A Review on the Quantum Drift Diffusion Model

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Abstract

We consider the quantum drift diffusion model for semiconductor devices and collect recent results on the stationary and transient equations. The stationary model including generation–recombination terms is studied for bipolar devices and the transient equations are considered in the unipolar case. We cover several topics, such as existence and uniqueness of solutions, asymptotic limits and convergence of a nonlinear iteration scheme in the stationary case as well convergence of a positivity preserving semidiscretization of the transient equations and the linear stability of stationary states.

Key words. quantum drift diffusion, generalized Gummel iteration, analysis, numerics, convergence, fourth order PDE, positivity

AMS(MOS) subject classification. 35J55, 35J60, 35K35, 65M12, 65M20, 76Y05

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1 Introduction

Modern semiconductor device modelling has to keep pace with the increasing speed of miniaturization, which poses many challenging problems concerning the modelling and the numerical point of view. As many devices, like HEMT's, MOSFET's or resonant tunneling structures (RTD's) already reached the decanano length scale, quantum effects play a dominant role and must be accurately resolved by modern simulation tools suitable for an engineering–oriented device analysis [20]. The Semiconductor Industry Association (SIA) projects that 2009 the leading edge MOS device will employ a 0.05μm 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 more negligible [19].

Clearly, microscopic models such as the Schrödinger–Poisson or the Wigner–Poisson system are capable of resolving correctly the quantum dominated device behaviour [48]. During the last years many results such as the well–posedness of the whole space problem as well as the semiclassical limit have been proved [16, 45]. However, from the numeral point of view these macroscopic models meet several problems: Firstly, the high computational costs especially in multidimensions [41, 60]. Secondly one computes a lot of redundant information, since the macroscopic quantities, such as current–voltage characteristics or particle densities are computed via microscopic auxiliary quantities, e.g. the wave function [42]. Further, quantum effects are only existing in small parts of the device, such as inversion layers, and almost negligible in the remaining part [3]. Lastly, their correct physical setting is based on an unbounded position domain, such that the prescription of appropriate boundary data poses severe problems [41]. Nevertheless, much research was spend on this question: Analytical and numerical methods for the Schrödinger–Poisson system on bounded position domains [52, 53], absorbing boundary conditions for the quantum kinetic Wigner equation [11] and also the coupling of microscopic models with different classical and kinetic model was studied [1].

In parallel much effort has been spend on the derivation of a 'classical' picture of quantum mechanics in terms of macroscopic fluid type unknowns. This idea goes back to the early beginnings of quantum mechanics, where macroscopic quantum models such as Bloch's equation for the density matrix [49] or Madelung's transform of the Schrödinger equation where invented [42]. These are however still direct reformulations of an underlying microscopic model. They are employed in many fields of application, e.g. semiconductor device modelling, superconductivity or recently superfluidity [43].

Influenced by the immense success of the macroscopic theory of charge transport in semiconductors in form of the drift diffusion model (DD) of Van Roosbroeck [50], *Ancona et al.* [3, 7, 4] proposed a quantum correction of this well understood system. They assume that the essential nonlocality of quantum mechanics can be approximated by the demanding that the equations of state for the charged particles depend not only on their respective densities but also on the density–gradient. This *density–gradient theory* is impressively capable of describing the correct device behaviour in the vicinity of strong inversion layers in MOS structures when compared to one–electron quantum mechanic simulations [3]. *Ancona et al.* started their considerations following ideas from gas dynamics and applied their model also to other applications such as field emission from metals and steady state tunneling in metal–insulator–metal structures (MIM), where Fowler–Nordheim tunneling plays a prominent role [5]. This theory has also significant computational advantages, such that during the last decade many people studied this approach analytically and numerically.

Not surprisingly also many applied mathematicians became interested in these new macroscopic quantum models. Starting from the Wigner–Poisson system [22] or the mixed state Schrödinger–Poisson system [27] they used the strong tool of asymptotic analysis to derive a whole hierarchy of macroscopic quantum models in analogy to the classical continuum models, ranging from the quantum hydrodynamic model over quantum energy transport to the quantum drift diffusion model:

$$
\begin{array}{c}
\boxed{\text{Wigner–Poisson/Schrödinger–Poisson}}\\
\Downarrow\\
\boxed{\text{Quantum Hydrodynamics (QHD)}}\\
\Downarrow\\
\boxed{\text{Quantum Energy Transport (QET)}}\\
\Downarrow\\
\boxed{\text{Quantum Drift Diffusion (QDD)}}
\end{array}
$$

They describe the electron flow in the semiconductor crystal in terms of fluid–type unknowns, such as electron density, current density and energy density, whose evolution is governed by corresponding conservation laws. Originally, the QHD is an infinite hierarchy of moment equations, which has to be supplemented with appropriate closure conditions [28]. Nowadays the full QHD consists of three balance laws, while the QDD is isothermal and thus two equations are sufficient. The QET was derived only recently and is not investigated so far [37]. Note that for the QHD and the QDD oftenly the synonyms *density–gradient theory* or *quantum moment equations* are used in the engineering literature.

Gardner [22] derives the full QHD from the Wigner equation and shows that it allows to simulate quantum devices, especially RTD's, numerically very efficiently. Note that the isothermal QHD, i.e. the equations of state for the electron density and the current density including inertia is already stated and numerically investigated in [30, 5]. *Zhou and Ferry* [20] employed the full QHD for the simulation of multiple devices, such as HEMT's, MESFET's and RTD's. They studied the influence of quantum effects on the velocity overshoot and did also report current oscillations in transient simulations [66, 67, 68].

Recently, *Gardner and Ringhofer* [23] derived a 'smooth' QHD, where the quantum term involves a smoothed potential which has the capability of handling the discontinuities in the classical potential energy occurring in the vicinity of heterojunction barriers in a mathematically rigorous way. Numerical simulations show that negative differential resistance is present in the simulation of RTD's [24]. Further analytical work on the QHD can be found in [15, 10, 26, 35, 36, 33, 21, 25, 57]. We note that the choice of appropriate boundary conditions and of the heat conductivity is delicate and influences strongly the numerical results [35, 55, 59].

Performing the zero relaxation time limit in the isothermal QHD the convective term vanishes and one obtains the QDD [56] (see also Section 1.1). These equations equal up to a quantum correction the classical DD [50]. The mathematical analysis and numerical understanding of this set of equations is now in a rather mature state. In this paper we are going to give a review on the results obtained so far.

The advantage of the QDD is threefold:

1. The perturbation character of the QDD equations promises a reduction of redundancy in regions where the device behaves 'almost' classical.
2. There is a natural way to describe boundary conditions.
3. Existing simulation codes for the classical DD can be easily adjusted.

The analysis for the thermal equilibrium problem (which is equal to the one for the QHD) was performed by *Unterreiter* in [62] via a variational approach. *Ben Abdallah and Unterreiter* [2] proved existence of solutions of a bipolar extension of the stationary equations incorporating generation–recombination effects. A generalized Gummel iteration for the efficient numerical treatment of the QDD is developed in [58] and also analyzed.

The study of the transient equations is much more involved due to their fourth order nature. Existence of a non–negative global solution in the case of vanishing temperature and zero electric field is proved in [38]. A positivity preserving numerical scheme is derived in [40], which proves to be convergent and also the optimal order of convergence can be shown [39]. The linear stability of stationary states is investigated in [56].

The QDD gained considerable attention not only mathematically but also from the engineering point of view. It was employed for the simulation of many quantum semiconductor devices and proved its numerical efficiency, especially in several space dimensions [9, 8, 12, 64]. Due to its numerical robustness it is already integrated in the 2d/3d PROPHET simulation code from *Lucent Technologies*. Encouraging comparisons with Schrödinger–Poisson simulations can be found in [6, 64].

To get a comprehensive impression of the capabilities of the QDD we also have to mention its limitations. As only low order quantum corrections are considered no quantum interference phenomena are included in the model. Further, the simulation of modern single–electron devices is out of reach due to the break down of the continuum hypotheses. Also the choice of the mobility coefficient and the effective tunneling mass is delicate [63, 8, 64]. Either, they are derived empirically or used as fitting parameters to get better quantitative agreement of computational and experimental results.

The paper is organized as follows. In Section 1.1 we derive the QDD via the zero relaxation time limit in the isothermal QHD. Results on the bipolar stationary equations are given in Section 2. We discuss the thermal equilibrium problem as well as the biased case and a generalized Gummel iteration. Recent results on the transient model are given in Section 3. There, the existence of global non–negative solutions, the convergence of a positivity–preserving numerical scheme and the linear stability of stationary states are discussed. Further, we give conclusions in Section 4.

1.1 Passage from QHD to QDD

It is well–known that quantum moment equations can be derived in various ways [22, 27, 23]. In this section we start from the isothermal QHD and deduce the QDD in the zero relaxation time limit. This asymptotic link is just in analogy to connection of the classical hydrodynamic equations to the DD [29].This *formal* derivation was first presented in [56].

The transient, isothermal QHD consists of conservation laws for the electron density and the current density [22]. The unscaled QHD equations stated on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or 3 read:

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

$$\frac{\partial J}{\partial t} + \frac{1}{q} \operatorname{div} \left(\frac{J \otimes J}{n} \right) + \frac{q\, k_B\, T_0}{m} \nabla n + \frac{q^2}{m} n\, \nabla V - \frac{q\, \hbar^2}{2\, m^2} n\, \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = -\frac{J}{\tau}, \tag{1.1b}$$

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

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

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 to [48]. Physical parameters are the permittivity ϵ, the ambient temperature T_0 and the relaxation time τ, which depend on the material and on the operating conditions of the device. The time–independent doping profile $C_{dot} = C_{dot}(x)$ represents the distribution of charged background ions.

For the zero relaxation time limit is it convenient to introduce in (1.1) the following diffusion scaling, where the new dimensionless quantities are marked by a tilde:

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

Here, C_m denotes the maximal absolute value of the doping profile C_{dot} and L is a characteristic device length, e.g. the diameter. Defining the scaled Planck constant ε, the scaled Debye length λ and the scaled relaxation time τ_0 by

$$\varepsilon^2 = \frac{\hbar^2}{2\, m\, k_B\, T_0\, L^2}, \quad \lambda^2 = \frac{\epsilon\, k_B\, T_0}{q^2\, C_m\, L^2}, \quad \tau_0^2 = \frac{k_B\, T_0\, \tau^2}{m\, L^2},$$

we end up with the scaled QHD equations

$$\frac{\partial n}{\partial t} + \operatorname{div} J = 0, \tag{1.2a}$$

$$\tau_0^2\, \frac{\partial J}{\partial t} + \tau_0^2 \operatorname{div} \left(\frac{J \otimes J}{n} \right) + \nabla n + n\, \nabla V - \varepsilon^2\, n\, \nabla \left(\frac{\Delta \sqrt{n}}{\sqrt{n}} \right) = -J, \tag{1.2b}$$

$$-\lambda^2\, \Delta V = n - C_{dot}, \tag{1.2c}$$

where we omitted the tilde for notational convenience.

In applications the following data of a quantum semiconductor device [6, 64] is realistic:

$$L = 100\,\mathrm{nm}, \quad \tau = 10^{-13}\,\mathrm{s}, \quad \mathrm{T}_0 = 77\,\mathrm{K},$$

where the relaxation time τ corresponds to the low field mobility of GaAs [61]. The squared scaled relaxation time is $\tau_0^2 \approx 10^{-4}$, which justifies the relaxation limit $\tau_0 \to 0$ in (1.2). This *formally* yields the system

$$\frac{\partial n}{\partial t} + \operatorname{div} J = 0, \tag{1.3a}$$

$$-\varepsilon^2\, n\, \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right) + \nabla n + n\,\nabla V = -J, \tag{1.3b}$$

$$-\lambda^2\,\Delta V = n - C_{dot}. \tag{1.3c}$$

System (1.3) differs from the classical drift diffusion equations [48] only in the quantum correction '$-\varepsilon^2\, n\, \nabla\left(\frac{\Delta\sqrt{n}}{\sqrt{n}}\right)$'.

Inserting (1.3b) into (1.3a) we can eliminate the current density J. From the identity

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

we get the scaled transient QDD:

$$\frac{\partial n}{\partial t} = -\frac{\varepsilon^2}{2}\,\Delta^2 n + \frac{\varepsilon^2}{2}\sum_{i,j=1}^{d} \partial_{x_i}\partial_{x_j}\left(\frac{\partial_{x_i} n\,\partial_{x_j} n}{n}\right) + \Delta n + \operatorname{div}(n\,\nabla V), \tag{1.4a}$$

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

Hence, the transient QDD consists of a nonlinear fourth–order parabolic equation for the electron density n, which is self–consistently coupled to the Poisson equation for the potential V.

Especially, for the stationary equations there exist various formulations. These range from second order [2] via third [21] to fourth order systems [15], which all have their specific advantages and drawbacks. In the next section we concentrate on the stationary second order system.

2 The Stationary Equations

In Section 1.1 we derived the unipolar QDD. As all classical models involve two types of carriers, namely electrons and holes, it is only natural to extend the QDD to handle also bipolar quantum devices. This extension is proposed by *Ben Abdallah and Unterreiter* in [2] and reads in its scaled, stationary form stated on a bounded domain $\Omega \subset \mathbb{R}^d$, $d = 1, 2$ or $d = 3$:

$$-\varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V + B_n = F, \tag{2.1a}$$

$$-\xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}} + \log(p) - V + B_p = G, \tag{2.1b}$$

$$\operatorname{div}(\mu_n\, n \nabla F) = R(n,p)\left(\exp(F+G) - \delta^2\right), \tag{2.1c}$$

$$\operatorname{div}(\mu_p\, p \nabla G) = R(n,p)\left(\exp(F+G) - \delta^2\right), \tag{2.1d}$$

$$-\lambda^2 \Delta V = n - p - C_{dot}. \tag{2.1e}$$

The *scaled* physical parameters are the Planck constant ε, the ratio ξ of the effective masses of electrons and holes and the mobilities μ_n, μ_p of electrons and holes, respectively, and the Debye length λ. All these quantities are assumed to be positive constants, excluding especially field dependent mobilities. The doping profile $C_{dot} = C_{dot}(x)$ (where x is the spatial variable ranging in Ω) representing a fixed charge distribution and the non-negative quantum well potentials $B_{n,p} = B_{n,p}(x)$ are assumed to be fixed. Equation (2.1) also includes generation-recombination processes of the form $R(n,p)\,(\exp(F+G) - \delta^2)$, where $R : \mathbb{R}^2 \to \mathbb{R}$ and $\delta > 0$. In thermal equilibrium there is no generation-recombination process. Hence, $\delta^2 = \exp(F_{eq} + G_{eq})$, where F_{eq}, G_{eq} are the (constant!) equilibrium values of the quantum quasi Fermi levels, see [62]. The model includes Shockley–Read–Hall and Auger generation-recombination processes but excludes generation through impact ionization [44].

In (2.1) the electron density $n = n(x) \geq 0$, the hole density $p = p(x) \geq 0$, the quantum quasi Fermi levels $F = F(x), G = G(x)$ and the electrostatic potential $V = V(x)$ are unknown. The current densities of electrons and holes are determined by the charge densities, the quantum quasi Fermi levels F, G and the mobilities:

$$J_n = \mu_n\, n \nabla F, \quad J_p = -\mu_p\, p \nabla G. \tag{2.2}$$

The model equations (2.1) are supplemented with mixed Dirichlet-Neumann boundary conditions

$$n = n_D, \quad p = p_D, \quad V = V_D + V_{ext} \text{ on } \Gamma_D, \tag{2.3a}$$

$$F = F_{eq} + V_{ext}, \quad G = G_{eq} - V_{ext} \text{ on } \Gamma_D, \tag{2.3b}$$

$$\nabla n \cdot \nu = \nabla p \cdot \nu = \nabla V \cdot \nu = 0 \text{ on } \Gamma_N, \tag{2.3c}$$

$$\nabla F \cdot \nu = \nabla G \cdot \nu = 0 \text{ on } \Gamma_N, \tag{2.3d}$$

where Γ_D and Γ_N are disjoint parts of the boundary of Ω with $\Gamma_D \cup \Gamma_N = \partial\Omega$ and ν is the unit outward normal vector along Γ_N. Here, Γ_D models the Ohmic contacts of the device, while the insulating parts of the boundary are described by Γ_N.

This set of boundary conditions is motivated by its analogy to the classical DD. Nevertheless, the choice of the Dirichlet data n_D, p_D and V_D is still an open problem, since up to now no rigorous derivation from microscopic quantum models is available [55, 40].

Some authors assume charge neutrality and vanishing quantum effects at the boundary and sometimes only homogeneous Neumann data is employed [38, 40]. Clearly, the thermal equilibrium densities n_{eq} and p_{eq} are possible candidates for n_D and p_D and the built–in potential V_{eq} for V_D, respectively.

2.1 Thermal Equilibrium

The thermal equilibrium problem is of great interest for itself, as in the variational approach by Unterreiter [62] one needs not to prescribe any boundary data for the particle densities. Instead one assumes the *total charge neutrality* of the device and finds the thermal equilibrium state as the state of minimal total energy [53, 62]

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

in the set

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

where $H(t) = t\log(t) - t + 1$ is a primitive of $h(t) = \log t$ and

$$N \stackrel{\text{def}}{=} \int_\Omega C^+_{dot}\, dx, \quad P \stackrel{\text{def}}{=} \int_\Omega C^-_{dot}\, dx$$

are the densities of donator and acceptor atoms. Further, $V = V[n - p - C_{dot}]$ is the self consistent electrostatic potential defined via $-\lambda^2\Delta V = n - p - C_{dot}$ with $\int_\Omega V(x)\, dx = 0$. We note that

$$\int_\Omega (n - p - C_{dot})\, dx = 0 \quad \text{ for all } (n,p) \in \mathcal{C},$$

which yields the desired charge neutrality of the device.

The existence and uniqueness of a minimizer $(n_{eq}, p_{eq}) \in \mathcal{C}$ is proved by *Unterreiter* in [62] by means of variational calculus, where he also identifies the Euler–Lagrange equations.

Theorem 2.1. *Assume*

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

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

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

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

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

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

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

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

Further, he investigates the semiclassical limit $\varepsilon \to 0$ and the small Debye length limit $\lambda \to 0$.

There exist various possibilities for the numerical calculation of the minimizer. In [58] a projected quasi–gradient method is presented and its convergence proved, both on the continuous level and for the discretized problem.

Numerical investigations give evidence that for the thermal equilibrium state charge neutrality at the boundary holds [55] , at least as long as the devices is not to small. By means of asymptotic analysis the author shows in [55] that this cannot hold for ultra–small devices, whereas the assumption of vanishing quantum effects at the boundary can be justified.

2.2 QDD with Bias

The full system (2.1) supplemented with boundary conditions (2.3) is analytically investigated by *Ben Abdallah and Unterreiter* in [2]. They show the following existence result.

Theorem 2.2. *Assume*

A.1 $\Omega \subset \mathbb{R}^d, d = 1, 2$ *or* $d = 3$ *is a bounded domain and* $\partial\Omega$ *is* $C^{0,1}$ *and piecewise regular.*

A.2 $R \in C^0(\mathbb{R} \times \mathbb{R}; [0, \infty))$.

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

Then the system (2.1) *supplemented with boundary data* (2.3) *possesses a solution* $n, p, V, F, G \in H^1(\Omega) \cap L^\infty(\Omega)$. *Further,* $n, p, V, F, G \in C^0(\Omega)$ *and* $n(x), p(x) > 0$ *for all* $x \in \Omega$.

The proof is done by means of variational methods combined with Schauder's fixed point theorem. They also tackle the case of vanishing charge density at the boundary occurring at inversion layers. *Ancona* [3] emphasized this issue as one of the main advantages of the QDD, since here such kind of boundary conditions can be incorporated in contrast to the classical DD.

The question of uniqueness of solutions was left open in this paper and finally answered in [58] (see also Section 2.3). There it is shown that the solution is unique as long as the device is operated near the thermal equilibrium state, i.e. for small applied biasing voltages V_{ext}. This is in analogy to the result for the classical model [44, 51].

In [2] also the semiclassical limit is established, i.e. the solutions of the QDD converge to solutions of the classical DD as $\varepsilon \to 0$. We give the precise convergence result.

Theorem 2.3. *Let the assumptions of Theorem 2.2 hold and assume* $n_D, p_D > 0$. *Then there exist functions* $n, p, V, F, G \in C^0(\Omega) \cap H^1(\Omega)$ *satisfying*

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

and (2.3) *such that a solution* $n^\varepsilon, p^\varepsilon, V^\varepsilon, F^\varepsilon, G^\varepsilon \in C^0(\Omega) \cap H^1(\Omega)$ *of system* (2.1) *supplemented with* (2.3) *fulfils* $\sqrt{n^\varepsilon} \to \sqrt{n}$, $\sqrt{p^\varepsilon} \to \sqrt{p}$, $V^\varepsilon \to V$, $F^\varepsilon \to F$, $G^\varepsilon \to G$ *strongly in* $H^1(\Omega)$, *weak-$*$ in* $L^\infty(\Omega)$ *as* $\varepsilon \to 0$.

In this sense the QDD behaves well for small ε despite of its singular perturbation character. Clearly, this will be different if heterojunction barriers are present or in the vicinity of strong inversion layers (see [6]).

2.3 A Generalized Gummel–Iteration

In this section we consider a decoupling algorithm for the numerical solution of (2.1), which proves to work in a stable and efficient manner. For the classical DD an iteration introduced by *Gummel* [32] is most commonly employed and proved to be rather well suited for many problems of practical relevance. There exist a vast literature in which the Gummel–iteration is thoroughly studied from a numerical and an analytical point of view (for an excellent overview see [44, 34] and the references therein).

In [58] a fixed point mapping is constructed which yields a *generalized Gummel–iteration* for the QDD. This algorithm relies on a fixed point iteration decoupling the current equations from the rest of the system. In each iteration step two semi linear elliptic systems are solved. The fixed point mapping T is defined via: Let (F_0, G_0) be a pair of quantum quasi Fermi levels from an appropriately chosen set. Then, $T(F_0, G_0) := (F_1, G_1)$, where (F_1, G_1) is computed from (F_0, G_0) as follows:

Algorithm 1. (Generalized Gummel–iteration)

1. *Solve the semi linear elliptic system*

$$-\varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V + B_n = F_0, \tag{2.4a}$$

$$-\xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}} + \log(p) - V + B_p = G_0, \tag{2.4b}$$

$$-\lambda^2 \Delta V = n - p - C_{dot}, \tag{2.4c}$$

subject to the boundary conditions (2.3) *for* (n_1, p_1, V_1).

2. *Solve*

$$\operatorname{div}\left(\mu_n\, n_1\, \nabla F\right) = R(n_1, p_1)\, \left(\exp\left(F + G\right) - \delta^2\right), \tag{2.5a}$$

$$\operatorname{div}\left(\mu_p\, p_1\, \nabla G\right) = R(n_1, p_1)\, \left(\exp\left(F + G\right) - \delta^2\right), \tag{2.5b}$$

subject to the boundary conditions (2.3) *for* (F_1, G_1).

Clearly, every fixed point of T is a solution of the original problem (2.1) with boundary conditions (2.3). The unique solvability of the above boundary value problems and thus the well–posedness of the fixed point mapping is also shown in [58]. From the numerical point of view it is advantageous not to deal with a coupled system of five semi linear elliptic equations, but with two much more tractable problems: System (2.4) is similar to the thermal equilibrium problem [62], which has been intensively investigated and system (2.5) fits into the theory of monotone operators [65]. Further, if the device is operated near thermal equilibrium, even convergence of the iterating sequence $(n^k, p^k, V^k, F^k, G^k)$ defined via Algorithm 1 can be proved. The precise result reads.

Theorem 2.4. *There exists a constant $U_\circ > 0$, depending on various device parameters, such that*

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

implies:

a) There exists a unique solution $(n_\circ, p_\circ, V_\circ, F_\circ, G_\circ)$ of (2.1), (2.3).

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

In fact one shows that T is a contraction on an appropriately chosen set. Then Theorem 2.4 follows from Banach's fixed point theorem.

The proof of the contractivity of T heavily relies on the Lipschitz–continuity of the first step in Algorithm 1, which is a consequence of the following Poicaré–type estimate.

Lemma 2.5. *Assume* **A.1** *of Theorem 2.2. Then there exists for all $\beta \in \mathbb{R}$ and all $\theta \in (0,1)$ a constant $K = K(\Omega, \beta, \theta, s) \in (0, \infty)$ such that for all $u \in H^1(\Omega) \cap L^\infty(\Omega)$ with $\theta \le u \le 1/\theta$ and all $\phi \in H_0^1(\Omega \cup \Gamma_N) \cap L^\infty(\Omega)$:*

$$\int_\Omega u^\beta \left| \nabla \left(\frac{\phi}{u} \right) \right|^2 dx \ge K \|\phi\|^2_{L^s(\Omega)}. \tag{2.6}$$

Lemma 2.5 assures that the quantum operators $A(\rho) = \Delta\sqrt{\rho}/\sqrt{\rho}$, $\rho = n$ or $\rho = p$, are monotonic with respect to the $L^s(\Omega)$–norm. Alternatively, one can deduce that the second variation of the quantum energy term

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

is positive definite with respect to the $L^s(\Omega)$–norm. In this sense the Bohm potential is much easier to handle numerically than the third order operator in (1.1), which seems to be responsible for dispersive effects in the QHD [46, 33] and also yields analytical problems [21]. In [56] it is shown that also the fourth order operator in the transient QDD (1.4) has such a monotonicity property.

Theorem 2.4 applies in cases where F and G are close to their corresponding equilibrium values F_{eq}, G_{eq} on Γ_D. This corresponds to the uniqueness result for the classical DD [51]: For small applied bias voltages the current-voltage characteristics is uniquely defined. This is physically reasonable. For higher applied voltages no uniqueness result is available. But it may be assumed that uniqueness does not hold in general: The performance of many devices (thyristors) relies on the existence of multiple solutions [48].

Note that in the engineering literature [6, 9, 66, 64] also other numerical schemes are reported, such as a damped Newton–iteration or a hybrid method, which combines the robustness of the Gummel–iteration with the second order convergence of Newton's iteration. There the Gummel iteration is used to compute a good starting point for the first Newton step. Up to know there is no numerical analysis available for these methods. However, it is assumed that this encounters the same difficulties as the one for the classical model, since the invertibility of the linearization of (2.1) strongly depends on the size of the off–diagonal terms [44, 34]. Nevertheless, a Newton iteration is the method of choice for (2.4) due to the monotonicity of the quantum operator.

For all numerical approaches voltage continuation, i.e. the applied voltage is incremented and in each step the previous solution is used as an initial guess for the next iteration, proved to be necessary to stabilize the numerics for large applied biasing voltages.

3 The Transient QDD

While the stationary QDD was investigated thoroughly and its analysis is now in a rather mature state, only recently some results on the transient equations (1.4) are available [38, 40, 39]. This is due to the fact that the equation for the electron density is of fourth order, such that no maximum principle is available to ensure the positivity of the density. In [38] the main part of (1.4a) is investigated:

$$n_t = -(n(\log(n))_{xx})_{xx} \tag{3.1a}$$

for $t > 0$, subject to the initial condition

$$n(0, x) = n_0(x) \tag{3.1b}$$

and the boundary conditions

$$n(0) = n(1) = 1, \quad n_x(0) = n_x(1) = 0. \tag{3.1c}$$

Note that (3.1a) can be equivalently written as

$$n_t = -n_{xxxx} + \left(\frac{n_x^2}{n}\right)_{xx}, \tag{3.2}$$

This is exactly (1.4a) in the case of zero temperature and zero electric field. Surprisingly, this equation also arises as a scaling limit in the study of interface fluctuations in a certain spin system [18]. The variable n describes the scaling limit of probabilities for a random variable. Problem (3.1a)–(3.1b) with periodic boundary conditions was first studied by Bleher *et al.* in [14]. Assuming (strictly) positive $H^1(\Omega)$–data, they showed that there exists a unique positive classical solution locally in time. For "small" initial data, the solution is even global in time. However, the problem whether non–negative solutions for general (non–negative) initial data exist *globally* in time remained open. This was recently answered: In [40] it is proved that for general initial data a non–negative solution exists *globally* in time. Note that the equivalent formulation of (3.1a) is not degenerate such that the techniques developed for the so–called thin film equations [13, 31, 54], especially the concept of nonlinear entropy dissipation, are not applicable.

In fact, it is shown that for non–negative initial data satisfying a certain integrability condition, there exists a generalized *non–negative* solution *globally* in time. As only weak assumptions are imposed on the data , it can be a priorily not expected that the solutions have $L^2_{loc}(0,\infty;H^2(\Omega))$–regularity. But similar to [13] a new solution concept is introduced, which is given in the following existence result.

Theorem 3.1. *Assume that the initial datum n_0 is measurable and satisfies the condition*

$$\int_\Omega n_0 - \log(n_0)\; dx < +\infty. \tag{3.3}$$

Then there exists a solution n of (3.1a)–(3.1c) *satisfying*

$$n(x,t) \geq 0 \quad a.e.\ in\ (0,\infty)\times\Omega, \tag{3.4a}$$

$$n \in L^2_{loc}(0,\infty;W^{1,1}(\Omega)), \quad n_t \in L^1_{loc}(0,\infty;H^{-2}(\Omega)), \tag{3.4b}$$

$$\log(n) \in L^2_{loc}(0,\infty;H^2(\Omega)) \cap L^\infty(0,\infty;L^1(\Omega)). \tag{3.4c}$$

Further, $n(\cdot,0) = n_0$ in the sense of $H^{-2}(\Omega)$ and it holds for any $T>0$ and any smooth test function $\phi \in C_c^\infty((0,\infty)\times\Omega)$,

$$\int_0^T \langle n_t, \phi\rangle_{H^{-2},H_0^2}\; dt = -\int_0^T \int_\Omega n\,(\log(n))_{xx}\,\phi_{xx}\; dx\,dt.$$

The proof of Theorem 3.1 is based on two ideas. The first one is to perform an exponential transformation of variables. Setting $n = e^{2u}$, equation (3.1a) reads in the new variable:

$$\left(e^{2u}\right)_t = -2\, \left(e^{2u}\, u_{xx}\right)_{xx}. \tag{3.5}$$

Hence, the existence of a (generalized) solution u of (3.5) implies the existence of a non–negative solution n of (3.1a). Exponential transformations were already successfully employed in the study of the stationary QHD [33, 15].

Clearly, a solution $u \in L^\infty((0,\infty)\times\Omega)$ to (3.5) provides a *positive* solution n to (3.1a). However, only the regularity $u \in L^2_{loc}(0,\infty; L^\infty(\Omega))$ (see (3.4)) can be deduced such that only the existence of *non–negative* solutions to (3.1a) can be concluded. This is in contrast to the stationary problem, where the positivity property immediately follows from an $H^s(\Omega)$–bound for the corresponding stationary variable u and the Sobolev embedding $H^s(\Omega) \hookrightarrow L^\infty(\Omega)$ when $s > d/2$, d being the space dimension (see [33]).

This observation gave the motivation to discretize (3.5) in time, which is the second main idea for the proof, yielding a sequence of elliptic problems. The existence of solutions $u(t_k,\cdot)$ in $H^2(\Omega)$ to the resulting elliptic problems can be proved. Hence, the approximate solutions $u(t_k,\cdot)$ are in $L^\infty(\Omega)$ and expressions like $e^{u(t_k,x)}$ are well defined.

It is worth noting that equation (3.1a) possesses several Lyapunov functionals [14] which provide a priori estimates in the existence proof. It can be easily seen that the *entropy*

$$S(t) = \int_\Omega n(t)\,(\log(n(t)) - 1) + 1\; dx$$

is (formally) non–increasing in time. In the case of periodic boundary conditions, also the *Fisher information*

$$\int_\Omega \left|(\sqrt{n})_x\right|^2\; dx$$

is non–increasing in time.

3.1 A Positivity–preserving Semidiscretization

The techniques developed in [38] are also suitable to treat the coupled system (1.4). As for the moment analytically only the non–negativity of solutions can be expected, the question arises, if at least the construction of a positivity preserving numerical scheme is possible. This is of great practical relevance as the engineering–oriented device analysis is focused on numerical simulations for which the positivity of particle densities is essential to ensure the stability of the numerical schemes.

Following the ideas stated in [38, 40] an implicit semidiscretization of (1.4) is derived and an existence and stability result for the discretized system at each time level is proved.

Influenced by the results for the stationary QDD again the quantum quasi Fermi level F and the new variable $\rho = \sqrt{n}$ are introduced. Then (1.4) reads:

$$\left(\rho^2\right)_t = \operatorname{div}(\rho^2 \nabla F), \tag{3.6a}$$

$$-\varepsilon^2 \frac{\Delta\rho}{\rho} + \theta \log(\rho^2) + V = F, \tag{3.6b}$$

$$-\lambda^2 \Delta V = \rho^2 - C_{dot}. \tag{3.6c}$$

Here, θ denotes the scaled lattice temperature. For the numerical treatment of (3.6) a horizontal line method is employed and the transient problem is replaced by a sequence of elliptic problems for $0 = t_0 < t_1 < \ldots < t_N = T$. In fact, system (3.6) is discretized using an implicit Euler scheme:

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

$$\frac{1}{\tau_k}\left(\rho_k^2 - \rho_{k-1}^2\right) = \operatorname{div}(\rho_k^2 \nabla F_k), \tag{3.7a}$$

$$-\varepsilon^2 \frac{\Delta\rho_k}{\rho_k} + \theta \log(\rho_k^2) + V_k = F_k, \tag{3.7b}$$

$$-\lambda^2 \Delta V_k = \rho_k^2 - C_{dot}, \tag{3.7c}$$

subject to the boundary conditions

$$\rho_k = \rho_D, \quad F_k = F_D, \quad V_k = V_D \quad \text{on } \Gamma_D, \tag{3.7d}$$

$$\nabla\rho_k \cdot \nu = \nabla F_k \cdot \nu = \nabla V_k \cdot \nu = 0 \quad \text{on } \Gamma_N, \tag{3.7e}$$

where

$$\rho_D = \sqrt{C_{dot}}, \quad F_D = U, \quad V_D = -\theta \log\left(C_{dot}\right) + U. \tag{3.8}$$

Here, f_k is an approximation for $f(t_k)$ and $\tau_k \stackrel{\text{def}}{=} t_k - t_{k-1}$. Then the approximate solution to (3.6) is given by $(\rho^\tau, F^\tau, V^\tau)$, where $\rho^\tau|_{(t_{k-1},t_k]} \equiv const$ for $k = 1, \ldots, N$ and F^τ, V^τ respectively.

In [40] an existence theorem for (3.7) is proved. It is assumed that the boundary $\partial\Omega$ and the data are sufficiently smooth, such that an elliptic Schauder estimate holds. Further, the lattice temperature has to be sufficiently large, which ensures the positivity of the semidiscrete solution. This is necessary, since the boundary data (3.7d), (3.7e) does not allow for the usage of the techniques developed in [38]. The precise existence and positivity result reads:

Proposition 3.2. *Let $k \in \{1, \dots, N\}$ 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* (3.7) *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 [40, Corollary 2.5]).

Lemma 3.3. *For $k = 1, \dots, N$ let (ρ_k, F_k, V_k) be the recursively defined solution of* (3.7) *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*

$$\|\rho^\tau\|_{L^\infty(H^1)} + \|V^\tau\|_{L^\infty(H^1)} + \|\rho^\tau \nabla F^\tau\|_{L^2(L^2)} \leq c. \tag{3.9}$$

In the one–dimensional case it is possible to prove (see [40, 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 (3.6).

Here, the a priori bounds on the approximate solution in Lemma 3.3 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 [40]). In one space dimension this is an immediate consequence of the estimate (3.9) and the embedding $H^1(\Omega) \hookrightarrow L^\infty(\Omega)$. In fact, no analytical results on system (3.6) are available in several space dimensions. Thus, one has to state additional assumptions on the sequence of approximating solutions. These even yield explicit error estimates, which exhibit the optimal order of convergence for the implicit Euler scheme.

Theorem 3.4. *For $k = 1, \dots, N$ let (ρ_k, F_k, V_k) be the recursively defined solution of* (3.7) *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*

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

as $\tau \to 0$, *where* (ρ, F, V) *is a solution of the continuous problem* (3.6). *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*

$$\|\rho^\tau - \rho\|_{L^\infty(L^2)} + \varepsilon^2 \|\rho^\tau - \rho\|_{L^2(W^{m,p})} + \|F^\tau - F\|_{L^\infty(H^2)} + \|V^\tau - V\|_{L^\infty(H^2)} \leq C\, e^{\alpha T}\, \tau, \quad (3.10)$$

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

The uniform lower bound for ρ^τ is necessary to verify the strong convergence of the quantum quasi Fermi level $F^\tau \to F$, which allows for the identification of the limiting current density $J = \rho^2 \nabla F$. This was in one space dimension out of reach due to the weaker assumptions and convergence properties. Note that the assumption on the time regularity of ρ, i.e. $\rho_{tt} \in L^2(\Omega)$, seems to be quite strong only at a first glance. Comparing the result for the classical transient DD given in [17], this regularity was already used there to derive the optimal order of convergence in one space dimension. Most remarkably, it is also sufficient to guarantee for the optimal convergence rate of this fourth order system in several space dimensions.

3.2 Linear Stability of Stationary States

Another interesting question is how does the transient QDD behave close to a steady state. This is investigated in [56], where the author studies small perturbations of the stationary state and derives conditions which ensure their linear stability.

One can prove that the stationary fourth order system allows for a solution $(n, V) \in H^2(\Omega) \times H^1(\Omega)$, where the lower bound on n is strictly positive and independent of ε. At such a state the operator G defined by

$$G(n) \stackrel{\text{def}}{=} \operatorname{div}(n \nabla A(n)),$$

where

$$A(n) \stackrel{\text{def}}{=} -\varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}} + \log(n) + V[n - C_{dot}],$$

and $V[n - C_{dot}]$ denotes the solution of $-\lambda^2 \Delta V = n - C_{dot}, V - V_D \in H_0^1(\Omega \cup \Gamma_N)$, is Fréchet–differentiable.

Assume that a solution z of the perturbed problem

$$\frac{\partial z}{\partial t} = G(z) \quad \text{in } \Omega \times (0,T), \tag{3.11a}$$

$$z = n_D, \quad \nabla z \cdot \nu = 0 \quad \text{on } \partial\Omega \times (0,T), \tag{3.11b}$$

$$z(\cdot, 0) = n(\cdot) + \delta\, g(\cdot) \quad \text{in } \Omega, \tag{3.11c}$$

where $\delta > 0$ is a small parameter and $g \in L^2(\Omega)$, can be written as $z(x,t) = n(x) + \delta\, \Theta(x,t)$. Then, Θ satisfies the linear first order approximation

$$\frac{\partial \Theta}{\partial t} = G'(n)[\Theta] \quad \text{in } \Omega \times (0,T),$$

$$\Theta = 0, \quad \nabla\Theta \cdot \nu = 0 \quad \text{on } \partial\Omega \times (0,T),$$

$$\Theta(\cdot, 0) = g(\cdot) \quad \text{in } \Omega,$$

which is nothing than the linearized transient QDD.

Employing Hilbert space methods for linear parabolic PDE's and exploiting the monotonicity of the quantum operator the author shows the existence of a unique solution Θ satisfying some stability estimate [56]. More precisely:

Theorem 3.5. *Assume that Ω is sufficiently regular. Let $f \in L^2(0,T; L^2(\Omega))$ and $g \in L^2(\Omega)$. Then there exists a unique solution $\Theta \in L^2(0,T; H_0^2(\Omega))$ of the inhomogeneous problem*

$$\frac{\partial \Theta}{\partial t} = G'(n)[\Theta] + f \quad \textit{in } \Omega \times (0,T), \tag{3.12a}$$

$$\Theta = 0, \quad \nabla\Theta \cdot \nu = 0 \quad \textit{on } \partial\Omega \times (0,T), \tag{3.12b}$$

$$\Theta(\cdot, 0) = g(\cdot) \quad \textit{in } \Omega. \tag{3.12c}$$

For $t \in (0,T)$ the solution Θ satisfies the stability estimate

$$\|\Theta(t)\|_{L^2(\Omega)} \le A\, e^{a\,t} \left\{ \|g\|_{L^2(\Omega)} + \|f\|_{L^2(L^2)} \right\}, \tag{3.13}$$

with constants $a, A > 0$, which only depend on $\Omega, \varepsilon, \lambda, n$ and J.

In fact, one can precise the constant a in Theorem 3.5 and derive conditions under which it is negative, such that any perturbation g is exponentially damped and the corresponding state is linearly stable.

Theorem 3.6. *Let the assumptions of Theorem 3.5 hold. Then there exists a constant $J_0 = J_0(\Omega, \varepsilon, \lambda, n) > 0$ such that for*

$$\left\| \frac{J}{n} \right\|_{L^\infty(\Omega)} \leq J_0$$

the unique solution $\Theta \in L^2(0, T; H_0^2(\Omega))$ of problem (3.12) satisfies

$$\|\Theta(t)\|_{L^2(\Omega)} \to 0, \qquad \textit{as } t \to \infty,$$

i.e. the corresponding stationary state n is linearly stable.

An analogous result is given by *Markowich and Ringhofer* in [47] for the classical DD. For the transient QDD the smallness of ε is a purely technical assumption and is needed to derive the desired estimates. Nevertheless, we have an improvement due to the quantum regularization, as it allows to assure the linear stability of stationary states for a wider range of applied biasing voltages.

4 Conclusions

We gave an overview of the results available in the mathematical literature on the QDD for semiconductor devices. The analysis is now in a rather mature state even for the transient model. It covers proofs of existence and uniqueness as well as asymptotic limits and stability estimates. Also some numerical results are at hand concerning convergence of a generalized Gummel iteration and of a positivity preserving semidiscretization for the fourth order transient system. The vast applicability of the QDD for various devices is impressively evidenced in the engineering literature. Future work will focus on the derivation of stable nonlinear discretization schemes, coupling with other semiconductor models and generalizations in the spirit of 'smooth' QHD.

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