SIAM J. Numer. Anal.
Vol. 42, No. 4, pp. 1648–1668

UNIFORM CONVERGENCE OF AN EXPONENTIALLY FITTED SCHEME FOR THE QUANTUM DRIFT DIFFUSION MODEL*

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Abstract. We analyze an exponentially fitted finite element scheme for the unipolar quantum drift diffusion model in one-dimensional space. The existence of discrete solutions is shown under very mild assumptions, and convergence of a subsequence is proved by compactness arguments. The scheme is constructed in such a way that it reduces in the semiclassical limit to the well-known Scharfetter–Gummel discretization for the classical drift diffusion model. We derive uniform error bounds which allow for the semiclassical limit on the discrete level. Numerical tests underlining the analytical results are presented.

Key words. quantum drift diffusion, generalized Scharfetter–Gummel discretization, mixed finite elements, exponential fitting, uniform convergence, semiclassical limit, semiconductor

AMS subject classifications. 35J60, 35J70, 65N12, 65N15, 65N30, 76Y05

DOI. 10.1137/S0036142903429961

1. Introduction.

From the earliest days of semiconductor industry there has been a never-ending drive towards increased miniaturization. The original aim was to produce more devices per unit area, but now scientists and engineers are exploiting quantum size effects to introduce new electronic properties into existing materials. Many devices, like MOSFETs or resonant tunneling structures, already reached the decanano length scale [19]. The Semiconductor Industry Association (SIA) projects that by 2009 the leading edge MOS device will employ a 0.05 μm length scale and an oxide thickness of 1.5 nm or less. But already today quantum mechanical effects, like confinement in barrier structures or inversion layers as well as direct tunneling through the oxide causing gate leakage in MOS structures are no longer negligible [18]. Hence, scientists are in charge to develop "correct" models which can be easily incorporated into existing modern simulation tools.

During the last years much effort has been spent on the derivation and analysis of *macroscopic* quantum models, which allow for an accurate description of the underlying physics of the devices by reasonable numerical costs. Nowadays, there exists a whole hierarchy of macroscopic models leading from the quantum hydrodynamic (QHD) models [25, 20] over the quantum energy transport (QET) model to the quantum drift diffusion (QDD) model, which can be derived from a moment expansion of the Wigner–Poisson system (see [26, 31] and the references therein for a comprehensive overview). Recently, extensions of these models were derived, which are better suited to deal with quantum tunneling and coherence effects [21, 22, 13, 17].

In this work we analyze a new numerical scheme for the QDD model. The mathematical analysis and numerical understanding of this model is in a rather mature state [31]. Essentially, this model is a dispersive regularization of the classical drift diffusion (DD) model of Van Roosbroeck [29], which accounted for the immense success of the macroscopic theory of charge transport in semiconductors and is commonly

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*Received by the editors June 20, 2003; accepted for publication (in revised form) May 18, 2004; published electronically December 27, 2004. This work was supported by European network HYKE, funded by the EC under contract HPRN-CT-2002-00282.

http://www.siam.org/journals/sinum/42-4/42996.html

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used (with all its enhancements) in modern simulation tools. First, Ancona [8], Ancona and Tiersten [5], and Ancona and Iafrate [10] proposed a quantum correction of this well-understood system. This *density-gradient theory* is impressively capable of describing the correct device behavior in the vicinity of strong inversion layers in MOS structures when compared to one-electron quantum mechanic simulations [8]. But already the shrinking device size poses severe numerical problems, since the local field strength increases and interior layers in the solution become more abrupt [14]. The QDD model was employed for the simulation of many quantum semiconductor devices and has proved its numerical efficiency, especially in several space dimensions [7, 11, 37]. Due to its numerical robustness it is already programmed into the 2d/3d PROPHET simulation code from *Lucent Technologies* as well as into various commercial device simulators, e.g., those from *ISE* and *Silvaco*. Encouraging comparisons with Schrödinger–Poisson simulations can be found in [3, 37].

The unscaled QDD model equations stated on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$, or 3, read as

$$\frac{\partial n}{\partial t} + \frac{1}{q}\,\mathrm{div}\,J = 0, \tag{1.1a}$$

$$\frac{q\,k_B\,T_0}{m}\nabla n + \frac{q^2}{m}\,n\,\nabla V - \frac{q\,\hbar^2}{2\,m^2}\,n\,\nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) = -\frac{J}{\tau_0}, \tag{1.1b}$$

which are self-consistently coupled with the Poisson equation for the electrostatic potential

$$-\epsilon\,\Delta V = q\,(n - C_{dop})\,. \tag{1.1c}$$

The variables are the electron density $n = n(x,t)$, the current density $J = J(x,t)$, and the electrostatic potential $V = V(x,t)$. The physical constants are the elementary charge q, the Boltzmann constant k_B, the effective electron mass m, and the reduced Planck constant $\hbar$. For the values of these constants we refer the reader to [29]. Physical parameters are the permittivity ϵ, the relaxation time τ_0, and the lattice temperature T_0. The time-independent doping profile $C_{dop} = C_{dop}(x)$ represents the distribution of charged background ions.

In this paper we consider the stationary QDD model for unipolar devices in one-dimensional space. We introduce the diffusion scaling, where the new dimensionless quantities are marked by a tilde:

$$\begin{aligned} &n \to C_m\,\tilde{n}, && C_{dop} \to C_m\,\tilde{C}_{dop}, && x \to L\,\tilde{x}, \\ &t \to \frac{m\,L^2}{k_B\,T_0\,\tau_0}\tilde{t}, && V \to \frac{k_B\,T_0}{q}\tilde{V}, && J \to \frac{q\,k_B\,T_0\,C_m\,\tau_0}{L\,m}\tilde{J}. \end{aligned}$$

Here, C_m denotes the maximal absolute value of the doping profile C_{dop} and L is a characteristic device length, e.g., the diameter. Defining the scaled Planck constant ε and the scaled Debye length λ,

$$\varepsilon^2 = \frac{\hbar^2}{2\,m\,k_B\,T_0\,L^2}, \quad \lambda^2 = \frac{\epsilon\,k_B\,T_0}{q^2\,C_m\,L^2},$$

and introducing the quantum quasi-Fermi level F via $J = n\,\partial_x F$, we can divide equation (1.1b) by n and integrate once. This yields the scaled QDD model stated on the bounded domain $\Omega = (0, 1)$:

$$\partial_x (n\, \partial_x F) = 0, \tag{1.2a}$$

$$-\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + \log(n) + V = F, \tag{1.2b}$$

$$-\lambda^2 \partial_{xx} V = n - C_{dop}. \tag{1.2c}$$

Throughout the paper we assume that $C_{dop} \in L^\infty(\Omega)$. In (1.2) the electron density $n = n(x) \geq 0$, the quantum quasi-Fermi level $F = F(x)$, and the electrostatic potential $V = V(x)$ are unknown.

The model equations (1.2) are supplemented with Dirichlet boundary conditions modeling the Ohmic contacts of the device:

$$n = n_D > 0, \quad V = V_D \overset{\text{def}}{=} V_{eq} + V_{ext}, \quad F = F_D \overset{\text{def}}{=} F_{eq} + V_{ext} \quad \text{on } \partial\Omega, \tag{1.3}$$

where V_{ext} is the applied biasing voltage. This set of boundary conditions is motivated by its analogy to the classical DD model [30, 27, 28]. Nevertheless, the correct choice of the Dirichlet data is still an open problem. A recent discussion can be found in [6]. Clearly, the thermal equilibrium density n_{eq} is a possible candidate for n_D. The built-in potential is given by V_{eq}, and F_{eq} is chosen accordingly.

Remark 1. The restriction to the unipolar case is just to keep the notation simple. In fact, Ben Abdallah and Unterreiter [1] proved existence of solutions and considered the semiclassical limit for the bipolar case. The results of this paper are easily extendable to the bipolar setting.

So far, only standard discretization schemes were employed, which require very fine meshes to ensure an adequate resolution of the desired quantities. To account for this problems we want to generalize the classical Scharfetter–Gummel (SG) discretization for the DD equations [35] to this quantum model. A first step in this direction can be found in [9, 4] where a nonlinear discretization scheme is suggested. Here, we follow a different approach [33] since we are moreover interested in a scheme which is stable in the semiclassical limit $\varepsilon \to 0$ recovering the classical SG scheme. However, the SG method relies on the introduction of the so-called Slotboom variable which allows for the symmetrization of the continuity equation [29]. This is impossible in the formulation (1.2) of the QDD model, since we have the additional quantum Bohm potential. Nevertheless, we can deal with this problem by interpreting the Bohm potential as a correction of the classical electrostatic potential V and introducing the *corrected potential* G via

$$G = -\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + V$$

which yields for the current density $J = \partial_x n + n \partial_x G$; i.e., the drift is now given by G. Then, system (1.2) can be written as

$$\partial_x J = 0, \quad J = \partial_x n + n \partial_x G, \tag{1.4a}$$

$$-\varepsilon^2 \frac{\partial_{xx}\sqrt{n}}{\sqrt{n}} + V = G, \tag{1.4b}$$

$$-\lambda^2 \partial_{xx} V = n - C_{dop}. \tag{1.4c}$$

We introduce the generalized Slotboom variable $u = e^G n$, which yields for the current density $J = e^{-G}\partial_x u$. Assuming vanishing quantum effects and vanishing quantum current at the boundary, we get

$$G = V_D, \quad u = e^{V_D} n_D \quad \text{on } \partial\Omega. \tag{1.5}$$

This nonlinear system is discretized using a mixed finite element discretization for the current density J and the Slotboom variable u, and standard linear elements for n and V. For an overview of stabilized discretization schemes for the classical DD model see [23] and the references therein.

We prove under very mild assumptions that the resulting nonlinear discrete system possesses a solution and that at least a subsequence of the sequence of discrete solutions converges to a continuous solution. Since we have no uniqueness for the QDD model in general, we cannot expect convergence of the full sequence. The proof is based on a variational argument similar to the one used in [1] and the derivation of appropriate a priori bounds. Especially, we can show that a discrete solution fulfills the same maximum principle as a continuous solution.

Our mixed finite element scheme is chosen in such a way that in the case of vanishing quantum effects ($\varepsilon = 0$) one recovers the classical SG discretization of the DD model. By deriving a priori bounds on the discrete solutions which are independent of ε, we can even perform the semiclassical limit $\varepsilon \to 0$ on the discrete level and derive estimates on the convergence rate, which are uniform in ε.

We present simulations of a ballistic diode and a resonant tunneling structure which exactly reproduce the predicted accuracy results underlining the feasibility of our approach. Moreover, these simulations show that the asymptotic constant in the error estimate for the current density seems to be almost independent of the size of the scaled Planck constant ε, which is essential from the engineering point of view, since it allows for an accurate computation of the current density also in the semiclassical limit.

The paper is organized as follows. In section 2 we introduce our nonlinear discrete scheme and section 3 is devoted to the proof of the existence and convergence of discrete solutions. The semiclassical limit is performed in section 4, where also uniform convergence rates are given. Finally, simulations of a ballistic diode and a resonant tunneling structure are presented in section 5. Concluding remarks are given in section 6.

2. A generalized SG discretization.

In this section we present a discretization of system (1.4) in the spirit of the well-known SG discretization for the classical DD model [35]. Here the drift is given by the generalized potential G, such that we have to take additional care about (1.4b) which involves the quantum Bohm potential.

First, we write (1.4) in a weak form. For notational convenience we define the spaces

$$X = H_0^1(\Omega), \quad \Sigma = L^2(\Omega),$$

and testing appropriately we get the following:

Find $n \in n_D + X$, $V \in V_D + X$, $G \in G_D + X$, and $J \in \Sigma$ such that

$$\int_\Omega e^G J \cdot \tau \, dx - \int_\Omega \partial_x \left(e^G n\right) \cdot \tau \, dx = 0, \tag{2.1a}$$

$$\int_\Omega J \cdot \partial_x \phi \, dx = 0, \tag{2.1b}$$

$$\varepsilon^2 \int_\Omega \partial_x \sqrt{n} \partial_x \left(\frac{\phi}{\sqrt{n}} \right) \, dx = \int_\Omega (G - V)\phi \, dx, \tag{2.1c}$$

$$\lambda^2 \int_\Omega \partial_x V \partial_x \phi \, dx = \int_\Omega (n - C_{dop})\phi \, dx \tag{2.1d}$$

for all $\phi \in X$ *and* $\tau \in \Sigma$.

We discretize (2.1) on the possibly nonuniform grid $0 = x_0 < x_1 < \cdots < x_N = 1$ defining the subintervals and the grid spacing by

$$I_i = (x_{i-1}, x_i], \quad h_i = x_i - x_{i-1}, \quad h = \max_i h_i.$$

We employ finite-dimensional spaces of linear and constant finite elements:

$$X_h = \left\{ w \in H_0^1(\Omega) : w|_{I_i} \in P_1, i = 1, \dots, N \right\},$$
$$\Sigma_h = \left\{ w \in L^2(\Omega) : w|_{I_i} \in P_0, i = 1, \dots, N \right\}.$$

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 $i = 0, \dots, N$. We will make frequent use of the following interpolation result [23].

PROPOSITION 2.1. *There exists a constant* $c > 0$, *independent of* h, *such that*

$$\left| w - w^I \right|_{H^1(\Omega)} \le c\, h \left(\sum_i |w|^2_{H^2(I_i)} \right)^{1/2},$$
$$\left| w - w^I \right|_{L^2(\Omega)} \le c\, h^2 \left(\sum_i |w|^2_{H^2(I_i)} \right)^{1/2}$$

for all $w \in H^1(\Omega) \cap \left\{ H^2(I_i), \text{ for all } i = 1, \dots, N \right\}$.

Let $(\cdot, \cdot)$ denote the standard inner product on $L^2(\Omega)$. We define its discrete analogue using the trapezoidal rule

$$(u, v)_h \overset{\text{def}}{=} \int_\Omega (uv)^I \, dx = \sum_{i=0}^N \omega_i \, u(x_i) v(x_i),$$

where $\omega_i > 0$ denotes the corresponding weights of the quadrature formula. We have the following consistency result for the discrete inner product.

LEMMA 2.2. *Let* $f, g \in X_h$. *Then there exists a constant* $c > 0$, *independent of* h, *such that*

$$|(f, g) - (f, g)_h| \le ch^2 \left\| \partial_x f \right\|_{L^2(\Omega)} \left\| \partial_x g \right\|_{L^2(\Omega)}.$$

The corresponding discretization of (2.1) reads as follows:

Find $n_h \in n_D + X_h$, $V_h \in V_D + X_h$, $G_h \in G_D + X_h$, *and* $J_h \in \Sigma_h$ *such that*

$$\left(e^{G_h} J_h, \tau_h \right) - \left(\partial_x \left(e^{G_h} n_h \right)^I, \tau_h \right) = 0, \tag{2.2a}$$

$$(J_h, \partial_x \phi_h) = 0, \tag{2.2b}$$

$$\varepsilon^2 \left(\partial_x (\sqrt{n_h})^I, \partial_x \left(\frac{\phi_h}{\sqrt{n_h}} \right)^I \right) = (G_h - V_h, \phi_h)_h, \tag{2.2c}$$

$$\lambda^2 \left(\partial_x V_h, \partial_x \phi_h \right) = \left(n_h - C_{dop}, \phi_h \right)_h \tag{2.2d}$$

for all $\phi_h \in X_h$ *and* $\tau_h \in \Sigma_h$.

The discretization of the generalized Slotboom variable u is given by $u_h = \left(e^{G_h} n_h\right)^I$.

We define the piecewise constant function $\bar{G}_h$ by

$$e^{\bar{G}_h}|_{I_i} = \frac{1}{h_i} \int_{I_i} e^{G_h}\, dx.$$

Using that the discrete current density J_h is constant on each element and the identity

$$G_h = \log \left(\frac{u_h}{n_h} \right)^I = \log(u_h)^I - \log(n_h)^I,$$

we can rewrite (2.2) equivalently as follows:

Find $n_h \in n_D + X_h$, $V_h \in V_D + X_h$, $u_h \in u_D + X_h$, *and* $G_h \in G_D + X_h$ *such that*

$$\left(e^{-\bar{G}_h} \partial_x u_h, \partial_x \phi_h \right) = 0, \tag{2.3a}$$

$$\varepsilon^2 \left(\partial_x (\sqrt{n_h})^I, \partial_x \left(\frac{\phi_h}{\sqrt{n_h}} \right)^I \right) + \left(\log(n_h)^I, \phi_h \right)_h = \left(\log(u_h)^I - V_h, \phi_h \right)_h, \tag{2.3b}$$

$$\lambda^2 \left(\partial_x V_h, \partial_x \phi_h \right) = \left(n_h - C_{dop}, \phi_h \right)_h. \tag{2.3c}$$

Remark 2. Formally, we deduce from (2.2c) that for $\varepsilon = 0$ it holds that $G_h \equiv V_h$ and the mixed finite element scheme reduces to the classical one. Note that in contrast to the classical SG scheme, (2.3a) determines the unknown corrected potential G_h, while (2.3b) is now the one for the electron density n_h.

Remark 3. The *nonlinear discretization scheme* developed in [9, 4] is based on finite differences and differs in the discretization of (2.3b). There, additionally some kind of exponential fitting is used for this equation; i.e., the electron density is approximated by an exponential function on each element. The scheme performs extremely well especially for large grid-spacings, but so far no numerical analysis is available. It is worth noting that an exponential transformation ($n = \exp(w)$) was also employed in the study of the transient problem [27, 28], but a numerical analysis for the fully discrete tranformed system is left for future research.

3. Existence and convergence of discrete solutions.

We show that the nonlinear discrete system (2.3) possesses at least one solution and we derive a priori bounds on the sequence of discrete solution which ensure that there exists a subsequence converging to the continuous solution. The existence proof is based on a variational argument, which also allows to derive the desired a priori bounds.

We state the main theorem of this section establishing existence of a discrete solution and its convergence.

THEOREM 3.1. *For each* $h > 0$ *there exists a discrete solution* $(n_h, V_h, G_h, u_h) \in (n_D, V_D, G_D, u_D) + X_h^4$ *of* (2.3). *Further, there exists a subsequence, again denoted by* (n_h, V_h, G_h, u_h), *such that*

$$\left((\sqrt{n_h})^I, V_h, G_h, u_h \right) \to \left(\sqrt{n}, V, G, u \right) \qquad \text{in } \left[H^1(\Omega) \right]^4,$$

for $h \to 0$, *where* $(n, V, G, u) \in (n_D, V_D, G_D, u_D) + X^4$ *solves the continuous problem* (2.1).

Corollary 3.2. *The sequence of discrete current densities* (J_h) *possesses a subsequence such that* $J_h \to J$ *in* $L^2(\Omega)$ *for* $h \to 0$.

Remark 4. Generally, we cannot expect convergence of the whole sequence, since the continuous as well as the discrete QDD model may admit for multiple solutions. Uniqueness can only be proven near to the thermal equilibrium state, i.e., for small applied biasing voltages V_{ext} [34].

For the existence proof we employ Brouwer's fixed point theorem. We define the closed, bounded, and convex set

$$\mathcal{U}_h \overset{\text{def}}{=} \left\{ u_h \in u_D + X_h : \underline{u} \le u_h \le \overline{u} \right\},$$

where the lower and upper bound are given by

$$\underline{u} \overset{\text{def}}{=} \min_{\partial\Omega} e^{V_D} n_D, \quad \overline{u} \overset{\text{def}}{=} \max_{\partial\Omega} e^{V_D} n_D.$$

On this set we define the fixed point mapping $T_h : \mathcal{U}_h \to \mathcal{U}_h$, where $u_h = T_h(w_h)$ is calculated via the following iteration:

1. *Find* $(n_h, V_h) \in (n_D, V_D) + X_h^2$ *as the solution of*

(3.1a)
$$\varepsilon^2 \left(\partial_x (\sqrt{n_h})^I, \partial_x \left(\frac{\phi_h}{\sqrt{n_h}} \right)^I \right) + \left(\log(n_h)^I, \phi_h \right)_h = \left(\log(w_h)^I - V_h, \phi_h \right)_h,$$

(3.1b)
$$\lambda^2 \left(\partial_x V_h, \partial_x \phi_h \right) = \left(n_h - C_{dop}, \phi_h \right)_h$$

for all $\phi_h \in X_h$.

2. *Set* $G_h = \log(w_h)^I - \log(n_h)^I$.
3. *Find* $u_h \in u_D + X_h$ *as the solution of*

(3.2)
$$\left(e^{-\bar{G}_h} \partial_x u_h, \partial_x \phi_h \right) = 0$$

for all $\phi_h \in X_h$.

3.1. Well-posedness of the fixed point mapping. The well-posedness of the first step is the content of the following result, which also provides uniform bounds on the electron density n_h and the potential V_h.

Lemma 3.3. *Let* $w_h \in \mathcal{U}_h$ *be given. Then there exists a unique solution* $(n_h, V_h) \in (n_D, V_D) + X_h^2$ *of the nonlinear system* (3.1). *Further, there exists a constant* $\theta \in (0,1)$, *independent of* h, *such that*

(3.3)
$$\theta \le n_h \le 1/\theta, \quad \left\| (\sqrt{n_h})^I \right\|_{H^1(\Omega)} \le 1/\theta, \quad \|V_h\|_{H^1(\Omega)} \le 1/\theta.$$

Proof. For the proof we employ a variational argument following the ideas in [36]. Let $H(s)$ be a primitive of $\log(s)^I$ with $H \ge 0$. We introduce the auxiliary variable $\rho_h \overset{\text{def}}{=} \sqrt{n_h}$. On the closed set

$$\mathcal{R}_h \overset{\text{def}}{=} \left\{ \rho_h : \rho_h^2 \in n_D + X_h, \rho_h \ge 0 \right\},$$

we define the functional

$$E(\rho) \overset{\text{def}}{=} \varepsilon^2 \int_\Omega \left| \partial_x \rho^I \right|^2 dx + \sum_{i=0}^N \omega_i H(\rho_i^2) + \frac{\lambda^2}{2} \int_\Omega \left| \partial_x V_h[\rho^2 - C_{dop}] \right|^2 dx - \sum_{i=0}^N \omega_i \log(w_i)\, \rho_i^2,$$

where $V_h \overset{\text{def}}{=} V_h[\rho^2 - C_{dop}] \in V_D + X_h$ is the unique discrete solution of Poisson's equation $\lambda^2(\partial_x V_h, \partial_x \phi_h) = (\rho^2 - C_{dop}, \phi_h)_h$ for all $\phi_h \in X_h$. Identifying ρ with its vector of nodal values in $\mathbb{R}^{N+1}$ one easily verifies that E possesses a unique minimizer $\rho_h \in \mathcal{R}_h$, since E is bounded from below, continuous, and convex with respect to ρ_h^2 [34]. The minimizer also satisfies the Euler–Lagrange equation

$$\varepsilon^2 \left(\partial_x \rho_h^I, \partial_x \phi_h\right) + \left(\rho_h \log(\rho_h^2)^I, \phi_h\right)_h = \left(\rho_h(\log(w_h)^I - V_h[\rho^2 - C_{dop}]), \phi_h\right)_h \tag{3.4}$$

for all $\phi_h \in X_h$.

Now we derive uniform estimates on the solution. In the following let $\theta \in (0,1)$ denote not necessarily identical constants, which are assumed to be independent of h. Choosing $\rho_D \overset{\text{def}}{=} \sqrt{n_D} \in \mathcal{R}_h$ as a comparison function we clearly have $E(\rho_h) \leq E(\rho_D)$, from which we deduce

$$\varepsilon^2 \int_\Omega \left|\partial_x \rho_h^I\right|^2 \, dx + \frac{\lambda^2}{2} \int_\Omega \left|\partial_x V_h[\rho_h^2 - C_{dop}]\right|^2 \, dx + \sum_{i=0}^{N} \omega_i H(\rho_i^2) \\ \leq E(\rho_D) + |\log(\overline{u})| \left(\rho_h, \rho_h\right)_h .$$

This yields immediately the existence of a constant $\theta \in (0,1)$, independent of h, such that

$$\left\|\partial_x \rho_h^I\right\|_{L^2(\Omega)} \leq 1/\theta \quad \text{and} \quad \|\partial_x V_h\|_{L^2(\Omega)} \leq 1/\theta.$$

Employing Sobolev's embedding theorem in one-dimensional space [2], i.e., $H^1(\Omega) \hookrightarrow C^{0,\beta}(\bar{\Omega})$, $\beta \in [0, 1/2)$, we find a uniform constant $\theta \in (0,1)$ with

$$\left\|\rho_h^I\right\|_{C^{0,\beta}(\bar{\Omega})} \leq 1/\theta \quad \text{and} \quad \|V_h\|_{C^{0,\beta}(\bar{\Omega})} \leq 1/\theta.$$

A direct calculation finally yields $\|n_h\|_{L^\infty(\Omega)} \leq 1/\theta$, for some uniform constant $\theta \in (0,1)$.

Next we prove the uniform positivity of ρ_h. Let $[\phi]^-$ denote the linear interpolant of $\phi^- \overset{\text{def}}{=} \min(0, \phi)$. Testing (3.4) with $\phi_h = [\rho_h - \underline{\rho}]^-$ for $\underline{\rho} > 0$ yields

$$\varepsilon^2 \left(\partial_x \rho_h^I, \partial_x [\rho_h - \underline{\rho}]^-\right) = \left(\left[-\log(\rho_h^2)^I + \log(w_h)^I - V_h[\rho_h^2 - C_{dop}]\right] \rho_h, [\rho_h - \underline{\rho}]^-\right)_h ,$$

which can be estimated as follows:

$$\varepsilon^2 \left(\partial_x \rho_h^I, \partial_x [\rho_h - \underline{\rho}]^-\right) \leq \sum_{i=0}^{N} \left[\omega_i (-\log(\rho_i^2) + \log(\underline{u}) - 1/\theta) \rho_i (\rho_i - \underline{\rho})^-\right] \\ \leq 0$$

if we choose $\underline{\rho}^2 = e^{-1/\theta} \underline{u}$. Further we calculate

$$\left(\partial_x \rho_h^I, \partial_x [\rho_h - \underline{\rho}]^-\right) = \sum_{i=0}^{N} h_i (\rho_{i+1} - \rho_i) \left[(\rho_{i+1} - \underline{\rho})^- - (\rho_i - \underline{\rho})^-\right] \\ \geq \sum_{i=0}^{N} h_i \left|(\rho_{i+1} - \underline{\rho})^- - (\rho_i - \underline{\rho})^-\right|^2 .$$

Hence,

$$\sum_{i=0}^{N} h_i \left|(\rho_{i+1} - \underline{\rho})^- - (\rho_i - \underline{\rho})^-\right|^2 \leq 0,$$

which implies $(\rho_{i+1} - \underline{\rho})^- = (\rho_i - \underline{\rho})^-, i \in \{0, \dots, N-1\}$, and due to the positivity of ρ_D we have

$$(\rho_i - \underline{\rho})^- \equiv 0 \quad \text{for all } i \in \{0, \dots, N\}.$$

Thus, it holds that, $\rho_h \geq \underline{\rho}$ and $n_h \geq \underline{\rho}^2$, respectively. ∎

An easy consequence of Lemma 3.3 is the following result, which establishes uniform $L^\infty(\Omega)$-bounds on the discrete generalized potential G_h.

COROLLARY 3.4. *Let $w_h \in \mathcal{U}_h$ be given. Then there exist uniform bounds $\underline{G}, \overline{G} > 0$, independent of h, such that*

$$\underline{G} \leq G_h \leq \overline{G}. \tag{3.5}$$

Further, Corollary 3.4 and standard results from elliptic theory [16, 24] yield the unique solvability of (3.2).

LEMMA 3.5. *Let $G_h \in G_D + X_h$ be given with $G_h > \underline{G}$ uniformly in h. Then there exists a unique solution $u_h \in \mathcal{U}_h$ of* (3.2). *Further, there exists a constant $\theta \in (0,1)$, independent of h, such that*

$$\|u_h\|_{H^1(\Omega)} \leq 1/\theta. \tag{3.6}$$

3.2. Proof of the existence theorem. The results derived so far ensure the well-posedness of the fixed point mapping and we are now in the position to prove the convergence theorem.

Proof of Theorem 3.1. First we note that the fixed point mapping T_h is well defined and continuous due to Lemma 3.3, Corollary 3.4, and Lemma 3.5.

Identifying u_h with its vector of nodal values in $\mathbb{R}^{N+1}$ we deduce the existence of a fixed point $u_h \in \mathcal{U}_h$ from Brouwer's fixed point theorem [38], since $\mathcal{U}_h$ is a closed, convex and compact subset of $\mathbb{R}^{N+1}$.

The uniform bounds given in Lemma 3.3, Corollary 3.4, and Lemma 3.5 imply the existence of a subsequence $(\rho_{h_k}, V_{h_k}, G_{h_k}, u_{h_k})$ such that

$$\left(\rho^I_{h_k}, V_{h_k}, G_{h_k}, u_{h_k}\right) \rightharpoonup (\rho, V, G, u) \quad \text{weakly in } \left[H^1(\Omega)\right]^4,$$

for $h_k \to 0$, where $(\rho^2, V, G, u) \in (n_D, V_D, G_D, u_D) + X_h^2$.

These convergences are by far sufficient to pass to the limit in (2.3): due to Sobolev's embedding theorem we have $\rho^I_{h_k} \to \rho$ and also $\rho_{h_k} \to \rho$ in $L^\infty(\Omega)$, such that we can deduce the strong $H^1(\Omega)$ convergence of $(\rho^I_{h_k})$ from (3.4). Standard results from elliptic theory [24] yield

$$V_{h_k} \to V \quad \text{in } H^1(\Omega),$$
$$u_{h_k} \to u \quad \text{in } H^1(\Omega),$$

and finally $G_{h_k} \to G$ in $H^1(\Omega)$ for $h_k \to 0$.

Hence, (ρ^2, V, G, u) is in fact a solution of (2.3), which ends the proof. ∎

3.3. Convergence rates. For completeness we also state a result establishing convergence rates for the finite element discretization (2.2). Since we consider a fully nonlinear system of equations which may admit multiple solutions, we have to impose an additional assumption on the isolatedness of the continuous solution.

THEOREM 3.6. *Let* $(n, V, G, u) \in \left[H^2(\Omega)\right]^4$ *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* (n_h, V_h, G_h, u_h) *of the discrete problem* (2.3). *Further, there exists a constant* $c > 0$*, independent of* h*, such that*

$$\|n - n_h\|_{H^1(\Omega)} + \|V - V_h\|_{H^1(\Omega)} + \|u - u_h\|_{H^1(\Omega)} \leq c\, h. \tag{3.7}$$

The proof can be found in [32]. Note that here the constant c generally depends on ε, such that the performance of the semiclassical limit is not possible on this level. In the next section we will use different techniques to overcome this problem.

4. Semiclassical limit—Uniform convergence. In this section we provide estimates independent of the parameter ε, which allow to perform the semiclassical limit in the numerical scheme recovering the classical SG discretization.

We need estimates on the discrete solution, which are independent of ε and h, generalizing the estimates given in section 3. Examining carefully the proofs of that section, we conclude that they crucially depend on ε, since we exploited the monotonicity of the quantum Bohm potential. But in fact we can introduce a different fixed point mapping. The key idea is to reinterpret the equation for n as the one for G and vice versa. This yields the fixed point map $N : n_D + X \to n_D + X$ with $N(m) = n$, where given $m \in n_D + X$ the solution n is calculated via the following iteration:

1. *Find* $V \in V_D + X$ *such that*

$$\lambda^2 \int_\Omega \partial_x V \, \partial_x \phi \, dx = \int_\Omega (m - C_{dop})\phi \, dx \tag{4.1a}$$

for all $\phi \in X$.

2. *Find* $(n, G) \in (n_D, G_D) + X^2$ *such that*

$$-\int_\Omega n \, \partial_x G \, \partial_x \phi \, dx - \int_\Omega \partial_x n \, \partial_x \phi \, dx = 0, \tag{4.1b}$$

$$\varepsilon^2 \int_\Omega \partial_x \sqrt{n} \, \partial_x \left(\frac{\phi}{\sqrt{n}}\right) \, dx = \int_\Omega (G - V)\phi \, dx \tag{4.1c}$$

for all $\phi \in X$.

Remark 5. The reader easily verifies that the fixed point mapping N is well defined and possesses a fixed point exploiting the relation $G = F - \log(n)$. Hence, (4.1) is just a reformulation of (1.2).

Also the discrete system (2.2) can be reformulated in the former manner:

Find $n_h \in n_D + X_h$, $V_h \in V_D + X_h$, *and* $G_h \in G_D + X_h$ *such that,*

$$-\int_\Omega \partial_x n_h \, \partial_x \phi_h \, dx - \int_\Omega n_h \, \partial_x G_h \partial_x \phi_h \, dx = \langle f_h, \phi_h \rangle, \tag{4.2a}$$

$$\varepsilon^2 \int_\Omega \partial_x (\sqrt{n_h})^I \, \partial_x \left(\frac{\phi_h}{\sqrt{n_h}}\right)^I \, dx = (G_h - V_h, \phi_h)_h, \tag{4.2b}$$

$$\lambda^2 \int_\Omega \partial_x V_h \, \partial_x \phi_h \, dx = (n_h - C_{dop}, \phi_h)_h \tag{4.2c}$$

for all $\phi_h \in X_h$.

Here, the right-hand side f_h is given by

$$\langle f_h, \phi_h \rangle \overset{\text{def}}{=} \int_\Omega e^{-G_h} \partial_x \left(e^{G_h} n_h \right) \partial_x \phi_h \, dx - \int_\Omega e^{-\bar{G}_h} \partial_x \left(e^{G_h} n_h \right)^I \partial_x \phi_h \, dx.$$

The main result of this section reads as follows.

THEOREM 4.1. *Let* $(n, V, G, u) \in \left[H^2(\Omega) \right]^4$ *be a solution of the continuous problem* (1.2) *and assume that the Fréchet derivative* $(I - DN)(n) \in \mathcal{L}(H^1(\Omega), H^1(\Omega))$ *of the mapping* $I - N : H^1(\Omega) \to H^1(\Omega)$ *at a solution* n *is uniformly bounded invertible, i.e.,*

$$\left\| (I - DN)^{-1} \right\|_{\mathcal{L}(H^1(\Omega), H^1(\Omega))} \le M,$$

where $M > 0$ *is independent of* ε.

Then there exists a constant $c > 0$ *such that for each* $0 < \varepsilon < \varepsilon_0$ *with* $\varepsilon_0 = \varepsilon_0(h) > 0$ *we have the uniform estimates*

$$\|n - n_h\|_{H^1(\Omega)} \le c\, h, \tag{4.3a}$$

$$\|V - V_h\|_{H^1(\Omega)} \le c\, h, \tag{4.3b}$$

$$\|G - G_h\|_{H^1(\Omega)} \le c\, h, \tag{4.3c}$$

$$\|u - u_h\|_{H^1(\Omega)} \le c\, h, \tag{4.3d}$$

$$\|J - J_h\|_{L^2(\Omega)} \le c\, h. \tag{4.3e}$$

The proof of Theorem 4.1 is done in several steps.

4.1. Regularity of weak solutions. First, we show that a weak solution of system (2.1) is in fact in $\left[H^2(\Omega) \right]^4$ and that the stronger norm is also uniformly bounded in ε. This generalizes the results given in [1].

THEOREM 4.2. *Let* (n, V, G, J) *be a weak solution of* (2.1). *Then it holds that* $(n, V, G) \in \left[H^2(\Omega) \right]^3$ *and there exists a constant* $K > 0$, *independent of* ε, *such that*

$$\|n\|_{H^2(\Omega)} + \|V\|_{H^2(\Omega)} + \|G\|_{H^2(\Omega)} \le K.$$

Proof. We eliminate G and J in (1.4) and introduce the auxiliary $\rho = \sqrt{n}$, which yields the fourth-order equation

$$\varepsilon^2 \rho_{xxxx} - \varepsilon^2 \frac{\rho_{xx}^2}{\rho} - 2\rho_{xx} - 2\frac{\rho_x^2}{\rho} - 2\rho_x V_x - \rho V_{xx} = 0$$

supplemented with boundary conditions

$$\rho = \rho_D, \quad \rho_{xx} = 0 \quad \text{on } \partial\Omega.$$

This equation possesses a unique weak solution $\rho \in H^4(\Omega)$ (see [27]). Testing the fourth-order equation with $\phi = -\rho_{xx}$ we get

$$\varepsilon^2 \int_\Omega \rho_{xxx}^2 \, dx + \varepsilon^2 \int_\Omega \frac{\rho_{xx}^3}{\rho} \, dx + 2 \int_\Omega \rho_{xx}^2 \, dx + 2 \int_\Omega \frac{\rho_x^2}{\rho} \rho_{xx} \, dx$$
$$+ 2 \int_\Omega \rho_x V_x \rho_{xx} \, dx + \int_\Omega \rho V_{xx} \rho_{xx} \, dx = 0.$$

From the Gagliardo–Nierenberg inequality [24] we derive

$$\|\rho_x\|_{L^4(\Omega)} \leq c_1 \|\rho\|_{H^2(\Omega)}^{1/4} \|\rho\|_{H^1(\Omega)}^{3/4},$$

with $c_1 = c_1(\Omega) > 0$, which yields, using Poincaré's inequality,

$$\begin{aligned} 2\int_\Omega \frac{\rho_x^2}{\rho}\rho_{xx} &\leq \frac{2}{\underline{\rho}} \|\rho_x\|_{L^4(\Omega)}^2 \|\rho_{xx}\|_{L^2(\Omega)} \\ &\leq 2\frac{c_2(\Omega)}{\underline{\rho}} \|\rho\|_{H^2(\Omega)}^{3/2} \|\rho\|_{H^1(\Omega)}^{3/2} \\ &\leq \frac{1}{2}\|\rho\|_{H^2(\Omega)}^2 + 2\frac{c_2^2}{\underline{\rho}^2}\|\rho\|_{H^1(\Omega)}^6 . \end{aligned}$$

Note that the upper and lower bounds $\underline{\rho} \leq \rho \leq \overline{\rho}$ are also uniform in ε (see [1]). Further, the Gagliardo–Nierenberg inequality gives

$$\|\rho_{xx}\|_{L^3(\Omega)} \leq c_3(\Omega) \|\rho\|_{H^3(\Omega)}^{7/12} \|\rho\|_{H^1(\Omega)}^{5/12},$$

which yields

$$\begin{aligned} \varepsilon^2 \int_\Omega \frac{\rho_{xx}^3}{\rho} &\leq \frac{\varepsilon^2}{\underline{\rho}} \|\rho_{xx}\|_{L^3(\Omega)}^3 \\ &\leq \frac{\varepsilon^2 c_3}{\underline{\rho}} \|\rho\|_{H^3(\Omega)}^{7/4} \|\rho\|_{H^1(\Omega)}^{5/4} \\ &\leq \frac{\varepsilon^2}{2}\|\rho\|_{H^3(\Omega)}^2 + \frac{\varepsilon^2 c_3^2}{2\underline{\rho}}\|\rho\|_{H^1(\Omega)}^{10} . \end{aligned}$$

Finally, we derive from Sobolev's embedding theorem and standard regularity results [24]

$$\begin{aligned} 2\int_\Omega \rho_x V_x \rho_{xx} &\leq 2\|\rho_x\|_{L^2(\Omega)} \|\rho_{xx}\|_{L^2(\Omega)} \|V_x\|_{L^\infty(\Omega)} \\ &\leq \frac{1}{4}\|\rho_{xx}\|_{L^2(\Omega)}^2 + c_4 \|\rho\|_{H^1(\Omega)}^2 \|V\|_{H^2(\Omega)}^2 \\ &\leq \frac{1}{4}\|\rho_{xx}\|_{L^2(\Omega)}^2 + c_4 \|\rho\|_{H^1(\Omega)}^4 \end{aligned}$$

and

$$\begin{aligned} \int_\Omega \rho V_{xx} \rho_{xx} &= -\frac{1}{\lambda^2}\int_\Omega \rho\rho_{xx}(\rho^2 - C_{dop}) \\ &\leq \frac{1}{\lambda^2}\|\rho\|_{L^\infty(\Omega)} \left(\|\rho\|_{L^\infty(\Omega)}^2 + \|C_{dop}\|_{L^\infty(\Omega)}\right) \|\rho_{xx}\|_{L^2(\Omega)} \\ &\leq \frac{1}{8}\|\rho_{xx}\|_{L^2(\Omega)}^2 + c_5(\lambda, \overline{\rho}, C_{dop}). \end{aligned}$$

Combining these estimates and using Poincaré's inequality we get

$$\frac{\varepsilon^2}{2}\int_\Omega \rho_{xxx}^2 + \frac{1}{4}\int_\Omega \rho_{xx}^2 \leq c_6(\Omega, \lambda, \underline{\rho}, \|\rho\|_{H^1(\Omega)}),$$

where c_6 is independent of ε.

Hence, we established $\|\rho\|_{H^2(\Omega)} \le \tilde{K}$ for some $\tilde{K} > 0$ uniformly in ε and due to the uniform upper and lower bounds, it even holds that $\|n\|_{H^2(\Omega)} \le K$. The uniform boundedness of $\|V\|_{H^2(\Omega)}$ and $\|G\|_{H^2(\Omega)}$ follows now from the standard elliptic theory. ◻

4.2. Uniform bounds on the discrete solution. Secondly, we derive uniform bounds for the discrete solution of system (2.2).

LEMMA 4.3. *There exist constants $K > 0$ and $\theta \in (0,1)$, independent of ε and h, such that*

$$\left\|(\sqrt{n_h})^I\right\|_{H^1(\Omega)} + \|V_h\|_{H^1(\Omega)} + \|u_h\|_{H^1(\Omega)} + \|G_h\|_{H^1(\Omega)} \le K,$$
$$\theta \le n_h, u_h \le 1/\theta.$$

Proof. By construction we have $\underline{u} \le u_h \le \overline{u}$. Further, $\inf_{\mathcal{R}_h} E$ is also uniformly bounded in ε, such that each term of $E(\rho_h)$ is uniformly bounded. This implies $\|V_h\|_{H^1(\Omega)} \le K$, where the constant $K > 0$ is independent of ε and h. Mimicking the proof of Lemma 3.3 we get $\theta \le n_h$, where $\theta \in (0,1)$ is independent of ε and h. This yields $G_h \le 1/\theta$, which in turn implies $\|u_h\|_{H^1(\Omega)} \le K$.

Now let $\xi_h \in \mathcal{R}_h$ be the unique minimizer of the classical energy functional

$$E_{class}(\xi) = \int_\Omega H(\xi^2)\, dx + \frac{\lambda^2}{2}\int_\Omega \left|\partial_x V_h[\xi^2 - C_{dop}]\right|^2\, dx - \int_\Omega \log(u_h)^I\, \xi^2\, dx.$$

For $\rho_h = \sqrt{n_h}$ it holds that $E(\rho_h) \le E(\xi_h)$ and $E_{class}(\xi_h) \le E_{class}(\rho_h)$, which implies

$$\int_\Omega \left|\partial_x \rho_h^I\right|^2\, dx \le \int_\Omega \left|\partial_x \xi_h^I\right|^2\, dx.$$

In fact, we can calculate ξ_h explicitly from $\xi_h^2 = (u_h\, e^{-V_h})^I$. The bounds derived so far ensure the uniform boundedness of ξ_h in $H^1(\Omega)$ with respect to ε and h. Hence, we finally get $\left\|(\sqrt{n_h})^I\right\|_{H^1(\Omega)} \le K$ and $n_h \le 1/\theta$ as well as $-1/\theta \le G_h$. From $G_h = \log(u_h)^I - \log(n_h)^I$ we deduce that $\|G_h\|_{H^1(\Omega)} \le K$ by a direct calculation. ◻

4.3. Consistency of the discrete fixed point operator. Third, we introduce some auxiliary problems, which allow to derive the consistency of the two steps of the fixed point mapping N. Let $\hat{n} \overset{\text{def}}{=} N(n_h) \in n_D + X$ and define $\hat{n}_h \in n_D + X$ as the solution of

$$-\int_\Omega \partial_x \hat{n}_h\, \partial_x \phi\, dx - \int_\Omega \hat{n}_h\, \partial_x G_h\, \partial_x \phi\, dx = \langle f_h, \phi \rangle$$

for all $\phi \in X$. The functions $\hat{V}$ and $\hat{G}$ as well as $\hat{V}_h$ and $\hat{G}_h$ are defined in analogy.

Standard results for finite element approximations of linear elliptic equations directly yield the following result [16].

LEMMA 4.4. *Let $(\hat{n}_h, \hat{V}_h)$ be defined as above and (n_h, V_h) is a discrete solution of* (4.2). *Then there exists a constant $c > 0$, independent of ε and h, such that*

$$\|\hat{n}_h - n_h\|_{H^1(\Omega)} + \left\|\hat{V}_h - V_h\right\|_{H^1(\Omega)} \le ch.$$

Further, we introduce the auxiliary variables $\hat{u} \stackrel{\text{def}}{=} e^{\hat{G}}\hat{n} \in u_D + X$ and $\hat{u}_h \stackrel{\text{def}}{=} e^{G_h}\hat{n}_h \in u_D + X$, which fulfill

$$-\int_\Omega e^{-\hat{G}}\partial_x\hat{u}\,\partial_x\phi\,dx = 0 \quad \text{and} \quad -\int_\Omega e^{-G_h}\partial_x\hat{u}_h\,\partial_x\phi\,dx = \langle f_h, \phi\rangle$$

for all $\phi \in X$.

Taking the difference of these two equations and testing with $\phi = \hat{u} - \hat{u}_h \in X$ yield

$$e^{-\underline{\hat{G}}}\,\|\partial_x(\hat{u}-\hat{u}_h)\|_{L^2(\Omega)} \le \left\|e^{-\hat{G}} - e^{-G_h}\right\|_{L^\infty(\Omega)}\|\partial_x\hat{u}_h\|_{L^2(\Omega)} + \|f_h\|_{L^2(\Omega)},$$

from which we deduce

$$\|\hat{u}-\hat{u}_h\|_{H^1(\Omega)} \le c\left\{\left\|\hat{G}-G_h\right\|_{H^1(\Omega)} + h\right\}. \tag{4.4}$$

Further, we have by a direct calculation

$$\|\partial_x(\hat{n}-\hat{n}_h)\|_{L^2(\Omega)} \le c\left(\|\partial_x(\hat{u}-\hat{u}_h)\|_{L^2(\Omega)} + \left\|\hat{G}-G_h\right\|_{H^1(\Omega)}\right) \tag{4.5}$$

for some constant $c > 0$.

We need the following consistency result, which can be easily derived by cumbersome calculations and thus are omitted here for the sake of a compact presentation.

LEMMA 4.5. *There exists a constant $c > 0$, independent of ε and h, such that*

$$\sup_{\|\phi\|_{H^1(\Omega)}=1} |\langle f_h, \phi\rangle| \le ch.$$

Next, we prove the key estimate, which will finally allow for the derivation of the uniform convergence rates.

LEMMA 4.6. *Let $\hat{G}$ be defined as above and G_h a solution of* (4.2). *Then there exists a constant $c = c(\hat{n}, \hat{V}, \hat{G}) > 0$, independent of ε and h, such that*

$$\left\|G_h - \hat{G}^I\right\|_{L^2(\Omega)} \le c\left(h^2 + h^{-1}\varepsilon^2\|\hat{n}-n_h\|_{H^1(\Omega)} + \varepsilon^2\right).$$

Proof. We define

$$\langle A(n), \phi\rangle \stackrel{\text{def}}{=} \varepsilon^2\int_\Omega \partial_x(\sqrt{n})\,\partial_x\left(\frac{\phi}{\sqrt{n}}\right)\,dx,$$
$$\langle A_h(n_h), \phi\rangle \stackrel{\text{def}}{=} \varepsilon^2\int_\Omega \partial_x(\sqrt{n_h})^I\,\partial_x\left(\frac{\phi}{\sqrt{n_h}}\right)^I\,dx.$$

First, we estimate the difference $G_h - \hat{G}^I$. Due to (4.1) it holds that

$$\langle A_h(n_h), \phi_h\rangle = (G_h - V_h, \phi_h)_h \quad \text{for all } \phi_h \in X_h,$$
$$\langle A(\hat{n}), \phi\rangle = \int_\Omega(\hat{G}-\hat{V})\phi\,dx \quad \text{for all } \phi \in X.$$

Testing the difference of these two equations with $\phi = G_h - \hat{G}^I \in X_h$ yields

$$\begin{aligned}
&\langle A_h(n_h) - A(\hat{n}), \phi\rangle \\
&= \Big(G_h - \hat{G} - (V_h - \hat{V}), \phi\Big) + (G_h - V_h, \phi) - (G_h - V_h, \phi)_h \\
&= \Big(G_h - \hat{G}^I, \phi\Big) + \Big(\hat{G}^I - \hat{G}, \phi\Big) - \Big(V_h - \hat{V}, \phi\Big) + (G_h - V_h, \phi) - (G_h - V_h, \phi)_h\,,
\end{aligned}$$

which implies, due to Lemma 2.2,

$$\begin{aligned}
\left\|G_h - \hat{G}^I\right\|_{L^2(\Omega)}^2 \le{}& \left\|\hat{G}^I - \hat{G}\right\|_{L^2(\Omega)} \|\phi\|_{L^2(\Omega)} + \left\|V_h - \hat{V}\right\|_{L^2(\Omega)} \|\phi\|_{L^2(\Omega)} \\
&+ c_1 h^2 \|\partial_x(G_h - V_h)\|_{L^2(\Omega)} \|\partial_x \phi\|_{L^2(\Omega)} + \langle A_h(n_h) - A_h(\hat{n}), \phi\rangle \\
&+ \langle A_h(\hat{n}) - A(\hat{n}), \phi\rangle\,.
\end{aligned}$$

We estimate termwise. First,

$$\begin{aligned}
|\langle A_h(n_h) - A_h(\hat{n}), \phi\rangle| ={}& \varepsilon^2 \int_\Omega \partial_x \left(\sqrt{n_h} - \sqrt{\hat{n}}\right)^I \partial_x \left(\frac{\phi}{\sqrt{\hat{n}}}\right)^I dx \\
&+ \varepsilon^2 \int_\Omega \partial_x \left(\sqrt{n_h}\right)^I \partial_x \left(\frac{\phi}{\sqrt{n_h}} - \frac{\phi}{\sqrt{\hat{n}}}\right)^I dx \\
\le{}& \varepsilon^2 \left\|\partial_x \left(\sqrt{n_h} - \sqrt{\hat{n}}\right)^I\right\|_{L^2(\Omega)} \left\|\partial_x \left(\frac{\phi}{\sqrt{\hat{n}}}\right)^I\right\|_{L^2(\Omega)} \\
&+ \varepsilon^2 \left\|\partial_x \left(\sqrt{n_h}\right)^I\right\|_{L^2(\Omega)} \left\|\partial_x \left(\frac{\phi}{\sqrt{n_h}} - \frac{\phi}{\sqrt{\hat{n}}}\right)^I\right\|_{L^2(\Omega)}
\end{aligned}$$

which can be estimated using Proposition 2.1 by

$$\begin{aligned}
|\langle A_h(n_h) - A_h(\hat{n}), \phi\rangle| \le{}& \varepsilon^2 c_2 \left\|\partial_x \left(\sqrt{n_h} - \sqrt{\hat{n}}\right)\right\|_{L^2(\Omega)} \left\|\partial_x \left(\frac{\phi}{\sqrt{\hat{n}}}\right)\right\|_{L^2(\Omega)} \\
&+ \varepsilon^2 c_3 \left\|\partial_x \left(\sqrt{n_h}\right)\right\|_{L^2(\Omega)} \left\|\partial_x \left(\frac{\phi}{\sqrt{n_h}} - \frac{\phi}{\sqrt{\hat{n}}}\right)\right\|_{L^2(\Omega)}
\end{aligned}$$

and employing the uniform bounds derived so far

$$\begin{aligned}
|\langle A_h(n_h) - A_h(\hat{n}), \phi\rangle| &\le \|n_h - \hat{n}\|_{H^1(\Omega)} \Big\{\varepsilon^2 c_4 \|\phi\|_{H^1(\Omega)} + \varepsilon^2 c_5 \|\partial_x \phi\|_{L^2(\Omega)}\Big\} \\
&\le \varepsilon^2 c_6 \|n_h - \hat{n}\|_{H^1(\Omega)} \|\phi\|_{H^1(\Omega)}
\end{aligned}$$

for some uniform constants $c_i > 0$, $i = 1, \ldots, 6$.

Second, employing successively Proposition 2.1 we get

$$
\begin{aligned}
|\langle A_h(\hat{n}) - A(\hat{n}), \phi\rangle| &= \varepsilon^2 \int_\Omega \partial_x \left(\left(\sqrt{\hat{n}}\right)^I - \sqrt{\hat{n}} \right) \partial_x \left(\frac{\phi}{\sqrt{\hat{n}}} \right) \, dx \\
&\quad + \varepsilon^2 \int_\Omega \partial_x \left(\sqrt{\hat{n}}\right)^I \partial_x \left[\left(\frac{\phi}{\sqrt{\hat{n}}} \right)^I - \left(\frac{\phi}{\sqrt{\hat{n}}} \right) \right] \, dx \\
&\le \varepsilon^2 \left\| \partial_x \left(\left(\sqrt{\hat{n}}\right)^I - \sqrt{\hat{n}} \right) \right\|_{L^2(\Omega)} \left\| \partial_x \left(\frac{\phi}{\sqrt{\hat{n}}} \right) \right\|_{L^2(\Omega)} \\
&\quad + \varepsilon^2 \left\| \partial_x \left(\sqrt{\hat{n}}\right)^I \right\|_{L^2(\Omega)} \left\| \partial_x \left[\left(\frac{\phi}{\sqrt{\hat{n}}} \right)^I - \left(\frac{\phi}{\sqrt{\hat{n}}} \right) \right] \right\|_{L^2(\Omega)} \\
&\le \varepsilon^2 c_7 h \left\| \sqrt{\hat{n}} \right\|_{H^2(\Omega)} \|\phi\|_{H^1(\Omega)} + \varepsilon^2 c_8 h \left\| \frac{\phi}{\sqrt{\hat{n}}} \right\|_{H^2(\Omega)} \\
&\le c_9 \, \varepsilon^2 h \, \|\hat{n}\|_{H^2(\Omega)} \|\phi\|_{H^1(\Omega)}
\end{aligned}
$$

for some uniform constants $c_i > 0$, $i = 7, 8, 9$.

Combining the estimates derived so far we have

$$
\begin{aligned}
\left\| G_h - \hat{G}^I \right\|_{L^2(\Omega)} &\le \varepsilon^2 c_6 h^{-1} \|n_h - \hat{n}\|_{H^1(\Omega)} + c_9 \, \varepsilon^2 \\
&\quad + \left\| \hat{G}^I - \hat{G} \right\|_{L^2(\Omega)} + \left\| V_h - \hat{V} \right\|_{L^2(\Omega)} + c_1 h \, \|\partial_x (G_h - V_h)\|_{L^2(\Omega)},
\end{aligned}
$$

where we employed the inverse estimate $\|\phi_h\|_{H^1(\Omega)} \le c h^{-1} \|\phi_h\|_{L^2(\Omega)}$ for all $\phi_h \in X_h$. Finally, we use again Proposition 2.1 to end with

$$
\left\| G_h - \hat{G}^I \right\|_{L^2(\Omega)} \le c_{10} \left\{ \varepsilon^2 h^{-1} \|n_h - \hat{n}\|_{H^1(\Omega)} + \varepsilon^2 + h^2 + h \right\}. \qquad \square
$$

Next, we estimate the remaining difference $n_h - \hat{n}$.

LEMMA 4.7. *Let $\hat{n}$ be defined as above and n_h a solution of* (4.2). *Then there exist constants $c = c(\hat{n}, \hat{V}, \hat{G}, \hat{u}) > 0$, independent of ε and h, and $\varepsilon_0 = \varepsilon_0(h) > 0$ such that for $\varepsilon < \varepsilon_0$ it holds that*

$$
\|n_h - \hat{n}\|_{H^1(\Omega)} \le ch.
$$

Proof. We estimate

$$
\|n_h - \hat{n}\|_{H^1(\Omega)} \le \|n_h - \hat{n}_h\|_{H^1(\Omega)} + \|\hat{n}_h - \hat{n}\|_{H^1(\Omega)}
$$

and using Lemma 4.4 as well as (4.4) and (4.5)

$$
\begin{aligned}
\|n_h - \hat{n}\|_{H^1(\Omega)} &\le c_1 \left\{ \|\hat{u} - \hat{u}_h\|_{H^1(\Omega)} + \left\| G_h - \hat{G} \right\|_{H^1(\Omega)} + h \right\} \\
&\le c_2 \left\{ \left\| G_h - \hat{G} \right\|_{H^1(\Omega)} + h \right\} \\
&\le c_2 \left\{ \left\| G_h - \hat{G}^I \right\|_{H^1(\Omega)} + \left\| \hat{G}^I - \hat{G} \right\|_{H^1(\Omega)} + h \right\}
\end{aligned}
$$

and employing Proposition 2.1 and the inverse estimate $\|\phi_h\|_{H^1(\Omega)} \le ch^{-1} \|\phi_h\|_{L^2(\Omega)}$ for all $\phi_h \in X_h$, we have using Lemma 4.6

$$\begin{aligned}\|n_h - \hat{n}\|_{H^1(\Omega)} &\le c_3 \left\{ h \left\|\hat{G}\right\|_{H^2(\Omega)} + h^{-1} \left\|G_h - \hat{G}^I\right\|_{L^2(\Omega)} + h \right\} \\ &\le c_4 \left\{ h + h^{-2}\varepsilon^2 \|n_h - \hat{n}\|_{H^1(\Omega)} + h^{-1}\varepsilon^2 \right\}\end{aligned}$$

for some uniform constants $c_i > 0$, $i = 1, \dots, 4$. Now we assume

$$\varepsilon^2 \le \varepsilon_0^2 \overset{\text{def}}{=} \frac{h^2}{2c_4},$$

which yields the desired estimate $\|n_h - \hat{n}\|_{H^1(\Omega)} \le ch$, with $c = 2c_4 + 1$. ◻

4.4. Proof of the uniform convergence result. Now we are in the position to prove the main theorem of this section.

Proof of Theorem 4.1. We have the identity

$$n_h - n + N(n) - N(n_h) = (I - DN(\xi))(n_h - n) = n_h - \hat{n}_h + \hat{n}_h - \hat{n},$$

which yields

$$\|n - n_h\|_{H^1(\Omega)} \le \left\|(I - DN)^{-1}\right\|_{\mathcal{L}(H^1(\Omega), H^1(\Omega))} \|n_h - \hat{n}\|_{H^1(\Omega)} .$$

Hence, we have due to Lemma 4.7

$$\|n - n_h\|_{H^1(\Omega)} \le ch$$

for some constant $c > 0$, independent of ε and h. Finally, the other uniform estimates follow from standard results for the approximation of elliptic equations. ◻

5. Numerical results. In this section we present numerical simulations underlining the feasibility of the previously analyzed extended SG discretization. We study a ballistic n^+–n–n^+ diode fabricated of GaAs and a resonant tunneling structure. Both devices consist of a channel and source and drain contact regions, which are assumed to be equally long. The channel is moderately doped with a doping density of $5 \cdot 10^{21}\,\mathrm{m}^{-3}$, while the drain and source are highly doped with $10^{24}\,\mathrm{m}^{-3}$. The resonant tunneling diode has the same underlying structure, but the channel is replaced by a quantum well sandwiched between two barriers. This resonant barrier structure is itself sandwiched between two spacer layers (see Figure 5.1). The physical effect of the barriers is a shift in the Fermi level, which can be modeled by an additional step function B added to the electrostatic potential; i.e., V is replaced by $V + B$. Since, we need more smoothness of B for the numerical analysis, we used instead a smoothed function B, which is depicted together with the doping profile in Figure 5.2. We choose a scaled Debye length of $\lambda^2 = 10^{-2}$ and set the scaled biasing voltage to $V_{ext} = 5$. To emphasize the large gradients occurring in the electron density in the case of the resonant tunneling diode, we show in Figure 5.2 also the computed densities for the different values of the scaled Planck constant ε. These are in fact a consequence of the barrier function and can only be smoothed for large ε. Note that for $\varepsilon^2 = 10^{-5}$ there is already no visible difference to the classical solution.

Remark 6. There is numerical evidence that the QDD model shows negative differential resistance for some resonant tunneling diodes [34, 15], but one has to admit

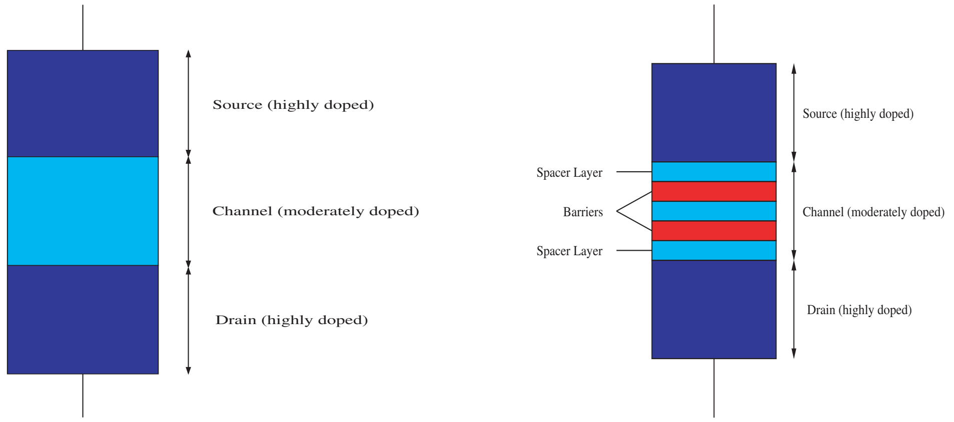

FIG. 5.1. *Diode structure (left: ballistic, right: RTD).*

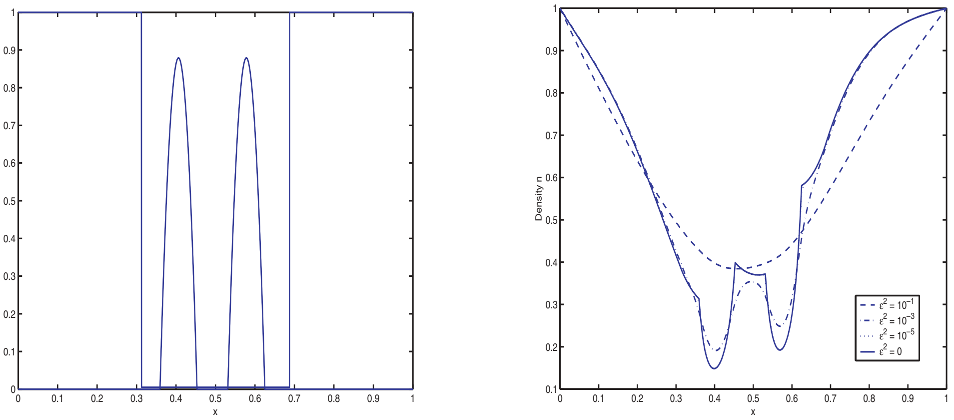

FIG. 5.2. *RTD (left: doping profile, barriers, right: electron densities).*

that the model is far from giving accurate quantitative results for this application. This stems from the fact that the model is mainly designed for scattering dominated transport and no quantum coherence is included. Nevertheless, this device is a good test example due to the large gradients in the electron density near to the barriers.

For the computations we used several uniform grids of variable size and the discretization (2.2). To investigate the semiclassical limit numerically we decreased the scaled squared Planck constant ε^2 from 10^{-1} to 0. The discrete nonlinear system is solved with a damped Newton iteration, which proved to be stable. In Figure 5.3 to Figure 5.5 we present the errors in the electron densities n, the electrostatic potentials V, and the generalized potentials G measured in the $H^1(\Omega)$-seminorm. Further, we depict in Figure 5.6 the error of the current densities J in the $L^2(\Omega)$-norm. The left picture always corresponds to the ballistic diode, while the right one shows the error for the resonant tunneling structure. Since in both cases an analytical solution is not available, we take the solution on the finest grid ($h = 1/4096$) as the "exact" solution.

The numerical results show in both cases that the error behaves like $\mathcal{O}(h)$ for all independent variables. Further, the scheme is stable in the semiclassical limit since the convergence rate is not affected by the size of ε. Note that the error in

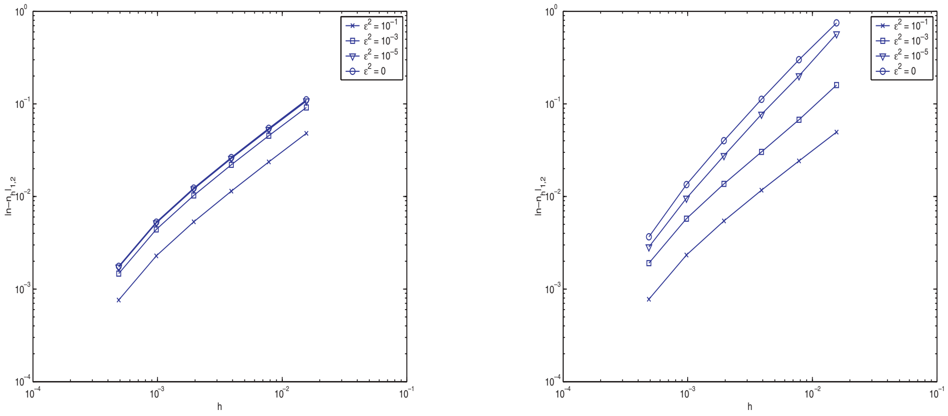

Fig. 5.3. *Error of the electron density (left: ballistic, right: RTD).*

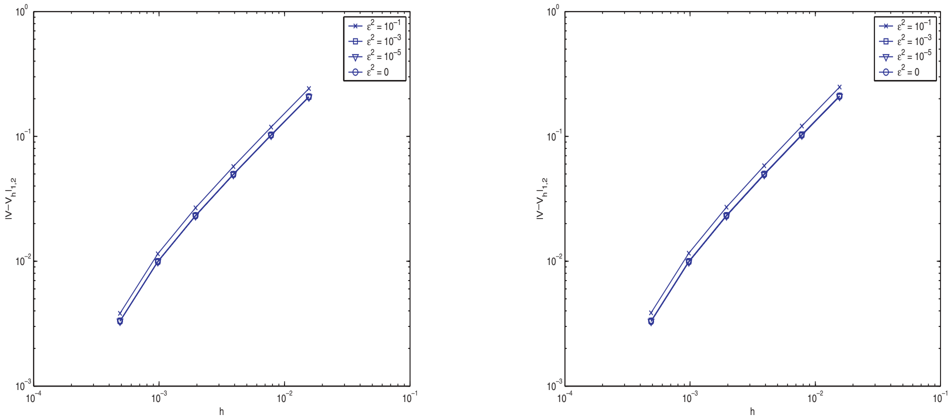

Fig. 5.4. *Error of the potential (left: ballistic, right: RTD).*

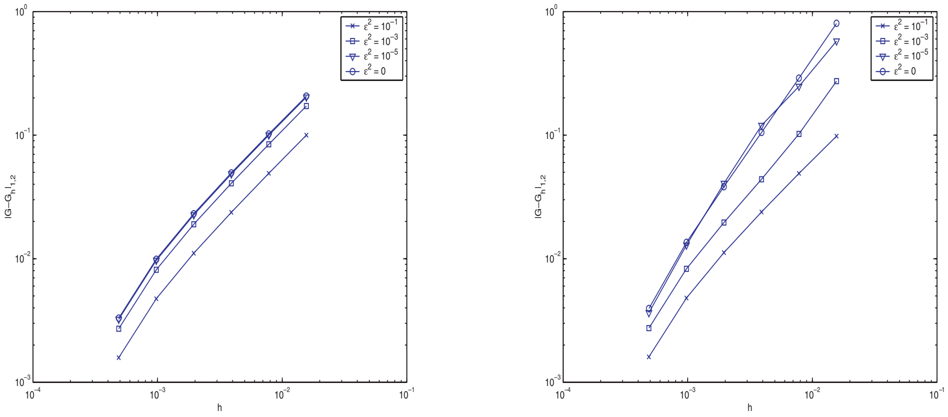

Fig. 5.5. *Error of the generalized potential (left: ballistic, right: RTD).*

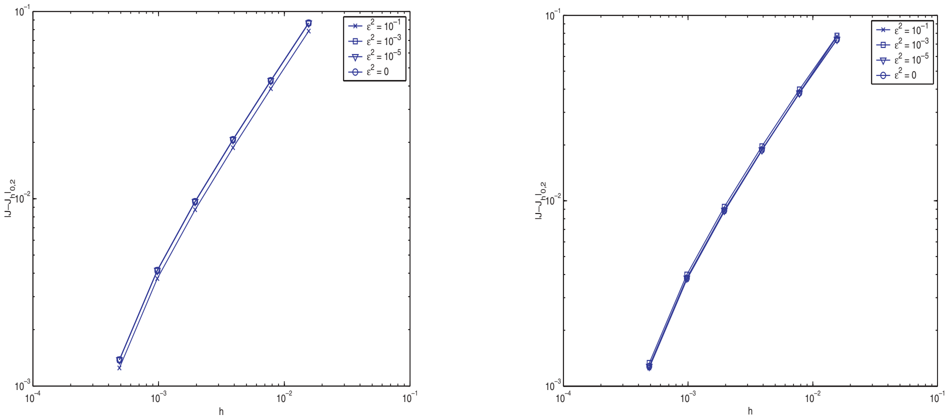

FIG. 5.6. *Error of the current density (left: ballistic, right: RTD).*

the electron density and the generalized potential of the RTD is much more affected by the size of ε, which is a consequence of the additional barrier function B. Most interestingly, in both cases the error in the current density even does not depend on ε. This observation is essential from the engineering point of view, since it allows for an accurate computation of current voltage characteristics also in the semiclassical limit.

6. Conclusions. We presented and analyzed a new stabilized finite element discretization for the quantum drift diffusion model, which is a generalization of the well-known Scharfetter–Gummel discretization for the classical drift diffusion model. The scheme yields the expected approximation errors and allows for the performance of the semiclassical limit on the discrete level, in such a way that the error estimates hold uniformly. The extension to bipolar devices is straightforward. Further, the numerical scheme can be easily extended to space dimensions larger than one using, e.g., the finite element spaces described in [12]. However, the proofs in this paper are not directly extendible, since we employed embedding theorems and inverse estimates, which crucially depend on the space dimension.

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