
Volume 253 Issue 1 July 1, 2012 ISSN 0022-0396
ELSEVIER
JOURNAL OF
DIFFERENTIAL
EQUATIONS
Editors-in-Chief
Alberto Bressan
Shui-Nee Chow
John Mallet-Paret
W.-M. Ni
Founding Editors
Jack K. Hale
J. P. LaSalle
Editorial Board
John Ball
Courtney Coleman
Avner Friedman
Yuan Lou
Kening Lu
Robert McCann
Konstantin Mischaikow
Czesław Olech
Denis Serre
James Serrin
Marshall Slemrod
Walter Strauss
Roger Temam
C. Eugene Wayne
Sijue Wu
Yingfei Yi
Chongchun Zeng
Enrique Zuazua

J. Differential Equations 253 (2012) 356–377

Contents lists available at SciVerse ScienceDirect

Journal of Differential Equations

www.elsevier.com/locate/jde

Boundary layer analysis in the semiclassical limit of a quantum drift–diffusion model

Shen Bian [a], Li Chen [a], Michael Dreher [b,*]

[a] Department of Mathematical Sciences, Tsinghua University, Beijing 100084, PR China
[b] Fachbereich Mathematik und Statistik, Universität Konstanz, 78457 Konstanz, Germany

ARTICLE INFO

Article history:
Received 16 February 2012
Revised 14 March 2012
Available online 30 March 2012

MSC:
35J50
76N20
81Q20

Keywords:
Quantum drift–diffusion model
Boundary layer
Elliptic system
Variational methods

ABSTRACT

We study a singularly perturbed elliptic second order system in one space variable as it appears in a stationary quantum drift–diffusion model of a semiconductor. We prove the existence of solutions and their uniqueness as minimizers of a certain functional and determine rigorously the principal part of an asymptotic expansion of a boundary layer of those solutions. We prove analytical estimates of the remainder terms of this asymptotic expansion, and confirm by means of numerical simulations that these remainder estimates are sharp.

1. Introduction and known results

The distribution of charged particles in a semiconductor can be described by various systems of partial differential equations, for instance the drift–diffusion equations. Typically, the relevant particles are the mobile electrons in the conduction band (which is an energy band at a higher level) and the so-called holes (which are vacant positions of positive charge in the next lower energy band, called valence band). Additionally, charged ions may have been placed at certain lattice positions in the semiconductor crystal, and these doping ions can carry positive or negative charge, depending on the desired electronical behavior. For small scaled devices, it may be necessary to consider also quantum effects. Then, in the stationary case, the *quantum drift–diffusion model* reads (after scaling)

* Corresponding author. Fax: +49 7531 884248.
E-mail addresses: bs09@mails.tsinghua.edu.cn (S. Bian), lchen@math.tsinghua.edu.cn (L. Chen), michael.dreher@uni-konstanz.de (M. Dreher).

0022-0396/$ – see front matter
http://dx.doi.org/10.1016/j.jde.2012.03.008

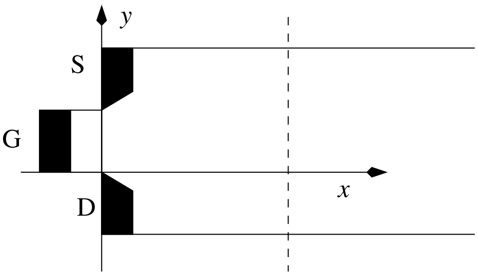

Fig. 1. A rough schematic sketch of a MOSFET, with horizontal variable x and vertical variable y, and with fictitious boundary in the bulk at $x = 1$.

$$F = V + h_n(n) - \varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}}, \tag{1.1}$$

$$G = -V + h_p(p) - \xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}}, \tag{1.2}$$

$$\operatorname{div}(\mu_n n \nabla F) = R_0(n, p) R_1(F, G), \tag{1.3}$$

$$\operatorname{div}(-\mu_p p \nabla G) = -R_0(n, p) R_1(F, G), \tag{1.4}$$

$$-\lambda^2 \Delta V = n - p - C(x), \tag{1.5}$$

for the unknowns n, p, F, G, V. The functions n and p describe the densities of electrons and holes, and F, G are the quantum quasi Fermi levels. Finally, V is the electric potential as generated from the charged particles via (1.5). Here C is the known density of positive ions. The functions h_n, h_p are called the enthalpy functions of the electrons and holes; typically they are of the form $h(s) = T \ln s$ with some positive temperature constant T. The positive parameter ε is proportional to the Planck constant $\hbar$ and describes quantum effects, and the positive constant ξ is related to the quotient of the effective masses of the electrons and the holes. Next, the functions R_0, R_1 are known expressions, which model generation–recombination effects. The constants μ_n, μ_p are related to the mobilities of the particles, and λ is known as the scaled Debye length. Typically, the above system is studied in a bounded domain with various boundary conditions, for instance Dirichlet boundary conditions of (n, p, V, F, G) on a boundary part Γ_+ (with n, p positive there), homogeneous Neumann boundary conditions of (n, p, V, F, G) on a boundary part Γ_N, and $(n, p, V) = (0, 0, V_{\text{extern}} + V_{\text{equil}})$ on a further boundary part Γ_0 (note that the elliptic equations (1.3) and (1.4) degenerate at points where $n = p = 0$).

The system (1.1)–(1.5), also known as the density gradient model, goes back to the works of Ancona [2,1]; and it can be understood as a combination of the Schrödinger and Gauss equations. Extensive mathematical studies can be found in [11,13,3]; and we also refer to [10,7] for reviews, to [6] and [9] for the transient case, and to [8] for a numerical scheme. Several results were proved in [3] under appropriate assumptions: the full system has a solution $(n, p, V, F, G) \in L^\infty(\Omega) \cap H^1(\Omega) \cap C(\Omega)$ with non-negative n and p. And if $F, G \in L^\infty(\Omega)$ are given, then a solution (n, p, V) to (1.1), (1.2), (1.5) exists which is uniquely determined by the condition that a certain functional shall be minimized. Finally, the semiclassical limit $\varepsilon \to 0$ has been performed, under the assumption that the boundary part Γ_0 is empty.

It is one of the goals of this article to remove this restriction on Γ_0, for a sub-class of the systems from [3].

Our studies are related to MOSFET[1] devices, whose structure is sketched in Fig. 1. At one end of the device, there are contacts called *source*, *gate*, *drain*, of which the gate contact is insulated by means of an oxide, explaining the name of the device. This insulator is quite thin, which then gives rise to the quantum effects. Depending on an applied voltage V_{GS} between gate and source, the density of

[1] Metal–oxide-semiconductor field-effect transistor.

movable charge carriers changes, and this effect decides whether a current can flow from source to drain. If such movable particles are available between source and drain in abundance, we say that an *inversion layer* has formed. In an opposite situation, when no movable particles are available in a certain region, we say that this region *depleted* of particles. Various asymptotic expansions for such layers have been proposed in [14,15,4]; we also refer to [5] for a model involving quantum effects. The modifications of [5] to the model (1.1)–(1.5) can be summarized as follows. The holes are supposed to be in thermal equilibrium, which implies $G \equiv 0$. In many situations, the parameter ξ from (1.2) is small, which motivates us to neglect quantum effects for the holes, and then (1.2) turns into

$$0 = -V + h_p(p),$$

or $p = \exp(V/T_p)$. Moreover, generation–recombination events are ignored: $R_0 \cdot R_1 \equiv 0$. Next we assume that the domain Ω of the device is a square $(0,1) \times (0,1) \subset \mathbb{R}^2$, and we write the spatial variable as (x, y), with x running from the contacts into the bulk of the crystal. Concerning the electron density n, we assume thermal equilibrium in direction of the x variable, which makes F a function of $y \in (0,1)$ only, and F is assumed to be known. The *quasi* 1*D approximation* is supposed, which says that all functions depend only weakly on the variable y. Hence we will neglect the derivatives with respect to y from now on, and the system becomes

$$F = V(x) + T_n \ln n(x) - \varepsilon^2 \frac{(\sqrt{n(x)}\,)_{xx}}{\sqrt{n(x)}}, \quad 0 < x \leqslant 1, \tag{1.6}$$

$$-\lambda^2 V_{xx}(x) = n(x) - \exp\big(V(x)/T_p\big) - C(x), \quad 0 \leqslant x \leqslant 1. \tag{1.7}$$

The boundary conditions at the fictitious boundary $x = 1$ in the bulk are

$$n(1) = n_B, \qquad V(1) = V_B, \tag{1.8}$$

and to express that quantum effects do not appear there, we assume that

$$F = V_B + T_n \ln n_B. \tag{1.9}$$

The boundary conditions at the location of the gate ($x = 0$) are, with given constants $\beta \geqslant 0$ and $V_{GS} \in \mathbb{R}$,

$$n(0) = 0, \qquad V_x(0) = \beta\big(V(0) - V_{GS}\big). \tag{1.10}$$

The vanishing of the particle density $n(x)$ at $x = 0$ makes two terms in (1.6) singular, and the formation of an additional layer inside the inversion layer is to be expected: the *quantum layer*. In the classical drift–diffusion model, where $\varepsilon = 0$, this boundary condition $n(0) = 0$ is not imposed, and then the number of mobile electrons near the interface is higher in the classical model. A precise understanding of this loss of electrons near the interface due to quantum effects is of high relevance for a valid circuit design. (See Fig. 2.)

The objective of this paper is to study this quantum layer with the rigor of analysis. Our modeling follows [5], where an asymptotic expansion was conjectured, and our paper gives an analytical proof of that expansion. The key improvement presented in this article is a precise discussion of the error terms, which enables us to perform the limit $\varepsilon \to 0$ rigorously, even in the presence of a zero boundary value of the electron density.

We sketch the results presented in this paper. First, we prove the existence of a solution to the system (1.6), (1.7), (1.8), (1.10), which is unique as a minimizer to a certain functional. Our approach builds upon [3]; however, the additional nonlinearity in our equation (1.7) which is not present in [3] requires several changes.

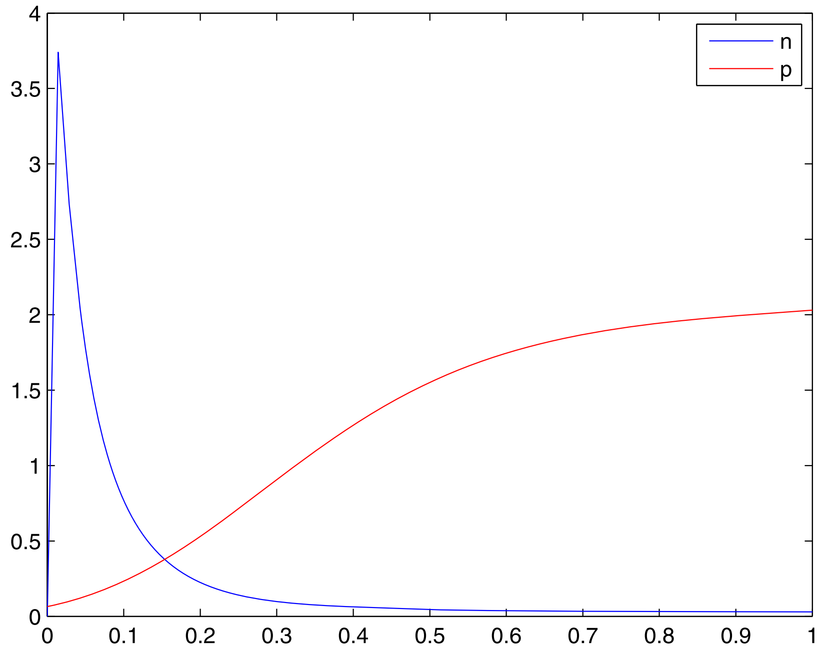

Fig. 2. Electron and hole densities in case of an inversion layer.

Second, we prove rigorously that the electric potential V_ε converges to the corresponding solution V_* of the classical model, with an analytic estimate of the error $V_\varepsilon - V_*$. We also determine the profile of the quantum layer of the electron density, again with several analytical error estimates.

And our third result are numerical simulations which confirm that our analytical error estimates are sharp.

2. Main results

Our first result is about the existence of solutions (n, V), which are constructed in such a way that $\varrho := \sqrt{n}$ is the unique non-negative minimizer of a certain functional, see Remark 3.6.

Theorem 2.1. *Let us be given positive constants T_n, T_p, ε, λ, n_B, and real constants F, V_{GS}, and V_B, and a non-negative constant β. Suppose that $C = C(x)$ is continuous and real-valued.*

Then the boundary-value problem (1.6), (1.7), (1.8), (1.10) *possesses a solution $(n, V) \in C^2([0,1])$ with $n(x) > 0$ for $0 < x \leqslant 1$, such that $\varrho := \sqrt{n}$ is the unique non-negative minimizer to $\mathcal{F}$ from* (3.8)*.*

And there is a constant C_0, independent of ε and of the solution (n, V), with

$$\varepsilon^2 \left\| (\sqrt{n})' \right\|^2_{L^2((0,1))} + \left\| V' \right\|^2_{L^2((0,1))} \leqslant C_0. \tag{2.1}$$

Our second result will describe the shape of n and V, in particular for small values of ε. The precise formulation requires some preparations.

By variational methods, we will show in Proposition 3.5 that $V_*, n_* \in C^2([0,1])$ exist uniquely which solve

$$\begin{cases} -\lambda^2 V_*''(x) = n_*(x) - \exp\bigl(V_*(x)/T_p\bigr) - C(x), & 0 \leqslant x \leqslant 1, \\ n_*(x) := \exp\bigl(\bigl(F - V_*(x)\bigr)/T_n\bigr), & 0 \leqslant x \leqslant 1, \\ V_*'(0) = \beta\bigl(V_*(0) - V_{GS}\bigr), \quad V_*(1) = V_B. \end{cases} \tag{2.2}$$

Let $Z = Z(y)$ be the unique function from $C^2([0,\infty))$ that solves

$$Z''(y) = Z(y)\ln Z(y), \quad 0 < y < \infty, \qquad Z(0) = 0, \qquad \lim_{y\to+\infty} Z(y) = 1. \tag{2.3}$$

As shown in [5], this function is strictly increasing with $Z'(0) = 1/\sqrt{2}$, and it approaches the value 1 exponentially for $y \to +\infty$, with the asymptotics $1 - Z(y) \approx \exp(C_Z - y)$, $C_Z \approx 0.244$.

Theorem 2.2. *Assume* (1.9). *Then there is a positive ε_0, such that, for $0 < \varepsilon \leqslant \varepsilon_0$, we have*

$$\|n - n_{(0)}\|_{L^2((0,1))} + \|V - V_{(0)}\|_{W_2^1((0,1))} \leqslant C\varepsilon,$$

where the zero-th order approximations $(n_{(0)}, V_{(0)})$ of (n, V) are defined as follows:

$$n_{(0)}(x) := n_*(x) Z^2\left(\sqrt{2T_n} \cdot \frac{x}{\varepsilon}\right), \qquad V_{(0)}(x) := V_*(x).$$

Theorem 2.3. *The approximations $n_{(0)}$ satisfy the uniform estimates*

$$\|n - n_{(0)}\|_{L^\infty((0,1))} \leqslant C\varepsilon^{3/4}, \quad 0 < \varepsilon \leqslant \varepsilon_0,$$

and in particular, we have

$$\left|n(x) - n_{(0)}(x)\right| \leqslant C\varepsilon^{3/4} \cdot \frac{x}{\varepsilon}, \quad 0 \leqslant x \leqslant \varepsilon. \tag{2.4}$$

Our notation is standard. In particular, C is a generic positive constant that is independent of the unknowns and may change its value from line to line.

3. Existence of solutions

Now we begin to demonstrate Theorem 2.1, and our strategy is as follows. Assuming that n were known, we then find V as the unique solution to (1.7) using variational methods. This dependence of V from n will be mainly described by the mapping Φ below. Then (1.6) becomes a differential equation of n alone, which turns out to be the Euler–Lagrange equation of a certain functional $\mathcal{F}$. Then it remains to show that $\mathcal{F}$ has a unique minimizer; here we will follow the approach of [3].

First we consider the boundary-value problem

$$\begin{cases} -\lambda^2 U''(x) = q(x) - p\big(x, U(x)\big), & 0 \leqslant x \leqslant 1, \\ U'(0) = \beta U(0), & \beta \geqslant 0, \\ U(1) = 0, \end{cases} \tag{3.1}$$

with a given $q \in C([0, 1])$, under some assumptions on the nonlinearity p:

$$\begin{cases} p \in C^1\big([0,1] \times \mathbb{R}\big), \\ p_U(x, U) > 0 & \forall (x, U) \in [0,1] \times \mathbb{R}, \\ P(x, U) := \displaystyle\int_{u=0}^{U} p(x, u)\,\mathrm{d}u \geqslant -C & \forall (x, U) \in [0,1] \times \mathbb{R}. \end{cases} \tag{3.2}$$

We start our considerations with the simple observation that solutions U to (3.1) are unique, by the theory of monotone operators.

To prove the existence of a solution to (3.1), we choose the variational space

$$X_U := \big\{U \in W_2^1\big((0,1)\big) \colon U(1) = 0\big\}.$$

Lemma 3.1. *For a fixed function $q \in C([0,1])$, define a functional*

$$\mathcal{F}^{(0)}(U) := \frac{\lambda^2}{2}\int_0^1 \big(U'(x)\big)^2\,\mathrm{d}x + \frac{\lambda^2}{2}\beta\big(U(0)\big)^2 + \int_0^1 -q(x)U(x) + P\big(x, U(x)\big)\,\mathrm{d}x. \tag{3.3}$$

This functional possesses a unique minimizer $U_0 \in X_U$, and this minimizer is a classical solution to the boundary-value problem (3.1)*.*

Proof. By Poincaré's inequality, (3.2), and $\beta \geqslant 0$, the functional $\mathcal{F}^{(0)}$ is coercive:

$$\mathcal{F}^{(0)}(U) \geqslant \frac{\lambda^2}{4}\|U\|^2_{W_2^1} - C, \quad \forall U \in X_U,$$

and then the existence of a minimizer $U_0 \in X_U$ follows by standard arguments, and $U_0 \in X_U \subset C([0,1])$ is bounded. Take $\varphi \in C^\infty([0,1])$ with $\varphi(1) = 0$. Then

$$\mathcal{F}^{(0)}(U_0 + \delta\varphi) = \mathcal{F}^{(0)}(U_0) - \delta\int_0^1 \big(\lambda^2 U_0'' + q - p(x, U_0)\big)\varphi\,\mathrm{d}x$$
$$+ \delta\lambda^2\big(-U_0'(0) + \beta U_0(0)\big)\varphi(0) + \mathcal{O}\big(\delta^2\big),$$

and therefore U_0 solves $-\lambda^2 U_0'' = q - p(x, U_0)$ in the distributional sense, and it follows that $U_0 \in C^2([0,1])$, as well as $-U_0'(0) + \beta U_0(0) = 0$. □

Next we discuss how this minimizer U_0 of $\mathcal{F}^{(0)}$ depends on q.

Lemma 3.2. *Define a mapping $\Phi : C([0,1]) \to C_B^2([0,1])$, with $C_B^2([0,1])$ as the vector space of all functions U from $C^2([0,1])$ with $U'(0) = \beta U(0)$ and $U(1) = 0$, via the relation $\Phi\{q\} := U_0$, and U_0 is defined as the unique minimizer of the functional $\mathcal{F}^{(0)}$ from* (3.3)*. Then Φ is a homeomorphism.*

Proof. Clearly, Φ is bijective, and Φ^{-1} is continuous. It remains to establish the continuity of Φ. To this end, let $q_1 \in C([0,1])$ be given, and $q_2 \in C([0,1])$ with $\|q_1 - q_2\|_{L^\infty} \leqslant 1$. Define $U_k := \Phi\{q_k\}$. Then $-\lambda^2 U_k'' + p(x, U_k) = q_k$, hence

$$\lambda^2\int_0^1 \big(U_1' - U_2'\big)^2\,\mathrm{d}x + \lambda^2\beta\big(U_1(0) - U_2(0)\big)^2 + \int_0^1 \big(p(x, U_1) - p(x, U_2)\big)(U_1 - U_2)\,\mathrm{d}x$$
$$= \int_0^1 (q_1 - q_2)(U_1 - U_2)\,\mathrm{d}x,$$

which implies, using $\beta \geqslant 0$, the monotonicity of p, and Poincaré's inequality, that $\|U_1 - U_2\|_{W_2^1} \leqslant C\|q_1 - q_2\|_{L^2}$, hence also $\|U_1 - U_2\|_{L^\infty} \leqslant C\|q_1 - q_2\|_{L^2}$. Next we have $\|p(\cdot, U_1) - p(\cdot, U_2)\|_{L^\infty} \leqslant C\|q_1 - q_2\|_{L^2}$, and then also $\|U_1'' - U_2''\|_{L^\infty} \leqslant C\|q_1 - q_2\|_{L^\infty}$. □

For more information, we determine the Fréchet derivative of Φ.

Lemma 3.3. *Fix $q_0 \in C([0,1])$. Then there is a C such that we have the expansion*

$$\Phi\{q\} = \Phi\{q_0\} + W + R$$

for all $q \in C([0,1])$ with $\|q - q_0\|_{C([0,1])} \leqslant 1$, where $W \in C^2([0,1])$ is the unique solution to

$$-\lambda^2 W'' + p_U\big(x, \Phi\{q_0\}\big)W = q - q_0, \qquad W'(0) = \beta W(0), \qquad W(1) = 0,$$

with $\|W\|_{C^2([0,1])} \leqslant C\|q - q_0\|_{C([0,1])}$, and $\|R\|_{C^2([0,1])} \leqslant C\|q - q_0\|^2_{C([0,1])}$.

Proof. From Lemma 3.2 we know $\|\Phi\{q\} - \Phi\{q_0\}\|_{C^2([0,1])} \leqslant C\|q - q_0\|_{C([0,1])}$. We define $R := \Phi\{q\} - \Phi\{q_0\} - W$ and have

$$\begin{aligned}
-\lambda^2 R'' &= -\lambda^2\big(\Phi\{q\}'' - \Phi\{q_0\}'' - W''\big) \\
&= -p_U\big(x, \Phi\{q_0\}\big) \cdot \big(\Phi\{q\} - \Phi\{q_0\} - W\big) + \mathcal{O}\big(\big\|\Phi\{q\} - \Phi\{q_0\}\big\|^2_{C([0,1])}\big) \\
&= -p_U\big(x, \Phi\{q_0\}\big)R + \mathcal{O}\big(\|q - q_0\|^2_{C([0,1])}\big).
\end{aligned}$$

Note that $p_U(x, \Phi\{q_0\}) > 0$, hence we get $\|R\|_{C^2([0,1])} \leqslant C\|q - q_0\|^2_{C([0,1])}$. □

Lemma 3.4. *Define a function $K = K(x, U) := Up(x, U) - P(x, U)$, and set*

$$\mathcal{F}^{(1)}(q) := \frac{\lambda^2}{2}\int_0^1 \big(\big(\Phi\{q\}\big)'(x)\big)^2\,\mathrm{d}x + \frac{\lambda^2}{2}\beta\big(\Phi\{q\}(0)\big)^2 + \int_0^1 K\big(x, \Phi\{q\}(x)\big)\,\mathrm{d}x.$$

Then $K(x, U) \geqslant 0$ for all $(x, U) \in [0,1] \times \mathbb{R}$, and the Fréchet derivative of $\mathcal{F}^{(1)}$ is given via

$$\mathcal{F}^{(1)}(q) = \mathcal{F}^{(1)}(q_0) + \int_0^1 \Phi\{q_0\} \cdot (q - q_0)\,\mathrm{d}x + \mathcal{O}\big(\|q - q_0\|^2_{C([0,1])}\big).$$

Here the remainder term is positive for $q \neq q_0$, and $\mathcal{F}^{(1)}$ is strictly convex.

Proof. Concerning the bound for K, we remark that $P(x, 0) = 0$, $p_U > 0$ and

$$K(x, U) = \int_{u=0}^{U} u p_U(x, u)\,\mathrm{d}u.$$

For the proof of the second claim, we put $U_0 = \Phi\{q_0\}$ and $U := \Phi\{q\}$. Then $U = U_0 + W + R$ with W and R as given in Lemma 3.3, and it follows that

$$\begin{aligned}
\mathcal{F}^{(1)}(q) = \mathcal{F}^{(1)}(q_0) &+ \lambda^2\int_0^1 U_0' \cdot (U - U_0)'\,\mathrm{d}x + \lambda^2\beta U_0(0) \cdot \big(U(0) - U_0(0)\big) \\
&+ \frac{\lambda^2}{2}\int_0^1 \big(U' - U_0'\big)^2\,\mathrm{d}x + \frac{\lambda^2}{2}\beta\big(U(0) - U_0(0)\big)^2 + \int_0^1 K(x, U) - K(x, U_0)\,\mathrm{d}x
\end{aligned}$$

$$\geqslant \mathcal{F}^{(1)}(q_0) + \int_0^1 U_0 \cdot (q - q_0)\,\mathrm{d}x$$

$$+ \int_0^1 -U_0 \cdot \big(p(x,U) - p(x,U_0)\big) + K(x,U) - K(x,U_0)\,\mathrm{d}x.$$

Now we have, with some $\tilde{U}$ between U and U_0,

$$-U_0\big(p(x,U) - p(x,U_0)\big) + K(x,U) - K(x,U_0) = \frac{1}{2} P_{UU}(x,\tilde{U}) \cdot (U_0 - U)^2 \geqslant 0,$$

because of $P_{UU} = p_U > 0$. □

Proposition 3.5. *Suppose that λ and T_p are positive, V_{GS}, V_B are real, and $n - C$ is a continuous given real-valued function on $[0,1]$. Then there is exactly one solution $V \in C^2([0,1])$ to (1.7) with the boundary conditions $V(1) = V_B$ and $V'(0) = \beta(V(0) - V_{GS})$. Moreover, the nonlinear boundary-value problem (2.2) possesses exactly one solution $V_* \in C^2([0,1])$.*

Proof. To find V, we put $V = V_{\mathrm{inh}} + U$ with V_{inh} as the unique solution to

$$\begin{cases} -\lambda^2 V''_{\mathrm{inh}}(x) = -C(x), & 0 \leqslant x \leqslant 1, \\ V'_{\mathrm{inh}}(0) = \beta\big(V_{\mathrm{inh}}(0) - V_{GS}\big), & V_{\mathrm{inh}}(1) = V_B. \end{cases} \tag{3.4}$$

We then have $U = \Phi\{n\}$, with Φ as defined in Lemma 3.2, and

$$p(x,U) := \exp\big(V_{\mathrm{inh}}(x)/T_p\big)\exp(U/T_p). \tag{3.5}$$

The uniqueness of V is proved by monotonicity arguments. The result concerning V_* solving (2.2) is proved likewise. □

For $n \geqslant 0$ we may write $n = \varrho^2$, and then we write (1.6)–(1.8), (1.10) as

$$\begin{cases} \varrho F = \varrho\big(V_{\mathrm{inh}} + \Phi\{\varrho^2\}\big) + 2T_n \varrho \ln \varrho - \varepsilon^2 \varrho'', & \varrho \geqslant 0, \text{ on } [0,1], \\ \varrho(0) = 0, \quad \varrho(1) = \varrho_B := \sqrt{n_B}, \end{cases} \tag{3.6}$$

with V_{inh} given by (3.4).

Set $h(s) = T_n \ln s$ for $s > 0$ and

$$H(s) := \int_{\sigma=1}^{s} h(\sigma)\,\mathrm{d}\sigma = T_n(s \ln s - s + 1). \tag{3.7}$$

Our intuition is to look for ϱ as a non-negative minimizer to the functional

$$\mathcal{F}(\varrho) := \int_0^1 \big(\varepsilon^2 |\varrho'|^2 + H(\varrho^2) + \varrho^2 V_{\mathrm{inh}} - \varrho^2 F\big)\,\mathrm{d}x + \mathcal{F}^{(1)}(\varrho^2),$$

over the set $X_\varrho := \{\varrho \in W_2^1((0,1)) : \varrho(0) = 0, \ \varrho(1) = \varrho_B\}$.

Remark 3.6. For the convenience of the reader, we collect all information about how to construct $\mathcal{F}$ in one place: for functions ϱ from X_ϱ we shall discuss

$$\mathcal{F}(\varrho) := \int_0^1 \left(\varepsilon^2|\varrho'|^2 + H\left(\varrho^2\right) + \varrho^2 V_{\mathrm{inh}} - \varrho^2 F\right) \mathrm{d}x + \frac{\lambda^2}{2} \int_0^1 \left(\left(\Phi\left\{\varrho^2\right\}\right)'\right)^2 \mathrm{d}x$$
$$+ \frac{\lambda^2}{2}\beta\left(\Phi\left\{\varrho^2\right\}(0)\right)^2 + \int_0^1 \Phi\left\{\varrho^2\right\}(x)\cdot p\left(x, \Phi\left\{\varrho^2\right\}(x)\right) - P\left(x, \Phi\left\{\varrho^2\right\}(x)\right) \mathrm{d}x, \quad (3.8)$$

with V_{inh} as the unique solution to (3.4), $p = p(x, U)$ defined in (3.5), and $P = P(x, U)$ from (3.2). Finally, $U = \Phi\{q\}$ is defined as the unique solution to (3.1). For the definition of $\mathcal{F}$, we take $q := \varrho^2$.

However, some problem occurs here. The pole of $h = h(s)$ at $s = 0$ and the boundary values of ϱ at $x = 0$ make the functional $\mathcal{F}$ irregular, and then the Euler–Lagrange equations cannot be derived. To overcome this difficulty, we perform a regularization step: for a parameter $\gamma \in (0, 1)$, we set

$$h_\gamma(s) := \begin{cases} h(\gamma): & 0 \leqslant s \leqslant \gamma, \\ h(s): & \gamma \leqslant s \leqslant \gamma^{-1}, \\ h(\gamma^{-1}): & \gamma^{-1} \leqslant s, \end{cases}$$

and then we put $H_\gamma(s) := \int_{\sigma=1}^s h_\gamma(\sigma)\,\mathrm{d}\sigma$. The functional for which we seek a non-negative minimizer is

$$\mathcal{F}_\gamma(\varrho) := \int_0^1 \left(\varepsilon^2|\varrho'|^2 + H_\gamma\left(\varrho^2\right) + \varrho^2 V_{\mathrm{inh}} - \varrho^2 F\right) \mathrm{d}x + \mathcal{F}^{(1)}\left(\varrho^2\right), \quad (3.9)$$

where we restrict γ to the interval $(0, \gamma_0)$, and γ_0 with $0 < \gamma_0 \ll 1$ is selected by the condition $H_\gamma(s) - s\|V_{\mathrm{inh}} - F\|_{L^\infty((0,1))} \geqslant s$ for $s \geqslant \gamma_0^{-1}$.

Lemma 3.7. *For functions ϱ taking only non-negative values, the functionals $\mathcal{F}$ and $\mathcal{F}_\gamma$ from* (3.8) *and* (3.9) *are strictly convex functionals of ϱ^2, in the following sense: if $\varrho_1, \varrho_2 \in X_\varrho$ with $\varrho_{1,2} \geqslant 0$ and $\varrho_1 \neq \varrho_2$, and if $0 < t < 1$, then*

$$\mathcal{F}\left(\sqrt{t\varrho_1^2 + (1-t)\varrho_2^2}\right) < t\mathcal{F}(\varrho_1) + (1-t)\mathcal{F}(\varrho_2),$$
$$\mathcal{F}_\gamma\left(\sqrt{t\varrho_1^2 + (1-t)\varrho_2^2}\right) < t\mathcal{F}_\gamma(\varrho_1) + (1-t)\mathcal{F}_\gamma(\varrho_2).$$

Non-negative minimizers of $\mathcal{F}$ or $\mathcal{F}_\gamma$ are unique.

Proof. First, the strict convexity of the functional $\varrho^2 \mapsto \int_0^1 |\nabla\varrho|^2\,\mathrm{d}x$ was shown in [11]. Second, the scalar functions H and H_γ are weakly convex functions. And third, we recall the strict convexity of $\mathcal{F}^{(1)}$ from Lemma 3.4. □

Lemma 3.8. *For $0 < \gamma < \gamma_0$, the functional $\mathcal{F}_\gamma$ possesses a non-negative minimizer $\varrho_\gamma \in C^2([0,1]) \cap X_\varrho$, and each such minimizer satisfies the uniform in γ estimate*

$$\varepsilon\|\varrho_\gamma\|_{W_2^1((0,1))} + \left\|\Phi\left\{\varrho_\gamma^2\right\}\right\|_{W_2^1((0,1))} \leqslant C. \quad (3.10)$$

Proof. We clearly have $\mathcal{F}_\gamma(\varrho) \geqslant \frac{\varepsilon^2}{2}\|\varrho\|^2_{W_2^1((0,1))} - C$ for all $\varrho \in X_\varrho$, with some $C \in \mathbb{R}_+$ depending only on $\|V_{\mathrm{inh}} - F\|_{L^\infty((0,1))}$, but not on γ. Then $m_\gamma := \inf\{\mathcal{F}_\gamma(\varrho)\colon \varrho \in X_\varrho\}$ exists. Let $(\varrho_1, \varrho_2, \ldots)$ be a sequence in X_ϱ with $\lim_{j\to\infty} \mathcal{F}_\gamma(\varrho_j) = m$. Then this sequence is bounded in $W_2^1((0,1))$, hence we can assume strong convergence in $C([0,1])$, and weak convergence in $W_2^1((0,1))$ of this sequence to some limit $\varrho_\gamma \in X_\varrho$. Then $\mathcal{F}^{(1)}(\varrho_j^2)$ has the limit $\mathcal{F}^{(1)}(\varrho_\gamma^2)$ for $j \to \infty$, because $\Phi : C([0,1]) \to C_B^2([0,1])$ is continuous, see Lemma 3.2. By classical arguments [12], we conclude that $\mathcal{F}_\gamma$ is weakly sequentially lower semi-continuous on X_ϱ, and consequently $\mathcal{F}_\gamma$ has a minimizer on X_ϱ. If $\varrho_\gamma \in X_\varrho$ is such a minimizer, then $|\varrho_\gamma|$ also belongs to X_ϱ, and it has the same value of $\mathcal{F}_\gamma$. Independent of γ estimates of such non-negative minimizers ϱ_γ can be found by choosing a non-negative function $\varrho^* \in X_\varrho$. Then $\mathcal{F}_\gamma(\varrho_\gamma) \leqslant \mathcal{F}_\gamma(\varrho^*)$, and the right-hand side is bounded from above independently of γ because H_γ is uniformly bounded from below. This gives us (3.10). □

Lemma 3.9. *Let $\varrho_\gamma \in C^2([0,1]) \cap X_\varrho$ be a non-negative minimizer of $\mathcal{F}_\gamma$, and $V_\gamma := V_{\mathrm{inh}} + \Phi\{\varrho_\gamma^2\}$. Then*

$$-\varepsilon^2 \varrho_\gamma'' + \big(h_\gamma\big(\varrho_\gamma^2\big) + V_\gamma - F\big)\varrho_\gamma = 0. \tag{3.11}$$

Proof. By Lemma 3.4, (3.11) is just the Euler–Lagrange equation for $\mathcal{F}_\gamma$. □

Proof of Theorem 2.1. By the uniform bound of $\|\varrho_\gamma\|_{W_2^1((0,1))}$ and the compact embedding $W_2^1((0,1)) \subset C([0,1])$, we can assume to have a sequence $(\varrho_\gamma)_{\gamma\to 0}$ of non-negative solutions to (3.11) that converges in $C([0,1])$ to a non-negative limit ϱ. Since the function $s \mapsto sh(s^2)$ is continuous on $[0,\infty)$, we deduce that

$$\big(h_\gamma\big(\varrho_\gamma^2\big) - V_\gamma + F\big)\varrho_\gamma \to \big(h\big(\varrho^2\big) - V + F\big)\varrho, \quad V := V_{\mathrm{inh}} + \Phi\big\{\varrho^2\big\},$$

with convergence in $C([0,1])$, for $\gamma \to 0$. Then $\varrho \geqslant 0$ is a distribution solution to (3.6), and by elliptic regularity, $\varrho \in C^2([0,1])$, and $\|\varrho_\gamma'' - \varrho''\|_{L^\infty((0,1))} \to 0$.

The positivity of $\varrho(x)$ at all $x \in (0,1)$ is shown as in [3, Section 2.4], and from $\mathcal{F}(\sigma) = \lim_{\gamma\to 0}\mathcal{F}_\gamma(\sigma)$, with $\mathcal{F}$ from (3.8) and any function $\sigma \in X_\varrho$, we learn that ϱ indeed minimizes $\mathcal{F}$. It remains to show (2.1). Choose any $\varrho^* \in X_\varrho$. Then $\mathcal{F}(\varrho) \leqslant \mathcal{F}(\varrho^*)$, which is bounded independently of $\varepsilon \in (0,1]$. Observe that there is a constant $C \in \mathbb{R}_+$ such that

$$\int_0^1 H\big(\psi^2\big) + \psi^2(V_{\mathrm{inh}} - F)\,\mathrm{d}x \geqslant -C, \qquad \mathcal{F}^{(1)}\big(\psi^2\big) \geqslant -C,$$

for all $\psi \in C([0,1])$, from which (2.1) quickly follows. □

4. Asymptotics of the solutions

Now we begin to demonstrate Theorem 2.2. From now on, let $(n_\varepsilon, V_\varepsilon)$ be the solution to (1.6), (1.7), (1.8), (1.10), as constructed in Theorem 2.1. We introduce the notation $\varrho_\varepsilon := \sqrt{n_\varepsilon}$. Then the pair $(\varrho_\varepsilon, V_\varepsilon)$ solves

$$\begin{cases} \varepsilon^2 \varrho_\varepsilon'' = g(\varrho_\varepsilon) + \varrho_\varepsilon \cdot (V_\varepsilon - F), \\ -\lambda^2 V_\varepsilon'' = \varrho_\varepsilon^2 - p(V_\varepsilon) - C(x), \end{cases} \tag{4.1}$$

with $g(s) := 2T_n s \ln s$ and $p(s) := \exp(s/T_p)$. And we have the boundary conditions

$$\begin{cases} \varrho_\varepsilon(0) = 0, \quad \varrho_\varepsilon(1) = \varrho_B := \sqrt{n_B}, \\ V_\varepsilon'(0) = \beta\big(V_\varepsilon(0) - V_{GS}\big), \quad V_\varepsilon(1) = V_B. \end{cases} \tag{4.2}$$

Since the proof of Theorem 2.2 will span almost the whole Section 4, we present its main steps. First we prove uniform bounds of V_ε, and of ϱ_ε from below (away from $x = 0$). In Section 4.2, we then show $V_\varepsilon \approx V_*$ on the whole interval (with an error of $\varepsilon^{1/2}$), and that $\varrho_\varepsilon \approx \varrho_*$ for $x > \sqrt{\varepsilon}$ with an error of $\varepsilon^{1/4}$. The next step (Proposition 4.5) then is a discussion of ϱ_ε for $x \in [0, 2\sqrt{\varepsilon}]$; here it is helpful to know the behavior of ϱ_ε for $x \in [\sqrt{\varepsilon}, 2\sqrt{\varepsilon}]$, as found out in the previous step. Then, in Section 4.3, a multiplier technique is used to improve the error estimates.

4.1. Properties of the solutions

We begin with some uniform estimates.

Lemma 4.1. *There is a constant C_1, independent of ε, such that*

$$\|V_\varepsilon\|_{C^2([0,1])} + \|n_\varepsilon\|_{C([0,1])} \leqslant C_1.$$

Proof. By the embedding $W_2^1((0,1)) \subset C([0,1])$, (2.1), and $V_\varepsilon(1) = V_B$, we find $\|V_\varepsilon\|_{C([0,1])} \leqslant C$. Suppose that ϱ_ε takes a local maximum at an inner point $x^* \in (0,1)$. Then $\varrho_\varepsilon''(x^*) \leqslant 0$, hence $h(\varrho_\varepsilon^2(x^*)) + V_\varepsilon(x^*) - F \leqslant 0$. We then have $\varrho_\varepsilon^2(x^*) \leqslant \exp((F - V_\varepsilon(x^*))/T_n)$, and then also $\|n_\varepsilon\|_{C([0,1])} \leqslant C$. Then (1.7) gives us the remaining bound for $\|V_\varepsilon\|_{C^2([0,1])}$. □

A first information on the graph of n is given by the next result.

Lemma 4.2. *There is a positive constant g_* such that*

$$\varrho_\varepsilon(x) \geqslant g_*, \quad \varepsilon \leqslant x \leqslant 1.$$

And there is a unique $x_1 \in (0,1)$ with $\varrho_\varepsilon(x_1) = g_*$, and $\varrho_\varepsilon'(x) > 0$ on $[0, x_1]$.

Proof. The function ϱ_ε solves (4.1) and (4.2). Define g_* as

$$g_* := \min\left\{\frac{\varrho_B}{2}, \exp\left(\frac{-32 - C_1}{2T_n} - 1\right)\right\}, \tag{4.3}$$

with C_1 from Lemma 4.1 as an upper estimate of $\|V_\varepsilon - F\|_{C([0,1])}$.

Then it follows that whenever $0 < \varrho_\varepsilon(\tilde{x}) \leqslant g_*$, then

$$2T_n \ln \varrho_\varepsilon(\tilde{x}) + V_\varepsilon(\tilde{x}) - F \leqslant -32,$$

and consequently $\varrho_\varepsilon''(\tilde{x}) < 0$. Then $\varrho_\varepsilon'(\tilde{x}) \leqslant 0$ is impossible because this would imply $\varrho_\varepsilon'(x) < 0$ for all $x \in (\tilde{x}, 1]$, contradicting $\varrho_\varepsilon(1) = \varrho_B > g_*$. Hence there is a uniquely determined number $x_1 \in (0,1)$ with

$$\varrho_\varepsilon(x) \begin{cases} < g_*: & 0 \leqslant x < x_1, \\ > g_*: & x_1 < x \leqslant 1. \end{cases}$$

Moreover, on the interval $[0, x_1]$, ϱ_ε is strictly increasing. It remains to show that $x_1 \leqslant \varepsilon$. Define $x_2 \in (0, x_1)$ by $\varrho_\varepsilon(x_2) = \frac{1}{2}g_*$. Then we have $x_2 \leqslant \frac{1}{2}x_1$, by the concavity of ϱ_ε on $(0, x_1)$. On the interval $[x_2, x_1]$, we have $\varrho_\varepsilon(x) \geqslant \frac{1}{2}g_*$, hence $\varepsilon^2 \varrho_\varepsilon'' \leqslant -16 g_*$. Now we make use of a simple fact: if

$|\psi''(x)| \geqslant d_0$ on $[a,b]$ for some $\psi \in C^2([a,b])$, then $\max_{[a,b]} \psi - \min_{[a,b]} \psi \geqslant d_0(b-a)^2/8$. Hence we conclude that

$$\frac{1}{2} g_* \geqslant \frac{16 g_*}{\varepsilon^2} \cdot \frac{(x_2 - x_1)^2}{8},$$

or $x_1 - x_2 \leqslant \frac{1}{2}\varepsilon$, implying $x_1 \leqslant \varepsilon$ as desired. □

The next result is a first step in showing that the quantum term $\varepsilon^2 \varrho_\varepsilon''$ is of less relevance for $x \geqslant \mathcal{O}(\sqrt{\varepsilon})$.

Lemma 4.3. *Assume* (1.9)*. Then there is a constant C, independent of $\varepsilon \in (0, 1/8]$, such that*

$$\|2T_n \ln \varrho_\varepsilon + V_\varepsilon - F\|_{L^\infty((\sqrt{\varepsilon},1))} \leqslant C\varepsilon^{1/4}, \tag{4.4}$$

$$\|2T_n \ln \varrho_\varepsilon + V_\varepsilon - F\|_{L^2((\sqrt{\varepsilon},1))} \leqslant C\varepsilon^{3/4}, \tag{4.5}$$

$$\big\|\varrho_\varepsilon^2 - \exp\big((F - V_\varepsilon)/T_n\big)\big\|_{L^2((2\varepsilon,1))} \leqslant C\varepsilon^{1/2}, \tag{4.6}$$

$$\big\|\varrho_\varepsilon'\big\|_{L^\infty((\sqrt{\varepsilon},1))} \leqslant C\varepsilon^{-3/4}. \tag{4.7}$$

Proof. Take a function $\chi \in C^\infty([0,1])$ with $0 \leqslant \chi \leqslant 1$, $\chi' \geqslant 0$, and define

$$\chi(x) := \begin{cases} 3x: & 0 \leqslant x \leqslant 1/4, \\ 1: & 1/3 \leqslant x \leqslant 1, \end{cases} \qquad \chi_\varepsilon(x) := \chi(x - \varepsilon), \quad x \in [\varepsilon, 1].$$

By $(2T_n \ln \varrho_\varepsilon + V_\varepsilon - F)|_{x=1} = 0$ because of (1.9), we find

$$\int_\varepsilon^1 \frac{\varepsilon^2 \chi_\varepsilon}{\varrho_\varepsilon} \big(\varrho_\varepsilon''\big)^2 \,\mathrm{d}x = \int_\varepsilon^1 \chi_\varepsilon \varrho_\varepsilon''(2T_n \ln \varrho_\varepsilon + V_\varepsilon - F)\,\mathrm{d}x$$
$$= -2T_n \int_\varepsilon^1 \frac{\chi_\varepsilon}{\varrho_\varepsilon}\big(\varrho_\varepsilon'\big)^2 \,\mathrm{d}x - \int_\varepsilon^1 \chi_\varepsilon \varrho_\varepsilon' V_\varepsilon' \,\mathrm{d}x - \int_\varepsilon^1 \chi_\varepsilon' \varrho_\varepsilon'(2T_n \ln \varrho_\varepsilon + V_\varepsilon - F)\,\mathrm{d}x.$$

Now we estimate

$$\big|\chi_\varepsilon \varrho_\varepsilon' V_\varepsilon'\big| \leqslant \chi_\varepsilon T_n \frac{(\varrho_\varepsilon')^2}{\varrho_\varepsilon} + C_{T_n} \chi_\varepsilon \varrho_\varepsilon \big(V_\varepsilon'\big)^2 \leqslant T_n \frac{\chi_\varepsilon}{\varrho_\varepsilon}\big(\varrho_\varepsilon'\big)^2 + C\big(V_\varepsilon'\big)^2,$$

$$\int_\varepsilon^1 \chi_\varepsilon' \varrho_\varepsilon' \ln \varrho_\varepsilon \,\mathrm{d}x = -\big(\chi_\varepsilon'(\varrho_\varepsilon \ln \varrho_\varepsilon - \varrho_\varepsilon)\big)\big|_{x=\varepsilon} - \int_\varepsilon^1 \chi_\varepsilon''(\varrho_\varepsilon \ln \varrho_\varepsilon - \varrho_\varepsilon)\,\mathrm{d}x,$$

$$\int_\varepsilon^1 \chi_\varepsilon' \varrho_\varepsilon' V_\varepsilon \,\mathrm{d}x = -\big(\chi_\varepsilon' \varrho_\varepsilon V_\varepsilon\big)\big|_{x=\varepsilon} - \int_\varepsilon^1 \varrho_\varepsilon\big(\chi_\varepsilon'' V_\varepsilon + \chi_\varepsilon' V_\varepsilon'\big)\,\mathrm{d}x,$$

and consequently we have

$$\int_{\varepsilon}^{1} \frac{\chi_\varepsilon}{\varrho_\varepsilon}\left(\left(\varepsilon\varrho_\varepsilon''\right)^2 + T_n\left(\varrho_\varepsilon'\right)^2\right) dx \leqslant C.$$

Choose a positive $\sigma(\varepsilon) \leqslant 1/2$. Then Lemma 4.2 brings us to

$$\int_{\varepsilon+\sigma(\varepsilon)}^{1} \left(\varepsilon\varrho_\varepsilon''\right)^2 + T_n\left(\varrho_\varepsilon'\right)^2 dx \leqslant \frac{C}{\sigma(\varepsilon)}.$$

We easily see $\varepsilon^2\varrho_\varepsilon''' = (\varrho_\varepsilon(2T_n \ln\varrho_\varepsilon + V_\varepsilon - F))'$, hence $\varepsilon^2\|\varrho_\varepsilon'''\|_{L^2((\varepsilon+\sigma(\varepsilon),1))} \leqslant C\sigma^{-1/2}(\varepsilon)$. Interpolating $\|\varrho_\varepsilon\|_{W_2^3} \leqslant C\varepsilon^{-2}\sigma^{-1/2}(\varepsilon)$ and $\|\varrho_\varepsilon\|_{W_2^1} \leqslant C\sigma^{-1/2}(\varepsilon)$, we then derive $\varepsilon^2\|\varrho_\varepsilon\|_{W_2^2((\varepsilon+\sigma(\varepsilon),1))} \leqslant C\varepsilon\sigma^{-1/2}(\varepsilon)$, and now the differential equation implies

$$\left\|\varrho_\varepsilon(2T_n \ln\varrho_\varepsilon + V_\varepsilon - F)\right\|_{L^2((\varepsilon+\sigma(\varepsilon),1))} \leqslant \frac{C\varepsilon}{\sigma^{1/2}(\varepsilon)},$$

which is (4.5) and (4.6) for the choices $\sigma(\varepsilon) = \frac{1}{2}\sqrt{\varepsilon}$ and $\sigma(\varepsilon) = \varepsilon$. And (4.4) follows with $\sigma(\varepsilon) = \frac{1}{2}\sqrt{\varepsilon}$ and the inequality $\|\varrho_\varepsilon(2T_n \ln\varrho_\varepsilon + V_\varepsilon - F)\|_{W_2^1((\sqrt{\varepsilon},1))} \leqslant C\varepsilon^{-1/4}$ using interpolation. Finally, (4.7) is proved by interpolation, too:

$$\left\|\varrho_\varepsilon'\right\|_{L^\infty} \leqslant C\left\|\varrho_\varepsilon'\right\|_{L^2}^{1/2}\left\|\varrho_\varepsilon'\right\|_{W_2^1}^{1/2} \leqslant \frac{C}{\varepsilon^{1/2}\sigma^{1/2}(\varepsilon)}. \qquad \square$$

4.2. First remainder estimates

We continue our preparations for the proof of Theorem 2.2.

Lemma 4.4. *The sequence $(V_\varepsilon)_{\varepsilon\to 0}$ converges to a limit $V_* \in C^2([0,1])$,*

$$\|V_\varepsilon - V_*\|_{W_2^1((0,1))} \leqslant C\varepsilon^{1/2}, \tag{4.8}$$

and V_* solves (2.2). Moreover, the sequence $(\varrho_\varepsilon)_{\varepsilon\to 0}$ converges uniformly on compact subsets of $(0,1)$ to the limit $\varrho_* := \sqrt{n_*}$ in the sense of

$$\|\varrho_\varepsilon - \varrho_*\|_{L^\infty((\sqrt{\varepsilon},1))} = \left\|\varrho_\varepsilon - \exp\left((F - V_*)/(2T_n)\right)\right\|_{L^\infty((\sqrt{\varepsilon},1))} \leqslant C\varepsilon^{1/4}. \tag{4.9}$$

See (2.2) for the definition of n_*.

Proof. For parameters $0 < \varepsilon_2 < \varepsilon_1 < 1/8$, we conclude that

$$\lambda^2 \int_0^1 \big((V_{\varepsilon_1} - V_{\varepsilon_2})'\big)^2 \,\mathrm{d}x + \lambda^2 \beta \big(V_{\varepsilon_1}(0) - V_{\varepsilon_2}(0)\big)^2$$

$$= -\int_0^1 \big(\exp(V_{\varepsilon_1}/T_p) - \exp(V_{\varepsilon_2}/T_p)\big)(V_{\varepsilon_1} - V_{\varepsilon_2})\,\mathrm{d}x$$

$$+ \int_0^{2\varepsilon_1} \big(\varrho_{\varepsilon_1}^2 - \varrho_{\varepsilon_2}^2\big)(V_{\varepsilon_1} - V_{\varepsilon_2})\,\mathrm{d}x + \int_{2\varepsilon_1}^1 \big(\varrho_{\varepsilon_1}^2 - \varrho_{\varepsilon_2}^2\big)(V_{\varepsilon_1} - V_{\varepsilon_2})\,\mathrm{d}x.$$

The first integral on the right is non-negative, by monotonicity. The second integral is bounded by $2\varepsilon_1 \cdot 2C_1^2$, see Lemma 4.1. And for the third integral on the right, we exploit (4.6), monotonicity arguments, and the inequalities of Poincaré and Young. The result then is $\lambda^2 \|(V_{\varepsilon_1} - V_{\varepsilon_2})'\|^2_{L^2((0,1))} \leqslant C\varepsilon_1$, hence there is a limit $V_* \in W_2^1((0,1))$, and (4.8) holds. Combined with the uniform bound $\|V_\varepsilon\|_{C^2([0,1])} \leqslant C$ from Lemma 4.1, then also $\lim_{\varepsilon\to 0} \|V_\varepsilon - V_*\|_{C^1([0,1])} = 0$. Now Lemmas 4.1, 4.2, and (4.4) give us

$$\big\|\varrho_\varepsilon - \exp\big((F - V_\varepsilon)/(2T_n)\big)\big\|_{L^\infty((\sqrt{\varepsilon},1))} \leqslant C\varepsilon^{1/4},$$

and joining this estimate with (4.8) then yields (4.9). It follows that V_* is a distributional solution to (2.2), and then $V_* \in C^2([0,1])$ by elliptic regularity. □

Next we discuss the behavior of ϱ_ε near the boundary $x = 0$:

Proposition 4.5. *Put $c_0 := g_*/(2\sqrt{T_n}\varrho_*(0))$. On the interval $[0, c_0\varepsilon]$, we have the uniform expansion*

$$\varrho_\varepsilon(x) = \varrho_*(x) Z\left(\sqrt{2T_n} \cdot \frac{x}{\varepsilon}\right) + \mathcal{O}\left(\varepsilon^{1/2} \cdot \frac{x}{\varepsilon}\right), \tag{4.10}$$

$$\left\|\varrho_\varepsilon - \varrho_*(0) Z\left(\frac{\sqrt{2T_n}}{\varepsilon}\cdot\right)\right\|_{L^\infty((0,c_0\varepsilon))} \leqslant C\varepsilon^{1/2}, \tag{4.11}$$

with Z as in (2.3). And on the middle interval $[c_0\varepsilon, 2\sqrt{\varepsilon}]$, we uniformly have

$$\varrho_\varepsilon(x) = \varrho_*(x) Z\left(\sqrt{2T_n} \cdot \frac{x}{\varepsilon}\right) + \mathcal{O}\big(\varepsilon^{1/4}\big). \tag{4.12}$$

Proof. We multiply the first equation of (4.1) by $2\varrho_\varepsilon'$ and integrate on $[0, x]$:

$$\big(\varepsilon\varrho_\varepsilon'(x)\big)^2 - \big(\varepsilon\varrho_\varepsilon'(0)\big)^2 = T_n \varrho_\varepsilon^2(x)\left(2\ln\varrho_\varepsilon(x) - 1 + \frac{V_\varepsilon(x) - F}{T_n}\right) - V_\varepsilon'(\xi)\int_0^x \varrho_\varepsilon^2(t)\,\mathrm{d}t,$$

with $\xi \in (0, x)$, by partial integration and the mean value theorem of integration. We can re-order this to

$$T_n\varrho_\varepsilon^2(x)-\bigl(\varepsilon\varrho_\varepsilon'(0)\bigr)^2=R_\varepsilon:=\varrho_\varepsilon^2(x)\bigl(2T_n\ln\varrho_\varepsilon(x)+V_\varepsilon(x)-F\bigr)\\ -\bigl(\varepsilon\varrho_\varepsilon'(x)\bigr)^2-V_\varepsilon'(\xi)\int_0^x\varrho_\varepsilon^2(t)\,\mathrm{d}t. \tag{4.13}$$

Now we apply (4.5), (4.7), and then we deduce that $\|R_\varepsilon\|_{L^2((\sqrt{\varepsilon},2\sqrt{\varepsilon}))}\leqslant C\varepsilon^{3/4}$. If $0\leqslant x\leqslant 2\sqrt{\varepsilon}$, then (4.8) and $V_*\in C^2([0,1])$ imply

$$V_\varepsilon(x)=V_*(0)+\bigl(V_\varepsilon(x)-V_*(x)\bigr)+\bigl(V_*(x)-V_*(0)\bigr)=V_*(0)+\mathcal{O}\bigl(\varepsilon^{1/2}\bigr)\\ =F-2T_n\ln\varrho_*(0)+\mathcal{O}\bigl(\varepsilon^{1/2}\bigr),$$

which then yield

$$\bigl\|\ln\varrho_*^2(0)-(F-V_\varepsilon)/T_n\bigr\|_{L^2((\sqrt{\varepsilon},2\sqrt{\varepsilon}))}\leqslant C\varepsilon^{3/4},\\ \bigl\|\varrho_*^2(0)-\exp\bigl((F-V_\varepsilon)/T_n\bigr)\bigr\|_{L^2((\sqrt{\varepsilon},2\sqrt{\varepsilon}))}\leqslant C\varepsilon^{3/4}.$$

Now we bring (4.5) into the game:

$$\varepsilon^{1/4}\bigl|T_n\varrho_*^2(0)-\bigl(\varepsilon\varrho_\varepsilon'(0)\bigr)^2\bigr|=\bigl\|T_n\varrho_*^2(0)-\bigl(\varepsilon\varrho_\varepsilon'(0)\bigr)^2\bigr\|_{L^2((\sqrt{\varepsilon},2\sqrt{\varepsilon}))}\\ \leqslant\|R_\varepsilon\|_{L^2((\sqrt{\varepsilon},2\sqrt{\varepsilon}))}+T_n\bigl\|\varrho_*^2(0)-\exp\bigl((F-V_\varepsilon)/T_n\bigr)\bigr\|_{L^2((\sqrt{\varepsilon},2\sqrt{\varepsilon}))}\\ +T_n\bigl\|\varrho_*^2(\cdot)-\exp\bigl((F-V_\varepsilon)/T_n\bigr)\bigr\|_{L^2((\sqrt{\varepsilon},2\sqrt{\varepsilon}))}\\ \leqslant C\varepsilon^{3/4},$$

and this delivers us an explicit description of the slope $\varrho_\varepsilon'(0)$:

$$\bigl(\varepsilon\varrho_\varepsilon'(0)\bigr)^2=T_n\varrho_*^2(0)+\mathcal{O}\bigl(\varepsilon^{1/2}\bigr).$$

Consequently, for $0\leqslant x\leqslant 2\sqrt{\varepsilon}$, the differential equation (4.13) becomes

$$\bigl(\varepsilon\varrho_\varepsilon'(x)\bigr)^2=T_n\varrho_*^2(0)\left(\frac{\varrho_\varepsilon^2(x)}{\varrho_*^2(0)}\ln\left(\frac{\varrho_\varepsilon^2(x)}{\varrho_*^2(0)}\right)-\frac{\varrho_\varepsilon^2(x)}{\varrho_*^2(0)}+1\right)+\mathcal{O}\bigl(\varepsilon^{1/2}\bigr). \tag{4.14}$$

Recall that $x_1\in(0,\varepsilon]$ was defined by the condition $\varrho_\varepsilon(x_1)=g_*$, compare Lemma 4.2. The definition of g_* in (4.3) guarantees that $(\varrho_\varepsilon(x)/\varrho_*(0))^2\leqslant e^{-1}$ on $[0,x_1]$, hence

$$\bigl(\varepsilon\varrho_\varepsilon'(x)\bigr)^2\geqslant T_n\varrho_*^2(0)\left(1-\frac{2}{e}\right)+\mathcal{O}\bigl(\varepsilon^{1/2}\bigr)\geqslant\frac{T_n\varrho_*^2(0)}{16},\quad 0\leqslant x\leqslant x_1. \tag{4.15}$$

Next we bound x_1 from below. By the mean value theorem, a ξ exists with

$$\frac{g_*}{x_1}=\frac{\varrho_\varepsilon(x_1)}{x_1}=\varrho_\varepsilon'(\xi)\leqslant\varepsilon^{-1}\sqrt{T_n\varrho_*^2(0)+\mathcal{O}\bigl(\varepsilon^{1/2}\bigr)}\leqslant 2\sqrt{T_n}\varrho_*(0)\varepsilon^{-1},$$

compare (4.14), and therefore $x_1\geqslant c_0\varepsilon$ with $c_0:=g_*/(2\sqrt{T_n}\varrho_*(0))$.

We introduce the scaling

$$y = \frac{x}{\varepsilon}, \qquad \varrho_\varepsilon(x) =: \varrho_{(I,\varepsilon)}(y) \cdot \varrho_*(0),$$

and then (4.14) turns into the differential equation

$$\big(\varrho'_{(I,\varepsilon)}(y)\big)^2 = H\big(\varrho^2_{(I,\varepsilon)}(y)\big) + \mathcal{O}\big(\varepsilon^{1/2}\big), \quad 0 \leqslant y \leqslant 2\varepsilon^{-1/2}, \tag{4.16}$$

compare (3.7) for H. Now consider the interval $[0, c_0]$. By (4.15), we have

$$\varrho'_{(I,\varepsilon)}(y) = \sqrt{H\big(\varrho^2_{I,\varepsilon}(y)\big)} + \mathcal{O}\big(\varepsilon^{1/2}\big), \quad 0 \leqslant y \leqslant c_0.$$

Note that $\varrho^2_{(I,\varepsilon)}(y) \in [0, e^{-1}]$ for $y \in [0, c_0]$, which makes the function $s \mapsto \sqrt{H(s^2)}$ uniformly Lipschitz continuous on the relevant interval.

The function $Z = Z(y)$ defined in (2.3) solves

$$Z'(y) = \frac{1}{\sqrt{2T_n}}\sqrt{H\big(Z^2(y)\big)}, \quad 0 \leqslant y < \infty, \qquad Z(0) = 0. \tag{4.17}$$

Put $W(y) = \varrho_{(I,\varepsilon)}(y) - Z(\sqrt{2T_n}y)$. Then we have, for $y \in [0, c_0]$,

$$\begin{aligned}\big(W^2(y)\big)' &= 2W(y) \cdot \Big(\sqrt{H\big(\varrho^2_{(I,\varepsilon)}(y)\big)} - \sqrt{H\big(Z^2(\sqrt{2T_n}y)\big)} + \mathcal{O}\big(\varepsilon^{1/2}\big)\Big) \\ &\leqslant C_0 W^2(y) + \mathcal{O}(\varepsilon),\end{aligned}$$

hence $|W(y)| \leqslant C\varepsilon^{1/2}$ by Gronwall's Lemma. From (4.11) we then obtain

$$\varrho_\varepsilon(x) = \varrho_*(0) Z\left(\sqrt{2T_n} \cdot \frac{x}{\varepsilon}\right) + \mathcal{O}\left(\varepsilon^{1/2} \cdot \frac{x}{\varepsilon}\right), \quad x \in [0, c_0\varepsilon],$$

which implies (4.10) via the Lipschitz continuity of ϱ_*.

Now we come to the proof of the uniform estimate of W on $[c_0, 2\varepsilon^{-1/2}]$, from which then (4.12) will follow. It is already known from (4.11) and (4.9) that $|W(c_0)| \leqslant C\varepsilon^{1/2}$ and $|W(2\varepsilon^{-1/2})| \leqslant C\varepsilon^{1/4}$. Assuming that $|W|$ attains its maximal value on $y_* \in (c_0, 2\varepsilon^{-1/2})$, we then get from (4.16) and (4.17) that

$$\Big|H\big(\varrho^2_{(I,\varepsilon)}(y_*)\big) - H\big(Z^2(\sqrt{2T_n}y_*)\big)\Big| \leqslant C\varepsilon^{1/2}. \tag{4.18}$$

Note that H is convex with $H(1) = H'(1) = 0$ and $H''(1) = T_n$. If $\varrho^2_{(I,\varepsilon)}(y_*) \leqslant 1$ then it follows that $|\varrho^2_{(I,\varepsilon)}(y_*) - Z^2(\sqrt{2T_n}y_*)| \leqslant C\varepsilon^{1/4}$ with the consequence of $|W(y^*)| \leqslant C\varepsilon^{1/4}$, because of $Z(\sqrt{2T_n}y) \geqslant \text{const} > 0$ for $y \in [c_0, \infty)$.

The other case, where $\varrho^2_{(I,\varepsilon)}(y_*) > 1$, is a bit harder. Let y_0 denote the point in $[c_0, 2\varepsilon^{-1/2}]$ where $\varrho_{(I,\varepsilon)}$ attains its maximal value. Then $y_0 > c_0$ due to $\varrho'_{(I,\varepsilon)}(c_0) > 0$. And also $\varrho_{(I,\varepsilon)}(2\varepsilon^{-1/2}) \leqslant$

$1+W(2\varepsilon^{-1/2}) \leqslant 1+C\varepsilon^{1/4}$. If $y_0 < 2\varepsilon^{-1/2}$, then $\varrho'_{(I,\varepsilon)}(y_0)=0$, (4.16), and the convexity of H together imply

$$\left|\varrho_{(I,\varepsilon)}(y_0)-1\right|^2 \leqslant CH\left(\varrho^2_{(I,\varepsilon)}(y_0)\right) \leqslant C\varepsilon^{1/2}.$$

The result then is $\varrho_{(I,\varepsilon)}(y) \leqslant 1+C\varepsilon^{1/4}$ for $y \in [c_0, 2\varepsilon^{-1/2}]$, which brings us to $H(\varrho^2_{(I,\varepsilon)}(y_*)) \leqslant C\varepsilon^{1/2}$. We utilize (4.18) and recall that $Z(\sqrt{2T_n}y_*) < 1 \leqslant \varrho^2_{(I,\varepsilon)}(y_*)$:

$$\begin{aligned}
\left|\varrho^2_{(I,\varepsilon)}(y_*) - Z^2(\sqrt{2T_n}y_*)\right| &= \left|\varrho^2_{(I,\varepsilon)}(y_*)-1\right| + \left|1-Z^2(\sqrt{2T_n}y_*)\right| \\
&\leqslant C\left(\sqrt{H\left(\varrho^2_{(I,\varepsilon)}(y_*)\right)} + \sqrt{H\left(Z^2(\sqrt{2T_n}y_*)\right)}\right) \\
&\leqslant C\sqrt{H\left(\varrho^2_{(I,\varepsilon)}(y_*)\right)+\varepsilon^{1/2}} \\
&\leqslant C\varepsilon^{1/4},
\end{aligned}$$

and therefore $|W(y_*)| \leqslant C\varepsilon^{1/4}$. $\square$

4.3. *Proof of Theorem 2.2*

The zero-th order approximations are

$$\varrho_{(0)}(x) := \varrho_*(x)Z(\alpha x/\varepsilon), \qquad V_{(0)}(x) := V_*(x),$$

with $\alpha := \sqrt{2T_n}$, and the remainders $R_{0,\varrho} := \varrho_\varepsilon - \varrho_{(0)}$, $R_{0,V} := V_\varepsilon - V_{(0)}$ fulfill

$$\begin{aligned}
&R_{0,\varrho}(0)=0, \qquad R'_{0,\varrho}(0)=\mathcal{O}\left(\varepsilon^{1/2}\right), \qquad R'_{0,V}(0)=\beta R_{0,V}(0), \\
&R_{0,\varrho}(1)=\mathcal{O}\left(e^{-c/\varepsilon}\right), \qquad R'_{0,\varrho}(1)=\mathcal{O}\left(\varepsilon^{-3/4}\right), \qquad R_{0,V}(1)=0,
\end{aligned}$$

compare (4.7) and (4.11). The estimates of Lemma 4.4 and Proposition 4.5 are

$$\|R_{0,\varrho}\|_{L^\infty((0,1))} \leqslant C\varepsilon^{1/4}, \qquad \|R_{0,V}\|_{L^\infty((0,1))} \leqslant C\varepsilon^{1/2}.$$

The next lemma is proved by direct calculation.

Lemma 4.6. *The remainders satisfy the differential equations*

$$\varepsilon^2 R''_{0,\varrho} = \alpha^2\varrho_\varepsilon(\ln\varrho_\varepsilon - \ln\varrho_{(0)}) + R_{0,\varrho}\alpha^2\ln Z + \varrho_\varepsilon R_{0,V} - \frac{\varepsilon^2}{Z}\left(Z^2\varrho'_*\right)', \tag{4.19}$$

$$-\lambda^2 R''_{0,V} = 2\varrho_\varepsilon R_{0,\varrho} - R^2_{0,\varrho} + \varrho^2_*\cdot\left(Z^2-1\right) - p(V_\varepsilon) + p(V_{(0)}), \tag{4.20}$$

with $p(V)=\exp(V/T_p)$. *And* (4.19) *can be re-ordered to*

$$\frac{\varepsilon^2}{Z}\left(Z^2\left(\frac{R_{0,\varrho}}{Z}\right)'\right)' = \alpha^2\varrho_\varepsilon(\ln\varrho_\varepsilon - \ln\varrho_{(0)}) + \varrho_\varepsilon R_{0,V} - \frac{\varepsilon^2}{Z}\left(Z^2\varrho'_*\right)'. \tag{4.21}$$

Lemma 4.7. *For ε_0 sufficiently small, we have the estimate*

$$\int_0^1 \left(\varepsilon Z\left(\frac{R_{0,\varrho}}{Z}\right)'\right)^2 \mathrm{d}x + \alpha^2 \|R_{0,\varrho}\|^2_{L^2((0,1))} + \lambda^2 \|R'_{0,V}\|^2_{L^2((0,1))} \leqslant C\varepsilon^2. \tag{4.22}$$

Proof. We multiply (4.21) by $R_{0,\varrho}$ and integrate over $[0,1]$:

$$\varepsilon^2 \int_0^1 \left(Z^2\left(\frac{R_{0,\varrho}}{Z}\right)'\right)' \frac{R_{0,\varrho}}{Z} \,\mathrm{d}x = \alpha^2 \int_0^1 \varrho_\varepsilon(\ln\varrho_\varepsilon - \ln\varrho_{(0)})(\varrho_\varepsilon - \varrho_{(0)})\,\mathrm{d}x + \int_0^1 \varrho_\varepsilon R_{0,V} R_{0,\varrho}\,\mathrm{d}x - \varepsilon^2 \int_0^1 \left(Z^2\varrho'_*\right)' \frac{R_{0,\varrho}}{Z}\,\mathrm{d}x.$$

Now we have $\varrho_\varepsilon(\ln\varrho_\varepsilon - \ln\varrho_{(0)})(\varrho_\varepsilon - \varrho_{(0)}) \geqslant R^2_{0,\varrho}/2$ on $[0,1]$ if $0 < \varepsilon \leqslant \varepsilon_0 \ll 1$, and therefore partial integration brings us to

$$\frac{1}{2}\int_0^1 \left(\varepsilon Z\left(\frac{R_{0,\varrho}}{Z}\right)'\right)^2 \mathrm{d}x + \frac{\alpha^2}{2}\|R_{0,\varrho}\|^2_{L^2((0,1))} \leqslant -\int_0^1 \varrho_\varepsilon R_{0,V} R_{0,\varrho}\,\mathrm{d}x + C\varepsilon^2. \tag{4.23}$$

Next we multiply (4.20) by $R_{0,V}/2$, integrate over $[0,1]$, and then we get

$$\begin{aligned}
&\frac{\lambda^2}{2}\|R'_{0,V}\|^2_{L^2((0,1))} + \frac{\lambda^2\beta}{2}\big(R_{0,V}(0)\big)^2 + \int_0^1 \big(p(V_\varepsilon) - p(V_{(0)})\big)\cdot(V_\varepsilon - V_{(0)})\,\mathrm{d}x \\
&= \int_0^1 \varrho_\varepsilon R_{0,\varrho}R_{0,V} - R^2_{0,\varrho}R_{0,V} + \varrho^2_*\cdot\big(Z^2-1\big)R_{0,V}\,\mathrm{d}x \\
&\leqslant \int_0^1 \varrho_\varepsilon R_{0,\varrho}R_{0,V}\,\mathrm{d}x + \|R_{0,V}\|_{L^\infty((0,1))}\big(\|R_{0,\varrho}\|^2_{L^2((0,1))} + \|Z-1\|_{L^1((0,1))}\big).
\end{aligned}$$

Adding this to (4.23), $\|R_{0,V}\|_{L^\infty((0,1))} \leqslant C\varepsilon^{1/2}$, $\|Z-1\|_{L^1((0,1))} = \mathcal{O}(\varepsilon)$ and Young's inequality then conclude the proof. □

4.4. Proof of Theorem 2.3

For simpler notation, we define $\overline{R}_{0,\varrho} := R_{0,\varrho}/Z$, for which we have, by Proposition 4.5, the auxiliary estimates

$$\|\overline{R}_{0,\varrho}\|_{L^\infty((0,1))} \leqslant C\varepsilon^{1/4}, \qquad \|Z\overline{R}'_{0,\varrho}\|_{L^\infty((0,c_0\varepsilon))} \leqslant C\varepsilon^{-1/2},$$
$$\overline{R}_{0,\varrho}(1) = \mathcal{O}\big(e^{-c/\varepsilon}\big), \qquad \overline{R}'_{0,\varrho}(1) = \mathcal{O}\big(\varepsilon^{-3/4}\big).$$

We will also make use of $\varrho_\varepsilon = (\varrho_* + \bar{R}_{0,\varrho})Z$. To (4.21), we choose its left-hand side (without one factor ε^2) as a multiplier, and then we have

$$\begin{aligned}
&\int_0^1 \left(\frac{\varepsilon}{Z}\left(Z^2\bar{R}'_{0,\varrho}\right)'\right)^2 \mathrm{d}x \\
&\quad = \alpha^2 \int_0^1 \bar{R}_{0,\varrho}\left(Z^2\bar{R}'_{0,\varrho}\right)' \mathrm{d}x \\
&\qquad + \alpha^2 \int_0^1 \left((\varrho_* + \bar{R}_{0,\varrho})\ln(\varrho_* + \bar{R}_{0,\varrho}) - \bar{R}_{0,\varrho} - (\varrho_* + \bar{R}_{0,\varrho})\ln \varrho_*\right) \cdot \left(Z^2\bar{R}'_{0,\varrho}\right)' \mathrm{d}x \\
&\qquad + \int_0^1 (\varrho_* + \bar{R}_{0,\varrho})R_{0,V}\left(Z^2\bar{R}'_{0,\varrho}\right)' \mathrm{d}x - \int_0^1 \frac{\varepsilon}{Z}\left(Z^2\varrho'_*\right)' \cdot \frac{\varepsilon}{Z}\left(Z^2\bar{R}'_{0,\varrho}\right)' \mathrm{d}x \\
&\quad = -\alpha^2 \left\|Z\bar{R}'_{0,\varrho}\right\|_{L^2}^2 + \mathcal{O}\left(e^{-c/\varepsilon}\right) \\
&\qquad - \alpha^2 \int_0^1 Z\left[\varrho'_*\left(\ln\left(1 + \frac{\bar{R}_{0,\varrho}}{\varrho_*}\right) - \frac{\bar{R}_{0,\varrho}}{\varrho_*}\right) + \bar{R}'_{0,\varrho}\ln\left(1 + \frac{\bar{R}_{0,\varrho}}{\varrho_*}\right)\right] \cdot Z\bar{R}'_{0,\varrho}\, \mathrm{d}x \\
&\qquad - \int_0^1 Z\left((\varrho_* + \bar{R}_{0,\varrho})R_{0,V}\right)' \cdot Z\bar{R}'_{0,\varrho}\, \mathrm{d}x - \int_0^1 \frac{\varepsilon}{Z}\left(Z^2\varrho'_*\right)' \cdot \frac{\varepsilon}{Z}\left(Z^2\bar{R}'_{0,\varrho}\right)' \mathrm{d}x.
\end{aligned}$$

Now we estimate

$$\begin{aligned}
&\left\|Z\left[\varrho'_*\left(\ln\left(1 + \frac{\bar{R}_{0,\varrho}}{\varrho_*}\right) - \frac{\bar{R}_{0,\varrho}}{\varrho_*}\right) + \bar{R}'_{0,\varrho}\ln\left(1 + \frac{\bar{R}_{0,\varrho}}{\varrho_*}\right)\right]\right\|_{L^2} \\
&\quad \leqslant C\left\|Z\bar{R}^2_{0,\varrho}\right\|_{L^2} + C\left\|Z\bar{R}'_{0,\varrho}\bar{R}_{0,\varrho}\right\|_{L^2} \\
&\quad \leqslant C\|\bar{R}_{0,\varrho}\|_{L^\infty}\left(\|R_{0,\varrho}\|_{L^2} + \left\|Z\bar{R}'_{0,\varrho}\right\|_{L^2}\right), \\
&\left\|Z\left((\varrho_* + \bar{R}_{0,\varrho})R_{0,V}\right)'\right\|_{L^2((0,1))} \leqslant C\|R_{0,V}\|_{W_2^1}\left(1 + \left\|Z\bar{R}'_{0,\varrho}\right\|_{L^2}\right), \\
&\left\|\frac{\varepsilon}{Z}\left(Z^2\varrho'_*\right)'\right\|_{L^2} \leqslant C\sqrt{\varepsilon},
\end{aligned}$$

and we find (using $\|\bar{R}_{0,\varrho}\|_{L^\infty} \leqslant C\varepsilon^{1/4}$, $\|R_{0,\varrho}\|_{L^2} \leqslant C\varepsilon$ and $\|R_{0,V}\|_{W_2^1} \leqslant C\varepsilon$)

$$\begin{aligned}
&\left\|\frac{\varepsilon}{Z}\left(Z^2\bar{R}'_{0,\varrho}\right)'\right\|_{L^2((0,1))}^2 + \alpha^2\left\|Z\bar{R}'_{0,\varrho}\right\|_{L^2((0,1))}^2 \\
&\quad \leqslant C\left(\varepsilon^{1/4}\left(\varepsilon + \left\|Z\bar{R}'_{0,\varrho}\right\|_{L^2}\right) + \varepsilon^{1/2}\right)\left\|Z\bar{R}'_{0,\varrho}\right\|_{L^2} + \mathcal{O}\left(e^{-c/\varepsilon}\right),
\end{aligned}$$

hence Young's inequality implies

$$\left\| \frac{\varepsilon}{Z}\left(Z^2 \bar{R}'_{0,\varrho}\right)' \right\|^2_{L^2((0,1))} + \alpha^2 \left\| Z \bar{R}'_{0,\varrho} \right\|^2_{L^2((0,1))} \leqslant C\varepsilon.$$

Consequently, $\|\bar{R}'_{0,\varrho}\|_{L^2((c_0\varepsilon,1))} \leqslant C\varepsilon^{1/2}$, and (4.22) gives us $\|\bar{R}_{0,\varrho}\|_{L^2((c_0\varepsilon,1))} \leqslant C\varepsilon$. Interpolating these two estimates, we find $\|\bar{R}_{0,\varrho}\|_{L^\infty((c_0\varepsilon,1))} \leqslant C\varepsilon^{3/4}$, hence

$$\|R_{0,\varrho}\|_{L^\infty((c_0\varepsilon,1))} \leqslant C\varepsilon^{3/4}.$$

By (4.19) we then have $\|R_{0,\varrho}\|_{C^2([c_0\varepsilon,1])} \leqslant C\varepsilon^{-5/4}$, hence $\|R'_{0,\varrho}\|_{L^\infty((c_0\varepsilon,1))} \leqslant C\varepsilon^{-1/4}$, by interpolation. Now we go back to (4.13), which we write as

$$T_n \varrho_\varepsilon^2(x) - \left(\varepsilon \varrho'_\varepsilon(0)\right)^2 = \varrho_\varepsilon^2(x)\left(2T_n \ln \varrho_\varepsilon(x) + V_\varepsilon(x) - F\right) - V'_\varepsilon(\xi) \int_0^x \varrho_\varepsilon^2(t)\,\mathrm{d}t - \left(\varepsilon \varrho'_{(0)}(x) + \varepsilon R'_{0,\varrho}(x)\right)^2.$$

We choose $x \in [\varepsilon^{3/4}, 2\varepsilon^{3/4}]$ and find that then $\varepsilon^2(\varrho'_\varepsilon(0))^2 = T_n\varrho_\varepsilon^2(x) + \mathcal{O}(\varepsilon^{3/4})$, hence also $\varepsilon^2(\varrho'_\varepsilon(0))^2 = T_n\varrho_*^2(0) + \mathcal{O}(\varepsilon^{3/4})$. In the same way as during the proof of Proposition 4.5, we then show (2.4). This completes the proof of Theorem 2.3.

5. Numerical simulations

In this section, we will evaluate the remainder terms $R_{0,\varrho}$ and $R_{0,V}$ numerically. To find an approximate solution to (2.2), we apply a finite difference method on an equidistant grid and solve the resulting nonlinear system by Newton's method. The obtained zero-th order approximate solution can be used as initial values when we attack (4.1); and since (4.1) is a singularly perturbed system, we now choose a grid which is refined near the gate, where the quantum layer and the inversion layer are to be expected.

We choose the following scaled parameters:

$-V_{GS}$	T_n	T_p	λ	β	C	ϱ_B
1.5	0.04	0.06	1.0	0.75	−2.0	$\sqrt{0.03}$

Here we assume that the device is negatively doped (hence $C = -2$), and therefore the equilibrium value of the electron density is small ($\varrho_B^2 = 0.03$). The scaling we utilize in our paper follows [5] and goes back to [15]. We refer to Section 2.4 of [5], and in particular, our equations (1.6), (1.7), (1.10) correspond to Eqs. (2.19), (2.17), (2.20) there. This also motivates the choices of the other parameters in the table. Then we fix V_B from (1.7) by the condition that $V''(1)$ shall vanish, and $F = -0.0978$ is then given by (1.9).

Results for $\varepsilon = 0.0032$ are in Figs. 3, 4. We see that our zero-th order approximation $n_{(0)}$ matches the exact solution n everywhere at least as good as the classical solution n_*. In the interior layer ($0 \leqslant x \lesssim 0.02$), where the quantum effect is to be expected, $n_{(0)}$ approximates n very well (naturally, n_* gives the wrong prediction there), and in the intermediate region ($0.02 \lesssim x \lesssim 0.1$), the quality of approximation is reduced, but still acceptable. We have the expectation that a discussion of further terms of the asymptotic expansion may shed some light on this issue.

The numerically computed errors are as follows. We observe that the numerically computed values of $\|R_{0,V}\|_{L^\infty}$ indeed are proportional to ε. On the other hand, the values for $\|R_{0,\varrho}\|_{L^\infty}$

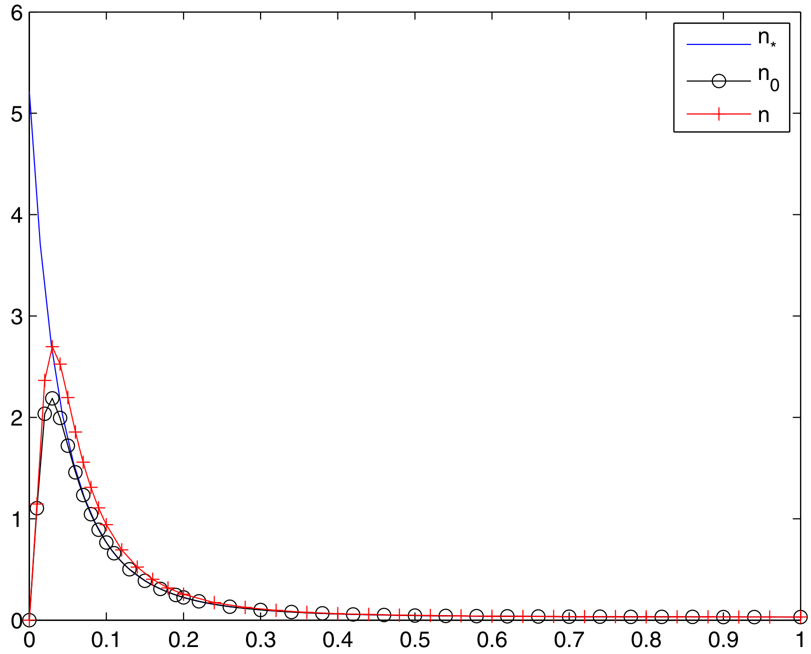

Fig. 3. The electron densities n, n_*, and $n_{(0)}$, as given in Theorem 2.1, (2.2), and Theorem 2.2, respectively.

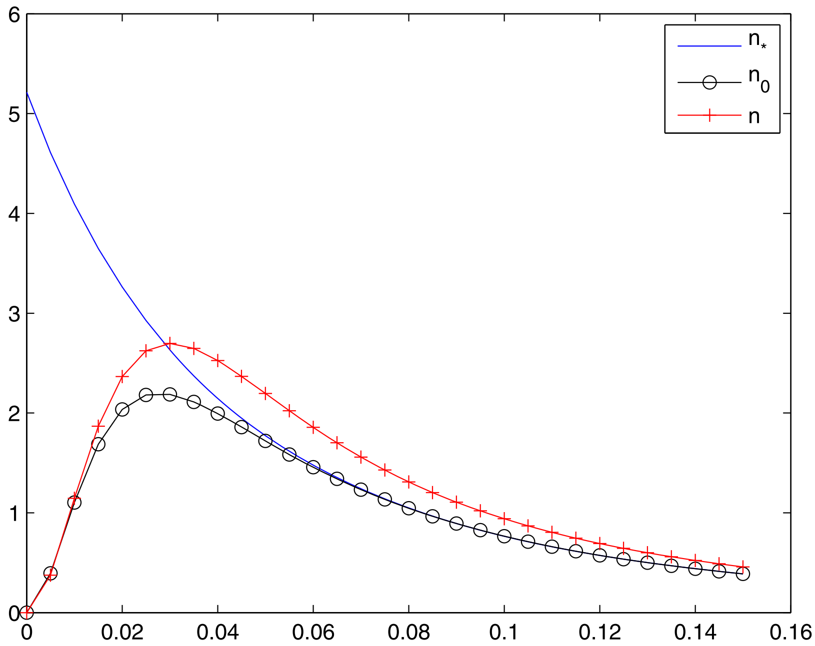

Fig. 4. A zoom into Fig. 3.

are worse, which of course also corresponds to our increased effort in finding an analytical error bound.

ε	$\|n - n_{(0)}\|_{L^2}$	$\|n - n_{(0)}\|_{L^\infty}$	$\|V - V_{(0)}\|_{L^2}$	$\|V - V_{(0)}\|_{L^\infty}$
0.0256	0.0840	0.2127	0.02274	0.0548
0.0128	0.1374	0.4381	0.01360	0.0357
0.0064	0.1458	0.5656	0.00738	0.0208
0.0032	0.1166	0.5372	0.00383	0.0113
0.0016	0.0772	0.4114	0.00195	0.0059
0.0008	0.0453	0.2706	0.000987	0.0030
0.0004	0.0247	0.1603	0.000495	0.00154
0.0002	0.0129	0.0886	0.000248	0.00078
0.0001	0.0066	0.0468	0.000123	0.00039

Acknowledgments

Li Chen is partially supported by the National Natural Science Foundation of China (NSFC), grant numbers 10871112 and 11011130029. Michael Dreher is supported by DFG (446 CHV 113/170/0-2) and by the Center of Evolution Equations of the University of Konstanz. Both authors thank Johannes Schnur for discussions on the manuscript, and the referee for helpful remarks.

References

[1] M.G. Ancona, Macroscopic description of quantum-mechanical tunneling, Phys. Rev. B 42 (2) (1990) 1222–1233.
[2] M.G. Ancona, H. Tiersten, Macroscopic physics of the silicon inversion layer, Phys. Rev. B 35 (15) (1987) 7959–7965.
[3] N. Ben Abdallah, A. Unterreiter, On the stationary quantum drift–diffusion model, Z. Angew. Math. Phys. 49 (1998) 251–275.
[4] E. Cumberbatch, H. Abebe, H. Morris, Current–voltage characteristics from an asymptotic analysis of the MOSFET equations, J. Engrg. Math. 39 (2001) 25–46.
[5] E. Cumberbatch, S. Uno, H. Abebe, Nano-scale MOSFET device modelling with quantum mechanical effects, European J. Appl. Math. 17 (2006) 465–489.
[6] U. Gianazza, G. Savaré, G. Toscani, The Wasserstein gradient flow of the Fisher information and the quantum drift–diffusion equation, Arch. Ration. Mech. Anal. 194 (2009) 133–220.
[7] A. Jüngel, Transport Equations for Semiconductors, Lecture Notes in Phys., vol. 773, Springer-Verlag, Berlin, 2009.
[8] A. Jüngel, R. Pinnau, Convergent semidiscretization of a nonlinear fourth order parabolic system, M2AN Math. Model. Numer. Anal. 37 (2) (2003) 277–289.
[9] A. Jüngel, I. Violet, The quasineutral limit in the quantum drift–diffusion equation, Asymptot. Anal. 53 (3) (2007) 139–157.
[10] P.A. Markowich, C.A. Ringhofer, C. Schmeiser, Semiconductor Equations, Springer-Verlag, Berlin, 1990.
[11] F. Pacard, A. Unterreiter, A variational analysis of the thermal equilibrium state of charged quantum fluids, Comm. Partial Differential Equations 20 (1995) 885–900.
[12] M. Struwe, Variational Methods, 2nd edition, Springer-Verlag, 1996.
[13] A. Unterreiter, The thermal equilibrium solution of a generic bipolar quantum hydrodynamic model, Comm. Math. Phys. 188 (1997) 69–88.
[14] M.J. Ward, Singular perturbations and a free boundary problem in the modeling of field-effect transistors, SIAM J. Appl. Math. 52 (1) (1992) 112–139.
[15] M.J. Ward, F.M. Odeh, D.S. Cohen, Asymptotic methods for metal oxide semiconductor field effect transistor modeling, SIAM J. Appl. Math. 50 (4) (1990) 1099–1125.