Convergent Semidiscretization of a Nonlinear Fourth Order Parabolic System

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Abstract

A semidiscretization in time of a fourth order nonlinear parabolic system in several space dimensions arising in quantum semiconductor modelling is studied. The system is numerically treated by introducing an additional nonlinear potential. The resulting sequence of nonlinear second order elliptic systems admits at each time level *strictly positive* solutions as long as the lattice temperature is sufficiently large. Exploiting the stability of the discretization, convergence is shown in the multi–dimensional case. Under some assumptions on the regularity of the solution the rate of convergence proves to be optimal.

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

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

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1 Introduction

The ongoing miniaturization of semiconductor devices reached nowadays a length scale at which quantum effects play a dominant role. Thus, standard models like the classical drift diffusion equations are physically inaccurate and have to be replaced by equations which incorporate the relevant quantum effects. 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].

During the last years a whole hierarchy of macroscopic models has been derived. They deal with macroscopic, fluid–type unknowns which allow for a natural interpretation of boundary conditions [Pin99]. The models consist of balance equations 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, Jun01].

Most analytical and numerical work on these models was spend on the stationary equations, since the main interest was focused on the stationary current–voltage characteristics. Particularly for stationary simulations, a first moment version of the isothermal QHD, the quantum drift diffusion model (QDD) [Anc87, AU98], proved to be quite promising since it allows a very effective numerical treatment [PU99]. Only recently some results on the transient equations are available. The transient quantum drift diffusion model can be derived as a zero relaxation time limit in the rescaled QHD, which reads

$$
\begin{gathered}
n_t + \operatorname{div} J = 0, \\
\tau_{relax}^2\, J_t + \tau_{relax}^2 \operatorname{div}\left(\frac{J \otimes J}{n}\right) + \theta\, \nabla n + n\, \nabla V - \varepsilon^2 n\, \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -J, \\
-\lambda^2 \Delta V = n - C_{dot}.
\end{gathered}
$$

Here, the parameters are the scaled Planck constant ε, the scaled Debye length λ, the scaled temperature θ and the scaled relaxation time τ_{relax}. 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 [Pin00]). 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 ($\tau_{relax} = 0$), stated on a bounded domain Ω, can be written as

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

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

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, 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 conditons are physically motivated and commonly employed in quantum semiconductor modelling. The numerical investigations in [Pin99] underline the reasonability of this choice.

System (1.4) is supplemented by the initial condition

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

Let us collect some results available for system (1.1). In [Pin00] the dynamic stability of stationary states with a slightly different set of boundary conditions 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 ($\theta = 0$) and vanishing electric field (1.1) simplifies to

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

Surprisingly, 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 [JP00] deduced under much weaker assumptions the existence of a non–negative *global* solution n in one space dimension.

In the last years the question of positivity preservation for the dynamics of fourth order equations was thoroughly investigated in the context of lubrication–type equations [BF90, BP98, PGG98], 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). Numerically, there are two ways of dealing with Equation (1.3): *Bertozzi et al.* [BZ00] designed a space discretization using finite differences, which exhibits the same properties as the continuous equation. *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 system (1.1) in one space dimension a different numerical scheme was introduced by the authors, which proved to be stable and convergent [JP01]: Writing Equation (1.1a) in conservation form

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

and introducing the quantum quasi Fermi level

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

yields the system

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

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

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

Here, $-\varepsilon^2\Delta\sqrt{n}/\sqrt{n}$ is the so–called quantum Bohm potential. The additional boundary conditions

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

are consistent with (1.1c)–(1.1f).

Then, an implicit time discretization by a backward Euler scheme for system (1.4) is suggested. The resulting sequence of elliptic systems proves to be uniquely solvable at each time step and moreover the semidiscrete solution is *strictly positive*. However, the positivity property relaxes in the limit to non–negativity.

In this paper we generalize this convergence result to the multi–dimensional case. From Remark 2.3 in [JP01] we learn that even for several space dimensions the semidiscretization possesses a strictly positive solution $n(x, t_k)$ as long as the lattice temperature θ is sufficiently large. Since there is no uniform lower bound on the electron density available we will assume this property and some regularity of the continuous solution. This has the benefit that we cannot only prove the desired convergence result but get also estimates on the rate of convergence which proves to be optimal for the Euler scheme.

The proof is based on a stability estimate which is a consequence of the boundedness of the *entropy* (or free energy)

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

In fact, S is non–increasing in time (see [JP01]). Here, $H(s) \stackrel{\text{def}}{=} s\left(\log(s) - 1\right) + 1$ denotes a primitive of the logarithm.

The paper is organized as follows. In Section 2 we introduce the semidiscretization of (1.4). Section 3 is devoted to the proof of convergence in the multi–dimensional case, which relies on an energy estimate for the discrete solution. Imposing some natural assumptions we show that the scheme is convergent with the optimal order in some suitable norm.

2 Semidiscretization

In this section we derive the implicit semidiscretization of (1.4) and state an existence and stability result for the discretized system at each time level. In particular, the positivity of the electron density is guaranteed.

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

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

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

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

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 $\{t_k : k = 0, \dots, N\}$, where $0 = t_0 < t_1 < \dots < t_N = T$. We set $\tau_k \stackrel{\text{def}}{=} t_k - t_{k-1}$ and define the maximal subinterval length $\tau \stackrel{\text{def}}{=} \max_{k=1,\dots,N} \tau_k$. We assume that the partition fulfills

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

For any Banach space B we define

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

and introduce the abreviation $v_k = v^\tau(t)$ for $t \in (t_{k-1}, t_k]$ and $k = 1, \dots, N$. 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 $k = 1, \dots, N$ solve recursively the elliptic systems

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

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

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

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

$$\rho_D = \sqrt{C_{dot}}, \quad F_D = U, \quad V_D = -\theta \log(C_{dot}) + U. \tag{2.4}$$

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

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 and let $H_0^1(\Omega \cup \Gamma_N)$ for $\Gamma_N \subset \partial\Omega$ be the closure of $C_c^\infty(\Omega \cup \Gamma_N)$ with respect to the $H^1(\Omega)$ norm [Tro87]. 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 $\|\cdot\|_{L^p(B)}$.

Naturally, we have to assume some regularity properties on the data. 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 (2.4) and

$$\rho_D \in H^4(\Omega), \quad \inf_\Omega \rho_D > 0, \quad \nabla\rho_D \cdot \nu = 0 \text{ on } \Gamma_N,$$
$$F_D \in C^{2,\gamma}(\bar\Omega) \quad \text{for } \gamma \in \left(0, \frac{1}{2}\right), \quad F_D \le -\overline{F}_D < 0,$$
$$V_D \in C^{2,\gamma}(\bar\Omega),$$

and the initial datum satisfies $\rho_0 \in H^2(\Omega)$. 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 $a \ge \underline{a} > 0$. 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

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

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 $F_D \le -\overline{F}_D$ 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.

In [JP01] an existence theorem for (2.3) is proved, which reads in the multi–dimensional case:

Proposition 2.2. *Assume* **A.1**—**A.3**. *Furthermore, let* $k \in \{1, \ldots, N\}$ *and let* $\rho_{k-1} \in C^{0,\gamma}(\bar{\Omega})$. *Then there exists a constant* $\theta_0 > 0$ *such that for all* $\theta > \theta_0$ *system* (2.3) *possesses a solution* (ρ_k, F_k, V_k), *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.

Furthermore, the approximate solution is stable in the following sense (see [JP01, Corollary 2.5]).

Lemma 2.3. *Assume* **A.1**—**A.3**. *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*

$$\|\rho^\tau\|_{L^\infty(H^1)} + \|V^\tau\|_{L^\infty(H^1)} + \|\rho^\tau \nabla F^\tau\|_{L^2(L^2)} \leq c. \tag{2.5}$$

Remark 2.4. In the one–dimensional case it is possible to prove (see [JP01, Theorem 3.3]) the existence of 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 weak solution of the continuous problem (2.1).

3 Convergence in Several Space Dimension

In this section we prove the convergence of the numerical scheme given by (2.3) in the multi–dimensional case. Here, the a priori bounds on the approximate solution in Lemma 2.3 are not sufficient to guarantee convergence, since the argument depends strongly on an $L^\infty(0, T; L^\infty(\Omega))$–bound on ρ^τ (see [JP01]). In one space dimension this is an immediate consequence of the estimate (2.5) and the embedding $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$. In fact, no analytical results on system

(1.4) are available in several space dimensions. 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 3.1. *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 $\exists \delta \in (0,1) \quad \forall \tau > 0: \quad \delta \leq \rho^\tau \leq \delta^{-1}, \quad \|\rho^\tau\|_{L^\infty(0,T;H^2(\Omega))} \leq \delta^{-1}$,

there exists a subsequence, again denoted by $(\rho^\tau, F^\tau, V^\tau)$, *such that*

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

as $\tau \to 0$, *where* (ρ, F, V) *is a solution of the continuous problem* (2.1).

Furthermore, if the embedding $H^2(\Omega) \hookrightarrow W^{m,p}(\Omega)$ *is continuous for some* $m \geq 0$, $p \geq 1$ *and*

A.5 $\rho \in H^2(0,T;L^2(\Omega))$,

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*

$$\|\rho^\tau - \rho\|_{L^\infty(L^2)} + \varepsilon^2 \|\rho^\tau - \rho\|_{L^2(W^{m,p})} + \|F^\tau - F\|_{L^\infty(H^2)} + \|V^\tau - V\|_{L^\infty(H^2)} \leq C\, e^{\alpha T}\, \tau, \quad (3.1)$$

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

Remark 3.2.

(a) Assumption **A.4** allows us to verify the strong convergence $F^\tau \to F$ which yields the identification $J = \rho^2 \nabla F$ for the limiting current density. Notice that this extends the one–dimensional result (see Remark 2.4).

(b) Already in the classical regime ($\varepsilon = 0$) assumption **A.5** is employed for the derivation of the optimal order of convergence in one space dimension [CJ90]. Remarkably, it is also sufficient in this higher order system in several space dimensions.

(c) An inspection of the proof of Theorem 3.1 shows that the last assumption in **A.4** can be replaced by the weaker condition $\|\rho^\tau\|_{L^\infty(0,T;Z)} \le \delta^{-1}$, and Z is a Sobolev space which embeddes compactly into $W^{1,3}(\Omega)$.

For the convergence result we also need some bound in the energy norm and 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

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

Following the outlines of the proof of Lemma 3.1 and Lemma 3.2 in [JP01] one verifies that **A.4** is sufficient to derive the following additional stability estimates.

Lemma 3.3. *Assume* **A.1**—**A.4**. *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 $\tilde{n}^\tau \in H^1(0,T;\,H^{-1}(\Omega))$. Further, there exists a positive constant c, independent of τ, such that*

$$\|\rho^\tau\|_{L^2(H^2)} \le c \quad \textit{and} \quad \|\tilde{n}_t^\tau\|_{L^2(H^{-1})} \le c. \tag{3.2}$$

For the proof of Theorem 3.1 we need the monotonicity of the quantum "operator"

$$A(\rho) = \frac{1}{\rho}\operatorname{div}\Big(\rho^2 \nabla \frac{\Delta\rho}{\rho}\Big), \qquad \rho \in H^4(\Omega).$$

Lemma 3.4. *Assume* **A.1** *and* **A.3**. *Choose $m \ge 0$, $p \ge 1$ such that the continuous embedding $H^2(\Omega) \hookrightarrow W^{m,p}(\Omega)$ 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 $\phi \in H^2(\Omega) \cap H_0^1(\Omega \cup \Gamma_N)$ it holds*

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

The proof of Lemma 3.4 is a slight generalization of the one in [Pin00, Theorem 3.7]. It follows the monotonicity result.

Lemma 3.5. *Assume* **A.1**. *Let u, $v \in H^4(\Omega)$ be such that u, $v \ge \delta > 0$ in Ω and*

$$\begin{aligned} u - v = 0, \quad & \Delta u = \Delta v = 0 && \textit{on } \Gamma_D, \\ \nabla(u-v)\cdot\nu = 0, \quad & \nabla\frac{\Delta u}{u}\cdot\nu = \nabla\frac{\Delta v}{v}\cdot\nu = 0 && \textit{on } \Gamma_N. \end{aligned}$$

Then

$$\int_\Omega (A(u) - A(v))(u-v)dx = \int_\Omega \frac{1}{uv}\left|\operatorname{div}\left(u^2 \nabla \frac{u-v}{u}\right)\right|^2 dx. \tag{3.3}$$

Proof. By integration by parts we obtain

$$
\begin{aligned}
&\int_\Omega (A(u)-A(v))(u-v)dx \\
&= \int_\Omega \left(\frac{\Delta u}{u} \operatorname{div}\Big(u^2 \nabla \frac{u-v}{u}\Big) - \frac{\Delta v}{v} \operatorname{div}\Big(v^2 \nabla \frac{u-v}{v}\Big)\right) dx \\
&= \int_\Omega \left(\frac{v\Delta u - u\Delta v}{uv} \operatorname{div}\Big(u^2 \nabla \frac{u-v}{u}\Big) - \frac{\Delta v}{v} \operatorname{div}\Big(v^2 \nabla \frac{u-v}{v} - u^2 \nabla \frac{u-v}{u}\Big)\right) dx.
\end{aligned}
$$

Since

$$v^2 \nabla \frac{u-v}{v} - u^2 \nabla \frac{u-v}{u} = 0 \qquad \text{in } \Omega,$$

this implies

$$\int_\Omega (A(u)-A(v))(u-v)dx = \int_\Omega \frac{1}{uv} \left| \operatorname{div}\left(u^2 \nabla \frac{u-v}{u}\right)\right|^2 dx.$$

□

Now we are in the position to prove Theorem 3.1. The first part of proof is a slight generalization of the one for Theorem 3.3 in [JP01]. However, we include it for the sake of a completeness.

Proof of Theorem 3.1. We choose a sequence of partitions of $[0,T]$ satisfying (2.2). According to Lemma 3.3 (ρ^τ) is bounded in $L^2(0,T;H^2(\Omega))$. We may choose a subsequence, again denoted by (ρ^τ), such that, as $\tau \to 0$,

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

Further, we have due to Lemma 3.3 and Lemma 2.3 that $\tilde{n}^\tau \in H^1(0,T;H^{-1}(\Omega))$. Since the embedding $H^2(\Omega) \hookrightarrow C^{0,\gamma}(\bar{\Omega})$ is compact for $1 \le d \le 3$ and $0 < \gamma < 1/2$ we deduce from Aubin's Lemma [Sim87] that

$$L^\infty(0,T;H^2(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)) \hookrightarrow C^0(0,T;C^{0,\gamma}(\bar{\Omega})) \quad \text{ compactly.}$$

Hence, using assumption **A.4**, 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 $n = \rho^2$. By assumption **A.4** and inequality (2.5), we get a uniform estimate for $\tilde{\rho}^\tau_t$ in $L^2(0,T;H^{-1}(\Omega))$. Hence, 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)

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

and consequently,

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

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 Lemma 2.3 that (J^τ) is bounded in $L^2(0,T,L^2(\Omega))$, such that

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

Now, the convergence of (F^τ) to F follows from the uniform bound $\rho^\tau \geq \delta$ combined with standard elliptic theory. Further, $J = \rho^2 \nabla F$.

The derived convergence properties are by far sufficient to pass to the limit in the weak formulation of (2.3).

In order to estimate the rate of convergence, we need some regularity properties for ρ_k and $\rho(t_k)$. From

$$-\varepsilon^2 \Delta \rho_k = \rho_k (F_k - \theta \log(\rho_k^2) - V_k) \in H^2(\Omega)$$

and assumption **A.2** we obtain $\rho_k \in H^4(\Omega)$. The compact embedding

$$L^\infty(0,T;H^2(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)) \hookrightarrow C^0([0,T];C^{0,\gamma}(\bar{\Omega}))$$

implies that ρ is continuous in $C^0([0,T];C^{0,\gamma}(\bar{\Omega}))$ and hence,

$$-\varepsilon^2 \Delta \rho = \rho(F - \theta \log(\rho^2) - V) \in C^0([0,T];C^{0,\gamma}(\bar{\Omega})).$$

By a bootstrapping argument, it follows $\rho \in C^0([0,T];H^4(\Omega))$.

Now let $k \in \{1,\dots,N\}$ be fixed. We take the difference of

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

and

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

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

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

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

$$\begin{aligned}
&2\int_\Omega (e_k - e_{k-1})e_k\;dx - \int_\Omega \frac{(\rho_k - \rho_{k-1})^2}{\rho_k} e_k\;dx + 2\int_\Omega f_k\, e_k\;dx \\
&= \tau_k \int_\Omega \left[\frac{1}{\rho_k}\operatorname{div}\left(\rho_k^2\,\nabla F_k\right) - \frac{1}{\rho(t_k)}\operatorname{div}\left(\rho(t_k)^2\,\nabla F(t_k)\right)\right] e_k\;dx.
\end{aligned} \tag{3.4}$$

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

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

The right hand side of (3.4) can be estimated using integration by parts.

$$\begin{aligned}
\tau_k \int_\Omega &\left[\frac{1}{\rho_k}\,\mathrm{div}\,\big(\rho_k^2\,\nabla F_k\big) - \frac{1}{\rho(t_k)}\,\mathrm{div}\,\big(\rho(t_k)^2\,\nabla F(t_k)\big)\right] e_k\; dx = \\
&\qquad - \tau_k\,\varepsilon^2 \int_\Omega (A(\rho_k) - A(\rho(t_k)))(\rho_k - \rho(t_k))dx \\
&\qquad + 2\,\tau_k\,\theta \int_\Omega \left[\Delta\rho_k + \frac{|\nabla\rho_k|^2}{\rho_k} - \Delta\rho(t_k) - \frac{|\nabla\rho(t_k)|^2}{\rho(t_k)}\right] e_k\; dx \\
&+ \tau_k \int_\Omega [2\,\nabla\rho_k\,\nabla V_k - 2\,\nabla\rho(t_k)\,\nabla V(t_k) + \rho_k\,\Delta V_k - \rho(t_k)\,\Delta V(t_k)]\, e_k\; dx \\
&\qquad \le -\tau_k\,\varepsilon^2 \int_\Omega (A(\rho_k) - A(\rho(t_k)))(\rho_k - \rho(t_k))dx \\
&\qquad - 2\,\tau_k\,\theta \int_\Omega \left|\frac{\rho(t_k)}{\rho_k}\,\nabla\rho_k - \frac{\rho_k}{\rho(t_k)}\,\nabla\rho(t_k)\right|^2\; dx \\
&+ \tau_k \int_\Omega [2\,\nabla\rho_k\,\nabla V_k - 2\,\nabla\rho(t_k)\,\nabla V(t_k) + \rho_k\,\Delta V_k - \rho(t_k)\,\Delta V(t_k)]\, e_k\; dx.
\end{aligned}$$

The last term can be handled as follows.

$$\begin{aligned}
\tau_k &\int_\Omega [2\,\nabla\rho_k\,\nabla V_k - 2\,\nabla\rho(t_k)\,\nabla V(t_k) + \rho_k\,\Delta V_k - \rho(t_k)\,\Delta V(t_k)]\, e_k\; dx \\
&= \tau_k \int_\Omega [2\,\nabla e_k\,\nabla V_k - 2\,\nabla\rho(t_k)\,\nabla(V(t_k) - V_k) + \rho_k\,\Delta V_k - \rho(t_k)\,\Delta V(t_k)]\, e_k\; dx \\
&\qquad = \tau_k \int_\Omega \big[-e_k^2\,\Delta V_k - 2\,\nabla\rho(t_k)\,\nabla(V(t_k) - V_k)\, e_k + e_k^2\,\Delta V_k \\
&\qquad\qquad -\rho(t_k)\Delta(V(t_k) - V_k)\, e_k\big]\; dx \\
&= -2\,\tau_k \int_\Omega \nabla\rho(t_k)\,\nabla(V(t_k) - V_k)\, e_k\; dx - \tau_k \int_\Omega \rho(t_k)(\rho(t_k) + \rho_k)\, e_k^2\; dx \\
&\qquad \le -2\,\tau_k \int_\Omega \nabla\rho(t_k)\,\nabla(V(t_k) - V_k)\, e_k\; dx \\
&\qquad\qquad \le 2\,\tau_k\,\|\nabla\rho(t_k)\|_{L^3(\Omega)}\,\|\nabla(V(t_k) - V_k)\|_{L^6(\Omega)}\,\|e_k\|_{L^2(\Omega)}\,.
\end{aligned}$$

The compact embedding

$$L^\infty(0,T;H^2(\Omega)) \cap H^1(0,T;H^{-1}(\Omega)) \hookrightarrow C^0([0,T];W^{1,3}(\Omega))$$

yields the uniform bound $\|\nabla \rho(t_k)\|_{L^3(\Omega)} \le c_0$.

From the boundary conditions for ρ_k, F_k and V_k (see (2.3d), (2.3e) and (2.4)) we conclude that

$$\begin{aligned} \nabla \rho_k \cdot \nu = \nabla \frac{\Delta \rho_k}{\rho_k} \cdot \nu = 0 \qquad & \text{in the sense of } L^2(\Gamma_N), \\ \rho_k = \rho_D, \quad \Delta \rho_k = 0 \qquad & \text{in the sense of } L^2(\Gamma_D). \end{aligned}$$

Similarly,

$$\begin{aligned} \nabla \rho(t_k) \cdot \nu = \nabla \frac{\Delta \rho(t_k)}{\rho(t_k)} \cdot \nu = 0 \qquad & \text{in the sense of } L^2(\Gamma_N), \\ \rho(t_k) = \rho_D, \quad \Delta \rho(t_k) = 0 \qquad & \text{in the sense of } L^2(\Gamma_D). \end{aligned}$$

Combining all these estimates, together with the monotonicity of A (see (3.3)) and Lemma 3.4 gives after summation

$$\begin{aligned} \frac{1}{2} \|e_k\|^2_{L^2(\Omega)} + M\, \varepsilon^2 \sum_{l=1}^{k} \tau_l \, \|e_k\|^2_{W^{m,p}(\Omega)} \le \frac{1-\eta}{\eta} \sum_{l=1}^{k} \int_\Omega \left(\rho_t(t_l)\, \tau_l + f_l\right)^2 \, dx \\ + 2 \sum_{l=1}^{k} \|f_l\|^2_{L^2(\Omega)} + 2\, c_0 \sum_{l=1}^{k} \tau_l \, \|\nabla (V(t_l) - V_l)\|_{L^6(\Omega)} \, \|e_l\|_{L^2(\Omega)} \,, \end{aligned}$$

where $M = M(\Omega, \delta) > 0$ is the constant specified in Lemma 3.5. Estimating

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

and

$$\|\nabla (V(t_k) - V_k)\|_{L^6(\Omega)} \le c_1 \, \delta^{-1} \, \|e_k\|_{L^2(\Omega)} \,,$$

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

$$\begin{aligned} & \frac{1}{2} \|e_k\|^2_{L^2(\Omega)} + M\, \varepsilon^2 \sum_{l=1}^{k} \tau_l \, \|e_k\|^2_{W^{m,p}(\Omega)} \\ & \qquad \le c_2 \sum_{l=1}^{k} \tau_l^2 \, \left(\|\rho_t\|^2_{L^\infty(t_{l-1}, t_l; L^2(\Omega))} + \|\rho_{tt}\|^2_{L^2(\Omega \times (t_{l-1}, t_l))} \right) \\ & \qquad\qquad + 2\, c_0\, c_1\, \delta^{-1} \sum_{l=1}^{k} \tau_l \, \|e_l\|^2_{L^2(\Omega)} \,, \end{aligned}$$

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

$$\left(\frac{1}{2} - 2\,c_1\,\delta^{-2}\,\tau_0\right) \|e_k\|^2_{L^2(\Omega)} + M\,\varepsilon^2 \sum_{l=1}^{k} \tau_l\,\|e_k\|^2_{W^{m,p}(\Omega)}$$
$$\leq c_2\,\|\rho\|^2_{H^2(0,T;L^2(\Omega))}\tau^2 + 2\,c_0\,c_1\,\delta^{-1} \sum_{l=1}^{k-1} \tau_l\ \|e_l\|^2_{L^2(\Omega)}\,.$$

Now it follows from the discrete Gronwall Lemma that

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

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

Remark 3.6. Although we do not get an 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).

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