Convergent Finite Element Discretizations of the Density Gradient Equation for Quantum Semiconductors

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Abstract

We study nonlinear finite element discretizations for the density gradient equation in the quantum drift diffusion model. Especially, we give a finite element description of the so–called nonlinear scheme introduced by *Ancona*. We prove the existence of discrete solutions and provide a consistency and convergence analysis, which yields the optimal order of convergence for both discretizations. The performance of both schemes is compared numerically, especially with respect to the influence of approximate vacuum boundary conditions.

Key words. Quantum semiconductors, density gradient equation, nonlinear finite element method, consistency, convergence, numerics

AMS(MOS) subject classification. 35J60, 35J70, 65N12, 65N15, 65N30, 76Y05

1 Introduction

During the last decade quantum corrections of the well–known drift diffusion (DD) model for semiconductor devices [15, 16, 17] gained considerable attention in the mathematics and engineering community [19, 9, 29]. Most common is the so–called quantum drift diffusion (QDD) model proposed by *Ancona and Iafrate* [5, 8, 3], which is also known as the density gradient (DG) model. It proved its reliability especially in the simulation of MOSFET devices [29, 10, 9, 7, 6] and is also well understood from the mathematical point of view [28, 1, 21, 18, 13, 14, 19]. This great success is also underlined by its inclusion into commercial software packages, e.g. by *Silvaco* or *Lucent.* Hence, the QDD model is a good candidate to be the successor of the classical DD model, since it adds quantum effects to the DD model in a general, compact and computationally efficient manner [9, 29].

The scaled unipolar, stationary QDD model on the bounded domain $\Omega = (0, 1)$ reads [19]

$$-\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + \log(n) + V = F, \tag{1.1a}$$

$$\partial_x(n\partial_x F) = 0, \tag{1.1b}$$

$$-\lambda^2 \partial_{xx} V = n - C_{dop} \tag{1.1c}$$

for the electron density n, the quantum quasi–Fermi potential F and the electrostatic potential V. The parameter ε is the scaled Planck constant, λ is the scaled Debye length and the function C_{dop} represents the concentration of fixed background ions. The system (1.1a)–(1.1c) is subject to Dirichlet boundary conditions modeling the Ohmic contacts of the device

$$n = n_D, \quad V = V_D := V_{eq} + V_{ext} \quad F = F_D := F_{eq} + V_{ext} \quad \text{on } \partial\Omega, \tag{1.1d}$$

where n_D, V_{eq} and F_{eq} are the equilibrium values of the charge concentrations, the potential and the quasi–Fermi level, respectively, and V_{ext} is the external applied voltage. Note, that the scaled constants are in general quite small, i.e. $\varepsilon^2, \lambda^2 = O(10^{-2\ldots-4})$, such that boundary or internal layers might occur [3].

Several discretization schemes have been proposed for solution of the coupled, nonlinear partial differential equations (1.1). These can be classified into linear and nonlinear schemes, depending on the respective discretization of (1.1a). Among the linear schemes are the piecewise linear finite element discretization developed in [24], where also its stability properties are studied. In addition, a linear conservative scheme based on finite differences is presented in [4]. However, due to the quantum effects that occur inside the device, the density might change by several orders of magnitude. Thus, such schemes require very fine grids in order to obtain reliable results, which implies a significant computational cost. To cope with such difficulties nonlinear schemes have to be used, like the finite difference nonlinear scheme [4], which has been proved its efficiency in solving on coarse grids device examples involving quantum effects. Another line of research is presented in [20, 22], where the existence of a discrete solution for the coupled problem, as well as error bounds and uniform convergence for a Scharfetter–Gummel type discretization are investigated [12, 25].

Although, the finite difference nonlinear scheme has been applied with success [4, 9], no numerical analysis is so far available. In this paper, we embed this question into the context of finite element discretizations and study their respective consistency and convergence. Choosing appropriate quadrature rules we recover *Ancona's* nonlinear scheme [4]. In [27] the effect of approximate vacuum boundary conditions is studied and an improved scheme is suggested. Here, we present a different approach based on finite elements, which is also not affected by the boundary condition and yields even simpler discrete nonlinear systems.

This paper is organized as follows. In Section 2 we present the two different discretization schemes for the DG equation (1.1a). The existence of discrete solutions, as well as consistency and convergence results for the discretization schemes are discussed in Section 3. Finally, numerical tests for a MIS diode, underlining the theoretical results, are presented in Section 4. Concluding remarks are given in Section 5.

2 The Finite Element Approach

In this section we introduce an exponential variable transform for the density, which already proved very helpful in the analysis of the transient problem [13, 14]. The construction of the nonlinear difference scheme in [4] relies on the same idea and is there motivated by replacing the "‘fast"’ density variable n with the "‘slow"’ one $u = log(n)$. In the following we write the transformed DG equation in weak form and perform the finite element discretization.

We consider here only the boundary value problem for the DG equation

$$-\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + \log(n) + V = 0, \tag{2.1a}$$

$$n(0) = \alpha \qquad n(1) = \beta. \tag{2.1b}$$

on the bounded domain $\Omega = (0,1)$ and for a given potential $V \in H^1(\Omega)$.

After multiplication with $\sqrt{n}$ and using an exponential transformation $n = e^{2u}$, in order to resolve better the large variations of the carrier density in the vicinity of inversion layers [3], we get the transformed problem in terms of the new unknown u

$$- \varepsilon^2 \partial_{xx} e^u + e^u(2u + V) = 0, \tag{2.2a}$$

$$u(0) = \frac{1}{2}\log(\alpha) \qquad u(1) = \frac{1}{2}\log(\beta). \tag{2.2b}$$

The weak formulation reads now: Find $u \in u_D + H_0^1(\Omega)$ such that

$$\varepsilon^2 \int_\Omega e^u \, \partial_x u \, \partial_x \phi \, dx \; + \int_\Omega (2u + V) e^u \, \phi \, dx = 0 \quad \text{for all } \phi \in H_0^1(\Omega), \tag{2.3}$$

where u_D is an $H^1(\Omega)$–extension of the boundary data.

Concerning the existence and uniqueness of solutions to the DG equation, different results are available in the literature [19], which depend on the specific formulation of the problem. In terms of the logarithmic variable u we have the following.

Proposition 2.1 *Let $V \in H^1(\Omega)$ and choose constants $\overline{V}$, $\underline{V} \in \mathbb{R}$ such that*

$$\underline{V} \; \leq V(x) \; \leq \overline{V} \quad \textit{for all } x \in \Omega.$$

Then, there exists a unique solution $u \in u_D + H_0^1(\Omega)$ for

$$\varepsilon^2 \int_\Omega e^u \, \partial_x u \, \partial_x \phi \, dx \; + \int_\Omega (2u + V) e^u \, \phi \, dx = 0, \quad \textit{for all } \phi \in H_0^1(\Omega). \tag{2.4}$$

In addition u is bounded from below and above, i.e.

$$\underline{u} \; \leq u(x) \; \leq \overline{u} \quad \textit{for all } x \in \Omega$$

where $\underline{u} = -\overline{V}/2$ and $\overline{u} = -\underline{V}\;/2$.

Remark 2.1 *The existence proof is based on Schauder's fixed point theorem [30]in combination with Stampacchia's truncation method for the derivation of the uniform bounds. Uniqueness follows from the monotonicity of the quantum Bohm potential [21, 13].*

Remark 2.2 *In fact, the solution u has a higher regularity. The identity $-\varepsilon^2 \partial_{xx} u = \varepsilon^2 (\partial_x u)^2 - 2u - V \in L^1(\Omega)$ yields $u \in W^{2,1}(\Omega)$. Now, Sobolev's embedding theorem [2] implies $\partial_x u \in L^4(\Omega)$ and hence we have $u \in H^2(\Omega)$.*

In order to discretize (2.3), the interval $[0, 1]$ is splitted into N subintervals $I_i = (x_{i-1}, x_i]$, $i = 1, ..., N$ with

$$0 = x_0 < x_1 < ... < x_{N-1} < x_N = 1.$$

We define the length of the intervals h_i and the maximal mesh spacing h by

$$h_i := x_i - x_{i-1} \quad i = 1, ..., N \quad \text{and} \quad h := \max_{i=1,\dots,N} h_i.$$

As a finite dimensional subspace of $H_0^1(\Omega)$ we use the space of piecewise linear functions

$$H_h := \{\phi \in C^0(\bar{\Omega}) : \ \phi|_{I_i} \in \mathbb{P}_1, \ i = 1, ..., N\}$$

with basis $\{b_0, ..., b_{N-1}\}$, where

$$b_i(x) = \begin{cases} \frac{x - x_i}{h_i} & \text{if } x \in I_i, \\ \frac{x_{i+1} - x}{h_i} & \text{if } x \in I_{i+1}, \\ 0 & \text{otherwise} . \end{cases}$$

The discretized problem may then be written in the form: Find $u_h \in u_D + H_h$ such that

$$\varepsilon^2 \int_\Omega e^{u_h} \ \partial_x u_h \ \partial_x b_i(x) \ dx \ + \int_\Omega (2u_h + V) e^{u_h} \ b_i(x) \ dx = 0, \tag{2.5}$$

for $i = 1, ..., N - 1$.

To solve this nonlinear system of equations we need to evaluate first the integrals in (2.5). This can be done exactly or approximately, but the exact calculation of these integrals yields a highly nonlinear system. This encourages us to use quadrature rules instead.

We now describe two alternative ways to compute approximately the integral in (2.5). The first approach leads us to the same exponential ansatz proposed by *Ancona* [4], which shows that Ancona's discretization can be studied from the finite element theory point of view. The second method is based on the linear interpolation of a part of the integrand and has the advantage that it allows for an easy treatment of the discrete nonlinear system. Since both quadrature rules do not affect the consistency of the discretization, we get finally convergence for both schemes.

2.1 Finite Element Derivation of Ancona's Scheme.

To obtain a finite element version of Ancona's nonlinear scheme [4] we approximate both integrals in (2.5). For the first integral we use the midpoint rule and get

$$\begin{aligned} \varepsilon^2 \int_\Omega e^u \ \partial_x u \ \partial_x b_i(x) \ dx &= \varepsilon^2 \Big(\frac{u_i - u_{i-1}}{h_i^2}\Big) \int_{I_i} e^{u_h(x)} dx - \varepsilon^2 \Big(\frac{u_{i+1} - u_i}{h_{i+1}^2}\Big) \int_{I_{i+1}} e^{u_h(x)} dx \\ &\approx \varepsilon^2 \Big(\frac{u_i - u_{i-1}}{h_i}\Big) e^{u(x_{i-1/2})} - \varepsilon^2 \Big(\frac{u_{i+1} - u_i}{h_{i+1}}\Big) e^{u(x_{i+1/2})} \\ &= \varepsilon^2 \left(\frac{u_i - u_{i-1}}{h_i}\right) e^{(u_{i-1} \ + \ u_i)/2} \ - \ \varepsilon^2 \left(\frac{u_{i+1} - u_i}{h_{i+1}}\right) e^{(u_i \ + \ u_{i+1})/2} \end{aligned} \tag{2.6}$$

where $x_{i-1/2} = \dfrac{x_i + x_{i-1}}{2}$ for $i = 1, \ldots, N$.

For the approximation of the second integral in (2.5) we proceed as follows

$$\begin{aligned}
\int_\Omega (2u+V)e^u b_i \, dx &= \int_{x_{(i-1)-1/2}}^{x_{(i-1)+1/2}} e^u(2u+V)b_i \, dx + \int_{x_{i-1/2}}^{x_{i+1/2}} e^u(2u+V)b_i \, dx \\
&+ \int_{x_{(i+1)-1/2}}^{x_{(i+1)+1/2}} e^u(2u+V)b_i \, dx, && \text{(2.7a)} \\
&\approx \int_{x_{i-1/2}}^{x_{i+1/2}} e^u(2u+V)b_i \, dx, && \text{(2.7b)} \\
&\approx (2u_i + V_i) \int_{x_{i-1/2}}^{x_{i+1/2}} e^u \, dx. && \text{(2.7c)}
\end{aligned}$$

The above approach considers the integrals between the midpoints of each subinterval I_i and uses an open quadrature rule obtaining (2.7b). Next, since e^u never changes sign in $[x_{i-1/2}, x_{i+1/2}]$, we can apply the weighted mean value theorem for integrals to replace (2.7b) by (2.7c).

The integral (2.7c) can be computed exactly which yields finally

$$\begin{aligned}
0 \;=\; &\varepsilon^2 \left(\frac{u_i - u_{i-1}}{h_i}\right) e^{(u_{i-1} \,+\, u_i)/2} \;-\; \varepsilon^2 \left(\frac{u_{i+1} - u_i}{h_{i+1}}\right) e^{(u_i \,+\, u_{i+1})/2} && \text{(2.8)} \\
&+ (2u_i + V_i)\; e^{u_i} \left(\frac{h_i}{u_i - u_{i-1}} \Big(1 - e^{(u_{i-1}-u_i)/2}\Big) + \frac{h_{i+1}}{u_{i+1} - u_i} \Big(e^{(u_{i+1}-u_i)/2} - 1\Big) \right).
\end{aligned}$$

Remark 2.3 *From equation (2.7b) it is observed that the terms* $\int_{x_0}^{x_{0+1/2}} e^u(2u+V)b_i \, dx$ *and* $\int_{x_{N+1/2}}^{x_{N+1}} e^u(2u+V)b_i \, dx$*, which contain the information given by the boundary condition are neglected. This is the cause for the sensitive behavior of the approximate solution near to the boundary (see also the discussion in [27] and Section 4).*

Remark 2.4 *If we introduce*

$$e^{u(x)}|_{I_i} = A_i e^{\alpha_i x}$$

where

$$A_i := \exp\left(\frac{u_{i-1}\; x_i - u_i\; x_{i-1}}{h_i}\right) \quad \textit{and} \quad \alpha_i := \frac{u_i - u_{i-1}}{h_i} \tag{2.9}$$

for $i = 1, \ldots, N$ *and set* $s_i := e^{u_i}$*, then the discretization scheme (2.8) is equivalent to the nonlinear discretization scheme developed in [4]. More precisely, plugging (2.9) in (2.8) we get*

$$\begin{aligned}
&\varepsilon^2 \; \frac{\sqrt{s_i s_{i-1}}}{h_i} \; \log\left(\frac{s_i}{s_{i-1}}\right) - \varepsilon^2 \; \frac{\sqrt{s_i s_{i+1}}}{h_{i+1}} \; \log\left(\frac{s_{i+1}}{s_i}\right) = && \text{(2.10)} \\
&\frac{1}{2} \; (2u_i + V_i) \; s_i \left[\; \frac{2h_i}{\log(\frac{s_i}{s_{i-1}})} \; \left(1 - \sqrt{\frac{s_{i-1}}{s_i}} \;\right) \; + \; \frac{2h_{i+1}}{\log(\frac{s_{i+1}}{s_i})} \; \left(\sqrt{\frac{s_{i+1}}{s_i}} - 1\right) \; \right].
\end{aligned}$$

After some algebraic operations, (2.10) becomes

$$
\begin{aligned}
&\Big\{ \Big[\varepsilon^2 F\Big(\frac{s_{i+1}}{s_i}\Big) - \frac{h_{i+1}^2}{8}\ (\log s_i^2 + V_i)\ W\Big(\frac{s_{i+1}}{s_i}\Big)\Big]\ \frac{s_{i+1}-s_i}{h_{i+1}} \\
&\quad - \Big[\varepsilon^2 F\Big(\frac{s_i}{s_{i-1}}\Big) - \frac{h_i^2}{8}\ (\log s_i^2 + V_i)\ W\Big(\frac{s_{i-1}}{s_i}\Big)\Big]\ \frac{s_i - s_{i-1}}{h_i} \Big\} \Big/ \frac{1}{2}(h_i + h_{i+1}) \\
&\quad = -(\log s_i^2 + V_i)\ s_i
\end{aligned}
\tag{2.11}
$$

where the functions $F(z)$ and $W(z)$ are defined by

$$
F(z) := \frac{\sqrt{z}}{z-1}\log z \qquad\qquad W(z) := \frac{4}{z-1}\Big(2\frac{\sqrt{z}-1}{\log z} - 1\Big).
$$

Equation (2.11) is just the nonlinear discretization of the DG equation (2.1a) obtained in [4].

2.2 The FE Scheme with Linear Interpolation

The second alternative to approximate (2.5) is as follows. We replace (2.5) by: Find $u_h \in u_D + H_h$ such that

$$
\varepsilon^2 \int_\Omega e^{u_h}\ \partial_x u_h\ \partial_x b_i(x)\ dx\ + \int_\Omega (e^{u_h}\ (2u_h + V))^I\ b_i(x)\ dx = 0, \tag{2.12}
$$

for $i = 1, ..., N-1$, where $(\cdot)^I$ denotes the linear interpolant on the grid.
Now, we compute these integrals exactly and get

$$
\begin{aligned}
&-\varepsilon^2 \frac{1}{h_i}\ e^{u_{i-1}} + \varepsilon^2\Big(\frac{1}{h_i} + \frac{1}{h_{i+1}}\Big)\ e^{u_i} - \varepsilon^2 \frac{1}{h_{i+1}}\ e^{u_{i+1}} + \frac{1}{6} h_i\ e^{u_{i-1}}\ (2u_{i-1} + V_{i-1}) \\
&\quad + \frac{1}{3}(h_i + h_{i+1})\ e^{u_i}\ (2u_i + V_i)\ +\ \frac{1}{6} h_{i+1}\ e^{u_{i+1}}\ (2u_{i+1} + V_{i+1})\ =\ 0,
\end{aligned}
\tag{2.13}
$$

for $i = 1, \ldots, N-1$.

Remark 2.5 *Rewriting equation (2.13) in terms of the variable s_i we get*

$$
\begin{aligned}
&-\varepsilon^2 \frac{s_i}{h_i} + \varepsilon^2\Big(\frac{1}{h_i} + \frac{1}{h_{i+1}}\Big)\ s_i - \varepsilon^2 \frac{s_i}{h_{i+1}}\ + \frac{1}{6} h_i\ s_{i-1}\ (2\log(s_{i-1}) + V_{i-1}) \\
&\quad + \frac{1}{3}(h_i + h_{i+1})\ s_i\ (2\log(s_i) + V_i)\ +\ \frac{1}{6} h_{i+1}\ s_{i+1}\ (2\log(s_{i+1}) + V_{i+1})\ =\ 0.
\end{aligned}
$$

We observe that our approach is closer to the linear conservative scheme proposed in [4]. The difference lies in the treatment of the second term.

3 Numerical Analysis

In this section we perform the numerical analysis of the finite element approximations introduced in Section 2. Especially, we show the existence of discrete solutions, analyze the consistency error of the discretization and prove that the method converges with optimal rate.

3.1 Auxiliary Results

In the following analysis we use several interpolation estimates, which we state here for later reference.

For every function $w \in C^0(\bar{\Omega})$ let w^I denote the linear interpolant verifying $w^I(x_i) = w(x_i)$ for $i = 0, \ldots, N$. Then the approximation theory in Sobolev spaces yields the following results [11].

Proposition 3.1 *There exist a constant $c > 0$, independent of h, such that*

$$|w - w^I|_{H^1(\Omega)} \leq ch\Big(\sum_{i=1}^{N} |w|^2_{H^2(I_i)}\Big)^{1/2}$$
$$|w - w^I|_{L^2(\Omega)} \leq ch^2\Big(\sum_{i=1}^{N} |w|^2_{H^2(I_i)}\Big)^{1/2}$$

for all $w \in H^1(\Omega) \cap \{H^2(I_i), \forall i = 1, \ldots, N\}$

The proof can be found in [23]. A simple application of Hölder's inequality and Proposition 3.1 lead us to the following estimate.

Proposition 3.2 *There exists a constant $c > 0$, independent of h, such that*

$$\left|\int_\Omega fg\ dx - \int_\Omega f^I g\ dx\right| \ \leq\ ch^2\Big(\sum_{i=1}^{N} |f|^2_{H^2(I_i)}\Big)^{1/2} \|g\|_{L^2(\Omega)}.$$

for all $f \in H^1(\Omega) \cap \{H^2(I_i), \forall i = 1, \ldots, N\}$ and $g \in L^2(\Omega)$.

3.2 Consistency

In this section we derive the order of consistency for the finite element discretization (2.13). Let $u \in H^2(\Omega)$ be the solution of (2.2a). For $r \in (0, r_0)$, $r_0 = 2\|u\|_{H^1(\Omega)}$, we define

$$B_r(u^I) := \{w_h \in u_D + H_h : \|u^I - w_h\|_{H^1(\Omega)} \leq r\},$$

and, further, for given $w_h \in B_r(u^I)$ the auxiliary functions $\hat{u} := T(w_h) \in u_D + H_0^1(\Omega)$ and $\hat{u}_h := T_h(w_h) \in u_D + H_h$, where $\hat{u}$ and $\hat{u}_h$ fulfill

$$\langle A(\hat{u}), \phi \rangle = \langle W, \phi \rangle \qquad \text{and} \qquad \langle A_h(\hat{u}_h), \phi \rangle = \langle W_h, \phi \rangle \,,$$

for all ϕ in $H_0^1(\Omega)$ or in H_h, respectively.

The corresponding operators A and A_h are defined as follows

$$\begin{aligned}
\langle A(u), \phi \rangle &:= \varepsilon^2 \int_\Omega e^{w_h} \partial_x u \; \partial_x \phi \; dx \; + 2 \int_\Omega e^{w_h} u \; \phi \; dx, \\
\langle A_h(u_h), \phi \rangle &:= \varepsilon^2 \int_\Omega e^{w_h} \partial_x u_h \; \partial_x \phi \; dx \; + 2 \int_\Omega (e^{w_h} u_h)^I \; \phi \; dx,
\end{aligned}$$

and for W and W_h we set

$$\langle W, \phi \rangle := - \int_\Omega e^{w_h} V \phi \; dx, \qquad \langle W_h, \phi \rangle := - \int_\Omega (e^{w_h} V)^I \phi \; dx.$$

Then, we can derive the following consistency result for the discrete operator T_h.

Theorem 3.1 *Let $u \in H^2(\Omega)$ be the solution of* (2.2a). *There exists a constant $c = c(u) > 0$, independent of h, such that*

$$\| T_h(w_h) - T(w_h) \|_{H^1(\Omega)} \leq ch$$

for all $w_h \in B_r(u^I)$.

Proof: Since w_h is fixed, both operators A and A_h are linear. First, we show that the operator A_h is H_h*–elliptic*. For fixed $w_h \in B_r(u^I) \subset H_h \subset C^0(\bar{\Omega})$, there are real constants m and M, only dependent on r, such that $m \leq w_h(x) \leq M$ for all $x \in \Omega$. Then, the first integral in the definition of the operator A_h satisfies the inequality

$$\varepsilon^2 \int_\Omega e^{w_h} |\partial_x u_h|^2 dx \geq \varepsilon^2 e^m \| \partial_x u_h \|^2_{L^2(\Omega)}$$

The second integral of A_h is just a numerical integration, where $(e^{w_h} u_h)^I$ is the piecewise linear interpolant of $e^{w_h} u_h$ in each subinterval $I_i := [x_{i-1}, x_i]$. Then

$$\begin{aligned}
\int_\Omega (e^{w_h} u_h)^I \; u_h \; dx &= \sum_{i=1}^N \int_{I_i} \Big(e^{w_{i-1}} u_{i-1} b_{i-1}(x) + e^{w_i} u_i b_i(x) \Big) (u_{i-1} b_{i-1}(x) + u_i b_i(x)) dx \\
&= \sum_{i=1}^N \frac{h_i}{6} \Big(2 e^{w_{i-1}} u_{i-1}^2 + u_i u_{i-1} (e^{w_{i-1}} + e^{w_i}) + 2 e^{w_i} u_i^2 \Big) \\
&\geq \sum_{i=1}^N \frac{h_i}{6} e^m \Big((u_{i-1}^2 + u_i^2) + (u_{i-1} + u_i)^2 \Big) \\
&\geq c_1 \| u_h \|^2_{L_2(\Omega)},
\end{aligned}$$

where $c_1 = c_1(m) > 0$ is independent of h. Hence, there exists a real constant $c_2 = c_2(m, \varepsilon) > 0$ such that

$$\langle A_h(u_h), u_h \rangle \geq c_2 \|u_h\|^2_{H^1(\Omega)} \tag{3.1}$$

i.e., A_h is a H_h–elliptic operator.

For $m_h := \hat{u}_h - \hat{u}^I \in H_h$ we get

$$\begin{aligned} c_2\|\hat{u}_h - \hat{u}^I\|^2_{H^1(\Omega)} &\leq \left\langle A_h(\hat{u}_h) - A_h(\hat{u}^I), m_h \right\rangle \\ &= \langle A_h(\hat{u}_h) - A(\hat{u}), m_h \rangle + \left\langle A(\hat{u}^I) - A_h(\hat{u}^I), m_h \right\rangle + \left\langle A(\hat{u}) - A(\hat{u}^I), m_h \right\rangle \end{aligned}$$

Now, we proceed to estimate each term. For the first term we have

$$\begin{aligned} |\langle A_h(\hat{u}_h) - A(\hat{u}), m_h \rangle| &= |\langle W_h - W, m_h \rangle| \\ &= \left| \int_\Omega (e^{w_h} V - (e^{w_h} V)^I) \; m_h \; dx \right|, \\ &\leq c_3 \, h \|V\|_{H^1(\Omega)} \|m_h\|_{L^2(\Omega)}, \end{aligned}$$

for some constant $c_3 = c_3(M) > 0$, independent of h.

Furthermore, the second term can be estimated as follows

$$\begin{aligned} |\left\langle A(\hat{u}^I) - A_h(\hat{u}^I), m_h \right\rangle| &= \left|2 \int_\Omega e^{w_h} \hat{u}^I \; m_h \; dx - 2 \int_\Omega (e^{w_h} \hat{u}^I)^I \; m_h \; dx \right|, \\ &\leq 2\|e^{w_h}\hat{u}^I - (e^{w_h}\hat{u}^I)^I\|_{L^2(\Omega)} \|m_h\|_{L^2(\Omega)} \\ &\leq 2c_4 \, h \|\hat{u}\|_{H^1(\Omega)} \|m_h\|_{L^2(\Omega)}, \end{aligned}$$

for some $c_4 = c_4(M) > 0$, independent of h. The last term allows for the following estimate:

$$\begin{aligned} |\left\langle A(\hat{u}) - A(\hat{u}^I), m_h \right\rangle| &= \varepsilon^2 \int_\Omega e^{w_h} \partial_x(\hat{u} - \hat{u}^I) \partial_x m_h dx \; + 2 \int_\Omega e^{w_h} (\hat{u} - \hat{u}^I) \; m_h \; dx, \\ &\leq \varepsilon^2 e^M \|\partial_x(\hat{u} - \hat{u}^I)\|_{L^2(\Omega)} \|\partial_x m_h\|_{L^2(\Omega)} + 2e^M \|\hat{u} - \hat{u}^I\|_{L^2(\Omega)} \|m_h\|_{L^2(\Omega)} \\ &\leq c_5 h \|\hat{u}\|_{H^2(\Omega)} \; \|m_h\|_{H^1(\Omega)}, \end{aligned}$$

for some constant $c_5(M, \varepsilon) > 0$, independent of h. Combining all three estimates we get

$$\|\hat{u}_h - \hat{u}^I\|_{H^1(\Omega)} \leq K_1 \, h \left(\|\hat{u}\|_{H^2(\Omega)} + \|V\|_{H^1(\Omega)} \right).$$

with $K_1 = K_1(u, \varepsilon) > 0$, independent of h.

Finally, using the triangle inequality and standard interpolation results [11] we obtain

$$\begin{aligned} \|T_h(w_h) - T(w_h)\|_{H^1(\Omega)} &= \|\hat{u}_h - \hat{u}\|_{H^1(\Omega)} \\ &\leq \|\hat{u}_h - \hat{u}^I\|_{H^1(\Omega)} + \|\hat{u}^I - \hat{u}\|_{H^1(\Omega)} \\ &\leq K_2 \, h \left(\|\hat{u}\|_{H^2(\Omega)} + \|V\|_{H^1(\Omega)} \right). \end{aligned}$$

□

3.3 Existence of the Discrete Solution and Convergence Rates

The previous consistency result in combination with Brouwer's fixed point theorem allows now to prove the existence of a discrete solution and the optimal convergence rate.

Theorem 3.2 *Let $u \in H^2(\Omega)$ be a solution of the continuous problem and assume that the Fréchet derivative $(I-DT)(u) \in \mathcal{L}(H^1(\Omega), H^1(\Omega))$ of $I-T : H^1(\Omega) \to H^1(\Omega)$ at u is boundedly invertible. Then there exists a constant $h_0 > 0$, such that for $h < h_0$ there exists a solution $u_h \in u_D + H_h$ of the discrete problem (2.12). Further, there exists a constant $c > 0$, independent of h, such that*

$$\|u - u_h\|_{H^1(\Omega)} \leq ch.$$

Proof: We employ Brouwer's fixed point theorem [30] and define the fixed point operator $S : B_r(u^I) \to B_r(u^I)$ via

$$S(w) := w + (I - DT(u))^{-1}(T_h(w) - w).$$

It holds

$$\begin{aligned} S(w) - u^I &= w - u^I + (I - DT(u))^{-1}(T_h(w) - w) \\ &= (I - DT(u))^{-1}[(I - DT(u))(w - u^I) + T_h(w) - w] \\ &= (I - DT(u))^{-1}[(I - DT(u))(w - u) + T(w) - w \\ &\qquad\qquad + (I - DT(u))(u - u^I) + T_h(w) - T(w) - T(u) + u] \\ &= (I - DT(u))^{-1}[\, o(\|u - w\|_{H^1(\Omega)}) + T_h(w) - T(w)] + u - u^I. \end{aligned}$$

Let $L := \|(I - DT(u))^{-1}\|_{\mathcal{L}(H^1(\Omega),H^1(\Omega))}$. Due to Theorem 3.1 we have

$$\|T_h(w) - T(w)\|_{H^1(\Omega)} \leq \frac{c}{L}h,$$

and, further, standard interpolation results give

$$\|u - u^I\|_{H^1(\Omega)} \leq ch.$$

If we choose $r = \min(3ch, r_0)$, it holds for all $w \in B_r(u^I)$

$$\|u - w\|_{H^1(\Omega)} \leq \|u - u^I\|_{H^1(\Omega)} + \|u^I - w\|_{H^1(\Omega)} \leq 4ch. \tag{3.2}$$

Moreover, we can choose $h_0 > 0$ such that for all $h < h_0$ it holds

$$\|u - w\|_{H^1(\Omega)} \leq 4ch \qquad \Rightarrow \qquad o(\|u - w\|_{H^1(\Omega)}) \leq \frac{c}{L}h.$$

This implies

$$\|S(w) - u^I\|_{H^1(\Omega)} \leq ch + ch + ch = r,$$

i.e. S maps $B_r(u^I)$ into itself.

Now, we apply Brouwer's fixed point theorem [30] and derive the existence of a fixed point $u_h \in B_r(u^I)$ of S fulfilling

$$u_h = S(u_h) = u_h + (I - DT(u))^{-1}(T_h(u_h) - u_h).$$

or $u_h = T_h(u_h)$, i.e. u_h is also a fixed point of T_h. Finally, we deduce from (3.2) the estimate

$$\|u - u_h\|_{H^1(\Omega)} \leq 4ch.$$

□

Remark 3.1 *Note, that an analogous analysis holds for the nonlinear scheme (2.11). In order to find the convergence rate it is only necessary to realize that for $f \in H^1(\Omega)$ and $s = \sum_{i=1}^N s_i \chi_{I_i}$, i.e. a step function with*

$$s_i = f\Big(\frac{x_{i-1} + x_i}{2}\Big), \qquad i = 1, ..., N$$

and χ_{I_i} denoting the characteristic function of I_i, it holds that

$$\|f - s\|_{L^2(\Omega)} \leq h\|\partial_x f\|_{L^2(\Omega)}. \tag{3.3}$$

For $f \in H^1(\Omega)$ and $g \in L^2(I_i)$ and s being the step function defined above, we have

$$\left| \int_{I_i} fg \; dx - \int_{I_i} sg \; dx \right| \;\leq\; h\|f\|_{H^1(I_i)}\|g\|_{L^2(I_i)}.$$

Replacing the respective estimates in the proof of Theorem 3.1, we deduce that also the nonlinear scheme of Ancona [4] is also converging with optimal rate.

4 Numerical results

In this section we present a numerical comparison of the proposed finite element methods. In particular, we check the theoretically predicted convergence rates and, moreover, the influence of the boundary data on both schemes, which is crucial in the simulation of MOS devices [6]. To compare both discretizations, we study a MIS (Metal Insulator Semiconductor) diode in thermal equilibrium. The MIS diode consists of a uniformly doped piece of semiconductor coated with a thin layer of insulating material which carriers a metal gate contact [16, 15, 26].

In particular, we study the behavior of the electron density in the semiconductor part of the device. Such behavior is described by the following boundary value problem for the electron density $n(x)$

$$-\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + \log(n) + V(x) = 0, \qquad \text{in } x \in (0,1) \tag{4.1}$$

$$n(0) = 0, \qquad n(1) = 1 \tag{4.2}$$

and the potential function V is given by

$$V(x) = x(\alpha x - \beta)e^{-\delta x};$$

where $\alpha = -47.57$, $\beta = 5.42$ and $\delta = 19.45$. This explicit form of $V(x)$ was obtained by performing an exponential fitting on precomputed data for the fully coupled problem.

Remark 4.1 *In [1] one finds an existence result for vacuum boundary conditions, which ensures that the solution stays positive in the interior of the domain. It is clear that the discretization schemes presented here cannot fulfill the boundary condition at* $x = 0$ *due to their exponential character. For this reason we use a very small value close to zero for the boundary value* $n(0)$*. For our numerical simulations we have considered several values of* $n(0)$ *and used different uniform grids.*

4.1 Influence of Approximate Boundary Conditions

From Figures 4.1 to 4.3 we see that the proposed finite element scheme is very stable with respect to the imposed approximate boundary conditions for any grid size. On the other hand, the nonlinear scheme shows a poor performance, which improves for decreasing grid spacings as Figure 4.3 shows. This sensitivity problem of the nonlinear scheme has been also reported in [27] and can be directly explained by Remark 2.3.

4.2 Convergence Rates

For both discretization schemes with different values of $n(0)$, we present in Figure 4.4 and Figure 4.5 the $L^2(\Omega)$ and $H^1(\Omega)$ norm of the error for the electron density n as the grid is refined. As 'exact solution', we choose the solution on a very fine grid (h=1/4500) for each method. From Figure 4.4, the sensitivity of the nonlinear scheme to the boundary condition is observed, the smaller $n(0)$ is taken the larger the error gets. The FEM scheme behaves well and is less sensitive to the respective approximate choice of the boundary condition (see Figure 4.5).

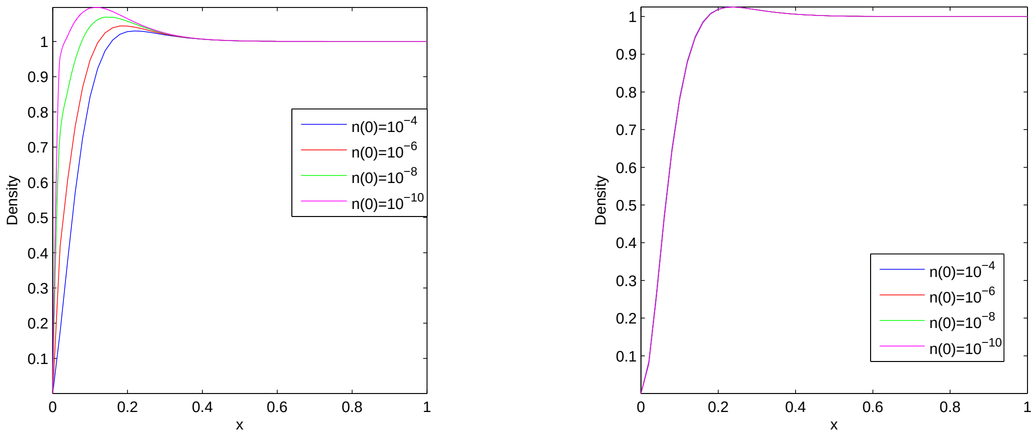

Figure 4.1: Electron density obtained by the nonlinear (left) and the finite element (right) scheme with $N = 50$ grid points and different boundary conditions at $x = 0$

In addition, the numerical results underline the theoretical consistency error of Section 3.3. In both cases the convergence rates behave like $\mathcal{O}(h)$ in the $H^1(\Omega)$–norm and $\mathcal{O}(h^2)$ in the $L^2(\Omega)$–norm (see Figure 4.4 and Figure 4.5, respectively).

5 Conclusions

We gave a finite element interpretation of Ancona's nonlinear scheme [4] and proposed a second approach based on an exponential transformation of variables and linear interpolation. Numerical tests indicate that the second approach is more stable on coarser grids. Both schemes are convergent with the optimal order of convergence.

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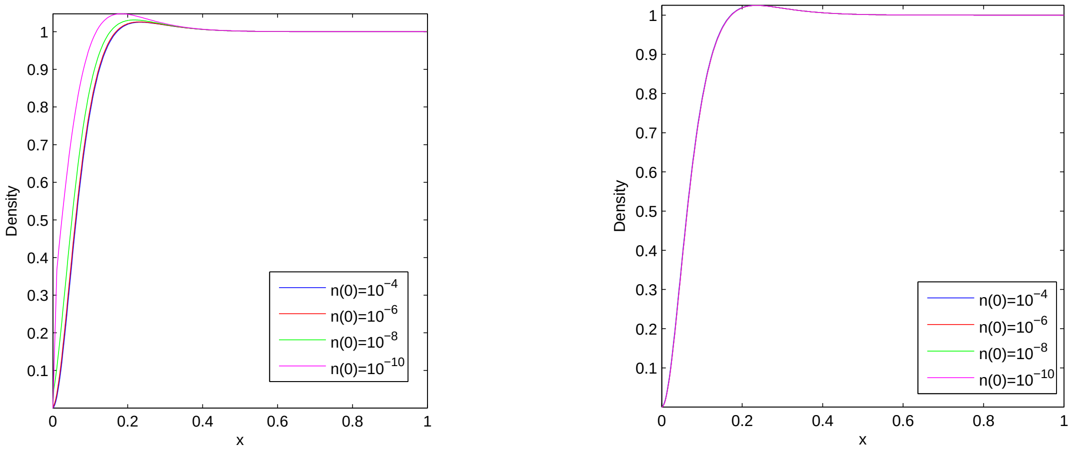

Figure 4.2: Electron density obtained by the nonlinear (left) and the finite element (right) scheme with $N = 375$ grid points and different boundary conditions at $x = 0$

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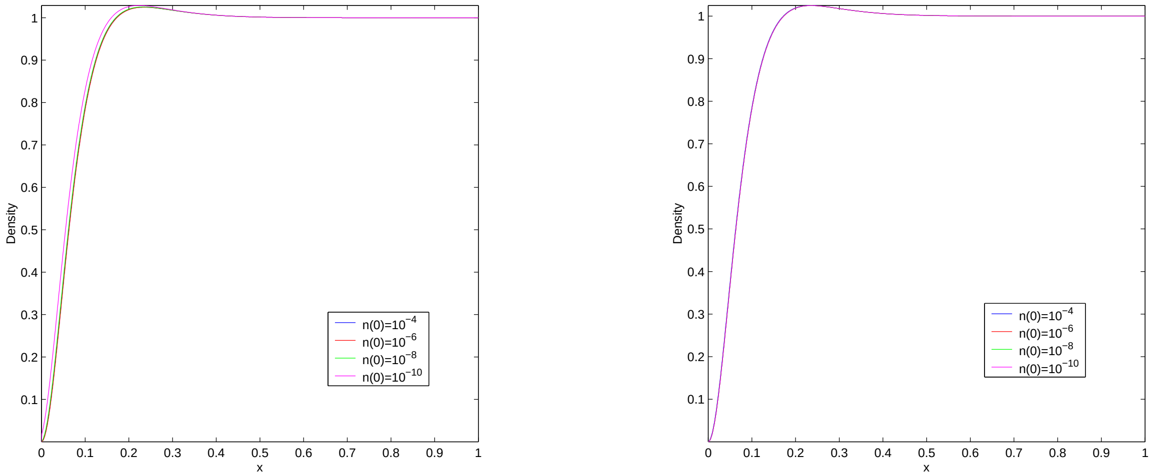

Figure 4.3: Electron density obtained by the nonlinear (left) and the finite element (right) scheme with $N = 1000$ grid points and different boundary conditions at $x = 0$

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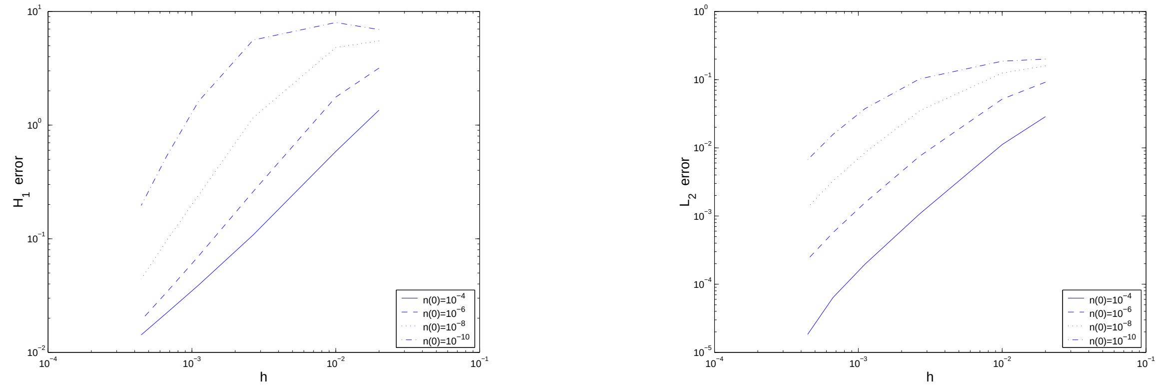

Figure 4.4: Consistency error of the nonlinear scheme with different boundary values at $x = 0$

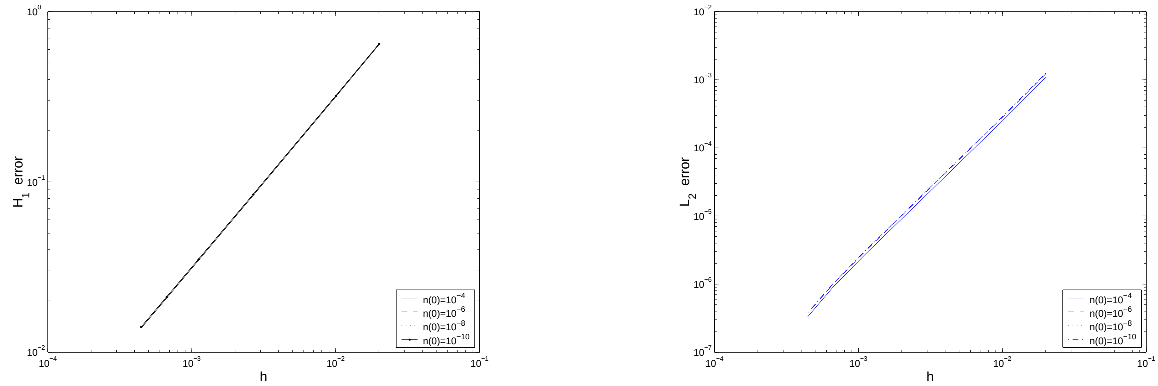

Figure 4.5: Consistency error of the finite element scheme with different boundary values at $x = 0$

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