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Abstract

A positivity–preserving numerical scheme for a fourth order nonlinear parabolic system arising in quantum semiconductor modelling is studied. The system is numerically treated by introducing an additional nonlinear potential and a subsequent semidiscretization in time. The resulting sequence of nonlinear second order elliptic systems admits at each time level *strictly positive* solutions, which is proved by an exponential transformation of variables. The stability of the scheme is shown and convergence is proved in one space dimension. The results extend under additional assumptions to the multi–dimensional case. Assuming enough regularity on the solution the rate of convergence proves to be optimal. Numerical results concerning the switching behaviour of a resonant tunneling diode are presented.

Key words. Higher order parabolic PDE, positivity, semidiscretization, stability, convergence, semiconductor.

AMS(MOS) subject classification. 35K35, 65M12, 65M15, 65M20, 76Y05

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1 Introduction

During the last years there was a fast progress in the miniaturization of semiconductor devices, reaching a length scale at which quantum effects play a dominant role. As classical simulation codes are no more capable of resolving the correct device behaviour, applied mathematicians have to keep pace by deriving accurate quantum models, which allow for an efficient numerical treatment.

The state of the art in quantum semiconductor device modelling ranges from *microscopic* models such as Schrödinger–Poisson systems [PU95] to *macroscopic* equations such as the quantum hydrodynamic model (QHD) [Gar94, GJ97, GR98]. While the former incorporate all relevant quantum phenomena they have two drawbacks: Firstly, the high computational costs which result from the extreme oscillatory behaviour of the wave function [MPP99] and secondly, the lack of appropriate boundary conditions as the Schrödinger equation is stated on an unbounded position domain [KKFR89, RFK89].

In contrast, the QHD deals with macroscopic, fluid–type unknowns which allow for a natural interpretation of boundary conditions [Pin99b]. The model consists of conservation laws for the particle density, current density and energy density and can be derived via a moment expansion from a many particle Schrödinger–Poisson system [GM97]. Although only a few moments are considered, numerical investigations underline the capability of the QHD to resolve the relevant quantum mechanical effects, e.g. negative differential resistance in the stationary current–voltage characteristic of resonant tunneling structures [Gar94, GR98]. A lot of information concerning the device behaviour can already be deduced from the stationary characteristics, but there are applications when one has to employ the transient equations, e.g. when a diode is switched from forward to reverse bias or when one studies the response time of several coupled devices or high frequency oscillation circuits.

Especially for stationary simulations a first moment version of the isothermal QHD, the quantum drift diffusion model (QDD) [Anc87, AU98], proved to quite promising since it allows a very effective numerical treatment [PU99]. The transient equations are a result of a zero relaxation time limit in the QHD [Pin99a], which reads in the diffusion scaling

$$n_t + \operatorname{div} J = 0,$$

$$\tau^2 J_t + \tau^2 \operatorname{div}\left(\frac{J \otimes J}{n}\right) + \nabla n + n \nabla V - \varepsilon^2 n \nabla \left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -J,$$

$$-\lambda^2 \Delta V = n - C_{dot}.$$

Here, the parameters are the scaled Planck constant ε, the scaled Debye length λ and the scaled relaxation time τ. The distribution of charged background ions is described by the doping profile $C_{dot}(x)$, which is assumed to be independent of time (for details see [Pin99a]). The variables are the electron density $n(x,t)$, the current density $J(x,t)$ and the electrostatic potential $V(x,t)$. The limiting system ($\tau = 0$), stated on a bounded domain Ω, can be written as

$$n_t = -\frac{\varepsilon^2}{2}\Delta^2 n + \frac{\varepsilon^2}{2}\sum_{i,j=1}^{d} \partial_{x_i}\partial_{x_j}\left(\frac{\partial_{x_i} n\,\partial_{x_j} n}{n}\right) + \Delta n + \operatorname{div}\left(n\,\nabla V\right), \tag{1.1a}$$

$$-\lambda^2 \Delta V = n - C_{dot}, \tag{1.1b}$$

yielding a fourth order nonlinear parabolic equation for the electron density n, which is self–consistently coupled to Poisson's equation for the potential V.

To get a well posed problem, the system (1.1) has to be supplemented with appropriate boundary conditions. We assume that the boundary $\partial\Omega$ of the domain Ω splits into two disjoint parts Γ_D and Γ_N, where Γ_D models the Ohmic contacts of the device and Γ_N represents the insulating parts of the boundary. Let ν denote the unit outward normal vector along $\partial\Omega$. The electron density is assumed to fulfill local charge neutrality at the Ohmic contacts:

$$n = C_{dot} \quad \text{on } \Gamma_D. \tag{1.1c}$$

Concerning the potential we assume that it is a superposition of its equilibrium value and an applied biasing voltage U at the Ohmic contacts, and that the electric field vanishes along the Neumann part of the boundary:

$$V = V_{eq} + U \quad \text{on } \Gamma_D, \quad \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N. \tag{1.1d}$$

Further, it is natural to assume that there is no normal component of the current along the insulating part of the boundary and additionally the normal component of the quantum current has to vanish:

$$J \cdot \nu = 0, \quad \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) \cdot \nu = 0 \quad \text{on } \Gamma_N. \tag{1.1e}$$

Lastly, we require that no quantum effects occur at the contacts:

$$\Delta\sqrt{n} = 0 \quad \text{on } \Gamma_D. \tag{1.1f}$$

These boundary conditions are physically motivated and commonly employed in quantum semiconductor modelling. The numerical investigations in [Pin99b] underline the reasonability of this choice.

System (1.1) is supplemented by an initial condition

$$n(x,0) = n_0(x) \quad \text{in } \Omega. \tag{1.1g}$$

This model was first investigated in [Pin99a] with a slightly different set of boundary conditions. There, the dynamic stability of stationary states was established, at least for small scaled Planck constants and small applied biasing voltages. So far, there are only a few results available concerning the solvability of (1.1) due to the lack of an appropriate maximum principle ensuring the positivity of the electron density n. Nevertheless, for zero temperature and vanishing electric field (1.1) simplifies to

$$n_t = -\frac{\varepsilon^2}{2}\Delta^2 n + \frac{\varepsilon^2}{2}\sum_{i,j=1}^{d}\partial_{x_i}\partial_{x_j}\left(\frac{\partial_{x_i} n\,\partial_{x_j} n}{n}\right). \tag{1.2}$$

This equation also arises as a scaling limit in the study of interface fluctuations in a certain spin system. *Bleher, et al.* [BLS94] showed that there exists a unique positive classical solution locally in time in one space dimension, assuming strictly positive $H^1(\Omega)$–data and periodic boundary conditions. The authors [JP99] deduced under much weaker assumptions the existence of a non–negative *global* solution n in one space dimension.

The preservation of non–negativity or positivity is not only challenging from an analytical point of view, also the derivation of sign–preserving numerical schemes for fourth–order equations is a field of intensive research. Even for strictly positive analytical solutions, the solution of a naive discretization scheme may become negative, causing unwanted numerical instabilities [Ber98].

In the last years this question was thoroughly investigated in the context of lubrication–type equations [BF90, BP98, dPGG98], which read

$$h_t + \operatorname{div}\left(f(h)\,\nabla\Delta h\right) = 0. \tag{1.3}$$

They arise in the study of thin liquid films and spreading droplets (for an overview see [Ber98] and the references therein). Here, the main ingredient for the proof of the non–negativity or positivity property is to exploit the special nonlinear structure of (1.3), especially the degeneracy of the mobility $f(h)$, i.e. $f(h) = h^\alpha$ as $h \to 0$ for some $\alpha > 0$. Numerically, there are two ways of dealing with Equation (1.3): *Bertozzi et al.* [BZ99] designed a space discretization using finite differences, which exhibits the same properties as the continuous equation. While *Barrett et al.* [BBG98] proposed a non–negativity preserving finite element method, where the non–negativity property is imposed as a constraint such that at each time level a variational inequality has to be solved.

Concerning Equation (1.2) a different approach was used in the existence proof [JP99]. After an exponential transformation of variables, $n = e^{2u}$, a semi–discretization in time was performed for

$$\left(e^{2u}\right)_t = -\varepsilon^2\left(e^{2u}\,u_{xx}\right)_{xx}.$$

As the resulting sequence of elliptic problems is uniquely solvable in each time step, this yields intrinsically a global non–negative solution. However, due to the introduced additional nonlinearity in the time derivative this scheme meets some difficulties in numerical simulations.

In this paper we introduce a totally new approach to the numerical solution of the fully coupled system (1.1), which consists of two main ideas: Firstly, we write Equation (1.1a) in conservation form

$$n_t = \operatorname{div}\left(n\,\nabla\left(-\varepsilon^2\frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V\right)\right)$$

and introduce the quantum quasi Fermi level

$$F = -\varepsilon^2\frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V.$$

Here, $-\varepsilon^2\Delta\sqrt{n}/\sqrt{n}$ is the so–called quantum Bohm potential. Employing the boundary conditions (1.1c)–(1.1f) we learn that the equilibrium value of the potential is given by $V_{eq} = -\log(C_{dot})$ and that F fulfills

$$F = U \quad \text{on } \Gamma_D, \quad \nabla F \cdot \nu = 0 \quad \text{on } \Gamma_N.$$

Secondly, motivated by the results for the stationary problem [AU98], we employ an implicit time discretization by a backward EULER scheme on the system

$$n_t = \operatorname{div}(n\,\nabla F), \tag{1.4a}$$

$$-\varepsilon^2\frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V = F, \tag{1.4b}$$

$$-\lambda^2\Delta V = n - C_{dot}. \tag{1.4c}$$

In the following we prove that in one space dimension the discretized version of (1.4) admits at each time level a *strictly positive* solution $n(x, t_k)$ and state conditions, which are sufficient to ensure the solvability in the multi–dimensional case. Unfortunately, we cannot derive a uniform lower bound on the electron density such that this property does not hold in the limit and weakens to non–negativity. Further, it is worth noting that the *entropy* (or free energy)

$$S(t) = \varepsilon^2\int_\Omega \left|\nabla\sqrt{n(t)}\right|^2\,dx + \int_\Omega H\left(n(t)\right)\,dx + \frac{\lambda^2}{2}\int_\Omega |\nabla V(t)|^2\,dx \tag{1.5}$$

is (formally) non–increasing in time, as long as the boundary data F_D for the quantum quasi Fermi level is non–positive. Here,

$$H(s) \stackrel{\text{def}}{=} s\left(\log(s) - 1\right) + 1$$

denotes a primitive of the logarithm. This observation allows us to derive a stability bound for the numerical scheme in arbitrary space dimensions. However, without additional assumptions, this is only sufficient to prove convergence of the scheme in one space dimension, since in the proof the Sobolev embedding $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$ plays a crucial role. Imposing stronger assumptions on the regularity of the continuous solutions we show convergence in arbitrary space dimensions and give an estimate on the order of convergence, which proves to be optimal.

Finally, let us give some comments on the numerical advantages of (1.4) compared with (1.1), which are twofold: On the one hand we do not have to discretize a higher order differential operator and on the other hand it is now possible to introduce an external potential, modelling discontinuities in the conduction band, which occur for example in resonant tunneling structures [Gar94, PU99]. It is common to replace in (1.4b) the potential $V \mapsto V+B$, where B is a step function. Clearly, such a replacement in (1.1a) causes extreme numerical problems due to the second derivative of B.

The paper is organized as follows. In Section 2 we introduce the semidiscretization of (1.4), prove the solvability of the discretized system in one space dimension and state additional conditions ensuring the solvability in multi–dimensions. Further, we derive a stability estimate on the discrete solution, which also holds for space dimensions larger than one. Section 3 is devoted to the proof of convergence in one space dimension, which relies on an energy estimate for the discrete solution. Imposing stronger assumptions we show in Section 4 that the scheme is convergent with the optimal order in some suitable norm. Finally, in Section 5 we apply the scheme for the simulation of a resonant tunneling diode and present numerical results concerning its switching behaviour. These are the first transient computations employing a *macroscopic* quantum model.

2 Semidiscretization

In this section we derive the implicit semidiscretization of (1.4) and prove the existence of solutions to the resulting system on each time level in the case $\Omega \subset \mathbb{R}$. Especially, we show that the approximation of the electron density is strictly positive. We discuss sufficient conditions guaranteeing the solvability in the multi–dimensional case. Further, we derive a stability estimate on the discrete solution, which is essentially a consequence of the boundedness of the entropy (1.5).

For the following investigations we introduce the new variable $\rho = \sqrt{n}$. Then (1.4) reads:

$$\left(\rho^2\right)_t = \operatorname{div}(\rho^2 \nabla F), \tag{2.1a}$$

$$-\varepsilon^2 \frac{\Delta\rho}{\rho} + \log(\rho^2) + V = F, \tag{2.1b}$$

$$-\lambda^2 \Delta V = \rho^2 - C_{dot}. \tag{2.1c}$$

For the numerical treatment of (2.1) we employ a vertical line method and replace the transient problem by a sequence of elliptic problems.

Let $T > 0$ be given. We divide the time interval $[0,T]$ into N subintervals by introducing the temporal mesh $\{t_k : k = 0, \ldots, N\}$, where $0 = t_0 < t_1 < \ldots < t_N = T$. We set $\tau_k \stackrel{\text{def}}{=} t_k - t_{k-1}$ and define the maximal subinterval length $\tau \stackrel{\text{def}}{=} \max_{k=1,\ldots,N} \tau_k$. We assume that the partition fulfills

$$\tau \to 0, \qquad \text{as } N \to \infty. \tag{2.2}$$

For any Banach space B we define

$$PC_N(0,T;B) \stackrel{\text{def}}{=} \left\{ v^\tau : (0,T] \to B : v^\tau|_{(t_{k-1},t_k]} \equiv \text{const. for } k = 1, \ldots, N \right\}$$

and introduce the short–cut $v_k = v^\tau(t)$ for $t \in (t_{k-1}, t_k]$ and $k = 1, \ldots, N$. Further, let $\tilde{v}^\tau$ denote the linear interpolant of $v^\tau \in PC_N(0,T;L^2(\Omega))$ given by

$$\tilde{v}^\tau(t,x) = \frac{t - t_{k-1}}{\tau_k}(v_k - v_{k-1}) + v_{k-1}, \qquad \text{for } x \in \Omega, \quad t \in (t_{k-1}, t_k].$$

Now we discretize (2.1) using an implicit EULER scheme:

Set $\rho_0 = \sqrt{n(0)}$. For $k = 1, \ldots, N$ solve recursively the elliptic systems

$$\frac{1}{\tau_k}\left(\rho_k^2 - \rho_{k-1}^2\right) = \operatorname{div}(\rho_k^2 \nabla F_k), \tag{2.3a}$$

$$-\varepsilon^2 \frac{\Delta \rho_k}{\rho_k} + \log(\rho_k^2) + V_k = F_k, \tag{2.3b}$$

$$-\lambda^2 \Delta V_k = \rho_k^2 - C_{dot}, \tag{2.3c}$$

subject to the boundary conditions

$$\rho_k = \rho_D, \quad F_k = F_D, \quad V_k = V_D \quad \text{on } \Gamma_D, \tag{2.3d}$$

$$\nabla \rho_k \cdot \nu = \nabla F_k \cdot \nu = \nabla V_k \cdot \nu = 0 \quad \text{on } \Gamma_N, \tag{2.3e}$$

where

$$\rho_D = \sqrt{C_{dot}}, \quad F_D = U, \quad V_D = -\log(C_{dot}) + U.$$

Then the approximate solution to (2.1) is given by $(\rho^\tau, F^\tau, V^\tau)$.

2.1 Solvability of the Discretized System

We use the standard notation for Sobolev spaces (see [Ada75]), denoting the norm of $W^{m,p}(\Omega)$ ($m \in \mathbb{R}_0^+, p \in [1,\infty]$) by $\|\cdot\|_{W^{m,p}(\Omega)}$. In the special case $p = 2$ we use

$H^m(\Omega)$ instead of $W^{m,2}(\Omega)$. Further, let $H_0^m(\Omega)$ be the closure of $C_c^\infty(\Omega)$ with respect to the $H^m(\Omega)$–norm. Its dual space $(H_0^m(\Omega))^*$ is denoted by $H^{-m}(\Omega)$ and the duality pairing of $H_0^m(\Omega)$ with its dual space is given by $\langle \cdot, \cdot \rangle_{H^{-m}, H_0^m}$. Moreover, for any Banach space B we define the space $L^p(0,T;B)$ with $p \in [1,\infty]$ consisting of all measurable functions $\varphi : (0,T) \to B$ for which the norm

$$\|\varphi\|_{L^p(0,T;B)} \stackrel{\text{def}}{=} \left(\int_0^T \|\varphi\|_B^p \; dt \right)^{1/p}, \quad p \in [1,\infty),$$
$$\|\varphi\|_{L^\infty(0,T;B)} \stackrel{\text{def}}{=} \sup_{t \in (0,T)} \|\varphi(t)\|_B, \quad p = \infty,$$

is finite. If the time interval is clear we shortly write $\|\cdot\|_{L^p(B)}$.

We can show the existence of a solution to the discrete system in one space dimension under natural assumptions on the data. The multi-dimensional case can be treated under additional assumptions (see Remark 2.3). For the subsequent considerations we impose the following assumptions.

A.1 Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or 3 be a bounded domain with boundary $\partial\Omega \in C^{1,1}$. The boundary $\partial\Omega$ is piecewise regular and splits into two disjoint parts Γ_N and Γ_D. The set Γ_D has nonvanishing $(d-1)$–dimensional Lebesgue–measure. Γ_N is closed.

A.2 The boundary data fulfills

$$\rho_D \in H^2(\Omega), \quad \inf_\Omega \rho_D > 0, \quad \nabla \rho_D \cdot \nu = 0 \text{ on } \Gamma_N,$$
$$F_D \in C^{2,\gamma}(\bar{\Omega}) \quad \text{for } \gamma \in \left(0, \frac{1}{2}\right), \quad F_D \leq -\overline{F}_D < 0,$$
$$V_D \in C^{2,\gamma}(\bar{\Omega})$$

and for the initial condition holds $\rho_0 \in H^2(\Omega)$. Further, $C_{dot} \in C^{0,\gamma}(\bar{\Omega})$.

A.3 Let $\gamma \in (0,1)$ and $a \in C^{0,\gamma}(\bar{\Omega})$ with $a \geq \underline{a} > 0$. Then there exists a constant $K = K(\Omega, \Gamma_D, \Gamma_N, a, d, \gamma) > 0$ such that for $f \in C^{0,\gamma}(\bar{\Omega})$ and $u_D \in C^{2,\gamma}(\bar{\Omega})$ there exists a solution $u \in C^{2,\gamma}(\bar{\Omega})$ of

$$\operatorname{div}(a \nabla u) = f, \quad u - u_D \in H_0^1(\Omega \cup \Gamma_N),$$

which fulfills

$$\|u\|_{C^{2,\gamma}(\bar{\Omega})} \leq K \left(\|u_D\|_{C^{2,\gamma}(\bar{\Omega})} + \|f\|_{C^{0,\gamma}(\bar{\Omega})} \right).$$

Remark 2.1.

(a) Assumption **A.3** is essentially a restriction on the geometry of Ω. It is fulfilled in the case where the Dirichlet and the Neumann boundary do not meet, i.e. $\overline{\Gamma}_D \cap \Gamma_N = \emptyset$ [Tro87].

(b) The restriction $F_D \leq -\overline{F}_D$ on the Quantum Quasi Fermi level is purely technical. From the physical point of view the device behaviour is independent of a shift $F \mapsto F + \alpha$, $V \mapsto V + \alpha$, $\alpha \in \mathbb{R}$.

(c) For a smoother presentation we assume that the boundary conditions are independent of time.

Now we state the main existence theorem for (2.3).

Theorem 2.2. *Assume* **A.2**—**A.3** *and* $d = 1$, $\partial\Omega = \Gamma_D$. *Furthermore, let* $k \in \{1, \ldots, N\}$ *and let* $\rho_{k-1} \in C^{0,\gamma}(\bar{\Omega})$. *Then there exists a solution* (ρ_k, F_k, V_k) *of the system* (2.3), *fulfilling*

(a) $(\rho_k, F_k, V_k) \in H^2(\Omega) \times C^{2,\gamma}(\bar{\Omega}) \times C^{2,\gamma}(\bar{\Omega})$ *for* $0 < \gamma < \frac{1}{2}$,

(b) $\exists c_k > 0 : \quad \rho_k \geq c_k > 0 \quad$ *in* Ω.

Proof. The proof is done in three steps: We eliminate F_k from (2.3), introduce an exponentional transformation of variables and employ Schauder's fixed point theorem on the resulting system. Elimination of F_k and some calculus yields (for positive ρ)

$$\frac{1}{\tau_k}(\rho^2 - \rho_{k-1}^2) = -\frac{\varepsilon^2}{2}(\rho^2(\log\rho^2)_{xx})_{xx} + (\rho^2(\log\rho^2)_x)_x + (\rho^2 V_x)_x, \tag{2.4a}$$

$$-\lambda^2 V_{xx} = \rho^2 - C_{dot} \quad \text{in } \Omega, \tag{2.4b}$$

$$\rho = \rho_D, \quad \rho_{xx} = 0, \quad V = V_D \quad \text{on } \partial\Omega, \tag{2.4c}$$

which has to be solved for (ρ, V).

Since there is no maximum principle available we employ the exponential transformation of variables $\rho = e^u$ as in [GJ99] and get the system

$$\frac{1}{\tau_k}(e^{2u} - \rho_{k-1}^2) = -\varepsilon^2(e^{2u}u_{xx})_{xx} + 2(e^{2u}u_x)_x + (e^{2u}V_x)_x, \tag{2.5a}$$

$$-\lambda^2 V_{xx} = e^{2u} - C_{dot} \quad \text{in } \Omega, \tag{2.5b}$$

$$u = u_D, \quad u_{xx} = -(u_x)^2, \qquad \text{on } \partial\Omega, \tag{2.5c}$$

where $u_D = \log\rho_D$. We show that there exists a solution $u \in H^2(\Omega)$ to (2.5). Since $H^2(\Omega) \hookrightarrow L^\infty(\Omega)$, we can set $\rho = e^u$ and ρ solves the system (2.4). Moreover, ρ is strictly positive in Ω.

To establish the existence of a solution to (2.5) we use Schauder's fixed point theorem. For this purpose we define a fixed point mapping $G : H^{3/2+\sigma}(\Omega) \to H^{3/2+\sigma}(\Omega)$, with $\sigma \in (0, \frac{1}{2})$ as follows. Let $w \in H^{3/2+\sigma}(\Omega)$ be given. Let $V \in H^1(\Omega)$ be the unique solution to

$$-\lambda^2 V_{xx} = e^{2w} - C_{dot} \text{ in } \Omega, \quad V = V_D \text{ on } \partial\Omega.$$

Furthermore, solve the linear problem

$$\frac{1}{\tau_k}(e^{2w} - \rho_{k-1}^2) = -\varepsilon^2 (e^{2w} u_{xx})_{xx} + 2(e^{2w} u_x)_x + (e^{2w} V_x)_x \quad \text{on } \Omega, \tag{2.6a}$$

$$u = u_D, \quad u_{xx} = -(w_x)^2 \quad \text{on } \partial\Omega. \tag{2.6b}$$

Notice that $H^{3/2+\sigma}(\Omega) \hookrightarrow C^1(\bar{\Omega})$ such that the above equation is strictly elliptic and w_x is well defined on $\partial\Omega$. It is easy to see that this problem has a unique solution $u \in H^2(\Omega)$. Then the mapping G, given by $G(w) = u$, is well defined.

Further, we have the following apriori estimate on u. Using $u - u_D$ as test function in (2.6a) and integration by parts give

$$\begin{aligned} &\varepsilon^2 \int_\Omega e^{2w} u_{xx}^2 \, dx + 2 \int_\Omega e^{2w} u_x^2 \, dx \qquad (2.7) \\ = \;& \varepsilon^2 \int_{\partial\Omega} e^{2w} u_{xx} (u - u_D)_x \, ds + \varepsilon^2 \int_\Omega e^{2w} u_{xx} u_{D,xx} \, dx + 2 \int_\Omega e^{2w} u_x u_{D,x} \, dx \\ & - \int_\Omega e^{2w} V_x (u - u_D)_x \, dx + \frac{1}{\tau_k} \int_\Omega (\rho_{k-1}^2 - e^{2w})(u - u_D) \, dx. \end{aligned}$$

In view of the boundary condition $u_{xx} = -(w_x)^2$, we can estimate the boundary term as follows:

$$\begin{aligned} & \left| \int_{\partial\Omega} e^{2w} u_{xx} (u - u_D)_x \, ds \right| \\ & \le \exp\left(2\|w\|_{L^\infty(\Omega)}\right) \|w_x\|_{L^\infty(\partial\Omega)}^2 \left(\|u_x\|_{L^1(\partial\Omega)} + \|u_{D,x}\|_{L^1(\partial\Omega)}\right) \\ & \le c_1(\|w\|_{C^1(\bar{\Omega})}) \left(\|u_x\|_{H^1(\Omega)} + 1\right) \\ & \le \exp\left(-2\|w\|_{L^\infty(\Omega)}\right) \left(\frac{\varepsilon^2}{2} \|u_{xx}\|_{L^2(\Omega)}^2 + \|u_x\|_{L^2(\Omega)}^2 \right) + c_2\left(\|w\|_{C^1(\bar{\Omega})}\right). \end{aligned}$$

Here, we have used the embedding $H^1(\Omega) \hookrightarrow L^1(\partial\Omega)$. Employing the elliptic estimate

$$\|V\|_{H^1(\Omega)} \le c_3 \|e^{2w} - C_{dot}\|_{L^2(\Omega)}$$

with $c_3 > 0$, Young's and Poincaré's inequality, we arrive at

$$\frac{\varepsilon^2}{2} \exp(-2\|w\|_{L^\infty(\Omega)}) \int_\Omega u_{xx}^2 \, dx + \exp(-2\|w\|_{L^\infty(\Omega)}) \int_\Omega u_x^2 \, dx \le c_3(\|w\|_{C^1(\bar{\Omega})}).$$

Thus, by Poincaré's inequality,

$$\|u\|_{H^2(\Omega)} \leq c_4(\|w\|_{H^{3/2+\sigma}(\Omega)}).$$

The constant $c_4 > 0$ also depends on k and the data.

Standard arguments now show that G is a continuous mapping. The compactness of G follows from the above estimate and the compact embedding $H^2(\Omega) \hookrightarrow H^{3/2+\sigma}(\Omega)$. Hence, the existence of a fixed point is now a consequence of Schauder's fixed point theorem.

Since $\rho = e^u$ and $\rho > 0$ in Ω, the Quantum Quasi Fermi level F in (2.3) is well defined and as F fulfills

$$\operatorname{div}\left(\rho^2 \nabla F\right) = \frac{1}{\tau_k}\left(\rho^2 - \rho_{k-1}^2\right) \in C^{0,\gamma}(\bar{\Omega})$$

we get from **A.3** the desired regularity $F \in C^{2,\gamma}(\bar{\Omega})$. An analoguous argument gives $V \in C^{2,\gamma}(\bar{\Omega})$. □

Remark 2.3. The same argument as in the previous proof does not work for the multi-dimensional problem. Indeed, the boundary condition $u_{xx} = -w_x^2$ on Γ_D has to be replaced by

$$\Delta u = -|\nabla w|^2 \quad \text{on } \Gamma_D,$$

and the boundary term in estimate (2.7) becomes

$$\varepsilon^2 \sum_{i,j=1}^{d} \int_{\partial\Omega} e^{2w}\, \partial_{ij} u\, \partial_i(u - u_D)\, \nu_j\, ds.$$

But now we cannot replace $\partial_{ij}u$ by an expression involving the derivatives of w and estimate as in the previous proof. Therefore, we have to consider another strategy.

Let **A.1**–**A.3** hold. Working directly with the system (2.3), where we replace $\log \rho^2$ by $\theta \log \rho^2$, $\theta > 0$ being a temperature constant, we can prove the existence of solutions if θ is sufficiently large. To see this, we define the fixed point operator as follows. Let $w \in H^{3/2+\sigma}(\Omega)$ $(0 < \sigma < 1/2)$ with $w \geq m > 0$ in Ω for some $m > 0$ to be determined, and let $V \in H^1(\Omega)$ be the unique solution to

$$-\lambda^2 \Delta V = w^2 - C_{dot} \quad \text{in } \Omega,$$
$$V = V_D \quad \text{on } \Gamma_D, \qquad \nabla V \cdot \nu = 0 \quad \text{on } \Gamma_N.$$

Since $w \in H^{3/2+\sigma}(\Omega) \hookrightarrow C^{0,\gamma}(\bar{\Omega})$ with $\gamma < \sigma$, we have $V \in C^{2,\gamma}(\bar{\Omega})$, in view of Assumption **A.3**. Further, the unique solution F to

$$\operatorname{div}(w^2 \nabla F) = \frac{1}{\tau_k}(w^2 - \rho_{k-1}^2) \quad \text{in } \Omega, \tag{2.8}$$
$$F = F_D \quad \text{on } \Gamma_D, \qquad \nabla F \cdot \nu = 0 \quad \text{on } \Gamma_N,$$

satisfies the regularity property $F \in C^{2,\gamma}(\bar{\Omega})$. Finally, let $\rho \in H^1(\Omega)$ be the unique solution to

$$\begin{gathered}\varepsilon^2 \Delta \rho = \rho\,(\theta \log \rho^2 + V - F) \quad \text{in } \Omega, \\ \rho = \rho_D \quad \text{on } \Gamma_D, \qquad \nabla\rho\cdot\nu = 0 \quad \text{on } \Gamma_N.\end{gathered} \tag{2.9}$$

The main difficulty now is to prove that $\rho \geq m > 0$ holds in Ω. Assuming a regularity assumption for $W^{2,p}(\Omega)$ spaces, similar to **A.3**, we obtain $\rho \in W^{2,p}(\Omega) \hookrightarrow C^1(\bar{\Omega})$ for $p > d$ and then, using Assumption **A.3**, $\rho \in C^{2,\gamma}(\bar{\Omega})$. Moreover, the fixed point operator $w \mapsto \rho$ is well defined.

In order to obtain the lower bound for ρ, we can use $(\rho - m)^- = \min(0, \rho - m)$ as a test function in (2.9) if $0 < m \leq \inf_{\Gamma_D} \rho_D$. Then we can achieve $\rho \geq m$ if $\inf_\Omega F > -\infty$ is independent of m, by choosing $m > 0$ small enough. For an estimate for $\inf_\Omega F$ take $(F - f)^-$ for appropriate f as test function in (2.8). Using Stampacchia's method, however, it is only possible to show that $F \geq f - c(\|w\|_{L^q})/m^2$ (for some $q > 1$).

We need to choose $\theta > 0$ large enough in order to get the bound $\rho \geq m$. We proceed similar as in [Jün98]. Indeed, it is easy to check that $\sup_\Omega F \leq c_1(m)$. This gives $\rho \leq c_2(m)$, by the truncation method, and thus $\inf_\Omega F \geq -c_3(m)$ (defining the fixed point operator in an appropriate way). Furthermore, it holds $\sup_\Omega V \leq c_4(m)$. Hence, employing the test function $(\rho - m)^-$ in (2.9), we obtain

$$\begin{aligned}\varepsilon^2 \int_\Omega |\nabla(\rho - m)^-|^2 dx &\leq \int_\Omega \rho(\theta \log m^2 + V - F)(-(\rho - m)^-) dx \\ &\leq \int_\Omega \rho(\theta \log m^2 + c_4(m) + c_3(m))(-(\rho - m)^-) dx \\ &\leq 0,\end{aligned}$$

if we choose $m = \min(0, \inf_{\Gamma_D} \rho_D)$ and $\theta > 0$ large enough. Therefore, $\rho \geq m$ in Ω.

With these a priori bounds, it is not difficult to show the existence of a solution to (2.3) in the multi-dimensional case for sufficiently large $\theta > 0$.

2.2 Stability Bounds

Now we prove a stability estimate on the solution, which is essentially a consequence of the boundedness of the entropy (1.5).

Lemma 2.4. *Assume* **A.1**—**A.2**. *For fixed $k \in \{1, \ldots, N\}$ let $(\rho_k, F_k, V_k) \in H^2(\Omega) \times C^{2,\gamma}(\bar{\Omega}) \times C^{2,\gamma}(\bar{\Omega})$ be a solution of* (2.3). *Then the following discrete* *entropy estimate holds*

$$
\begin{aligned}
&\varepsilon^2 \int_\Omega |\nabla \rho_k|^2 \ dx + \int_\Omega H(\rho_k^2)\ dx + \frac{\lambda^2}{2}\int_\Omega |\nabla V_k|^2 \ dx - \int_\Omega F_D\, \rho_k^2\ dx \\
&\quad \le \varepsilon^2 \int_\Omega |\nabla \rho_{k-1}|^2 \ dx + \int_\Omega H(\rho_{k-1}^2)\ dx + \frac{\lambda^2}{2}\int_\Omega |\nabla V_{k-1}|^2 \ dx - \int_\Omega F_D\, \rho_{k-1}^2\ dx.
\end{aligned} \tag{2.10}
$$

Proof. We use $\phi = F_k - F_D = -\varepsilon^2 \Delta \rho_k/\rho_k + \log(\rho_k^2) + V_k - F_D$ as test function in (2.3a). Note that ϕ satisfies homogeneous boundary donditions. This yields

$$
\frac{1}{\tau_k}\int_\Omega \left(\rho_k^2 - \rho_{k-1}^2\right)\phi\ dx = -\int_\Omega \rho_k^2\, \nabla F_k\, \nabla\left(F_k - F_D\right)\ dx.
$$

First, we estimate the left hand side

$$
\begin{aligned}
\frac{1}{\tau_k}\int_\Omega \left(\rho_k^2 - \rho_{k-1}^2\right)\phi\ dx &= \frac{1}{\tau_k}\Bigg[-\varepsilon^2\int_\Omega \left(\rho_k^2 - \rho_{k-1}^2\right)\frac{\Delta\rho_k}{\rho_k}\ dx \\
&\quad + \int_\Omega \left(\rho_k^2 - \rho_{k-1}^2\right)\log(\rho_k^2)\ dx \\
&\quad + \int_\Omega \left(\rho_k^2 - \rho_{k-1}^2\right)V_k\ dx - \int_\Omega \left(\rho_k^2 - \rho_{k-1}^2\right)F_D\ dx\Bigg] \\
&= \frac{1}{\tau_k}\left[I_1 + I_2 + I_3 + I_4\right].
\end{aligned}
$$

We estimate termwise. Integration by parts yields

$$
\begin{aligned}
I_1 &= \varepsilon^2\int_\Omega |\nabla\rho_k|^2\ dx - \varepsilon^2\int_\Omega \nabla\rho_k\,\nabla\left(\frac{\rho_{k-1}^2}{\rho_k}\right)\ dx \\
&= \varepsilon^2\int_\Omega |\nabla\rho_k|^2\ dx - \varepsilon^2\int_\Omega |\nabla\rho_{k-1}|^2\ dx + \varepsilon^2\int_\Omega \left|\nabla\rho_{k-1} - \frac{\rho_{k-1}^2}{\rho_k^2}\nabla\rho_k\right|^2\ dx \\
&\ge \varepsilon^2\int_\Omega |\nabla\rho_k|^2\ dx - \varepsilon^2\int_\Omega |\nabla\rho_{k-1}|^2\ dx.
\end{aligned}
$$

Employing some straight–forward calculus we get

$$
\begin{aligned}
I_2 &= \int_\Omega \rho_k^2\left(\log(\rho_k^2) - 1\right) + 1\ dx - \int_\Omega \rho_{k-1}^2\left(\log(\rho_{k-1}^2) - 1\right) + 1\ dx \\
&\quad + \int_\Omega \underbrace{\rho_{k-1}^2\left(\log(\rho_{k-1}^2) - 1\right) - \rho_{k-1}^2\log(\rho_k^2) + \rho_k^2}_{\ge 0}\ dx \\
&\ge \int_\Omega H\left(\rho_k^2\right)\ dx - \int_\Omega H\left(\rho_{k-1}^2\right)\ dx.
\end{aligned}
$$

Integration by parts yields

$$
\begin{aligned}
I_3 &= -\lambda^2 \int_\Omega \Delta \left(V_k - V_{k-1}\right) V_k \, dx \\
&= \lambda^2 \int_\Omega \nabla \left(V_k - V_{k-1}\right) \nabla V_k \, dx
\end{aligned}
$$

and using the identity $2\,r\,(r-s) = r^2 - s^2 + (r-s)^2$

$$
\begin{aligned}
&= \frac{\lambda^2}{2} \int_\Omega |\nabla V_k|^2 \, dx - \frac{\lambda^2}{2} \int_\Omega |\nabla V_{k-1}|^2 \, dx + \frac{\lambda^2}{2} \int_\Omega |\nabla \left(V_k - V_{k-1}\right)|^2 \, dx \\
&\geq \frac{\lambda^2}{2} \int_\Omega |\nabla V_k|^2 \, dx - \frac{\lambda^2}{2} \int_\Omega |\nabla V_{k-1}|^2 \, dx.
\end{aligned}
$$

Now we estimate the right hand side by Young's inequality.

$$
\begin{aligned}
-\int_\Omega \rho_k^2 \, \nabla F_k \, \nabla \left(F_k - F_D\right) \, dx &= -\int_\Omega \rho_k^2 \, |\nabla F_k|^2 \, dx + \int_\Omega \rho_k^2 \nabla F_k \, \nabla F_D \, dx \\
&\leq -\frac{1}{2} \int_\Omega \rho_k^2 \, |\nabla F_k|^2 \, dx + \frac{1}{2} \int_\Omega \rho_k^2 \, |\nabla F_D|^2 \, dx.
\end{aligned}
$$

Define the entropy

$$
S(\rho_k) = \varepsilon^2 \int_\Omega |\nabla \rho_k|^2 \, dx + \int_\Omega H(\rho_k^2) \, dx + \frac{\lambda^2}{2} \int_\Omega |\nabla V_k|^2 \, dx.
$$

Combining the above estimates we get

$$
\begin{aligned}
S(\rho_k) - \int_\Omega F_D \, \rho_k^2 \, dx + \frac{\tau_k}{2} \int_\Omega \rho_k^2 \, |\nabla F_k|^2 \, dx &\leq S(\rho_{k-1}) \\
&\quad - \int_\Omega F_D \, \rho_{k-1}^2 \, dx + \frac{\tau_k}{2} \int_\Omega \rho_k^2 \, |\nabla F_D|^2 \, dx \\
&\leq S(\rho_{k-1}) - \int_\Omega F_D \, \rho_{k-1}^2 \, dx - c_1(F_D) \, \tau_k \int_\Omega F_D \, \rho_k^2 \, dx \quad (2.11)
\end{aligned}
$$

(notice that $F_D < 0$), where

$$
c_1(F_D) = \frac{\|F_D\|^2_{W^{1,\infty}(\Omega)}}{2\,\overline{F}_D}.
$$

Thus consecutively we get

$$
S(\rho_k) - \int_\Omega F_D \, \rho_k^2 \, dx \leq S(\rho_0) - \int_\Omega F_D \, \rho_0^2 \, dx - c_1(F_D) \sum_{l=1}^{k-1} \tau_l \int_\Omega F_D \, \rho_l^2 \, dx.
$$

Note that $S \geq 0$. Hence, it holds

$$-\int_\Omega F_D\, \rho_k^2 \, dx \leq c_0(\rho_0, F_D) - c_1(F_D) \sum_{l=1}^{k-1} \tau_l \int_\Omega F_D\, \rho_l^2 \, dx.$$

Now the discrete Gronwall Lemma implies

$$-\int_\Omega F_D\, \rho_k^2 \, dx \leq c_0(\rho_0, F_D) \exp\left(c_1(F_D)\, t_k\right),$$

from which we immediately deduce the uniform boundedness of the entropy

$$S(\rho_k) \leq c_2(\rho_0, F_D, T).$$

□

Hence, the approximate solution is stable in the following sense.

Corollary 2.5. *Assume* **A.1**—**A.2**. *For $k = 1, \ldots, N$ let (ρ_k, F_k, V_k) be the recursively defined solution of* (2.3) *and* $(\rho^\tau, F^\tau, V^\tau) \in PC_N(0,T; H^2(\Omega) \times C^{2,\gamma}(\bar{\Omega}) \times C^{2,\gamma}(\bar{\Omega}))$. *Then $\rho^\tau \in L^\infty(0,T; H^1(\Omega))$ and $\rho^\tau \nabla F^\tau \in L^2(0,T; L^2(\Omega))$. Further, there exists a positive constant c, independent of τ, such that*

$$\|\rho^\tau\|_{L^\infty(H^1)} + \|V^\tau\|_{L^\infty(H^1)} + \|\rho^\tau \nabla F^\tau\|_{L^2(L^2)} \leq c. \tag{2.12}$$

Proof. The bounds on ρ^τ and V^τ are an immediate consequence of Lemma 2.4, while the one on F^τ follows from (2.11). □

3 Convergence in One Space Dimension

In this section we prove convergence of the scheme in one space dimension. Our argument depends crucially on a uniform $L^\infty(\Omega)$–bound on ρ^τ, which follows a priori from Corollary 2.5 only in one space dimension due to the embedding $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$.

First, we derive the following energy estimate.

Lemma 3.1. *Assume* **A.1**—**A.2** *and let $d = 1$, $\partial\Omega = \Gamma_D$. For $k = 1, \ldots, N$ let (ρ_k, F_k, V_k) be the recursively defined solution of* (2.3) *and* $(\rho^\tau, F^\tau, V^\tau) \in PC_N(0,T; H^2(\Omega) \times C^{2,\gamma}(\bar{\Omega}) \times C^{2,\gamma}(\bar{\Omega}))$. *Then $\rho^\tau \in L^2(0,T; H^2(\Omega))$ and there exists a positive constant c, independent of τ, such that*

$$\|\rho^\tau\|_{L^2(H^2)} \leq c. \tag{3.1}$$

Proof. We start with (2.3a), which can be equivalently written as

$$\frac{2}{\tau_k}\rho_k\left(\rho_k-\rho_{k-1}\right)-\frac{1}{\tau_k}\left(\rho_k-\rho_{k-1}\right)^2=\operatorname{div}\left(\rho_k^2\,\nabla F_k\right).$$

Since $\rho_k>0$, we can divide by ρ_k, which yields

$$\frac{2}{\tau_k}\left(\rho_k-\rho_{k-1}\right)-\frac{1}{\tau_k}\frac{\left(\rho_k-\rho_{k-1}\right)^2}{\rho_k}=\frac{1}{\rho_k}\operatorname{div}\left(\rho_k^2\,\nabla F_k\right)$$

and after elimination of F_k

$$\begin{aligned}&\frac{2}{\tau_k}\left(\rho_k-\rho_{k-1}\right)-\frac{1}{\tau_k}\frac{\left(\rho_k-\rho_{k-1}\right)^2}{\rho_k}\\&\qquad=-\varepsilon^2\Delta^2\rho_k+\varepsilon^2\frac{\left(\Delta\rho_k\right)^2}{\rho_k}+2\,\Delta\rho_k+2\,\frac{\left|\nabla\rho_k\right|^2}{\rho_k}+2\,\nabla\rho_k\,\nabla V_k+\rho_k\,\Delta V_k.\end{aligned}$$

Now we use $\phi=\rho_k-\rho_D$ as test function, observing that, in view of **A.2**, $\nabla\rho_D\cdot\nu=0$ on Γ_N:

$$\begin{aligned}\frac{2}{\tau_k}\int_\Omega\left(\rho_k-\rho_{k-1}\right)\left(\rho_k-\rho_D\right)\,dx&=-\varepsilon^2\int_\Omega\Delta\rho_k\,\Delta\left(\rho_k-\rho_D\right)\,dx\\&\quad+\varepsilon^2\int_\Omega\frac{\left(\Delta\rho_k\right)^2}{\rho_k}\left(\rho_k-\rho_D\right)\,dx\\&\quad+\int_\Omega\left(2\,\Delta\rho_k+2\,\frac{\left|\nabla\rho_k\right|^2}{\rho_k}\right)\left(\rho_k-\rho_D\right)\,dx\\&\quad+\int_\Omega\left(2\,\nabla\rho_k\,\nabla V_k+\rho_k\,\Delta V_k\right)\left(\rho_k-\rho_D\right)\,dx\\&\quad+\frac{1}{\tau_k}\int_\Omega\left(\rho_k-\rho_{k-1}\right)^2\frac{\rho_k-\rho_D}{\rho_k}\,dx\\&=I_1+I_2+I_3+I_4+I_5.\end{aligned}$$

We estimate termwise. The left hand side can be written as

$$\begin{aligned}\frac{2}{\tau_k}\int_\Omega\left(\rho_k-\rho_{k-1}\right)\left(\rho_k-\rho_D\right)\,dx&=\frac{2}{\tau_k}\int_\Omega\left(\rho_k-\rho_D-\left(\rho_{k-1}-\rho_D\right)\right)\left(\rho_k-\rho_D\right)\,dx\\&=\frac{1}{\tau_k}\int_\Omega\left(\rho_k-\rho_D\right)^2\,dx-\frac{1}{\tau_k}\int_\Omega\left(\rho_{k-1}-\rho_D\right)^2\,dx\\&\quad+\frac{1}{\tau_k}\int_\Omega\left(\rho_k-\rho_{k-1}\right)^2\,dx\end{aligned}$$

Define

$$\eta\stackrel{\text{def}}{=}\frac{\min_\Omega\rho_D}{\max_{k=1,\ldots,N}\left\|\rho_k\right\|_{L^\infty(\Omega)}}>0,$$

which is independent of N due to Corollary 2.5 and the embedding $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$ in one space dimension. Note, that for $k = 1, \dots, N$ it holds

$$\frac{\rho_k - \rho_D}{\rho_k} \leq 1 - \eta.$$

Then we have the following estimates. Young's inequality yields

$$\begin{aligned}
I_1 + I_2 &= -\varepsilon^2 \int_\Omega \Delta\rho_k \, \Delta\left(\rho_k - \rho_D\right)\, dx + \varepsilon^2 \int_\Omega \left(\Delta\rho_k\right)^2 \left(\frac{\rho_k - \rho_D}{\rho_k}\right)\, dx \\
&\leq -\varepsilon^2 \int_\Omega \left(\Delta\rho_k\right)^2\, dx + \varepsilon^2 \int_\Omega \Delta\rho_k \, \Delta\rho_D \, dx + (1-\eta)\,\varepsilon^2 \int_\Omega \left(\Delta\rho_k\right)^2\, dx \\
&\leq -\frac{\eta\,\varepsilon^2}{2} \int_\Omega \left(\Delta\rho_k\right)^2\, dx + \frac{\varepsilon^2}{2\,\eta} \int_\Omega \left(\Delta\rho_D\right)^2\, dx.
\end{aligned}$$

By integration by parts and usage of Young's inequality we get

$$\begin{aligned}
I_3 &= -2 \int_\Omega \nabla\rho_k \, \nabla\left(\rho_k - \rho_D\right)\, dx + 2 \int_\Omega \left|\nabla\rho_k\right|^2 \left(\frac{\rho_k - \rho_D}{\rho_k}\right)\, dx \\
&\leq -2\,\eta \int_\Omega \left|\nabla\rho_k\right|^2\, dx + 2 \int_\Omega \nabla\rho_k \, \nabla\rho_D \, dx \\
&\leq -\eta \int_\Omega \left|\nabla\rho_k\right|^2\, dx + \frac{1}{\eta} \int_\Omega \left|\nabla\rho_D\right|^2\, dx.
\end{aligned}$$

From Hölder's inequality we derive

$$\begin{aligned}
I_4 &= \int_\Omega \nabla\left(\rho_k - \rho_D\right)^2\, \nabla V_k \, dx + 2 \int_\Omega \nabla\rho_D \, \nabla V_k \left(\rho_k - \rho_D\right)\, dx \\
&\quad + \int_\Omega \rho_k \left(\rho_k - \rho_D\right) \Delta V_k \, dx \\
&= -\int_\Omega \left(\rho_k - \rho_D\right)^2 \Delta V_k \, dx + 2 \int_\Omega \nabla\rho_D \, \nabla V_k \left(\rho_k - \rho_D\right)\, dx \\
&\quad + \int_\Omega \left(\rho_k - \rho_D\right)^2 \Delta V_k \, dx + \int_\Omega \rho_D \left(\rho_k - \rho_D\right) \Delta V_k \, dx \\
&\leq 2\, \left\|\nabla\rho_D\right\|_{L^\infty(\Omega)} \left\|\nabla V_k\right\|_{L^2(\Omega)} \left\|\rho_k - \rho_D\right\|_{L^2(\Omega)} \\
&\quad - \lambda^{-2} \int_\Omega \rho_D \left(\rho_k - \rho_D\right)\left(\rho_k^2 - C_{dot}\right)\, dx \\
&\leq c_1,
\end{aligned}$$

for some positive constant $c_1 = c_1(\lambda, \Omega, \rho_D, \rho_0, C_{dot})$. Note that in one space dimension the embedding $H^2(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$ holds.

Finally, we get directly

$$I_5 \leq \frac{1-\eta}{\tau_k} \int_\Omega \left(\rho_k - \rho_{k-1}\right)^2\, dx.$$

Combining these estimates we arrive at

$$\begin{aligned}\frac{1}{\tau_k}\int_\Omega (\rho_k-\rho_D)^2\ dx + \frac{\eta}{\tau_k}\int_\Omega (\rho_k-\rho_{k-1})^2\ dx \\ + \frac{\eta\,\varepsilon^2}{2}\int_\Omega (\Delta\rho_k)^2\ dx + \eta\int_\Omega |\nabla\rho_k|^2\ dx \\ \le \frac{1}{\tau_k}\int_\Omega (\rho_{k-1}-\rho_D)^2\ dx + \frac{\varepsilon^2}{2\,\eta}\int_\Omega (\Delta\rho_D)^2\ dx + \frac{1}{\eta}\int_\Omega |\nabla\rho_D|^2\ dx + c_1,\end{aligned}$$

from which we immediately deduce

$$\begin{aligned}\|\rho_k-\rho_D\|^2_{L^2(\Omega)} + \eta\,\|\rho_k-\rho_{k-1}\|^2_{L^2(\Omega)} + \frac{\eta\,\varepsilon^2\,\tau_k}{2}\,\|\Delta\,(\rho_k-\rho_D)\|^2_{L^2(\Omega)} \\ + \eta\,\tau_k\,\|\nabla\,(\rho_k-\rho_D)\|^2_{L^2(\Omega)} \le \|\rho_{k-1}-\rho_D\|^2_{L^2(\Omega)} + \tau_k\,c_2.\end{aligned}$$

Now (3.1) follows from Gronwall's Lemma. □

For the convergence result we also need some bound on the time derivative. To this purpose we introduce the linear interpolant of $(\rho^\tau)^2 \in PC_N(0,T;L^2(\Omega))$, defined by

$$\tilde{n}^\tau(t,x) \stackrel{\text{def}}{=} \frac{t-t_k}{\tau_k}\left(\rho_k^2(x)-\rho_{k-1}^2(x)\right) + \rho_{k-1}^2(x), \quad x\in\Omega, \quad t\in(t_{k-1},t_k].$$

Lemma 3.2. *Let the assumptions of Lemma 3.1 hold. Then $\tilde{n}^\tau \in L^2(0,T;H^{-1}(\Omega))$, and there exists a positive constant c, independent of τ, such that*

$$\|\tilde{n}^\tau_t\|_{L^2(H^{-1})} \le c.$$

Proof. We supply $H^{-1}(\Omega)$ with the norm $\|\nabla\Delta^{-1}\cdot\|_{L^2(\Omega)}$, where $\Delta^{-1}: H^{-1}(\Omega)\to H^1_0(\Omega)$ is the inverse Laplacian [Tem97]. Using $\phi = -\Delta^{-1}\tilde{n}^\tau_t$ as test function in (2.3a) yields after integration by parts

$$\int_\Omega \left|\nabla\Delta^{-1}\tilde{n}^\tau_t\right|^2\ dx = \int_\Omega \rho_k^2\,\nabla F_k\,\nabla\Delta^{-1}\tilde{n}^\tau_t\ dx.$$

Employing Hölder's inequality we get

$$\left\|\nabla\Delta^{-1}\tilde{n}^\tau_t\right\|_{L^2(\Omega)} \le \|\rho^\tau\|^2_{L^\infty(L^\infty)}\,\|\rho^\tau\,\nabla F^\tau\|_{L^2(L^2)},$$

which is uniformly bounded according to Corollary 2.5. □

We state the desired convergence result.

Theorem 3.3. *Assume* **A.1**—**A.2** *and let* $d = 1$, $\partial\Omega = \Gamma_D$. *For* $k = 1, \dots, N$ *let* (ρ_k, F_k, V_k) *be the recursively defined solution of* (2.3) *and* $(\rho^\tau, F^\tau, V^\tau) \in PC_N(0,T; H^2(\Omega) \times C^{2,\gamma}(\bar{\Omega}) \times C^{2,\gamma}(\bar{\Omega}))$. *Then, there exists a subsequence, again denoted by* $(\rho^\tau, F^\tau, V^\tau)$, *such that*

$$\begin{aligned}
\rho^\tau &\rightharpoonup \rho \quad \text{weakly in } L^2(0,T,H^2(\Omega)),\\
\rho^\tau &\to \rho \quad \text{strongly in } C^0(0,T,C^{0,\gamma}(\bar{\Omega})),\\
(\rho^\tau)^2 F_x^\tau &\rightharpoonup J \quad \text{weakly in } L^2(0,T,L^2(\Omega)),\\
V^\tau &\to V \quad \text{strongly in } C^0(0,T,C^{2,\gamma}(\bar{\Omega})),
\end{aligned}$$

as $\tau \to 0$, *where* (ρ, J, V) *is a solution of*

$$\int_{Q_T} \rho^2\, \partial_t \phi \; dx\,dt + \int_{Q_T} J\, \phi_x \; dx\,dt = 0, \tag{3.2a}$$

$$\int_{Q_T} \left[\varepsilon^2 \rho_{xx}(2\rho_x\, \phi + \rho\, \phi_x) - \rho^2 \phi_x - V\left(\rho^2 \phi\right)_x\right]\, dx\,dt = \int_{Q_T} J\, \phi\; dx\,dt, \tag{3.2b}$$

$$\lambda^2 \int_{Q_T} V_x\, \phi_x \; dx\,dt = \int_{Q_T} \left(\rho^2 - C\right) \phi \; dx\,dt, \tag{3.2c}$$

for all $\phi \in C_0^\infty(\Omega \times (0,T))$, *where* $Q_T = \Omega \times (0,T)$.

Remark 3.4. The above result shows that (ρ, V) is a weak solution of the problem

$$\begin{gathered}
\partial_t(\rho^2) = -\left(\varepsilon^2 \rho^2 \left(\frac{\rho_{xx}}{\rho}\right)_x - (\rho^2)_x - \rho^2 V_x\right)_x,\\
-\lambda^2 V_{xx} = \rho^2 - C \qquad \text{in } Q_T,\\
\rho = \rho_D, \quad \rho_{xx} = 0, \quad V = V_D \qquad \text{on } \partial\Omega \times (0,T),\\
\rho(\cdot, 0) = \rho_0 \qquad \text{in } \Omega,
\end{gathered}$$

in the sense of Eqs. (3.2), satisfying $\rho \geq 0$ in Ω.

Proof. We choose a sequence of partitions of $[0,T]$ satisfying (2.2). According to Lemma 3.1 we have the boundedness of (ρ^τ) in $L^2(0,T;H^2(\Omega))$. We may choose a subsequence, again denoted by (ρ^τ), such that

$$\rho^\tau \rightharpoonup \rho \quad \text{weakly in } L^2(0,T,H^2(\Omega)).$$

Further, we have due to Lemma 3.2 and Corollary 2.5 that $\tilde{n}^\tau \in L^\infty(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$. Since the embedding $H^1(\Omega) \hookrightarrow C^{0,\gamma}(\bar{\Omega})$ is compact in one space dimension for $\gamma \in (0, 1/2)$ we deduce from Aubin's Lemma [Sim87] that

$$L^\infty(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)) \hookrightarrow C^0(0,T;C^{0,\gamma}(\bar{\Omega})) \quad \text{compactly.}$$

Hence, there exists a subsequence, not relabeled, such that

$$\tilde{n}^\tau \to n \quad \text{strongly in } C^0(0,T;C^{0,\gamma}(\bar{\Omega})).$$

The reader easily verifies the identification $n = \rho^2$. Moreover, the compact embedding

$$L^2(0,T;H^2(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)) \hookrightarrow L^2(0,T;H^1(\Omega))$$

implies that (up to a subsequence)

$$\rho^\tau \to \rho \quad \text{strongly in } L^2(0,T;H^1(\Omega)).$$

Standard results from elliptic theory and **A.2** imply now

$$V^\tau \to V \quad \text{strongly in } C^0(0,T,C^{2,\gamma}(\bar{\Omega})).$$

Defining $J^\tau = (\rho^\tau)^2 \nabla F^\tau$ we deduce from Corollary 2.5 that (J^τ) is bounded in $L^2(0,T,L^2(\Omega))$, such that

$$J^\tau \rightharpoonup J \quad \text{weakly in } L^2(0,T;L^2(\Omega)).$$

Note that the discrete solutions satisfy

$$\int_{Q_T} \left((\rho^\tau)^2\, \partial_t \phi + J^\tau\, \phi_x\right)\, dx\,dt = 0,$$

$$\int_{Q_T} \left[\varepsilon^2 \rho^\tau_{xx} (2\rho^\tau_x\, \phi + \rho^\tau\, \phi_x) - (\rho^\tau)^2 \phi_x - (\rho^\tau)^2 V_x\, \phi_x\right]\, dx\,dt = \int_{Q_T} J^\tau\, \phi\, dx\,dt,$$

$$\lambda^2 \int_{Q_T} V^\tau_x\, \phi_x\, dx\,dt = \int_{Q_T} ((\rho^\tau)^2 - C)\phi\, dx\,dt,$$

for all test functions $\phi \in C_0^\infty(Q_T)$. The derived convergence properties are by far sufficient to pass to the limit, which assures that (ρ, J, V) is a solution to (3.2). □

Remark 3.5. Note that one cannot derive the convergence of (F^τ), since (ρ^τ) may not be uniformly bounded from below away from zero. Under this additional assumption one also gets $F^\tau \to F$ strongly in $C^0(0,T;C^{2,\gamma}(\bar{\Omega}))$ and the identification $J = \rho^2\, \nabla F$ holds. From the physical point of view, the convergences stated in Theorem 3.3 are satisfactory, since in most applications one is interested in the current density J and not directly in the Quantum Quasi Fermi level.

4 Convergence in arbitrary Space Dimension

In this section we consider convergence of the numerical scheme given by (2.3) in higher dimensions. Unfortunately, the apriori bounds on the approximate solution in Corollary 2.5 are not sufficient to guarantee convergence in this case, since the argument depends strongly on an $L^\infty(0,T;L^\infty(\Omega))$–bound on ρ^τ. Thus, we have to state additional assumptions on the sequence of approximating solutions. These enable us to give even error estimates, which exhibit the optimal order of convergence for the implicit EULER scheme.

Theorem 4.1. *Assume* **A.1**—**A.3**. *For $k = 1, \dots, N$ let (ρ_k, F_k, V_k) be the recursively defined solution of* (2.3) *and $(\rho^\tau, F^\tau, V^\tau) \in PC_N(0,T;H^2(\Omega)\times C^{2,\gamma}(\bar\Omega)\times C^{2,\gamma}(\bar\Omega))$. Assuming*

A.4 $\exists\delta \in (0,1) \quad \forall\tau > 0: \quad \delta \le \rho^\tau \le \delta^{-1}, \quad \|\rho^\tau\|_{L^\infty(0,T;W^{1,4}(\Omega))} \le \delta^{-1}$,

there exists a subsequence in $L^2(0,T;H^2(\Omega))\times L^2(0,T;H^1(\Omega))\times L^\infty(0,T;H^1(\Omega))$, again denoted by $(\rho^\tau, F^\tau, V^\tau)$, such that

$$\begin{aligned} \rho^\tau &\rightharpoonup \rho \quad \text{weakly in } L^2(0,T,H^2(\Omega)),\\ \rho^\tau &\to \rho \quad \text{strongly in } C^0(0,T,C^{0,\gamma}(\bar\Omega)),\\ F^\tau &\to F \quad \text{strongly in } C^0(0,T,H^1(\Omega)),\\ V^\tau &\to V \quad \text{strongly in } C^0(0,T,C^{2,\gamma}(\bar\Omega)), \end{aligned}$$

as $\tau \to 0$, where (ρ, F, V) is a solution of the continuous problem (2.1).
Furthermore, if it holds $H^2(\Omega) \hookrightarrow W^{k,p}(\Omega)$ for $k \ge 0$, $p \ge 1$ and

A.5 $\rho_{tt} \in L^2(0,T;L^2(\Omega))$,

then there exists a constant $\tau_0 = \tau_0(\Omega,\lambda,\delta) > 0$ such that for $\tau \in [0,\tau_0)$ we have the following error estimate

$$\|\rho^\tau - \rho\|_{L^\infty(L^2)} + \varepsilon^2 \|\rho^\tau - \rho\|_{L^2(W^{k,p})} + \|F^\tau - F\|_{L^\infty(H^2)} + \|V^\tau - V\|_{L^\infty(H^2)} \le C\, e^{\alpha T}\, \tau \tag{4.1}$$

for positive constants $\alpha = \alpha(\Omega,\lambda,\delta,\tau_0)$ and $C = C(\Omega,\lambda,\delta,\tau_0)$.

For the proof of Theorem 4.1 we need the monotonicity of the quantum operator

$$A(\rho) = \Delta^2\rho - \frac{(\Delta\rho)^2}{\rho} = \frac{1}{\rho}\operatorname{div}\left(\rho^2\,\nabla\left(\frac{\Delta\rho}{\rho}\right)\right), \tag{4.2}$$

which is a consequence of the following result stating a generalized Poincaré–type inequality.

Lemma 4.2. *Assume* **A.1** *and* **A.3**. *Choose $k \ge 0$, $p \ge 1$ such that the embedding $H^2(\Omega) \hookrightarrow W^{k,p}(\Omega)$ holds. Then there exists for all $\beta \in \mathbb{R}$ and all $\delta \in (0,1)$ a constant $M = M(\Omega,\beta,\delta) > 0$ such that for all $\rho \in H^2(\Omega)$ with $\delta \le \rho \le 1/\delta$ and all $\phi \in H^2(\Omega) \cap H^1_0(\Omega \cup \Gamma_N)$ it holds*

$$\int_\Omega \rho^\beta \left|\operatorname{div}\left(\rho^2\,\nabla\left(\frac{\phi}{\rho}\right)\right)\right|^2\, dx \ge M\,\|\phi\|^2_{W^{k,p}(\Omega)}\,.$$

The proof of Lemma 4.2 is a slight generalization of the one in [Pin99a, Theorem 3.7]. It follows the monotonicity result.

Lemma 4.3. *Assume* **A.1** *and* **A.3**. *Choose $k \geq 0$, $p \geq 1$ such that the embedding $H^2(\Omega) \hookrightarrow W^{k,p}(\Omega)$ holds. Let $\rho^\tau \in PC_N(0,T;H^2(\Omega))$ and $\rho \in L^2(0,T;H^2(\Omega))$ be given as in Theorem 4.1. Then there exists a constant $M = M(\Omega,\delta) > 0$ such that*

$$\langle A(\rho^\tau) - A(\rho), \rho^\tau - \rho \rangle_{X^*,X} \geq M \left\| \rho^\tau - \rho \right\|^2_{W^{k,p}(\Omega)}, \tag{4.3}$$

where $X \stackrel{\text{def}}{=} H^2(\Omega) \cap H^1_0(\Omega \cup \Gamma_N)$.

Proof. The proof settles on the Gateaux–differentiability of A in certain directions and the mean value theorem. We set $\theta \stackrel{\text{def}}{=} \rho^\tau - \rho$ and

$$\rho_h \stackrel{\text{def}}{=} \rho + h\theta.$$

The mapping

$$\begin{aligned} [0,1] &\to \mathbb{R} \\ h &\mapsto \langle A(\rho_h), \theta \rangle_{X^*,X} \end{aligned}$$

is differentiable, which can be seen as follows. Set $Y = H^1_0(\Omega \cup \Gamma_N)$. Let $\sigma > 0$ and calculate, employing integration by parts,

$$\begin{aligned} \langle A(\rho_{h+\sigma}) - A(\rho_h), \theta \rangle_{X^*,X} &= \langle A(\rho_h + \sigma\theta) - A(\rho_h), \theta \rangle_{X^*,X} \\ = &- \left\langle \nabla \left(\frac{\Delta(\rho_h + \sigma\theta)}{\rho_h + \sigma\theta} \right), (\rho_h + \sigma\theta)^2 \nabla \left(\frac{\theta}{\rho_h + \sigma\theta} \right) \right\rangle_{Y^*,Y} \\ &+ \left\langle \nabla \left(\frac{\Delta(\rho_h + \sigma\theta)}{\rho_h + \sigma\theta} \right) \cdot \nu, (\rho_h + \sigma\theta)^2 \left(\frac{\theta}{\rho_h + \sigma\theta} \right) \right\rangle_{(H^{1/2}_{00}(\Gamma_N))^*, H^{1/2}_{00}(\Gamma_N)} \\ &+ \left\langle \nabla \left(\frac{\Delta\rho_h}{\rho_h} \right), \rho_h^2 \nabla \left(\frac{\theta}{\rho_h} \right) \right\rangle_{Y^*,Y} \\ &- \left\langle \nabla \left(\frac{\Delta\rho_h}{\rho_h} \right) \cdot \nu, \rho_h^2 \left(\frac{\theta}{\rho_h} \right) \right\rangle_{(H^{1/2}_{00}(\Gamma_N))^*, H^{1/2}_{00}(\Gamma_N)}. \end{aligned}$$

For the definition of the space $H^{1/2}_{00}(\Gamma_N)$, see [BaCa84]. The boundary terms vanish, since the second one for example fulfills

$$\begin{aligned} \nabla \left(\frac{\Delta\rho_h}{\rho_h} \right) \cdot \nu &= h \nabla \left(\frac{\Delta\rho^\tau}{\rho^\tau} \frac{\rho^\tau}{\rho_h} \right) \cdot \nu + (1-h) \nabla \left(\frac{\Delta\rho}{\rho} \frac{\rho}{\rho_h} \right) \cdot \nu \\ &= h \frac{\rho^\tau}{\rho_h} \nabla \left(\frac{\Delta\rho^\tau}{\rho^\tau} \right) \cdot \nu + h \frac{\Delta\rho^\tau}{\rho^\tau} \nabla \left(\frac{\rho^\tau}{\rho_h} \right) \cdot \nu \\ &\quad + (1-h) \frac{\rho}{\rho_h} \nabla \left(\frac{\Delta\rho}{\rho} \right) \cdot \nu + (1-h) \frac{\Delta\rho}{\rho} \nabla \left(\frac{\rho}{\rho_h} \right) \cdot \nu \\ &= 0 \end{aligned}$$

along Γ_N, see (1.1e).

Another integration by parts yields

$$
\begin{aligned}
-&\left\langle \nabla\left(\frac{\Delta(\rho_h+\sigma\theta)}{\rho_h+\sigma\theta}\right), (\rho_h+\sigma\theta)^2\,\nabla\left(\frac{\theta}{\rho_h+\sigma\theta}\right)\right\rangle_{Y^*,Y} \\
&+\left\langle \nabla\left(\frac{\Delta\rho_h}{\rho_h}\right), \rho_h^2\,\nabla\left(\frac{\theta}{\rho_h}\right)\right\rangle_{Y^*,Y} \\
&=\int_\Omega \frac{\Delta(\rho_h+\sigma\theta)}{\rho_h+\sigma\theta}\,\mathrm{div}\left((\rho_h+\sigma\theta)^2\,\nabla\left(\frac{\theta}{\rho_h+\sigma\theta}\right)\right)\,dx \\
&\quad-\int_\Omega \frac{\Delta\rho_h}{\rho_h}\,\mathrm{div}\left(\rho_h^2\,\nabla\left(\frac{\theta}{\rho_h}\right)\right)\,dx \\
&=\int_\Omega \left[\frac{\Delta(\rho_h+\sigma\theta)}{\rho_h+\sigma\theta}-\frac{\Delta\rho_h}{\rho_h}\right]\mathrm{div}\left((\rho_h+\sigma\theta)^2\,\nabla\left(\frac{\theta}{\rho_h+\sigma\theta}\right)\right)\,dx \\
&\quad-\int_\Omega \frac{\Delta\rho_h}{\rho_h}\underbrace{\left[\mathrm{div}\left(\rho_h^2\,\nabla\left(\frac{\theta}{\rho_h}\right)\right)-\mathrm{div}\left((\rho_h+\sigma\theta)^2\,\nabla\left(\frac{\theta}{\rho_h+\sigma\theta}\right)\right)\right]}_{=0}\,dx \\
&=\sigma\int_\Omega \frac{\rho_h\,\Delta\theta-\theta\,\Delta\rho_h}{(\rho_h+\sigma\theta)\rho_h}\,\mathrm{div}\left((\rho_h+\sigma\theta)^2\,\nabla\left(\frac{\theta}{\rho_h+\sigma\theta}\right)\right)\,dx.
\end{aligned}
$$

Now we easily derive

$$
\begin{aligned}
\lim_{\sigma\to 0}\frac{\langle A(\rho_{h+\sigma})-A(\rho_h),\theta\rangle_{X^*,X}}{\sigma} &= \int_\Omega \frac{\rho_h\,\Delta\theta-\theta\,\Delta\rho_h}{\rho_h^2}\,\mathrm{div}\left(\rho_h^2\,\nabla\left(\frac{\theta}{\rho_h}\right)\right)\,dx \\
&= \int_\Omega \rho_h^{-2}\left|\mathrm{div}\left(\rho_h^2\,\nabla\left(\frac{\theta}{\rho_h}\right)\right)\right|^2\,dx \\
&\geq M\,\|\theta\|^2_{W^{k,p}(\Omega)},
\end{aligned}
$$

by Lemma 4.3. The result follows from the mean value theorem. □

Now we are in the position to prove Theorem 4.1.

Proof *of Theorem 4.1.* From the proofs of Lemma 3.1 and Lemma 3.2 we learn that the uniform $L^\infty(0,T;L^\infty(\Omega))$–bound on ρ^τ is sufficient to guarantee the uniform boundedness of $\|\rho^\tau\|_{L^2(H^2)}$ and $\|\tilde{n}_t\|_{L^2(H^{-1})}$. Following now the outline of the proof of Theorem 3.3 we deduce, noting the compact embedding

$$
H^1(0,T;H^{-1}(\Omega))\cap L^\infty(0,T;W^{1,4}(\Omega))\hookrightarrow C^0(0,T;C^{0,\gamma}(\bar{\Omega}))
$$

for $1\leq d\leq 3$, that the desired convergence results hold. Here, the convergence of (F^τ) follows from the uniform bound $\rho^\tau\geq\delta$ combined with standard elliptic theory.

Now we estimate the rate of convergence. Let $k \in \{1, \dots, N\}$ be fixed. We take the difference of

$$2\,\rho_t = \frac{1}{\rho}\,\mathrm{div}\,\left(\rho^2\,\nabla F\right)$$

and

$$\frac{2}{\tau_k}\,(\rho_k - \rho_{k-1}) - \frac{1}{\tau_k}\frac{(\rho_k - \rho_{k-1})^2}{\rho_k} = \frac{1}{\rho_k}\,\mathrm{div}\,\left(\rho_k^2\,\nabla F_k\right).$$

Note that $\rho_k, \rho \geq \delta$. Further, by Taylor's expansion we have

$$\rho(t_k) = \rho(t_{k-1}) + \rho_t(t_k)\,\tau_k + \frac{1}{2}\int_{t_{k-1}}^{t_k} \rho_{tt}(s)(s - t_{k-1})\;ds.$$

Setting

$$f_k \stackrel{\text{def}}{=} \frac{1}{2}\int_{t_{k-1}}^{t_k} \rho_{tt}(s)(s - t_{k-1})\;ds$$

and defining the error

$$e_k \stackrel{\text{def}}{=} \rho_k - \rho(t_k)$$

we finally end up with

$$\begin{aligned} &\frac{2}{\tau_k}(e_k - e_{k-1}) - \frac{1}{\tau_k}\frac{(\rho_k - \rho_{k-1})^2}{\rho_k} + \frac{2}{\tau_k}f_k \\ =\;& \frac{1}{\rho_k}\,\mathrm{div}\,\left(\rho_k^2\,\nabla F_k\right) - \frac{1}{\rho(t_k)}\,\mathrm{div}\,\left(\rho(t_k)^2\,\nabla F(t_k)\right). \end{aligned}$$

Now we use $\phi = \tau_k\, e_k$ as test function, which yields

$$\begin{aligned} 2\int_\Omega (e_k - e_{k-1})e_k\;dx - \int_\Omega \frac{(\rho_k - \rho_{k-1})^2}{\rho_k}e_k\;dx + 2\int_\Omega f_k\,e_k\;dx \\ = \tau_k\int_\Omega \left[\frac{1}{\rho_k}\,\mathrm{div}\,\left(\rho_k^2\,\nabla F_k\right) - \frac{1}{\rho(t_k)}\,\mathrm{div}\,\left(\rho(t_k)^2\,\nabla F(t_k)\right)\right] e_k\;dx. \end{aligned}$$

We estimate termwise starting on the left–hand side.

Using the identity $2r(r - s) = r^2 - s^2 + (r - s)^2$ we get

$$2\int_\Omega (e_k - e_{k-1})e_k\;dx = \|e_k\|^2_{L^2(\Omega)} - \|e_{k-1}\|^2_{L^2(\Omega)} + \|e_k - e_{k-1}\|^2_{L^2(\Omega)}.$$

Let $\eta = \delta / \max_{k=1,\dots,N} \|\rho_k\|_{L^\infty(\Omega)} = \delta^2$. It holds

$$
\begin{aligned}
-\int_\Omega \frac{(\rho_k - \rho_{k-1})^2}{\rho_k}\, e_k\, dx &\geq -(1-\eta) \int_\Omega (\rho_k - \rho_{k-1})^2\, dx \\
&= -(1-\eta) \int_\Omega \left(e_k - e_{k-1} + \rho(t_k) - \rho(t_{k-1})\right)^2\, dx \\
&\geq - \|e_k - e_{k-1}\|^2_{L^2(\Omega)} \\
&\quad - \frac{1-\eta}{\eta} \int_\Omega \left(\rho_t(t_k)\, \tau_k + f_k\right)^2\, dx,
\end{aligned}
$$

where we used Taylor's expansion and Young's inequality. Trivially, it holds

$$
-2 \int_\Omega f_k\, e_k\, dx \leq 2\, \|f_k\|^2_{L^2(\Omega)} + \frac{1}{2} \|e_k\|^2_{L^2(\Omega)}\,.
$$

The right hand side can be estimated using integration by parts.

$$
\begin{aligned}
\tau_k \int_\Omega \left[\frac{1}{\rho_k} \operatorname{div}\left(\rho_k^2\, \nabla F_k\right) - \frac{1}{\rho(t_k)} \operatorname{div}\left(\rho(t_k)^2\, \nabla F(t_k)\right)\right] e_k\, dx = \\
- \tau_k\, \varepsilon^2 \left\langle A(\rho_k) - A(\rho(t_k)), \rho_k - \rho(t_k)\right\rangle_{X^*,X} \\
+ 2\, \tau_k \int_\Omega \left[\Delta\rho_k + \frac{|\nabla\rho_k|^2}{\rho_k} - \Delta\rho(t_k) - \frac{|\nabla\rho(t_k)|^2}{\rho(t_k)}\right] e_k\, dx \\
+ \tau_k \int_\Omega \left[2\, \nabla\rho_k\, \nabla V_k - 2\, \nabla\rho(t_k)\, \nabla V(t_k) + \rho_k\, \Delta V_k - \rho(t_k)\, \Delta V(t_k)\right] e_k\, dx \\
\leq -\tau_k\, \varepsilon^2 \left\langle A(\rho_k) - A(\rho(t_k)), \rho_k - \rho(t_k)\right\rangle_{X^*,X} \\
+ \int_\Omega \left|\frac{\rho(t_k)}{\rho_k}\, \nabla\rho_k - \frac{\rho_k}{\rho(t_k)}\, \nabla\rho(t_k)\right|^2\, dx \\
+ \tau_k \int_\Omega \left[2\, \nabla\rho_k\, \nabla V_k - 2\, \nabla\rho(t_k)\, \nabla V(t_k) + \rho_k\, \Delta V_k - \rho(t_k)\, \Delta V(t_k)\right] e_k\, dx.
\end{aligned}
$$

The last term can be handled as follows.

$$
\begin{aligned}
&\tau_k \int_\Omega [2\,\nabla\rho_k\,\nabla V_k - 2\,\nabla\rho(t_k)\,\nabla V(t_k) + \rho_k\,\Delta V_k - \rho(t_k)\,\Delta V(t_k)]\,e_k\,dx \\
&\le \tau_k \int_\Omega [2\,\nabla e_k\,\nabla V_k - 2\,\nabla\rho(t_k)\,\nabla(V(t_k)-V_k) + \rho_k\,\Delta V_k - \rho(t_k)\,\Delta V(t_k)]\,e_k\,dx \\
&\qquad = \tau_k \int_\Omega \big[-e_k^2\,\Delta V_k - 2\,\nabla\rho(t_k)\,\nabla(V(t_k)-V_k)\,e_k + e_k^2\,\Delta V_k \\
&\qquad\qquad - \rho(t_k)\Delta(V(t_k)-V_k)\,e_k\big]\;dx \\
&\quad = -2\,\tau_k \int_\Omega \nabla\rho(t_k)\,\nabla(V(t_k)-V_k)\,e_k\,dx - \tau_k\int_\Omega \rho(t_k)(\rho(t_k)+\rho_k)\,e_k^2\,dx \\
&\qquad\qquad \le -2\,\tau_k \int_\Omega \nabla\rho(t_k)\,\nabla(V(t_k)-V_k)\,e_k\,dx \\
&\qquad\qquad\quad \le 2\,\tau_k\,\|\nabla\rho(t_k)\|_{L^4(\Omega)}\,\|\nabla(V(t_k)-V_k)\|_{L^4(\Omega)}\,\|e_k\|_{L^2(\Omega)}\,.
\end{aligned}
$$

Combining all these estimates, together with the monotonicity of A (see (4.3)) and $\|\nabla\rho(t_k)\|_{L^4(\Omega)} \le \delta^{-1}$ yields after summation

$$
\begin{aligned}
\frac{1}{2}\,\|e_k\|_{L^2(\Omega)}^2 + M\,\varepsilon^2 \sum_{l=1}^k \tau_l\,\|e_k\|_{W^{k,p}(\Omega)}^2 &\le \frac{1-\eta}{\eta}\sum_{l=1}^k \int_\Omega (\rho_t(t_l)\,\tau_l + f_l)^2\;dx \\
&+ \sum_{l=1}^k \|f_l\|_{L^2(\Omega)} + 2\,\delta^{-1}\sum_{l=1}^k \tau_l\;\|\nabla(V(t_l)-V_l)\|_{L^4(\Omega)}\;\|e_l\|_{L^2(\Omega)}\,,
\end{aligned}
$$

where $M = M(\Omega,\delta) > 0$ is the constant specified in Lemma 4.3. Estimating

$$
\|f_k\|_{L^2(\Omega)}^2 \le \tau_k^3\,\|\rho_{tt}\|_{L^2(\Omega\times(t_{k-1},t_k))}^2\,,
$$

and

$$
\|\nabla(V(t_k)-V_k)\|_{L^4(\Omega)} \le c_1\,\delta^{-1}\,\|e_k\|_{L^2(\Omega)}\,,
$$

with $c_1 = c_1(\Omega,\lambda) > 0$, yields

$$
\begin{aligned}
&\frac{1}{2}\,\|e_k\|_{L^2(\Omega)}^2 + M\,\varepsilon^2 \sum_{l=1}^k \tau_l\,\|e_k\|_{W^{k,p}(\Omega)}^2 \\
&\qquad \le c_2 \sum_{l=1}^k \tau^2\;\Big(\|\rho_t\|_{L^2(\Omega\times(t_{l-1},t_l))}^2 + \|\rho_{tt}\|_{L^2(\Omega\times(t_{l-1},t_l))}^2\Big) \\
&\qquad\qquad + 2\,c_1\,\delta^{-2}\sum_{l=1}^k \tau_l\;\|e_l\|_{L^2(\Omega)}^2\,,
\end{aligned}
$$

where $c_2 = c_2(\delta) > 0$. Choose $\tau_0 < \frac{\delta^2}{4\,c_1}$. Then

$$\left(\frac{1}{2} - 2\,c_1\,\delta^{-2}\,\tau_0\right) \|e_k\|^2_{L^2(\Omega)} + M\,\varepsilon^2 \sum_{l=1}^{k} \tau_l \,\|e_k\|^2_{W^{k,p}(\Omega)}$$

$$\leq c_2 \left(\|\rho_t\|^2_{L^2(\Omega\times(0,T))} + \|\rho_{tt}\|^2_{L^2(\Omega\times(0,T))}\right) \tau^2 + 2\,c_1\,\delta^{-2} \sum_{l=1}^{k-1} \tau_l \,\|e_l\|^2_{L^2(\Omega)}\,.$$

Now it follows from the discrete Gronwall Lemma

$$\|e_k\|^2_{L^\infty(L^2)} + M\,\varepsilon^2\,\|e_k\|^2_{L^2(W^{k,p})} \leq c_3 e^{a t_k} \tau^2$$

for some $c_3, a > 0$. The estimates on $F^\tau - F$ and $V^\tau - V$ follow now from standard results of elliptic theory. □

Remark 4.4. Although we get no estimate on $\rho^\tau - \rho$ in $L^2(0, T, H^2(\Omega))$, the regularity in space is by far sufficient to define a suitable finite element discretization of (1.4).

5 Numerical Investigations

In this section we employ the transient quantum drift diffusion model for the simulation of the switching behaviour of a resonant tunneling diode (RTD). Such devices proved to be well suited for the validation of quantum models, since their performance is completely determined by quantum mechanical phenomena [KKFR89]. Their main characteristic is the appearance of negative differential resistance (NDR) in the stationary current voltage characteristic (IVC). During the last years most simulations focused on the stationary models and the computation of IVCs. There, NDR was recovered by many authors in a varying set of models, such as the QDD [PU99], the quantum hydrodynamic model (QHD) [Gar94] and recently the smoothed QHD [GR98]. A typical stationary IVC, which was computed using the QDD, is depicted in Figure 5.1. From experiments it is well–known that the switching time of the device is correlated with the peak–to–valley–ratio of the IVC, where a large ratio corresponds to a small switching time [MIO+86].

In the following we present the first simulations of the switching behaviour of a RTD computed by a *macroscopic* quantum model. The GaAs–AlGaAs double barrier structure consists of a quantum well GaAs–layer sandwiched between two $\mathrm{Al_xGa_{1-x}As}$–layers, each 5 nm thick. This resonant structure is itself sandwiched between two spacer layers of 5 nm thickness and supplemented with two contact GaAs–layers, each 25 nm thick. The contact region ist highly doped with $C_{dot} = 10^{24}\mathrm{m}^{-3}$, while the channel is moderately doped with $C_{dot} = 10^{21}\mathrm{m}^{-3}$. The

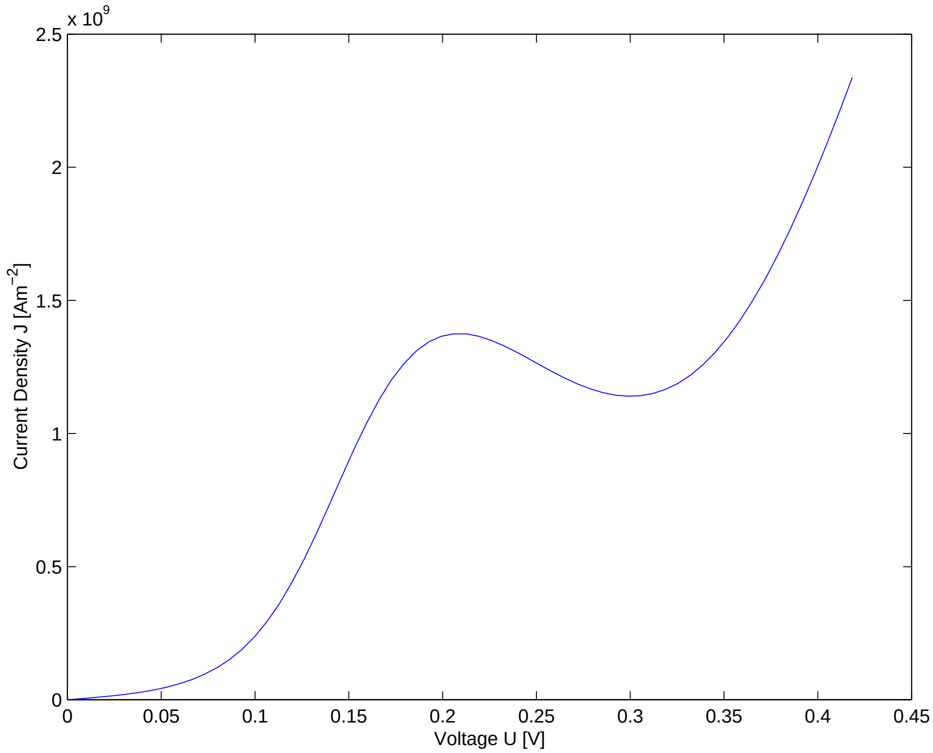

Figure 5.1: Stationary IVC of a RTD

barrier height is assumed to be $B = 0.4\text{eV}$ and the relaxation time is fixed at $\tau_{\text{relax}} \approx 10^{-12}\text{s}$. These device parameters yield for the scaled Planck constant and the scaled Debye length, respectively,

$$\varepsilon^2 = 5 \cdot 10^{-3}, \quad \lambda^2 = 8.6 \cdot 10^{-4}.$$

In the simulation we switched the RTD from the equilibrium state ($U = 0\text{V}$) to the valley state ($U = 0.3\text{V}$), see Figure 5.1. For the computations we used the one–dimensional version of (1.4) and replaced in (1.4b) the potential $V \mapsto V + B$, where B is a step function modelling the barriers. Then we employed the vertical line method given by (2.3) as time discretization. The discretization in space was done by finite differences on a uniform grid with 300 points.

To solve the resulting nonlinear systems we used a NEWTON–iteration, where the solution on the previous time level was used as initial guess. Due to this fact only two or three NEWTON–iterations were needed on each time level. The initial time step was set to $\tau_0 = 10^{-4}$ and afterwards a heuristic adjustment of the time step was used, which significantly reduced the total number of time steps required to reach the stationary state.

In Figure 5.2 we present the computed transient electron density over a period corresponding to the relaxation time. Note that the electrons move top–down.

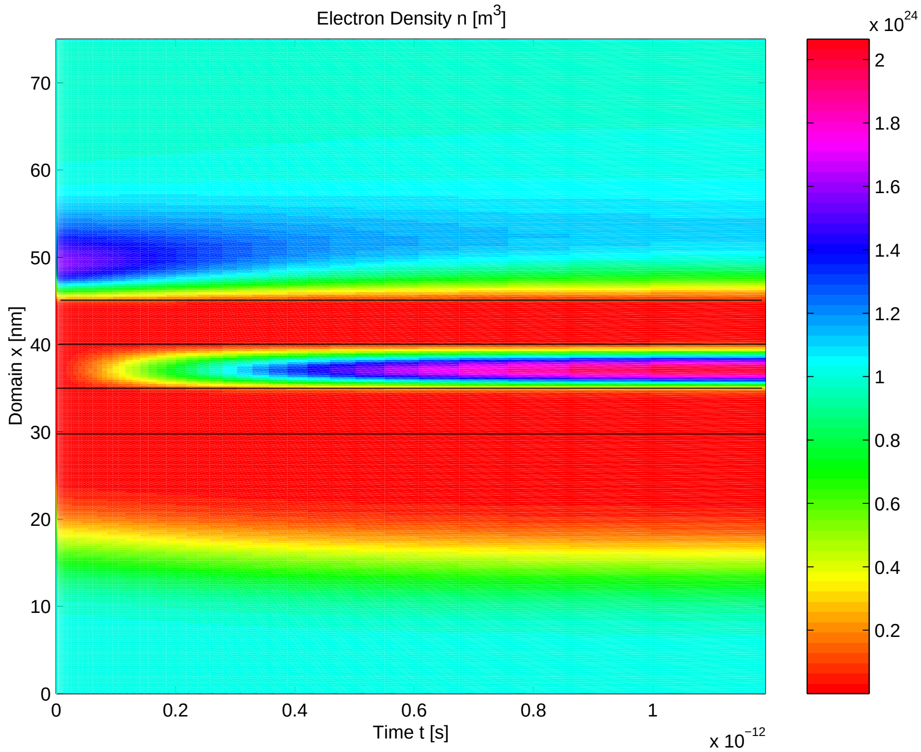

Figure 5.2: Transient Electron Density

One clearly identifies an initial time layer, where the electrons accumulate in front of the first barrier. After this short delay they start to tunnel through this barrier and accumulate dramatically in the quantum well. This charge build–up is more than three orders of magnitude larger than the background doping and was also reported by other authors [Gar94, Poh98, PU99].

Lastly we discuss the transient current density at the left contact ($x = 0$), which is depicted in Figure 5.3. As we switch at time $t = 0$ instantaneously out of the equlibrium state ($J = 0$) there is a jump in the current density. During the evolution to the stationary valley state the current density does not change monotonically, apparently an oscillation occurs. This oscillatory behaviour was also reported in [KKFR89], where the RTD was simulated by the (microscopic) Wigner–Poisson model. There the transient current density proved to be even highly oscillatory on account of ballistic effects. We cannot expect this in our case, since we are working in a diffusive regime [CGS99], where the small relaxation time prevents ballistic phenomena. Note that the stationary state is reached after 10^{-11} seconds, which is approximately ten times the relaxtion time.

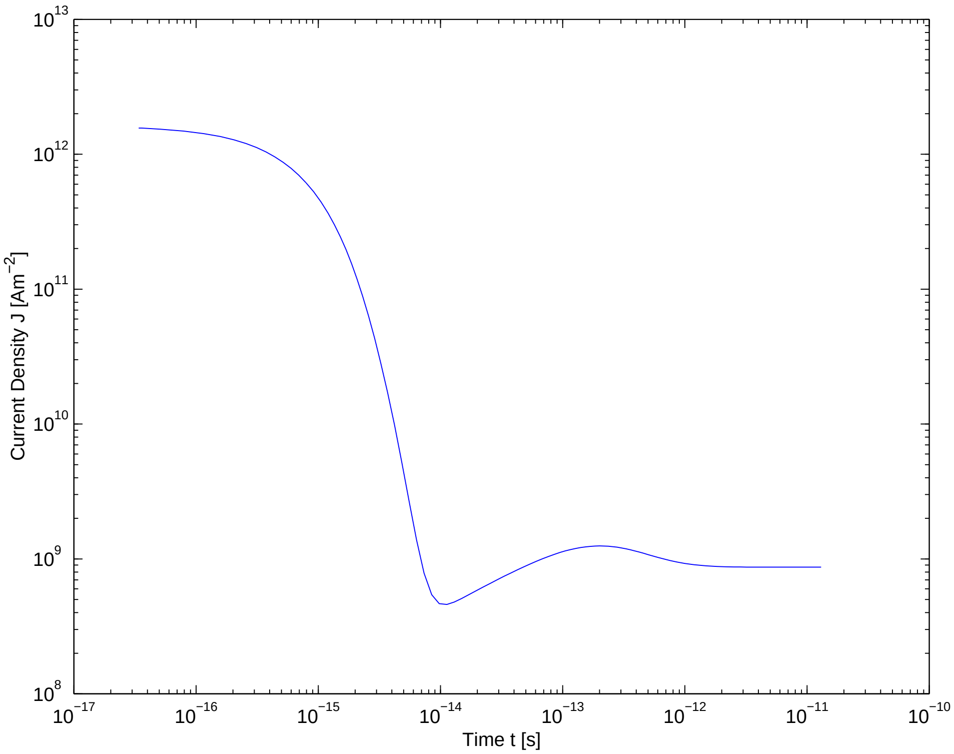

Figure 5.3: Transient Current Density

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