ numerically we have to discretize Algorithm 1. For this purpose let, by a slight abuse of notation, (h) denote a sequence of positive discretization parameters tending to zero.

Firstly, we shall be concerned with discretizations of X_h and C_h of X and C, respectively. Let $W \subseteq X$. We assume

D.1 For all h: X_h is a finite dimensional subspace of X. X_h is equipped with the inner product induced by X.
D.2 W is a dense subspace of X.
D.3 For all h: $\emptyset \neq C_h \subset X_h \cap M \cap W$. C_h is closed and convex.
D.4 For all h and all $\varphi_h \in X_h$ there is $t_h = t_h(\varphi_h) \in (0, \infty)$ such that $c_h + t\varphi_h \in X_h \cap M$ for all $c_h \in C_h$ and all $t \in [0, t_h]$

By assumption **D**.1 the projection Π_h of X onto X_h is well defined for all h. Due to **D**.3 the projection P_h of X onto C_h is well-defined. We assume

D.5 For all $c \in C$: $\lim\limits_{h\to 0} \|P_h c - c\|_X = 0$.
D.6 For all $r > 0$: $\lim\limits_{h\to 0} \sup\limits_{\substack{c_h \in C_h,\\ \|c_h\|_X \le r}} \|Pc_h - c_h\|_X = 0$.

Remark 13. *Note that neither $C_h \subset C$ nor $C \subset C_h$ is required and that the straight forward assumption $\lim\limits_{h\to 0} \sup\limits_{c_h \in C_h} \|Pc_h - c_h\|_X = 0$ does not even hold for quadratic finite elements, if $\mathcal{C}$ consists of functions $c \ge 0$ and $\mathcal{C}_h$ of elements with $c_h(x_i) \ge 0$ at the grid points x_i.*

Let $\{R_h, h > 0\}$ be a family of restrictions of X to X_h. We assume

D.7 For all h: $R_h : X \to X_h$ is linear, bounded and onto.
D.8 For all $w \in W$: $\lim\limits_{h\to 0} \|w - R_h w\|_X = 0$.

We deduce from the assumptions imposed so far

Lemma 14. *Assume **D**.0–**D**.8. Then:*

a) Let (c_h) be a sequence with $c_h \in C_h$ for all h. Assume that $c_h \rightharpoonup v \in X$ weakly in X as $h \to 0$. Then $v \in C$.
b) For all $u \in X$: $P_h u \to Pu$ strongly in X as $h \to 0$.
c) The norms $\|R_h\|_{L(W,X_h)}$ are uniformly bounded.
d) For all $u \in X$: $\Pi_h u \to u$ strongly in X as $h \to 0$.

Remark 15. *Due to **D**.8 and due to d) of Lemma 14 the pairs (X_h, R_h) and (X_h, Π_h) are convergent internal approximations W and X, respectively [5] .*

Secondly, $\mathcal{E}$ is discretized by a family of functionals $\mathcal{E}_h : X_h \cap M \to \mathbb{R}$ and we shall solve the finite dimensional optimization problems

$$\min_{c_h \in C_h} \mathcal{E}_h\left(c_h\right).$$

We make the following assumptions

D.9 For all h: $\mathcal{E}_h : M \cap X_h \to \mathbb{R}^+ \cup \{0\}$, $\mathcal{E}_h \not\equiv \infty$, is sequentially lower semi continuous, strictly convex and coercive.
D.10 For all h: The Gateâux derivative $\mathcal{E}_h(c_h)[\varphi]$ exists for all $c_h \in C_h$ and all directions $\varphi \in X_h$.
D.11 For all h and all $c_h \in C_h$: The mapping $\varphi \mapsto \mathcal{E}'_h(c_h)[\varphi]$ is linear.

Due to the assumptions **D**.0–**D**.11 we can proceed as in Subsection 2.2 to deduce that for all h: $\mathcal{E}_h$ has a unique minimizer $\tilde{c}_h \in C_h$ and the quasi-gradient $D\mathcal{E}_h(c_h)$ (which is again identified with its Riesz–representative) exists for all $c_h \in C_h$. We assume in similarity to Subsection 2.2

D.12 $D\mathcal{E}_h$ is Lipschitz-continuous uniformly in h, i.e. there is a constant $L_\circ \in (0, \infty)$ such that for all h and all $c_{h1}, c_{h2} \in C_h$:

$$\|D\mathcal{E}_h(c_{h1}) - D\mathcal{E}_h(c_{h2})\|_X \le L_\circ \|c_{h1} - c_{h2}\|_X.$$

D.13 For all h: $\mathcal{E}_h$ is uniformly convex at $\tilde{c}_h$.

The uniformity constant of **D**.13 may depend on h. Finally, let us assume that the following consistency conditions hold:

D.14 For all $u \in M$: $\lim\limits_{h\to 0} |\mathcal{E}_h\left(R_h u\right) - \mathcal{E}(u)| = 0$.
D.15 For all $c \in C$: $\lim\limits_{h\to 0} \|D\mathcal{E}_h\left(P_h c\right) - \delta\mathcal{E}(c)\|_X = 0$.

We are now in the position to discretize Algorithm 1:

Algorithm 2.

1. *Choose* $c_h^0 \in C_h$, $\gamma \in (0,1)$ *and* $\bar{a} > 0$.
2. *For* $k \in \mathbb{N}_0$ *compute the step length*

$$\alpha_h^k = \sup\left\{\alpha \in [0,\bar{a}] : \mathcal{E}_h\left(c_h^k\right) - \mathcal{E}_h\left(P_h\left(c_h^k - \alpha\, D\mathcal{E}_h(c_h^k)\right)\right) \geq \gamma\left\langle D\mathcal{E}_h\left(c_h^k\right), c_h^k - P_h\left(c_h^k - \alpha\, D\mathcal{E}_h(c_h^k)\right)\right\rangle\right\} \quad (2.4)$$

and set $c_h^{k+1} = P_h\left(c_h^k - \alpha_h^k\, D\mathcal{E}_h(c_h^k)\right)$.

It readily follows from Theorem 12:

Theorem 16. *Assume* **D**.*0*–**D**.*15*. *Then for all* h: *The sequence* $\left(c_h^k\right)_{k\in\mathbb{N}}$ *of Algorithm 2 converges to* $\tilde{c}_h$ *in* X_h *as* $k \to \infty$.

The main result of this section is

Theorem 17. *Assume* **V**.*1*–**V**.*9 and* **D**.*0*–**D**.*15*. *Let* $c^0 \in C$ *be the starting point of Algorithm 1. Assume for the respective starting points of Algorithm 2 holds*

$$\lim_{h\to 0}\left\|c_h^0 - R_h c^0\right\|_X = 0.$$

Then for all $k \in \mathbb{N}_0$:

$$\lim_{h\to 0}\left\|c_h^k - R_h c^k\right\|_X = 0.$$

The proof of Theorem 17 is deferred to the appendix.

Finally we observe that the results derived so far ensure that

Corollary 18. *Assume* **V**.*1*–**V**.*9 and* **D**.*0*–**D**.*15*. *Then* $\tilde{c}_h$ *converges to* $\tilde{c}$ *strongly in* X *as* $h \to 0$. The proof of Corollary 18 is deferred to the appendix.

2.4. Numerical Results. We employ Algorithm 1 to compute the thermal equilibrium state of a GaAs–AlGaAs double barrier structure. The device consists of a quantum well GaAs–layer sandwiched between two $\mathrm{Al_xGa_{1-x}As}$–layers, each 50 Å thick. This resonant barrier structure is itself sandwiched between two spacer layers of GaAs, each also 50 Å thick, and the whole channel lies in between the source and drain contact GaAs–layers of 250 Å thickness, respectively (see Figure 2.1).

The contact layers are n^+–doped with a doping density $C_{dot} = 10^{24}\,\mathrm{m}^{-3}$, while in the channel the doping is only $C_{dot} = 5\cdot 10^{21}\,\mathrm{m}^{-3}$. The barrier height B depends on the content of the content of aluminium, such that a low Al concentration implies a lower barrier height. As the equilibrium densities are crucial for the choice of 'correct' boundary conditions for the non–equilibrium problem, we will present numerical results for different heights B. These give numerical evidence that there is almost no influence of the barrier height B on the boundary values of the equilibrium densities.

We use a reduced one–dimensional version of (1.1) since the diode can be modeled as an unipolar device. Then, the unscaled QDD equations read

$$-\frac{\hbar^2}{6m}\frac{(\sqrt{n})_{xx}}{\sqrt{n}} + k_B\,T\log(n) + q\,V + B = F \quad (2.5a)$$

$$J = \mu_n\, n\, F_x, \quad J_x = 0 \quad (2.5b)$$

$$-\epsilon\, V_{xx} = q\,(n - C_{dot}) \quad (2.5c)$$

and they are considered on the interval $\Omega = (0, L)$.

The physical constants are the reduced Planck constant $\hbar = 1.05\cdot 10^{-34}\,\mathrm{V\,A\,s^2}$ the Boltzmann constant $k_B = 1.38\cdot 10^{-23}\,\mathrm{V\,A\,s\,K^{-1}}$, the elementary charge $q = 1.6\cdot 10^{-19}\,\mathrm{A\,s}$ and the permittivity of GaAs, $\epsilon = 12.9\cdot\epsilon_0 = 1.14\cdot 10^{-12}\,\mathrm{A\,s/V\,cm}$.

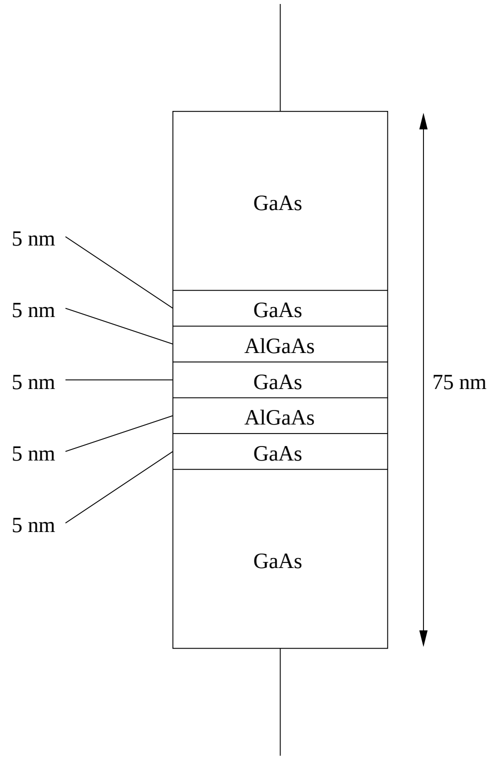

FIG. 2.1. *Resonant tunneling diode*

Furthermore, we have to specify the parameters of the device, as the device temperature $T = 77\,\mathrm{K}$, the device length $L = 750$ Å, the mobility of electrons $\mu_n = 25000\,\mathrm{cm}^2\,\mathrm{V}^{-1}\mathrm{s}^{-1}$ and the effective electron mass $m = 0.067 \cdot m_0 = 0.57 \cdot 10^{-31}\,\mathrm{kg}$.

We assume m to be constant along the device and ignore the effective jumps at the heterojunctions, although there are results giving evidence that their incorporation yields a higher accuracy of the device's current–voltage characteristics. This will be discussed more detailed in Section 3.5.

The variables are scaled in the following way:

$$x \to L\,\tilde{x}, \qquad n \to C_m\,\tilde{n}, \qquad F \to k_B\,T\,\tilde{F},$$
$$J \to \frac{\mu_n\,C_m\,k_B\,T}{L}\tilde{J}, \qquad V \to U_T\,\tilde{V}, \qquad C_{dot} \to C_m\,\tilde{C}_{dot}.$$

Here, C_m denotes the maximal density of charged background ions and $U_T = k_B T/q$ the thermal voltage. This scaling yields

$$\varepsilon^2 = \frac{\hbar^2}{6\,k_B\,T\,m_n\,L^2}, \quad \lambda^2 = \frac{\epsilon\,U_T}{q\,C_m\,L^2}.$$

To get a convergent internal approximation of $H^1(0,1)$ we define X_h as a space of linear finite elements with the canonical restriction R_h. The verification of Assumptions **D**.0—**D**.15 is straight forward and omitted here. We used a grid with 300 points and the computations were done for piecewise constant doping profile and barriers, but smoothing is possible and will improve the performance of the implemented code. The computed equilibrium densities can be found in Figure 2.2, where we also plotted the doping density for reference. One verifies that the influence of the barriers is only local in the resonant structure, such that the equilibrium densities fulfill the classical assumption of charge neutrality at the boundary (cf.

[24]). For a detailed discussion of boundary values for ultra small devices see [30]. Figure 2.3 shows the built–in potential and the computed Quantum Quasi Fermi Level. Note that these two coinci! de at the boundary points, which will be essential for the derivation of boundary values for the non–equilibrium problem.

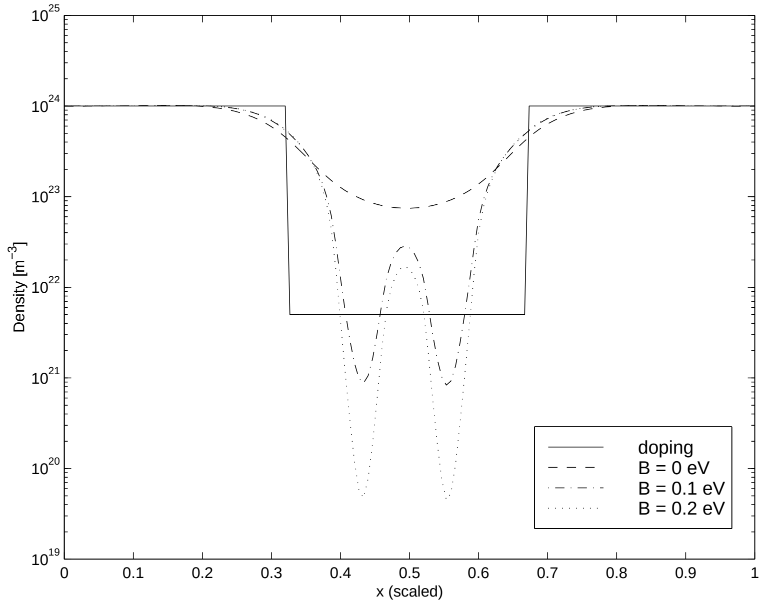

FIG. 2.2. *Equilibrium densities*

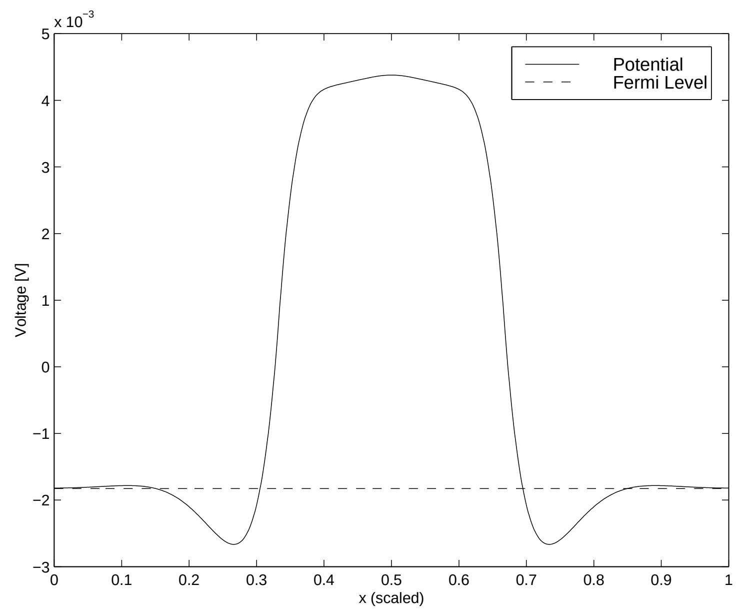

FIG. 2.3. *Built–in potential and Fermi Level for* $B = 0.1\text{eV}$

3. Computation of Current–Voltage Characteristics. In Subsection 3.1 we collect some assumptions required for the following investigations. The iteration scheme for the computation of the current–voltage characteristics is formally introduced in Subsection 3.2. The algorithm relies on a decoupling strategy generalizing the Gummel–iteration for the classical drift diffusion model. In Subsection 3.3 the well–posedness of the corresponding fixed point mapping is proven. A convergence analysis distinguishing between the cases $R \equiv 0$ and $R \not\equiv 0$ is carried out in Subsection 3.4. Numerical simulations of a RTD are presented in Subsection 3.5.

We introduce short-hands for spaces frequently used in the sequel:

$$\begin{aligned} \mathcal{V} &:= H_0^1(\Omega \cup \Gamma_N), \\ \mathcal{X} &:= H^1(\Omega) \cap L^\infty(\Omega), \\ \mathcal{X}_0 &:= H_0^1(\Omega \cup \Gamma_N) \cap L^\infty(\Omega), \\ L^\infty(\Delta;\Omega) &:= \{f \in \mathcal{X} : \ \Delta f \in L^\infty(\Omega)\}. \end{aligned}$$

Let us recall that $H_0^1(\Omega \cup \Gamma_N)$ is the closure of $C_c^\infty(\Omega \cup \Gamma_N)$ with respect to the $H^1(\Omega)$-norm. Equipped with the inner product of $H^1(\Omega)$, $H_0^1(\Omega \cup \Gamma_N)$ is a Hilbert-space.

3.1. Assumptions. We impose several assumptions on the data extending **A**.1–**A**.3 of Subsection 2.1. Let us recall

A.1 $\Omega \subset \mathbb{R}^d, d = 1, 2$ or $d = 3$ is a non-void, convex, bounded domain.

A.2 There exists a constant $K = K(\Omega) \in (0, \infty)$ such that for all $f \in L^2(\Omega)$,

$$\|V[f]\|_{L^\infty(\Omega)} \le K \|f\|_{L^2(\Omega)},$$

where $\Delta V[f] = f$.

A.3 $B_n, B_p, C_{dot} \in L^\infty(\Omega)$ and $B_{n,p} \ge 0$

We require some properties of the Dirichlet- and Neumann-boundary of Ω.

A.4 The boundary Γ of Ω is piecewise regular. Γ is the disjoint union of Γ_D and Γ_N. Γ_D has non vanishing $(d-1)$-dimensional Lebesgue measure. Γ_N is closed.

A.5 $\Gamma_D = \bigcup_{l=1}^M \Gamma_D^l$, where $M \ge 2$ and $\mathrm{dist}(\Gamma_D^{l_1}, \Gamma_D^{l_2}) > 0$ for $l_1 \neq l_2$ and $l_1, l_2 \in \{1, \dots, M\}$.

Remark 19.

a) Assumptions **A**.*1 and* **A**.*4 ensure the existence of a constant* $K = K(\Omega, \Gamma_D, \Gamma_N) \in (0, \infty)$ *such that for all* $u \in \mathcal{V}$ *[36]:*

$$\|u\|_{L^2(\Omega)} \le K \ \|\nabla u\|_{L^2(\Omega)}.$$

b) The sets $\Gamma_D^1, \dots, \Gamma_D^M$ *of* **A**.*5 are Ohmic contacts, while* Γ_N *are the insulating parts of the boundary. Due to* $M \ge 2$ *we have at least two Ohmic contacts. The assumption on the distance of two Ohmic contacts implies that they are pairwise separated by the insulating boundary* Γ_N. *This is realistic from the physical point of view (otherwise there could be short circuitin) and essential for the regularity of the solutions.*

The function R arising in the generation-recombination term is assumed to satisfy

A.6 $R \in C(\mathbb{R}^2)$ is non-negative and Lipschitz–continuous on closed intervals of $(0,\infty)^2$, i.e. for all $\theta \in (0,1)$ there exists a Lipschitz-constant $L_R(\theta) \in (0,\infty)$ such that for all $n_1, n_2, p_1, p_2 \in [\theta, 1/\theta]$

$$|R(n_1,p_1) - R(n_2,p_2)| \le L_R(\theta) \left(|n_1 - n_2| + |p_1 - p_2|\right).$$

Remark 20. *Clearly,* **A**.*6 is fulfilled for the Shockley–Read–Hall term*

$$R_{SRH}(n,p) = \frac{1}{a_0 + a_1 \ |n| + a_2 \ |p|},$$

and the Auger generation–recombination term

$$R_{AU}(n,p) = b_0 \ |n| + b_1 \ |p|,$$

with positive constants a_0, a_1, a_2, b_0 and b_1 [24].

As already mentioned in Subsection 2.1 the assumption **A**.1 imposed on Ω ensures the existence of $r, s \in (2, \infty]$ with $r^{-1} + s^{-1} = 2^{-1}$ and [2]

$$H^1(\Omega) \hookrightarrow L^s(\Omega) \quad , \quad H^2(\Omega) \hookrightarrow W^{1,r}(\Omega),$$

with $r > d$. In fact we can choose if $d = 1$: $r = 2, s = \infty$, and if $d = 2$: $s \in (2, \infty)$ and if $d = 3$: $s \in [3, 6)$. We require

A.7 For all $\theta \in (0, 1)$: There exists a constant $K = K(\Omega, \Gamma_D, \Gamma_N, \theta) \in (0, \infty)$ such that for all $a \in W^{1,r}(\Omega)$: If $\theta \leq a \leq 1/\theta$, then there exists for all $f \in L^\infty(\Omega)$ and all $u_D \in W^{1,r}(\Omega)$ a function $u \in W^{1,r}(\Omega)$ with

$$\operatorname{div}(a\nabla u) = f \quad , \quad u - u_D \in H_0^1(\Omega \cup \Gamma_N),$$
$$\|u\|_{W^{1,r}(\Omega)} \leq K \left(\|u_D\|_{W^{1,r}(\Omega)} + \|f\|_{L^\infty(\Omega)} \right).$$

Remark 21.

a) *The function u of* **A**.*7 equals u_D at Γ_D and satisfies homogeneous Neumann boundary conditions at Γ_N.*
b) *There exists at most one function u solving the mixed boundary value problem of* **A**.*7.*
c) *Assumption* **A**.*7 is essentially a requirement on the domain Ω and Γ_D, Γ_N. Especially the following cases are included (assuming* **A**.*1 and* **A**.*4): The boundary of Ω belongs to $C^{1,\delta}$ for a $\delta \in (0, 1)$ ([36]), or $\Omega \subseteq \mathbb{R}^2$ is polygonal convex and $r < 4$ ([15]), or $\Omega \subseteq \mathbb{R}$.*

We rewrite the boundary conditions (1.3) in the following form

$$n - n_D, \quad p - p_D, \quad V - (V_{eq} + V_{ext}) \in \mathcal{V}, \tag{3.1a}$$
$$F - (F_{eq} + V_{ext}), \quad G - (G_{eq} - V_{ext}) \in \mathcal{V}, \tag{3.1b}$$

where we assume that

A.8 $n_D, p_D \in W^{1,r}(\Omega)$ and there exists a constant $\theta_D \in (0, 1)$ such that $\theta_D \leq n_D, p_D \leq 1/\theta_D$.
A.9 $V_{ext} \in W^{2,\infty}(\Omega)$. $\|V_{ext}\|_{L^\infty(\Omega)} \leq \Phi_{max}$.
$V_{ext}|_{\Gamma_D^l} = U_l \in \mathbb{R}$ for $l = 1, \dots, M$.
$\min\{U_l : l = 1, \dots, M\} \leq V_{ext} \leq \max\{U_l : l = 1, \dots, M\}$.

Remark 22.

a) *If one chooses $n_D = n_{eq}$ and $p_D = p_{eq}$, then* **A**.*8 will be satisfied, see Subsection 2.1.*
b) *Assumption* **A**.*8 especially implies that $\sqrt{n_D}, \sqrt{p_D} \in L^\infty(\Delta; \Omega)$.*
c) *The constant Φ_{max} of* **A**.*9 limits the applied voltage. Such a limitation is necessary to prevent blasting.*
d) *Due to* **A**.*9 he externally applied voltage V_{ext} is constant at each Ohmic contact. This assumption is very natural in applications and simplifies the presentation. The reader may wish to verify that the subsequent results also hold - with obvious changes - also in cases where it is only assumed that $V_{ext} \in W^{2,\infty}(\Omega)$.*
e) *The assumed separation properties of Γ_D^l, $l = 1, \dots, M$ (see* **A**.*5) ensure that for given $U_1, \dots, U_M \in \mathbb{R}$ there exists an extension $V_{ext} \in W^{2,\infty}(\Omega)$ coinciding with U_l on Γ_D^l for $l = 1, \dots, M$ and satisfying the estimate of* **A**.*9.*

Let us recall that [1]

Theorem 23. *Assume* **A**.*1–***A**.*9. Then the system* (1.1), (3.1) *possesses a solution* $(n, p, V, F, G) \in \mathcal{X}^5$.

3.2. The Decoupling Algorithm. We introduce a decoupling algorithm for problem (1.1), (3.1). This algorithm relies on a fixed point iteration decoupling the current equations from the rest of the system. In each iteration step two semi linear elliptic systems are solved.

We formally introduce the fixed point mapping T. Let (F_0, G_0) be a pair of Quantum Quasi Fermi Levels from an appropriately chosen set. Then we set $T(F_0, G_0) := (F_1, G_1)$, where (F_1, G_1) is computed from (F_0, G_0) as follows:

Algorithm 3.

1. *Solve the semi linear elliptic system*

$$-\varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V + B_n = F_0, \tag{3.2a}$$

$$-\xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}} + \log(p) - V + B_p = G_0, \tag{3.2b}$$

$$-\lambda^2 \Delta V = n - p - C_{dot}, \tag{3.2c}$$

subject to the boundary conditions (3.1a) *for* (n_1, p_1, V_1).

2. *Solve*

$$\operatorname{div}(\mu_n\, n_1\, \nabla F) = R(n_1, p_1)\, \left(\exp(F+G) - \delta^2\right), \tag{3.3a}$$

$$\operatorname{div}(\mu_p\, p_1\, \nabla G) = R(n_1, p_1)\, \left(\exp(F+G) - \delta^2\right), \tag{3.3b}$$

subject to the boundary conditions (3.1b) *for* (F_1, G_1).

Clearly, every fixed point of T is a solution of the original problem (1.1) with boundary conditions (3.1).

From the numerical point of view it is advantageous not to deal with a coupled system of five semi linear elliptic equations, but with two much more tractable problems: System (3.2) is similar to the thermal equilibrium problem [37], which has been intensively investigated and system (3.3) fits into the theory of monotone operators [39].

Indeed, there are other possible decoupling strategies which result in even numerically more tractable iteration schemes, but a convergence analysis would be more involved.

3.3. Well–posedness of T and Algorithm 3. In the sequel several positive constants will be denoted as K. These constants will eventually depend — amongst others — on data which are assumed to be fixed. For the sake of a smoother presentation we shorthand these data as

$$\mathbf{D} := (\mathbf{D}_{dom}, \mathbf{D}_{pot}, \mathbf{D}_{par}, \mathbf{D}_{bdry}),$$

where $\mathbf{D}_{dom} := (\Omega, \Gamma_D, \Gamma_N)$, $\mathbf{D}_{pot} := (\|B_n\|_{L^\infty(\Omega)}, \|B_p\|_{L^\infty(\Omega)}, \|C_{dot}\|_{L^\infty(\Omega)})$, $\mathbf{D}_{par} := (\varepsilon, \xi, \lambda)$ and $\mathbf{D}_{bdry} := (\theta_D, \Phi_{max}, F_{eq}, G_{eq}, \|V_{eq}\|_{L^\infty(\Omega)})$.

We shall introduce an operator T acting on the set

$$\mathcal{C} = \left\{ (F, G) \in H^1(\Omega) \times H^1(\Omega) : \|F - F_{eq}\|_{L^\infty(\Omega)}, \|G - G_{eq}\|_{L^\infty(\Omega)} \le \Phi_{max} \right\}.$$

Obviously $\mathcal{C}$ is a closed and convex subset of $H^1(\Omega) \times H^1(\Omega)$. We wish to prove that T is well-defined on $\mathcal{C}$. Let us recall that

- $r = 2$ in one space dimension,
- $r > 2$ in two space dimensions,
- $r \in (3, 6]$ in three space dimensions,

and $s \in (2,\infty]$ satisfies $s^{-1} = 2^{-1} - r^{-1}$. We observe that $W^{1,r}(\Omega) \hookrightarrow L^s(\Omega)$.

We begin with investigations of the first boundary–value problem of Algorithm 3. Again a Poincaré–type inequality (compare Lemma 5) plays a prominent role.

Lemma 24. *Assume* **A**.*1 and* **A**.*4. Then there exists for all $\beta \in \mathbb{R}$ and all $\theta \in (0,1)$ a constant $K = K(\mathbf{D}_{dom}, \beta, \theta, s) \in (0,\infty)$ such that for all $u \in \mathcal{X}$ with $\theta \le u \le 1/\theta$ and all $\phi \in \mathcal{X}_0$:*

$$\int_\Omega u^\beta \left|\nabla\left(\frac{\phi}{u}\right)\right|^2 dx \ge K \|\phi\|^2_{L^s(\Omega)} . \tag{3.4}$$

The proof of Lemma 24 is deferred to the appendix.

Remark 25. *Lemma 24 assures (together with the estimates on n and p) that the quantum operators $A(\rho) = \Delta\sqrt{\rho}/\sqrt{\rho}$, $\rho = n$ or $\rho = p$, are monotonic with respect to the $L^s(\Omega)$–norm. Alternatively, one can deduce that the second variation of the quantum energy term*

$$\mathcal{E}_{quant}(\rho) = \int_\Omega |\nabla\sqrt{\rho}|^2 \, dx$$

is positive definite with respect to the $L^s(\Omega)$–norm. This property has already turned out to be essential for the understanding of the thermal equilibrium problem, see Subsection 2.1.

With the aid of Lemma 24 we can prove

Theorem 26. *Assume* **A**.*1–***A**.*9. Then:*

a) For all $(F,G) \in \mathcal{C}$: The system

$$-\varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V + B_n = F, \tag{3.5a}$$

$$-\xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}} + \log(p) - V + B_p = G, \tag{3.5b}$$

$$-\lambda^2 \Delta V = n - p - C_{dot}, \tag{3.5c}$$

subject to the boundary conditions (3.1a) *has a unique solution $(n_\circ, p_\circ, V_\circ) \in (n_D, p_D, V_{eq} + V_{ext}) + (\mathcal{V}\times\mathcal{V}\times\mathcal{V})$. Thus, there exist operators*

$$\begin{array}{rccl} S_1 & : & \mathcal{C}\times\mathcal{C} & \to & (n_D, p_D) + (\mathcal{V}\times\mathcal{V}) \\ & & (F,G) & \mapsto & S_1(F,G), \end{array}$$

$$\begin{array}{rccl} S_V & : & \mathcal{C}\times\mathcal{C} & \to & (V_{eq} + V_{ext}) + \mathcal{V} \\ & & (F,G) & \mapsto & S_V(F,G), \end{array}$$

such that for all $(F,G) \in \mathcal{C}$: The triple $(S_1(F,G), S_V(F,G))$ is the unique solution of (3.5),(3.1a).

b) There exists a constant $\theta = \theta(\mathbf{D}) \in (0,1)$ such that for all $(F,G) \in \mathcal{C}$: The unique solution $(n_\circ, p_\circ, V_\circ) = (S_1(F,G), S_V(F,G))$ of (3.5),(3.1a) *satisfies*

$$\begin{gathered} \theta \le n_\circ, p_\circ \le 1/\theta, \\ \|\Delta\sqrt{n_\circ}\|_{L^\infty(\Omega)}, \|\Delta\sqrt{p_\circ}\|_{L^\infty(\Omega)}, \|V_\circ\|_{L^\infty(\Omega)} \le 1/\theta. \end{gathered} \tag{3.6}$$

c) There exists a constant $K = K(\mathbf{D}, s) \in (0,\infty)$ such that for all $(F,G), (F_1,G_1) \in \mathcal{C}$:

$$\begin{aligned} &\|n_\circ - n_1\|_{L^s(\Omega)} + \|p_\circ - p_1\|_{L^s(\Omega)} \\ &\qquad \le K\left(\|F - F_1\|_{L^2(\Omega)} + \|G - G_1\|_{L^2(\Omega)}\right), \end{aligned} \tag{3.7}$$

where $(n_\circ, p_\circ) = S_1(F,G)$ and $(n_1, p_1) = S_1(F_1, G_1)$.

The proof of Theorem 26 (which is deferred to the appendix) heavily relies on the fact that S_1 is Lipschitz–continuous, see c). The Lipschitz–continuity of S_1 is a consequence of the Poincaré-type inequality of Lemma 24.

The definition of T is completed by the second step of Algorithm 3. We prove

Theorem 27. *Assume* **A**.*1*–**A**.*9. Then:*

a) For all $(n,p) \in S_1(\mathcal{C})$*: The system*

$$\operatorname{div}(n\,\nabla F) = R(n,p)\,\left(\exp(F+G) - \delta^2\right), \tag{3.8a}$$

$$\operatorname{div}(p\,\nabla G) = R(n,p)\,\left(\exp(F+G) - \delta^2\right), \tag{3.8b}$$

subject to the boundary conditions (3.1b) *has a unique solution* $(F_\circ, G_\circ) \in (F_{eq} + V_{ext}, G_{eq} - V_{ext}) + (\mathcal{V}\times\mathcal{V})$. *Thus, there exist an operator*

$$\begin{array}{rccl} S_2 & : & S_1(\mathcal{C}) & \rightarrow & (F_{eq}+V_{ext}, G_{eq}-V_{ext}) + (\mathcal{V}\times\mathcal{V}) \\ & & (n,p) & \mapsto & S_2(n,p), \end{array}$$

such that for all $(n,p) \in S_1(\mathcal{C})$*: The pair* $S_2(n,p)$ *is the unique solution of* (3.8),(3.1b).

b) For all $(n,p) \in S_1(\mathcal{C})$*: The unique solution* $(F_\circ, G_\circ) = S_2(n,p)$ *of* (3.8), (3.1b) *belongs to* $L^\infty(\Omega)\times L^\infty(\Omega)$ *and satisfies*

$$\min\left\{F_{eq}, F_{eq} + \inf_{\Gamma_D} V_{ext}\right\} \le F_\circ \le \max\left\{F_{eq}, F_{eq} + \sup_{\Gamma_D} V_{ext}\right\}, \tag{3.9a}$$

$$\min\left\{G_{eq}, G_{eq} - \sup_{\Gamma_D} V_{ext}\right\} \le G_\circ \le \max\left\{G_{eq}, G_{eq} - \inf_{\Gamma_D} V_{ext}\right\}. \tag{3.9b}$$

c) There exists a constant $K = K(\mathbf{D}_{dom}, \mathbf{D}_{bdry}, \theta(\mathbf{D}), L_R(\theta(\mathbf{D})), r, s) \in (0,\infty)$ *— where* $\theta(\mathbf{D})$ *is as in Theorem 26 — such that for all* (n_1,p_1), $(n_2,p_2) \in S_1(\mathcal{C})$*: The unique solutions* $(F_i,G_i) = S_2(n_i,p_i)$ *of* (3.8), (3.1b), $i=1,2$, *respectively, satisfy*

$$\begin{aligned} &\|\nabla(F_1 - F_2)\|_{L^2(\Omega)} + \|\nabla(G_1-G_2)\|_{L^2(\Omega)} \\ &\quad \le K\, e^{2\|V_{ext}\|_{L^\infty(\Omega)}}\, \|V_{ext}\|_{L^\infty(\Omega)} \left[\|n_1-n_2\|_{L^s(\Omega)} + \|p_1-p_2\|_{L^s(\Omega)}\right]. \end{aligned} \tag{3.10}$$

The proof of Theorem 27 is deferred to the appendix.

We set $T := S_2 \circ S_1$. Then T is due to Theorem 26 and Theorem 27 well–posed. Furthermore, due to the bounds (3.9) the operator T maps $\mathcal{C}$ into itself. Thus, Algorithm 3 defines a recursion formula: Choose $(F_0, G_0) \in \mathcal{C}$. For $k \in \mathbb{N}_0$ let

$$(n^{k+1}, p^{k+1}, V^{k+1}) := (S_1(F^k, G^k), S_V(F^k, G^k)),$$

$$(F^{k+1}, G^{k+1}) := S_2(n^{k+1}, p^{k+1}).$$

3.4. Convergence Analysis. In this subsection we investigate the convergence properties of a sequence $(n^k, p^k, V^k, F^k, G^k)_{k\in\mathbb{N}}$ generated by Algorithm 3. $(n^k, p^k, V^k, F^k, G^k)_{k\in\mathbb{N}}$ converges at least for sufficiently small values of the norm $\|V_{ext}\|_{L^\infty(\Omega)}$. In addition to this result convergence in case of $R \equiv 0$ is established whenever

$$\delta V_{ext} := \min_{1\le l_1\le M}\ \max_{1\le l_2\le M} |U_{l_1} - U_{l_2}|$$

is sufficiently small.

3.4.1. Convergence of $(n^k, p^k, V^k, F^k, G^k)_{k\in\mathbb{N}}$. The main result of this subsection is

Theorem 28. *Assume* **A**.*1*–**A**.*9. Then there exists a constant* $U_\circ = U_\circ(\mathbf{D}, \theta(\mathbf{D}), L_R(\theta(\mathbf{D})), r, s) \in (0, \infty)$ *— where* $\theta(\mathbf{D})$ *is as in Theorem 26 — such that*

$$\|V_{ext}\|_{L^\infty(\Omega)} < U_\circ$$

implies:

a) There exists a unique solution $(n_\circ, p_\circ, V_\circ, F_\circ, G_\circ)$ *of* (1.1), (1.3).

b) $T : (\mathcal{C}, \|.\|_{H^1(\Omega)}) \to (\mathcal{C}, \|.\|_{H^1(\Omega)})$ *is a contraction.*

c) $(n^k, p^k, V^k, F^k, G^k)$ *converges to* $(n_\circ, p_\circ, V_\circ, F_\circ, G_\circ)$ *strongly in* $(L^s(\Omega))^2 \times (H^1(\Omega))^3$ *as* $k \to \infty$.

The proof of Theorem 28 is deferred to the appendix.

Remark 29. *Theorem 28 applies in cases where*

$$\|F - F_{eq}\|_{L^\infty(\Gamma_D)}, \|G - G_{eq}\|_{L^\infty(\Gamma_D)} < U_\circ,$$

i.e. F *and* G *have to be close to* F_{eq}, G_{eq} *on* Γ_D. *This corresponds to the uniqueness result for the classical drift diffusion model [27]: For small applied bias voltages the current-voltage characteristics is uniquely defined. This is physically reasonable. For higher applied voltages no uniqueness result is available. But it may be assumed that uniqueness does not hold in general: The performance of many devices (thyristors) relies on the existence of multiple solutions [25].*

3.4.2. Convergence of $(n^k, p^k, V^k, F^k, G^k)_{k\in\mathbb{N}}$ in case of $R \equiv 0$. Let us recall that

$$\delta V_{ext} = \min_{1\le l_1 \le M} \max_{1 \le l_2 \le M} |U_{l_1} - U_{l_2}|.$$

By a close screening of the proof of Theorem 27 it is easy to verify

Theorem 30. *Assume* **A**.*1*–**A**.*9 and let* $R \equiv 0$ *Then there exists a constant* $K = K(\mathbf{D}_{dom}, \mathbf{D}_{bdry}, \theta(\mathbf{D}), r) \in (0, \infty)$ *— where* $\theta(\mathbf{D})$ *is as in Theorem 26 — such that for all* (n_1, p_1), $(n_2, p_2) \in S_1(\mathcal{C})$*: The unique solutions* $(F_i, G_i) = S_2(n_i, p_i)$ *of* (3.8), (3.1b), $i = 1, 2$, *respectively, satisfy*

$$\|\nabla (F_1 - F_2)\|_{L^2(\Omega)} + \|\nabla (G_1 - G_2)\|_{L^2(\Omega)} \le K\ \delta V_{ext} \left[\|n_1 - n_2\|_{L^s(\Omega)} + \|p_1 - p_2\|_{L^s(\Omega)} \right].$$

We can proceed along the lines of the proof of Theorem 28 to conclude

Theorem 31. *Assume* **A**.*1*–**A**.*9 and let* $R \equiv 0$. *Then there exists a constant* $U_1 = U_1(\mathbf{D}, \theta(\mathbf{D}), r, s) \in (0, \infty)$ *— where* $\theta(\mathbf{D})$ *is as in Theorem 26 — such that*

$$\delta V_{ext} < U_1$$

implies:

a) There exists a unique solution $(n_\circ, p_\circ, V_\circ, F_\circ, G_\circ)$ *of* (1.1), (1.3).

b) $T : (\mathcal{C}, \|.\|_{H^1(\Omega)}) \to (\mathcal{C}, \|.\|_{H^1(\Omega)})$ *is a contraction.*

c) $(n^k, p^k, V^k, F^k, G^k)$ *converges to* $(n_\circ, p_\circ, V_\circ, F_\circ, G_\circ)$ *strongly in* $(L^s(\Omega))^2 \times (H^1(\Omega))^3$ *as* $k \to \infty$.

3.5. Numerical Simulations of a Resonant Tunneling Diode. In this subsection we employ the generalized Gummel–iteration defined by Algorithm 3 to compute the stationary current–voltage characteristic (IVC) of the resonant tunneling diode depicted in Figure 2.1. For the calculations we supplement (2.5) with

the following boundary conditions which are in agreement with the boundary data for the computed equilibrium densities (see Section 2.4):
Assuming charge neutrality at the contacts gives rise to

$$n(0) = C_{dot}(0), \quad n(L) = C_{dot}(L).$$

As we have $V_{eq}(0) = V_{eq}(L) = F_{eq}$ we might choose without loss of generality $V_{eq} = F_{eq} = 0$ on $\partial\Omega$, since the system (2.5) does not change if one replaces V and F by $V + \alpha$ and $F + \alpha$, respectively, for some $\alpha \in \mathbb{R}$. This yields

$$V(0) = 0, \quad V(L) = U$$

and

$$F(0) = 0, \quad F(L) = U,$$

where U is the applied biasing voltage. This set of boundary conditions can also be motivated physically by employing the assumption of vanishing quantum effects at the boundary [18].

The values of the physical constants and parameters can be found in Section 2.4.. Furthermore, we assumed an effective electron mass $m = 0.126 \cdot m_0$, which correspond to a relaxation time $\tau = 0.18\,\mathrm{ps}$. The barrier height is assumed to be $B = 0.3\,\mathrm{eV}$, which is 65 % of the band gap.

For the numerical simulations we discretized system (2.5) using linear finite elements and decoupled the equations according to Algorithm 3. To compute the solution of the first step of Algorithm 3 we employed a Newton–iteration, since we control the linearization of the considered system due to Theorem 26. The second step was computed by standard techniques for linear elliptic equations.

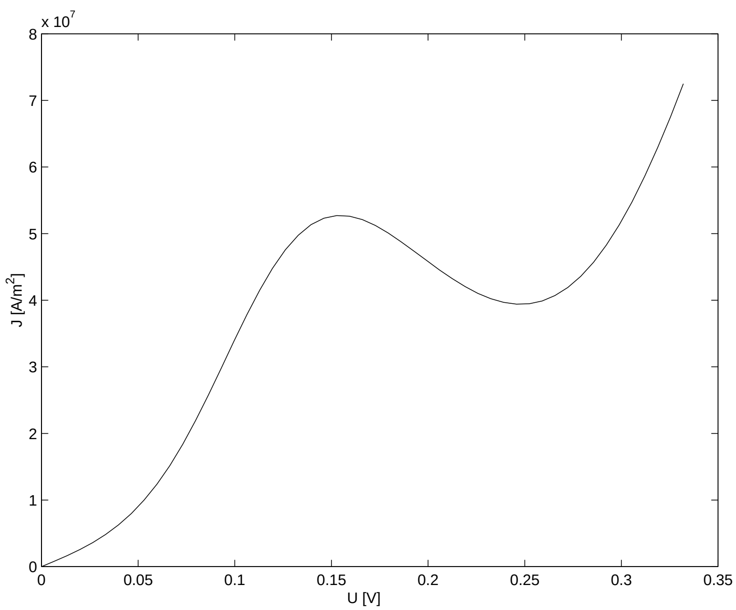

FIG. 3.1. *Current–voltage characteristic*

As expected the algorithm did behave very well for small voltages, in this special case up to 0.2 V, which could be even increased due to the usage of voltage continuation, i.e. the voltage was incremented and in each step the previous solutions was used as an initial guess for the iteration.

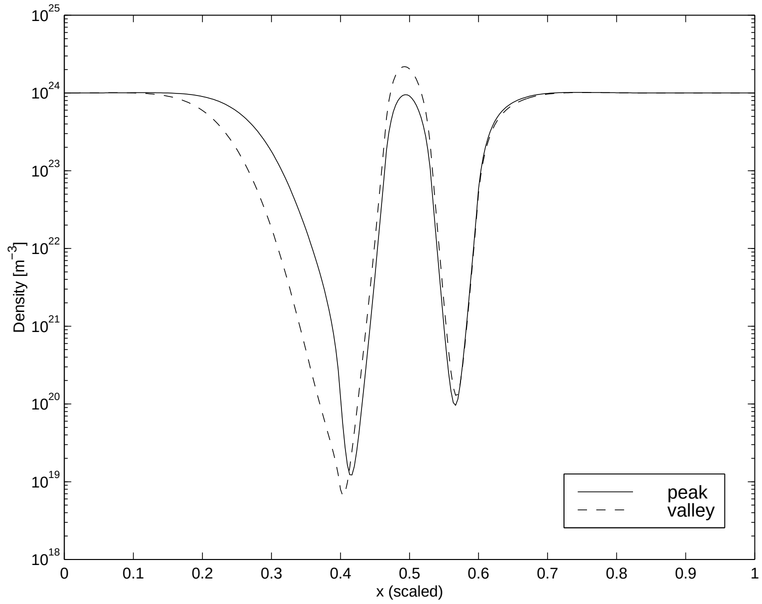

FIG. 3.2. *Electron densities at the peak ($U = 0.16$ V) and at the valley ($U = 0.25$ V)*

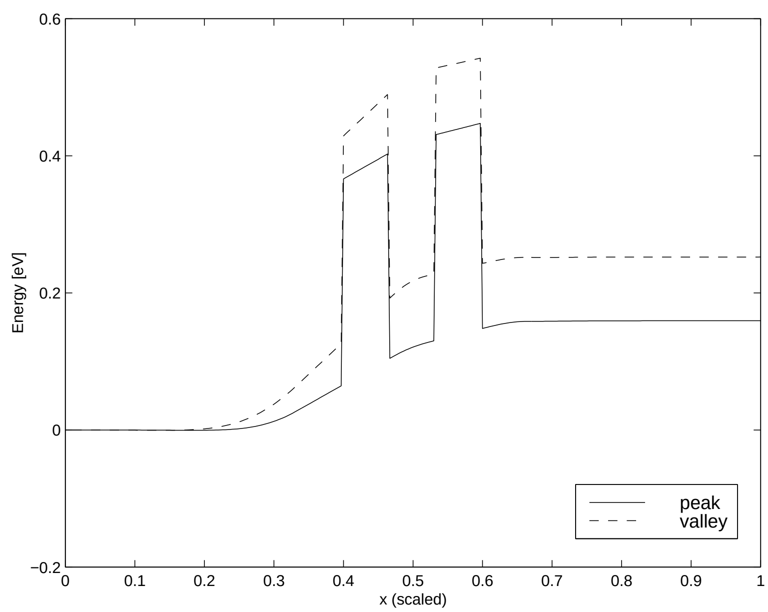

FIG. 3.3. *Conduction–band energy at the peak ($U = 0.16$ V) and at the valley ($U = 0.25$ V)*

Again, the computations were done for piecewise constant doping profile and barrier, but smoothing is possible and will improve the performance of the implemented code. The computations were done on a grid with 300 points.

The IVC depicted in Figure 3.1 has a prominent region of negative differential resistance and the peak to valley ratio is approximately 1.5:1. This is less than experimental values for similar devices [26, 28] and also the voltage at which the peak is observed (here 0.16 V) is lower than measured ones. But there are so many effects influencing the IVC, such as series resistance and contact resistance [26], which we did not include in our model. Furthermore, these values are very sensitive

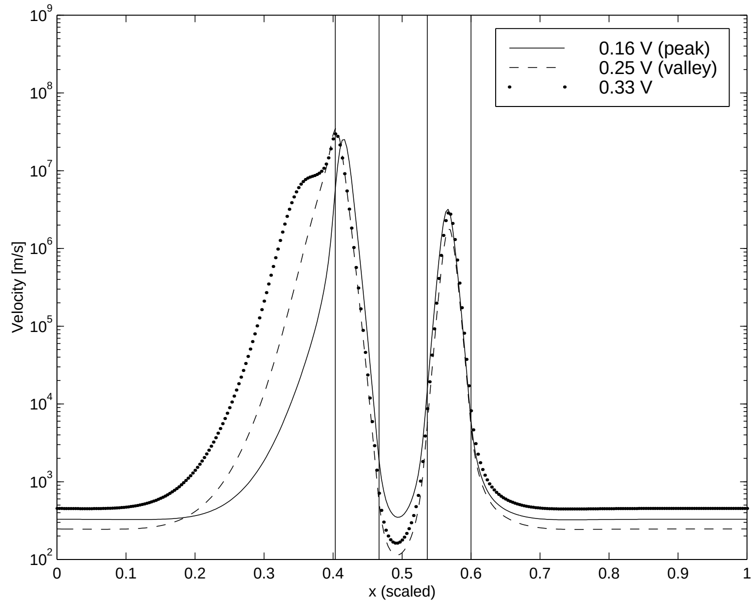

FIG. 3.4. *Electron velocities at the peak (U = 0.16 V), the valley (U = 0.25 V) and at* $U = 0.33$ *V*

to other parameters, as the barrier height and width, the effective electron mass or the relaxation time. The same holds for the peak current density, which strongly depends on the mobility of electrons, as can be seen from (2.5b) and which we assumed to be constant along the device, neglecting a dependence on the electric field. Thus, the choice of the intrinsic device parameters is crucial for the accurate quantitative simulation of resonant tunneling! structures. Especially, the imposed assumptions on the effective tunneling mass of the electrons is very restrictive, as Vanbésien et al. pointed out in [38].

Despite this quantitative deviations from experimental results, the QDD model is capable of predicting other effects of RTD structures. Figure 3.2 shows the computed electron densities in the device just for the applied voltages where the peak and the valley occur in the IVC. It illustrates the high concentration of electrons (more than two orders of magnitude higher than the background doping density) in the quantum well, which is typical for RTD structures and can also be seen in other QHD simulations [10, 16]. Note that concentration of electrons in the quantum well increases for increasing biasing voltages U.

The computed conduction–band energies $V + B$ can be found in Figure 3.3, showing clearly the effect of band bending near the resonant barrier, which decreases the effective voltage applied to the barrier.

Furthermore, we present the carrier velocities $J/(q\,n)$ in Figure 3.4, where additionally the barriers are indicated as vertical lines. The electrons are almost six orders of magnitude faster in the barriers than in the quantum well. Note that the lowest velocity in the quantum well occurs exactly when the valley current is flowing.

Appendix.

A.1. Proofs of Subsection 2.1.

Proof of Lemma 5. We introduce

$$S := \left\{ \phi \in H^1(\Omega) : \quad \int_\Omega \phi \, dx = 0, \quad \|\nabla \phi\|_{L^2(\Omega)} = 1 \right\}.$$

Due to the normalization condition $\int_\Omega \phi\ dx = 0$ and due to **A**.1 there exists a constant $\kappa \in (0,\infty)$ such that for all $\phi \in S$:

$$\|\phi\|_{H^1(\Omega)} \le \kappa \|\nabla \phi\|_{L^2(\Omega)} = \kappa. \tag{A.1}$$

For $\phi \in S$ let

$$\mathcal{F}(\phi) := \int_\Omega u^\beta \left|\nabla\left(\frac{\phi}{u}\right)\right|^2\ dx.$$

We observe that $\mathcal{F}$ maps S into $\mathbb{R}^+ \cup \{0,\infty\}$ and $\mathcal{F} \not\equiv \infty$. Since (2.1) is homogeneous with respect to ϕ it suffices to prove: There exists a $K \in (0,\infty)$ — which naturally depends on Ω, u, β — such that

$$\inf_{\phi\in S} \mathcal{F}(\phi) \ge K.$$

This estimate is shown in an indirect way: We assume that $\inf_{\phi\in S}\mathcal{F}(\phi) = 0$. Then there exists a minimizing sequence $(\phi_n)_{n\in\mathbb{N}}$ in C such that

$$\lim_{n\to\infty} \mathcal{F}(\phi_n) = \inf_{\phi\in S}\mathcal{F}(\phi) = 0.$$

Set $f_n = \frac{\phi_n}{u}$. With the aid of (A.1) we can assume without loss of generality that $\|f_n\|_{H^1(\Omega)}$ is uniformly bounded. Thus there exists a subsequence – again denoted by $(f_n)_{n\in\mathbb{N}}$ – such that $f_n \rightharpoonup f$ weakly in $H^1(\Omega)$ and $f_n \to f$ strongly in $L^2(\Omega)$ as $n\to\infty$. Due to sequentially lower semi continuity we have

$$\int_\Omega u^\beta \left|\nabla f\right|^2\ dx = 0$$

and therefore $f = c = \mathit{constant}$ and – since $H^1(\Omega)$ is strictly convex – $f_n \to c$ strongly in $H^1(\Omega)$ as $n\to\infty$. This implies $\phi_n \to c\,u$ strongly in $L^2(\Omega)$ as $n\to\infty$,

$$0 = \lim_{n\to\infty}\int_\Omega \phi_n\ dx = c\int_\Omega u\ dx$$

and therefore $c = f = 0$. Employing $\|\nabla\phi_n\|_{L^2(\Omega)} = 1$ we get

$$\begin{aligned}
1 &= \int_\Omega \left|\nabla(u\,f_n)\right|^2\ dx\\
&= \int_\Omega f_n^2\ |\nabla u|^2\ dx + 2\int_\Omega u\,f_n\,\nabla u\,\nabla f_n\ dx + \int_\Omega u^2\ |\nabla f_n|^2\ dx\\
&\le c(\Omega)\,\|u\|^2_{W^{1,r}(\Omega)}\,\|f_n\|^2_{H^1(\Omega)} + 2M\,\|u\|_{W^{1,r}(\Omega)}\,\|f_n\|_{L^s(\Omega)}\,\|\nabla f_n\|_{L^2(\Omega)}\\
&\quad + M^2\,\|f_n\|^2_{H^1(\Omega)}\,.
\end{aligned}$$

The right-hand side of this inequality tends to 0 as $n\to\infty$. Contradiction. □

Proof of Lemma 6. A straight-forward calculation gives

$$\begin{aligned}
\mathcal{E}\left(n_{eq},p_{eq}\right) &\le \mathcal{E}\left(\frac{n+n_{eq}}{2},\frac{p+p_{eq}}{2}\right)\\
&\le \frac{1}{2}\mathcal{E}\left(n,p\right) + \frac{1}{2}\mathcal{E}\left(n_{eq},p_{eq}\right)\\
&\quad - \frac{\varepsilon^2}{4}\int_\Omega\left[\frac{\left|n_{eq}\nabla n - n\nabla n_{eq}\right|^2}{n\,n_{eq}\left(n+n_{eq}\right)} + \xi\,\frac{\left|p_{eq}\nabla p - p\nabla p_{eq}\right|^2}{p\,p_{eq}\left(p+p_{eq}\right)}\right]dx\\
&\le \mathcal{E}\left(n,p\right) - \frac{\varepsilon^2}{4\,\overline{K}^2}\int_\Omega\left[n_{eq}^2\left|\nabla\left(\frac{n-n_{eq}}{n_{eq}}\right)\right|^2 + \xi\,p_{eq}^2\left|\nabla\left(\frac{p-p_{eq}}{p_{eq}}\right)\right|^2\right]dx
\end{aligned}$$

From Lemma 5 and Poincaré's inequality [2] we obtain the existence of constants $\kappa, \kappa_1 > 0$ such that for all $(n,p) \in C$:

$$\begin{aligned}\mathcal{E}(n,p) - \mathcal{E}(n_{eq},p_{eq}) &\ge \kappa_1 \left(\|\nabla(n-n_{eq})\|^2_{L^2(\Omega)} + \|\nabla(p-p_{eq})\|^2_{L^2(\Omega)} \right)\\ &\ge \kappa \, \|(n,p)-(n_{eq},p_{eq})\|^2_X \,.\end{aligned}$$

□

Proof of Lemma 7. a), b) and c) are obvious and d) can be derived after some cumbersome calculations. Concerning e) we immediately obtain the linearity of the mapping $(\varphi_1,\varphi_2) \mapsto \mathcal{E}'(n,p)[\varphi_1,\varphi_2]$. We estimate

$$\begin{aligned}|\mathcal{E}'(n,p)[\varphi_1,\varphi_2]| &\le \kappa_1\left(\underline{K},\overline{K}\right)\left(\|\nabla\varphi_1\|_{L^2(\Omega)} + \|\nabla\varphi_2\|_{L^2(\Omega)}\right)\\ &\quad + \kappa_2\left(\underline{K},\overline{K}\right)\left(\|\varphi_1\|_{L^s(\Omega)} + \|\varphi_2\|_{L^s(\Omega)}\right)\\ &\quad + \kappa_3\left(\underline{K},\overline{K},B_n,B_p\right)\left(\|\varphi_1\|_{L^1(\Omega)} + \|\varphi_2\|_{L^1(\Omega)}\right)\\ &\quad + \|V[n-p-C_{dot}]\|_{L^2(\Omega)}\left(\|\varphi_1\|_{L^2(\Omega)} + \|\varphi_2\|_{L^2(\Omega)}\right)\\ &\le \kappa_4(\underline{K},\overline{K},B_n,B_p,\Omega)\,\|\varphi\|_X \,,\end{aligned}$$

for some constants $\kappa_i \in (0,\infty)$, $i=1,\dots,4$, where we have used Hölder's inequality, standard results from the theory of elliptic PDE's and Sobolev's embedding theorems. Hence $\mathcal{E}'(n,p)$ is bounded for all $(n,p)\in C$. □

Proof of Lemma 8. Let $(n_1,p_1),(n_2,p_2)\in C$. We are only estimating the terms involving n_1 and n_2 since the others can be handled in analogy. Standard ellipticity results [14] imply

$$\begin{aligned}&\left|\int_\Omega V[n_1-n_2-p_1+p_2]\,(\varphi_1-\varphi_2)\;dx\right|\\ &\qquad \le \kappa_1\left(\|n_1-n_2\|_{L^2(\Omega)} + \|p_1-p_2\|_{L^2(\Omega)}\right)\left(\|\varphi_1\|_{L^2(\Omega)} + \|\varphi_2\|_{L^2(\Omega)}\right).\end{aligned}$$

Using the mean value theorem we get the following estimates:

$$\left|\int_\Omega (\log(n_1)-\log(n_2))\,\varphi_1\;dx\right| \le \kappa_2\,\|n_1-n_2\|_{L^2(\Omega)}\,\|\varphi_1\|_{L^2(\Omega)}\,,$$

$$\begin{aligned}&\left|\int_\Omega \left(\frac{\nabla n_1}{n_1} - \frac{\nabla n_2}{n_2}\right)\nabla\varphi_1\;dx\right|\\ &\qquad\le \int_\Omega \left|\nabla\left[\log(n_1)-\log(n_2)\right]\nabla\varphi_1\right|\;dx\\ &\qquad\le \kappa_3\left(\|\nabla(n_1-n_2)\|_{L^2(\Omega)} + \|n_1-n_2\|_{L^2(\Omega)}\right)\|\nabla\varphi_1\|_{L^2(\Omega)}\,,\end{aligned}$$

$$\begin{aligned}&\left|\int_\Omega \left[\left(\frac{\nabla n_1}{n_1}\right)^2 - \left(\frac{\nabla n_2}{n_2}\right)^2\right]\varphi_1\;dx\right|\\ &\qquad\le \int_\Omega \left|\nabla\left[\log(n_1)-\log(n_2)\right]\,\nabla\left[\log(n_1)+\log(n_2)\right]\varphi_1\right|\;dx\\ &\qquad\le \kappa_4\left(\|\nabla(n_1-n_2)\|_{L^2(\Omega)} + \|n_1-n_2\|_{L^s(\Omega)}\right)\|\varphi_1\|_{L^s(\Omega)}\,,\end{aligned}$$

for some constants $\kappa_i \in (0,\infty)$, $i = 1,\dots,4$, independent of (n_1,p_1) and (n_2,p_2). By Sobolev's embedding theorem there exists a constant $L > 0$ such that for all $(n_1,p_1),(n_2,p_2) \in C$:

$$\|\delta\mathcal{E}(n_1,p_1) - \delta\mathcal{E}(n_2,p_2)\|_{X'} \le L\,\|(n_1,p_1) - (n_2,p_2)\|_X$$

$\square$

A.2. Proof of Subsection 2.2.

Proof of Theorem 12. The proof of Theorem 12 is a modification of ideas that can be found in [9]. We shall make frequent use of the fact that $C - C \subset D$. For notational convenience we introduce

$$c(\alpha) = P\left(c - \alpha\,\delta\mathcal{E}(c)\right).$$

From the well known angle property

$$\forall u \in X \quad \forall c \in C: \quad \langle u - P(u), c - P(u)\rangle \le 0,$$

we deduce the following estimates. Setting $u = c^k - \alpha\,\delta\mathcal{E}\left(c^k\right)$ and $c = c^k$ gives

$$\left\langle \delta\mathcal{E}\left(c^k\right), c^k - c^{k+1}\right\rangle \ge \frac{1}{\alpha}\left\|c^k - c^{k+1}\right\|_X^2 \tag{A.2}$$

and by choosing instead $c = \tilde{c}$

$$\left\langle \delta\mathcal{E}\left(c^k\right), c^{k+1} - \tilde{c}\right\rangle \le \frac{1}{\alpha}\left\|c^k - c^{k+1}\right\|_X \left\|c^{k+1} - \tilde{c}\right\|_X. \tag{A.3}$$

First we establish the feasibility of Armijo's rule (2.3). This holds because of

$$\lim_{\alpha\to 0^+} \frac{\mathcal{E}(c) - \mathcal{E}\left(c(\alpha)\right)}{\langle \delta\mathcal{E}(c), c - c(\alpha)\rangle} = 1, \quad \text{for all } c \in C.$$

Employing the mean value theorem and the Lipschitz continuity of $\delta\mathcal{E}$ this can be seen as follows:

$$\begin{aligned}&|\mathcal{E}(c) - \mathcal{E}\left(c(\alpha)\right) - \langle\delta\mathcal{E}(c), c - c(\alpha)\rangle| = \\ &\qquad\left|\int_0^1 \langle \delta\mathcal{E}(c + t(c - c(\alpha))) - \delta\mathcal{E}(c), c - c(\alpha)\rangle\,dt\right| \le \frac{L}{2}\,\|c - c(\alpha)\|_X^2,\end{aligned}$$

which yields

$$\begin{aligned}\left|\frac{\mathcal{E}(c) - \mathcal{E}\left(c(\alpha)\right)}{\langle\delta\mathcal{E}(c), c - (c(\alpha))\rangle} - 1\right| &\le \frac{L}{2}\frac{\|c - c(\alpha)\|_X^2}{\langle\delta\mathcal{E}(c), c - (c(\alpha))\rangle} \\ &\le \frac{\alpha\,L}{2},\end{aligned}$$

because of (A.2). Next we show that the sequence of step sizes $\left(\alpha^k\right)_{k\in\mathbb{N}}$ generated by Algorithm 1 is bounded away from zero, which is an easy consequence of the following estimate [6]

$$\forall\sigma \in (0,1) \quad \forall\alpha \in \left[0, \frac{2(1-\sigma)}{L}\right]: \mathcal{E}(c) - \mathcal{E}(c(\alpha)) \ge \sigma\,\langle\delta\mathcal{E}(c), c - c(\alpha)\rangle,$$

which is derived as follows

$$\begin{aligned}\mathcal{E}(c)-\mathcal{E}(c(\alpha)) &= \int_0^1 \langle \delta\mathcal{E}(c+t(c-c(\alpha))), c-c(\alpha)\rangle\, dt \\ &\geq \langle \delta\mathcal{E}(c), c-c(\alpha)\rangle \\ &\quad - \int_0^1 |\langle \delta\mathcal{E}(c+t(c-c(\alpha)))-\delta\mathcal{E}(c), c-c(\alpha)\rangle|\, dt \\ &\geq \langle \delta\mathcal{E}(c), c-c(\alpha)\rangle - \frac{L}{2}\|c-c(\alpha)\|_X^2 \\ &\geq \left(1-\frac{\alpha L}{2}\right)\langle \delta\mathcal{E}(c), c-c(\alpha)\rangle,\end{aligned}$$

where we used a variant of (A.2). Hence, the construction of the step sizes $\left(\alpha^k\right)_{k\in\mathbb{N}}$ implies

$$\forall\, k\in\mathbb{N}_0: \quad \alpha^k \geq \frac{2(1-\gamma)}{L} =: \underline{a} > 0. \tag{A.4}$$

Now we are able to show the convergence of Algorithm 1. We set $\mathcal{E}^k := \mathcal{E}\left(c^k\right)$. Notice that we have

$$\begin{aligned}\mathcal{E}^k-\mathcal{E}^{k+1} &\geq \gamma\left\langle \delta\mathcal{E}\left(c^k\right), c^k-c^{k+1}\right\rangle \\ &= \gamma\,\mathcal{E}'\left(c^k\right)\left[c^k-c^{k+1}\right] \\ &\geq \frac{\gamma}{\bar{a}}\left\|c^k-c^{k+1}\right\|_X^2 \geq 0,\end{aligned}$$

due to (A.2). Hence, $\left(\mathcal{E}^k\right)_{k\in\mathbb{N}}$ is a non increasing bounded sequence and thus convergent with $\lim_{k\to\infty}\mathcal{E}^k = \hat{\mathcal{E}} \geq \mathcal{E}\left(\tilde{u}\right) > -\infty$. Consequently

$$\begin{aligned}&\lim_{k\to\infty}\mathcal{E}'\left(c^k\right)\left[c^k-c^{k+1}\right]=0 \\ &\text{and} \lim_{k\to\infty}\left\|c^k-c^{k+1}\right\|_X = 0.\end{aligned}$$

Due to the convexity of $\mathcal{E}$ we have

$$\begin{aligned}0 \leq \mathcal{E}^k-\mathcal{E}\left(\tilde{c}\right) &\leq \mathcal{E}'\left(c^k\right)\left[c^k-\tilde{c}\right] \\ &= \mathcal{E}'\left(c^k\right)\left[c^k-c^{k+1}\right]+\mathcal{E}'\left(c^k\right)\left[c^{k+1}-\tilde{c}\right] \\ &\leq \mathcal{E}'\left(c^k\right)\left[c^k-c^{k+1}\right]+\frac{1}{\underline{a}}\left\|c^k-c^{k+1}\right\|_X\left\|c^{k+1}-\tilde{c}\right\|_X,\end{aligned}$$

where we used (A.3). The coerciveness of $\mathcal{E}$ implies the boundedness of $\left(c^k\right)_{k\in\mathbb{N}}$ and thus $\lim_{k\to\infty}\mathcal{E}^k = \mathcal{E}\left(\tilde{c}\right)$ and it follows from the uniform convexity of $\mathcal{E}$ that $\lim_{k\to\infty}\left\|c^k-\tilde{c}\right\|_X = 0$. ☐

A.3. Proofs of Subsection 2.3.

Proof of Lemma 14. a) Since (c_h) is a weakly convergent sequence the norms $\|c_h\|_X$ are uniformly bounded. Hence it follows from **D**.6 that $\lim_{h\to 0}\|Pc_h - c_h\|_X = 0$. Therefore the sequence (Pc_h) is bounded, too. By passing to a subsequence $(Pc_{h'})$ we obtain $Pc_{h'} \rightharpoonup c \in X$ weakly in X as $h'\to 0$. Since C is closed and convex, C is weakly closed, too, see e.g. [31]. Hence $c\in C$. We furthermore have for all $x\in X$:

$$|\langle x, Pc_{h'}-v\rangle| \leq \|x\|_X\|Pc_{h'}-c_{h'}\|_X + |\langle x, c_{h'}-v\rangle|,$$

where both terms on the left-hand side converge to 0 as $h'\to 0$. Hence $Pc_{h'} \rightharpoonup v$ weakly in X as $h'\to 0$. This settles $v = c\in C$.

b) Step 1: We wish to prove that the sequence $(P_h u)$ is bounded for all $u \in X$. We observe that due to $P_h(Pu) \in C_h$,

$$\|u - P_h u\|_X \leq \|u - P_h(Pu)\|_X \leq \|u\|_X + \|P_h(Pu) - Pu\|_X + \|Pu\|_X,$$

and the middle term of the left-hand side of this inequality is uniformly bounded due to $Pu \in C$ and assumption **D**.5.

Step 2: We wish to prove that

$$\lim_{h \to 0} \|P_h u - u\|_X = \|Pu - u\|_X \tag{A.5}$$

for all $u \in X$. As shown in Step 1 the sequence $(P_h u)$ is uniformly bounded. It follows from **D**.6 that $\lim_{h\to 0} \|P(P_h u) - P_h u\|_X = 0$. We furthermore have $\|u - Pu\|_X \leq \|u - P_h u\|_X + \|P(P_h u) - P_h u\|_X$. Hence $\|u - Pu\|_X \leq \liminf_{h\to 0} \|u - P_h u\|_X$. On the other hand we have $\|u - P_h u\|_X \leq \|u - P_h(Pu)\|_X$ and therefore $\|u - P_h u\|_X \leq \|u - Pu\|_X + \|Pu - P_h(Pu)\|_X$, where due to **D**.5 the second term of this inequality tends to 0 as $h \to 0$. This gives $\|u - Pu\|_X \geq \limsup_{h\to 0} \|u - P_h u\|_X$.

Step 3: It suffices to prove that $P_h u - u \to Pu - u$ strongly in X as $h \to 0$. By Step 2 and due to the strict convexity of X it suffices to prove that $P_h u - u \rightharpoonup Pu - u$ weakly in X as $h \to 0$. Let (h') be a subsequence of (h). Since $(P_{h'} u)$ is bounded (Step 1) we may extract a subsequence $(P_{h''} u)$, such that $P_{h''} u \rightharpoonup c$ weakly in X as $h \to 0$. As already shown in a) we have $c \in C$. Using the weak sequentially lower semi continuity of the norm and Step 2 we get $\|c - u\|_X \leq \liminf_{h''\to 0} \|P_{h''} u - u\|_X = \|Pu - u\|_X$ and therefore $c = Pu$, which is independent of the choice of the subsequence (h'). Hence $P_h u \rightharpoonup Pu$ weakly in X as $h \to 0$ and therefore $P_h u - u \rightharpoonup Pu - u$ weakly in X as $h \to 0$, too.
c) follows immediately from **D**.7 and the Banach-Steinhaus theorem.
d) Let $u \in X$ and $\varepsilon > 0$ be arbitrary. Choose $w_\varepsilon \in W$ with $\|w_\varepsilon - u\|_X \leq \frac{\varepsilon}{2}$ and $h(\varepsilon) > 0$ such that $\|w_\varepsilon - R_h w_\varepsilon\|_X \leq \frac{\varepsilon}{2}$ for all $h < h(\varepsilon)$. Then for all $h < h(\varepsilon)$ the estimate $\|u - R_h w_\varepsilon\|_X \leq \|u - w_\varepsilon\|_X + \|w_\varepsilon - R_h w_\varepsilon\|_X \leq \varepsilon$ holds. This implies $\inf_{u_h \in X_h} \|u - u_h\|_X \leq \varepsilon$ for all $h < h(\varepsilon)$. □

Proof of Theorem 17. The proof is done by induction. For $k = 0$ there is nothing to do. Suppose we have

$$\lim_{h \to 0} \left\|c_h^k - R_h c^k\right\|_X = 0, \tag{I. A.}$$

for an iteration index $k \geq 0$. We calculate

$$\begin{aligned}\left\|c_h^{k+1} - R_h c^{k+1}\right\|_X &= \left\|P_h\left(c_h^k - \alpha_h^k\, D\mathcal{E}_h\left(c_h^k\right)\right) - R_h\left(P\left(c^k - \alpha^k\, \delta\mathcal{E}\left(c^k\right)\right)\right)\right\|_X \\ &\leq \sum_{l=1}^{5} \left\|I_h^l\right\|_X\end{aligned}$$

with

$$\begin{aligned}\left\|I_h^1\right\|_X &= \left\|c^k - c_h^k\right\|_X \\ \left\|I_h^2\right\|_X &= \alpha_h^k \left\|\delta\mathcal{E}\left(c^k\right) - D\mathcal{E}_h\left(c_h^k\right)\right\|_X \\ \left\|I_h^3\right\|_X &= \left|\alpha^k - \alpha_h^k\right| \left\|\delta\mathcal{E}\left(c^k\right)\right\|_X \\ \left\|I_h^4\right\|_X &= \left\|P_h\left(c^k - \alpha^k\delta\mathcal{E}\left(c^k\right)\right) - P\left(c^k - \alpha^k\delta\mathcal{E}\left(c^k\right)\right)\right\|_X \\ \left\|I_h^5\right\|_X &= \left\|P\left(c^k - \alpha^k\delta\mathcal{E}\left(c^k\right)\right) - R_h\left(P\left(c^k - \alpha^k\delta\mathcal{E}\left(c^k\right)\right)\right)\right\|_X\end{aligned}$$

These terms can be estimated as follows:

$$\left\|I_h^1\right\|_X \leq \left\|c^k - R_h c^k\right\|_X + \left\|R_h c^k - c_h^k\right\|_X$$

Thus we have $\lim_{h\to 0} \left\|I_h^1\right\|_X = 0$ due to (I. A.) and **D**.8. Since $\alpha_h^k \le \bar{a}$ and using the uniform Lipschitz continuity of $D\mathcal{E}_h$ we derive

$$\begin{aligned}\left\|I_h^2\right\|_X &\le \bar{a}\left\|\delta\mathcal{E}\left(c^k\right) - D\mathcal{E}_h\left(P_h c^k\right)\right\|_X + \bar{a}\left\|D\mathcal{E}_h\left(P_h c^k\right) - D\mathcal{E}_h\left(c_h^k\right)\right\|_X \\ &\le \bar{a}\left\|\delta\mathcal{E}\left(c^k\right) - D\mathcal{E}_h\left(P_h c^k\right)\right\|_X + \bar{a}\,L_\circ\,\left(\left\|c_h^k - R_h c^k\right\|_X + \right. \\ &\quad \left. + \left\|R_h c^k - c^k\right\|_X + \left\|c^k - P_h c^k\right\|_X\right)\end{aligned}$$

Employing (I. A.), **D**.5, **D**.6 and **D**.9–**D**.15 each of these terms converges to zero as $h \to 0$.

Next we show that $\lim_{h\to 0} \alpha_h^k = \alpha^k$. To this purpose choose an arbitrary subsequence of $\left(\alpha_h^k\right)$. Since $\left(\alpha_h^k\right)$ is bounded there exists another subsequence, again denoted by $\left(\alpha_h^k\right)$, such that $\lim_{h\to 0} \alpha_h^k = \tilde{\alpha}$. For this sequence one easily verifies that (2.4) becomes in the limit $h \to 0$:

$$\mathcal{E}\left(c^k\right) - \mathcal{E}\left(P\left(c^k - \tilde{\alpha}\,\delta\mathcal{E}\left(c^k\right)\right)\right) \ge \gamma\left\langle \delta\mathcal{E}\left(c^k\right), c^k - P\left(c^k - \tilde{\alpha}\,\delta\mathcal{E}\left(c^k\right)\right)\right\rangle.$$

Due to the definition of α^k we have $\tilde{\alpha} \le \alpha^k$. Assume by contradiction $\tilde{\alpha} < \alpha^k$. Then there exists an $\alpha_1 \in \left(\tilde{\alpha}, \alpha^k\right)$ such that for h small enough we have $\alpha_h^k < \alpha_1$ and

$$\mathcal{E}_h\left(c_h^k\right) - \mathcal{E}_h\left(P_h\left(c_h^k - \alpha_1\,D\mathcal{E}_h\left(c_h^k\right)\right)\right) \ge \gamma\left\langle D\mathcal{E}_h\left(c_h^k\right), c_h^k - P_h\left(c_h^k - \alpha_1\,D\mathcal{E}_h\left(c_h^k\right)\right)\right\rangle,$$

which is a consequence of the point wise convergence and of

$$\mathcal{E}\left(c^k\right) - \mathcal{E}\left(P\left(c^k - \alpha_1\,\delta\mathcal{E}\left(c^k\right)\right)\right) > \gamma\left\langle \delta\mathcal{E}\left(c^k\right), c^k - P\left(c^k - \alpha_1\,\delta\mathcal{E}\left(c^k\right)\right)\right\rangle.$$

But this is in contrast to the maximality of α_h^k and thus $\tilde{\alpha} = \alpha^k$. Together with the boundedness of $\left(\left\|\delta\mathcal{E}\left(c^k\right)\right\|_X\right)$ on C this implies $\lim_{h\to 0}\left\|I_h^3\right\|_X = 0$.

Finally, due to **D**.8 and Theorem 14, $\left\|I_h^4\right\|_X$ and $\left\|I_h^5\right\|_X$ are tending to zero as $h \to 0$. □

Proof of Corollary 18. Let $\varepsilon > 0$. Applying Theorems 12, 17 and 14 there exist constants $K_\varepsilon \in \mathbb{N}$ and $h_\varepsilon > 0$ such that

$$\left\|\tilde{c}_h - \tilde{c}\right\|_X \le \left\|\tilde{c}_h - c_h^k\right\|_X + \left\|c_h^k - c^k\right\|_X + \left\|c^k - \tilde{c}\right\|_X \le \varepsilon$$

for all $k \ge K_\varepsilon$ and $h \le h_\varepsilon$. □

A.4. Proofs of Subsection 3.2.

Proof of Lemma 24. We define $\mathcal{U} := \{u \in \mathcal{X} : \theta \le u \le 1/\theta\}$. Firstly we show that for each $u \in \mathcal{U}$ there exists a constant $K_u = K_u(\mathbf{D}_{dom}, \beta, \theta, s) \in (0, \infty)$ such that

$$\mathcal{F}_u(\phi) := \int_\Omega u^\beta |\nabla\phi|^2\,dx \ge K_u \tag{A.6}$$

for all

$$\phi \in \mathcal{B}_u := \left\{\phi \in \mathcal{X}_0 : \|\phi\,u\|_{L^s(\Omega)} = 1\right\}.$$

This is shown in an indirect way. Assume there exists a minimizing sequence $(\phi_k)_{k\in\mathbb{N}}$ such that $\lim_{k\to\infty} \mathcal{F}_u(\phi_k) = 0$. (We note that $\mathcal{F}_u(\phi) \not\equiv \infty$ for some $\phi \in \mathcal{B}_u$, i.e. $\inf_{\phi\in\mathcal{B}_u} \mathcal{F}_u(\phi) < \infty$.) Then — due to Poincaré's inequality — $\phi_k \to 0$ strongly in $H^1(\Omega)$ as $k \to \infty$. Since $H^1(\Omega) \hookrightarrow L^s(\Omega)$ we get $\lim_{k\to\infty} \|\phi_k\,u\|_{L^s(\Omega)} = 0$. Contradiction.

Hence for all $u \in \mathcal{U}$: $m_u := \inf_{\phi \in \mathcal{B}_u} \mathcal{F}_u(\phi) \in (0, \infty)$. We claim that $K := \inf_{u \in \mathcal{U}} m_u > 0$. (Certainly, $K \in [0, \infty)$.) We again proceed in an indirect way. Assume that $K = 0$. There exists a sequence $(u_k)_{k \in \mathbb{N}} \subset \mathcal{U}$ such that $\lim_{k \to \infty} m_{u_k} = 0$. Additionally, for each $k \in \mathbb{N}$ there exists a $\phi_k \in \mathcal{B}_{u_k}$ such that

$$\int_\Omega u_k^\beta \left|\nabla \phi_k\right|^2 \, dx \leq m_{u_k} + \frac{1}{k},$$

which again yields $\phi_k \to 0$ strongly in $H^1(\Omega)$ and $L^s(\Omega)$ as $k \to \infty$. But this implies

$$1 = \liminf_{k \to \infty} \|\phi_k \, u_k\|_{L^s(\Omega)} \leq 1/\theta \, \liminf_{k \to \infty} \|\phi_k\|_{L^s(\Omega} = 0.$$

Contradiction. Hence $K > 0$ holds. Now let $u \in \mathcal{U}$ and $\phi \in \mathcal{X}_0$ with $\phi \not\equiv 0$. Then $\tilde{\phi} = \phi / \|\phi \, u\|_{L^s(\Omega)}$ is an element of $\mathcal{B}_u$, which yields

$$\int_\Omega u^\beta \left|\nabla \phi\right|^2 \, dx \geq K \, \|\phi \, u\|^2_{L^s(\Omega)}.$$

Replacing ϕ by ϕ/u gives (3.4).□

Proof of Theorem 26. It readily follows from Theorem 2.1 in [1] that (3.5), (3.1a) possesses a solution $(n_\circ, p_\circ, V_\circ) \in \mathcal{X}^3$ which satisfies (3.6) for a $\theta = \theta(\mathbf{D}) \in (0,1)$. We will now prove (3.7) and thus show the uniqueness of the solution. Let $(F, G), (F_1, G_1) \in \mathcal{C}$ and let $(n_\circ, p_\circ, V_\circ), (n_1, p_1, V_1) \in (n_D, p_D, V_{eq} + V_{ext}) + (\mathcal{V} \times \mathcal{V} \times \mathcal{V})$ be any respective solutions of (3.5), (3.1a). We introduce an operator $\Phi : L^2(\Omega) \to H^1(\Omega)$ as follows. Given $f \in L^2(\Omega)$ we define $\Phi[f]$ as the unique $H^1(\Omega)$–solution of

$$-\lambda^2 \Delta \Phi = f, \quad \Phi - (V_{eq} + V_{ext}) \in \mathcal{V}.$$

We define the set

$$\mathcal{M} = \left\{(n, p) \in \mathcal{X}^2 : (n - n_D, p - p_D) \in \mathcal{X}_0^2, \quad \theta \leq n, p \leq 1/\theta\right\},$$

where we note that $(n_\circ, p_\circ), (n_1, p_1) \in \mathcal{M}$. We introduce the operator $A : \mathcal{M} \to H^{-1}(\Omega \cup \Gamma_N) \times H^{-1}(\Omega \cup \Gamma_N)$, which is given by

$$\begin{aligned}\langle A(n,p), \phi\rangle := &\int_\Omega \left[-\varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + \Phi[n - p - C] + B_n\right] \phi_1 \, dx \\ &+ \int_\Omega \left[-\xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}} + \log(p) - \Phi[n - p - C] + B_p\right] \phi_2 \, dx,\end{aligned}$$

for all $\phi = (\phi_1, \phi_2) \in \mathcal{V}^2$. We observe that A is actually well-defined on $\mathcal{M}$. Furthermore, for fixed $\phi = (\phi_1, \phi_2) \in \mathcal{V}^2$ and fixed $(n, p) \in \mathcal{M}$ the Gateâux–differential $\langle A'(n,p)[\Theta], \phi\rangle$ of $\langle A(.,.), \phi\rangle : \mathcal{M} \mapsto \mathbb{R}$ in a direction $\Theta = (\Theta_1, \Theta_2) \in (\mathcal{X}_0)^2$ exists and is given by

$$\begin{aligned}&\langle A'(n,p)[\Theta], \phi\rangle = \\ &\quad -\frac{\varepsilon^2}{2} \int_\Omega \left(\frac{\Delta\Theta_1}{n} - \frac{\Delta n}{n^2}\Theta_1 - \frac{\nabla n \nabla \Theta_1}{n^2} + \frac{|\nabla n|^2}{n^3}\Theta_1\right) \phi_1 \, dx \\ &\qquad + \int_\Omega \left(\frac{\Theta_1}{n} + \Phi\left[\Theta_1 - \Theta_2\right]\right) \phi_1 \, dx \\ &\quad -\xi\frac{\varepsilon^2}{2} \int_\Omega \left(\frac{\Delta\Theta_2}{p} - \frac{\Delta p}{p^2}\Theta_2 - \frac{\nabla p \nabla \Theta_2}{p^2} + \frac{|\nabla p|^2}{p^3}\Theta_2\right) \phi_2 \, dx \\ &\qquad + \int_\Omega \left(\frac{\Theta_2}{p} - \Phi\left[\Theta_1 - \Theta_2\right]\right) \phi_2 \, dx\end{aligned}$$

We also have for $i = \circ, 1$

$$\langle A(n_i, p_i), \phi\rangle = \langle (F_i, G_i), \phi\rangle, \quad \text{for all } \phi \in \mathcal{V}^2. \tag{A.7}$$

Let $\delta u = u_\circ - u_1$. Setting $\phi = (\delta n, \delta p)$ we obtain by subtraction from (A.7)

$$\langle A(n_\circ, p_\circ) - A(n_1, p_1), (\delta n, \delta p)\rangle = \langle (\delta F, \delta G), (\delta n, \delta p)\rangle$$

For $h \in [0,1]$ let

$$n_h := n_\circ - h\,\delta n \quad \text{and} \quad p_h := p_\circ - h\,\delta p.$$

We introduce the function $[0,1] \ni h \mapsto \langle A(n_h, p_h), (\delta n, \delta p)\rangle \in \mathbb{R}$, which is differentiable on $[0,1]$. By the mean value theorem there exists an $h \in (0,1)$ such that

$$\langle A'(n_h, p_h)[(\delta n, \delta p)], (\delta n, \delta p)\rangle = \langle (\delta F, \delta G), (\delta n, \delta p)\rangle. \tag{A.8}$$

Using Lemma 24 the left-hand side of (A.8) can be estimated as follows

$$\begin{aligned}\langle A'(n_h, p_h)[(\delta n, \delta p)], (\delta n, \delta p)\rangle &= \varepsilon^2 \int_\Omega n_h \left|\nabla\left(\frac{\delta n}{n_h}\right)\right|^2 dx \\ &\quad + \xi\varepsilon^2 \int_\Omega p_h \left|\nabla\left(\frac{\delta p}{p_h}\right)\right|^2 dx \\ &\quad + \int_\Omega \frac{(\delta n)^2}{n_h}\,dx + \int_\Omega \frac{(\delta p)^2}{p_h}\,dx \\ &\quad + \int_\Omega |\nabla\Phi[\delta n - \delta p]|^2\,dx \\ &\geq \varepsilon^2(1+\xi)K_1\left(\|\delta n\|^2_{L^s(\Omega)} + \|\delta p\|^2_{L^s(\Omega)}\right),\end{aligned}$$

where $K_1 = K_1(\mathbf{D}_{dom}, \theta(\mathbf{D}), s) \in (0,\infty)$. By the Cauchy–Schwarz–inequality we obtain

$$\begin{aligned}&\|\delta n\|^2_{L^s(\Omega)} + \|\delta p\|^2_{L^s(\Omega)} \\ &\qquad \leq \frac{K_2}{\varepsilon^2(1+\xi)K_1}\|(\delta F, \delta G)\|_{L^2(\Omega)}\left(\|\delta n\|^2_{L^s(\Omega)} + \|\delta p\|^2_{L^s(\Omega)}\right)^{1/2},\end{aligned}$$

where $K_2 = K_2(\Omega, s) \in (0,\infty)$. Canceling $\left(\|\delta n\|^2_{L^s(\Omega)} + \|\delta p\|^2_{L^s(\Omega)}\right)^{1/2}$ and using $(|a|+|b|)^{1/2} \leq |a|+|b| \leq 2^{1/2}\left(|a|^2+|b|^2\right)^{1/2}$ gives (3.7). $\square$

Proof of Theorem 27. a), b): We introduce for $m > 0$ a truncated exponential function

$$e_m(x) := \begin{cases}\exp(x), & x \leq \log(m),\\ m, & x \geq \log(m).\end{cases}$$

Instead of (3.8) we consider the modified system

$$\operatorname{div}(n\,\nabla F) = R(n,p)\left(e_m(F+G) - \delta^2\right), \tag{A.9a}$$

$$\operatorname{div}(p\,\nabla G) = R(n,p)\left(e_m(F+G) - \delta^2\right). \tag{A.9b}$$

For $u = (u_1, u_1) \in H^1(\Omega) \times H^1(\Omega)$ and $\phi = (\phi_1, \phi_2) \in \mathcal{V}^2$ we set

$$\begin{aligned}\langle A_m(u), \phi\rangle := &\int_\Omega n\,\nabla u_1\,\nabla\phi_1\,dx + \int_\Omega p\,\nabla u_2\,\nabla\phi_2\,dx \\ &+ \int_\Omega R(n,p)\left(e_m(u_1+u_2) - \delta^2\right)(\phi_1+\phi_2)\,dx.\end{aligned}$$

This defines an operator $A_m : H^1(\Omega) \times H^1(\Omega) \to H^{-1}(\Omega \cup \Gamma_N) \times H^{-1}(\Omega \cup \Gamma_N)$. We readily verify that A_m is bounded (takes bounded sets to bounded sets) and hemicontinuous. Furthermore, A_m is uniformly monotone, since for $u, v \in H^1(\Omega) \times H^1(\Omega)$ we have

$$\langle A_m(u) - A_m(v), u - v\rangle \geq \min\left\{\underline{n}, \underline{p}\right\} \|\nabla (u-v)\|^2_{L^2(\Omega)},$$

where we used $R \geq 0$ and the monotonicity $(e_m(x) - e_m(y))(x-y) \geq 0$ for all $x, y \in \mathbb{R}$. Due to Theorem 4.16 in [36] the equation

$$\langle A_m(F,G), \phi\rangle = 0, \qquad \text{for all } \phi \in \mathcal{V}^2$$

has a unique solution $(F_m, G_m) \in (F_{eq} + V_{ext}, G_{eq} - V_{ext}) + (\mathcal{V} \times \mathcal{V})$. This proves that (A.9) has a unique solution for all $m > 0$. Hence, it remains to establish (3.9) for all sufficiently large m. Let

$$\underline{F} = \min\left\{F_{eq}, F_{eq} + \inf_{\Gamma_D} V_{ext}\right\}, \qquad \overline{F} = \max\left\{F_{eq}, F_{eq} + \sup_{\Gamma_D} V_{ext}\right\},$$
$$\underline{G} = \min\left\{G_{eq}, G_{eq} - \sup_{\Gamma_D} V_{ext}\right\}, \qquad \overline{G} = \max\left\{G_{eq}, G_{eq} - \inf_{\Gamma_D} V_{ext}\right\}.$$

Let $m \geq \delta^2$. Then $\underline{F} + \overline{G} = \overline{F} + \underline{G} = F_{eq} + G_{eq}$ and thus

$$\delta^2 = \exp(\underline{F} + \overline{G}) = e_m(\underline{F} + \overline{G}) = \exp(\overline{F} + \underline{G}) = e_m(\overline{F} + \underline{G}).$$

One easily verifies that $(F - \overline{F})^+ = \max\{0, F - \overline{F}\}$ and $(G - \underline{G})^- = \min\{0, G - \underline{G}\}$ are admissible test functions in (A.9). This yields

$$\begin{aligned}
-\int_\Omega n \left|\nabla\left(F - \overline{F}\right)^+\right|^2 dx - \int_\Omega p \left|\nabla\left(G - \underline{G}\right)^-\right|^2 dx
&= \int_\Omega R(n,p)\left[e_m(F+G) - \delta^2\right] \\
&\qquad \cdot \left[\left(F - \overline{F}\right)^+ + \left(G - \underline{G}\right)^-\right] dx \\
&\geq 0
\end{aligned}$$

Thus, we have $(F - \overline{F})^+ \equiv 0$ and $(G - \underline{G})^- \equiv 0$ in the sense of $H^1(\Omega)$, which implies $F \leq \overline{F}$ and $\underline{G} \leq G$ a.e.. The other inequalities $\underline{F} \leq F$ and $G \leq \overline{G}$ can be shown analogously by choosing $(F - \underline{F})^-$ and $(G - \overline{G})^+$ as test functions, respectively.
c) We set $R_i = R(n_i, p_i)$ for $i = 1, 2$ and employ the weak formulation

$$-\int_\Omega n_i \nabla F_i \nabla \phi\, dx = \int_\Omega R_i \left(\exp(F_i + G_i) - \delta^2\right)\phi\, dx$$
$$-\int_\Omega p_i \nabla G_i \nabla \phi\, dx = \int_\Omega R_i \left(\exp(F_i + G_i) - \delta^2\right)\phi\, dx,$$

for all $\phi \in \mathcal{V}$. Using $\phi_1 = F_1 - F_2$ and $\phi_2 = G_1 - G_2$ as test functions, respectively, yields after subtraction

$$\begin{aligned}
&\int_\Omega n_1 \left|\nabla (F_1 - F_2)\right|^2 dx + \int_\Omega p_1 \left|\nabla (G_1 - G_2)\right|^2 dx = \\
&\quad -\int_\Omega (n_1 - n_2)\nabla F_2 \nabla (F_1 - F_2)\, dx - \int_\Omega (p_1 - p_2)\nabla G_2 \nabla (G_1 - G_2)\, dx \\
&\qquad -\int_\Omega R_1\left(e^{F_1+G_1} - e^{F_2+G_2}\right)\left((F_1 - F_2) + (G_1 - G_2)\right) dx \\
&\qquad\quad -\int_\Omega (R_1 - R_2)\left(e^{F_2+G_2} - e^{F_{eq}+G_{eq}}\right)\left((F_1 - F_2) + (G_1 - G_2)\right) dx
\end{aligned}$$

We estimate termwise. Employing Hölder's inequality we get

$$-\int_\Omega (n_1-n_2)\,\nabla F_2 \nabla\,(F_1-F_2)\ dx \qquad\qquad \leq \|n_1-n_2\|_{L^s(\Omega)}\,\|\nabla F_2\|_{L^r(\Omega)}\,\|\nabla(F_1-F_2)\|_{L^2(\Omega)}$$

and analogously

$$-\int_\Omega (p_1-p_2)\,\nabla G_2 \nabla\,(G_1-G_2)\ dx \qquad\qquad \leq \|p_1-p_2\|_{L^s(\Omega)}\,\|\nabla G_2\|_{L^r(\Omega)}\,\|\nabla(G_1-G_2)\|_{L^2(\Omega)}\,.$$

Next we use the fact that $R_i \geq 0$ and the monotonicity $(e^x-e^y)(x-y)\geq 0$, for all $x,y\in\mathbb{R}$, to derive

$$-\int_\Omega R_1\left(e^{F_1+G_1}-e^{F_2+G_2}\right)\left((F_1-F_2)+(G_1-G_2)\right)\ dx \leq 0.$$

The last term can be estimated as follows

$$\begin{aligned}-\int_\Omega (R_1-R_2)&\left(e^{F_2+G_2}-e^{F_{eq}+G_{eq}}\right)\left((F_1-F_2)+(G_1-G_2)\right)\ dx\\ &\leq \|R_1-R_2\|_{L^s(\Omega)}\left\|e^{F_2+G_2}-e^{F_{eq}+G_{eq}}\right\|_{L^r(\Omega)}\\ &\qquad\times\left[\|F_1-F_2\|_{L^2(\Omega)}+\|G_1-G_2\|_{L^2\Omega)}\right].\end{aligned}$$

Combining these estimates, using Young's inequality and Poincaré's inequality we obtain

$$\begin{aligned}\theta\,\|\nabla(F_1-F_2)\|^2_{L^2(\Omega)}&+\theta\,\|\nabla(G_1-G_2)\|^2_{L^2(\Omega)}\\ \leq\ &\frac{1}{\theta}\,\|n_1-n_2\|^2_{L^s(\Omega)}\,\|\nabla F_2\|^2_{L^r(\Omega)}+\frac{\theta}{4}\,\|\nabla(F_1-F_2)\|^2_{L^2(\Omega)}\\ +\ &\frac{1}{\theta}\,\|p_1-p_2\|^2_{L^s(\Omega)}\,\|\nabla G_2\|^2_{L^r(\Omega)}+\frac{\theta}{4}\,\|\nabla(G_1-G_2)\|^2_{L^2(\Omega)}\\ &+K_1^2\,\|R_1-R_2\|^2_{L^s(\Omega)}\left\|e^{F_2+G_2}-e^{F_{eq}+G_{eq}}\right\|^2_{L^r(\Omega)}\\ &\qquad+\frac{\theta}{4}\,\|\nabla(F_1-F_2)\|^2_{L^2(\Omega)}+\frac{\theta}{4}\,\|\nabla(G_1-G_2)\|^2_{L^2(\Omega)}\,,\end{aligned}$$

where $\theta=\theta(\mathbf{D})\in(0,1)$ is as in Theorem 26 and $K_1=K_1(\mathbf{D}_{dom},\theta)\in(0,\infty)$. Now we make use of the Lipschitz–continuity of R and the fact that $\|F_i-F_{eq}\|_{L^\infty(\Omega)}$, $\|G_i-G_{eq}\|_{L^\infty(\Omega)}\leq\|V_{ext}\|_{L^\infty(\Omega)}$ (see b)) to obtain after re-ordering

$$\begin{aligned}\frac{\theta}{2}\,\|\nabla(F_1-F_2)\|^2_{L^2(\Omega)}&+\frac{\theta}{2}\,\|\nabla(G_1-G_2)\|^2_{L^2(\Omega)}\leq\\ &\frac{1}{\theta}\,\|n_1-n_2\|^2_{L^s(\Omega)}\,\|\nabla F_2\|^2_{L^r(\Omega)}+\frac{1}{\theta}\,\|p_1-p_2\|^2_{L^s(\Omega)}\,\|\nabla G_2\|^2_{L^r(\Omega)}\\ &+K_1^2K_2\,e^{4\|V_{ext}\|_{L^\infty(\Omega)}}\|V_{ext}\|^2_{L^\infty(\Omega)}\left[\|n_1-n_2\|^2_{L^s(\Omega)}+\|p_1-p_2\|^2_{L^s(\Omega)}\right],\end{aligned}$$

where $K_2=K_2(\Omega;L_R(\theta),r,s)\in(0,\infty)$.
Next we wish to estimate $\|\nabla F_2\|^2_{L^r(\Omega)}$. (The term $\|\nabla G_2\|^2_{L^r(\Omega)}$ can be handled in analogy.) Setting $a:=n_2$ we easily verify that due to **A**.8 all assumptions required in **A**.7 are satisfied for a $\theta_\circ=\theta_\circ(\theta,\theta_D)$. Considering $U:=F_2-F_{eq}$ we have

$$\operatorname{div}(n_2\nabla U)=R_2\left(e^{U+F_{eq}+G_2}-e^{F_{eq}+G_{eq}}\right)\quad,\quad U-V_{ext}\in\mathcal{V}.$$

Hence, it follows from **A**.7 that there exists a constant $K_3 = K_3(\mathbf{D}_{dom}, \theta, \theta_D)$ such that

$$\begin{aligned}\|\nabla F_2\|_{L^r(\Omega)} &= \|\nabla U\|_{L^r(\Omega)} \\ &\le K_3 \, \left(\|V_{ext}\|_{W^{1,r}(\Omega)} + \left\|R_2 \, \left(e^{F_2+G_2} - e^{F_{eq}+G_{eq}}\right)\right\|_{L^\infty(\Omega)} \right) \\ &\qquad\qquad \le K_3 \, K_4 \, \|V_{ext}\|_{L^\infty(\Omega)} \, e^{2\|V_{ext}\|_{L^\infty(\Omega)}},\end{aligned}$$

where $K_4 = K_4(\mathbf{D}_{dom}, \theta, r) \in (0, \infty)$. Collecting all terms finally gives

$$\begin{aligned}&\|\nabla(F_1 - F_2)\|^2_{L^2(\Omega)} + \|\nabla(G_1 - G_2)\|^2_{L^2(\Omega)} \\ &\qquad \le K_5 \, e^{4\|V_{ext}\|_{L^\infty(\Omega)}} \, \|V_{ext}\|^2_{L^\infty(\Omega)} \, \left[\|n_1 - n_2\|^2_{L^s(\Omega)} + \|p_1 - p_2\|^2_{L^s(\Omega)}\right],\end{aligned}$$

where $K_5 = K_5(\mathbf{D}_{dom}, \mathbf{D}_{bdry}, \theta(\mathbf{D}), L_R(\theta(\mathbf{D})), r, s)$.

Now (3.10) immediately follows.□

A.5. Proof of Subsection 3.4.

Proof of Theorem 28. Let $(F_i, G_i) \in \mathcal{C}$, $i = \circ, 1$. We set $(n_i, p_i) := S_1(F_i, G_i)$, $i = \circ, 1$ and $(\tilde{F}_i, \tilde{G}_i) := S_2(n_i, p_i)$, $i = \circ, 1$. Then $(\tilde{F}_i, \tilde{G}_i) = T(F_i, G_i)$, $i = \circ, 1$.
b) Due to (3.7) there exists a $K_1 = K_1(\mathbf{D}, s) \in (0, \infty)$ such that

$$\begin{aligned}&\|n_\circ - n_1\|_{L^s(\Omega)} + \|p_\circ - p_1\|_{L^s(\Omega)} \\ &\qquad\qquad \le K \, \left(\|F_\circ - F_1\|_{L^2(\Omega)} + \|G_\circ - G_1\|_{L^2(\Omega)}\right). \qquad \text{(A.10)}\end{aligned}$$

Employing this estimate in (3.10) we get

$$\begin{aligned}&\left\|\nabla\left(\tilde{F}_\circ - \tilde{F}_1\right)\right\|_{L^2(\Omega)} + \left\|\nabla\left(\tilde{G}_\circ - \tilde{G}_1\right)\right\|_{L^2(\Omega)} \\ &\quad \le K_2 \, e^{2\|V_{ext}\|_{L^\infty(\Omega)}} \, \|V_{ext}\|_{L^\infty(\Omega)} \left[\|F_\circ - F_1\|_{L^2(\Omega)} + \|G_\circ - G_1\|_{L^2(\Omega)}\right], \qquad \text{(A.11)}\end{aligned}$$

for a constant $K_2 = K_2(\mathbf{D}, \theta(\mathbf{D}), L_R(\theta(\mathbf{D})), r, s) \in (0, \infty)$ and $\theta(\mathbf{D})$ is as in Theorem 26. Now we apply Poincaré's inequality to obtain

$$\begin{aligned}&\left\|\tilde{F}_\circ - \tilde{F}_1\right\|_{H^1(\Omega)} + \left\|\tilde{G}_\circ - \tilde{G}_1\right\|_{H^1(\Omega)} \\ &\quad \le K_3 \, e^{2\|V_{ext}\|_{L^\infty(\Omega)}} \, \|V_{ext}\|_{L^\infty(\Omega)} \left[\|F_\circ - F_1\|_{H^1(\Omega)} + \|G_\circ - G_1\|_{H^1(\Omega)}\right], \qquad \text{(A.12)}\end{aligned}$$

for a constant $K_3 = K_3(\mathbf{D}, \theta(\mathbf{D}), L_R(\theta(\mathbf{D})), r, s) \in (0, \infty)$. Hence b) follows by defining $U_\circ = U_\circ(\mathbf{D}, \theta(\mathbf{D}), L_R(\theta(\mathbf{D})), r, s) \in (0, \infty)$ via

$$K_3 \, e^{2U_\circ} \, U_\circ = 1.$$

a) follows immediately from b).
c) The stated convergence property of $(F^k, G^k)_{k\in\mathbb{N}}$ follows from b). The respective convergence property of $(n^k, p^k)_{k\in\mathbb{N}}$ follows from the convergence of $(F^k, G^k)_{k\in\mathbb{N}}$ and (3.7). This convergence of $(n^k, p^k)_{k\in\mathbb{N}}$ also ensures the stated convergence of $(V^k)_{k\in\mathbb{N}}$.□

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