Boundary Layers for Quantum Semiconductor Models

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Introduction

Throughout the last decades the miniaturisation of microelectronic semiconductor devices like metal oxide semiconductor field-effect transistors (MOSFETs) or tunneling diodes has progressed considerably. As a consequence, the necessity of modeling quantum effects in such devices became apparent. In this thesis, we will present two semiconductor models which are based on existing classical models. They have been extended to include quantum effects. Both models are macroscopic fluid-dynamical descriptions of the electron flow in semiconductors. We consider a variant of the viscous quantum hydrodynamic model

$$\begin{cases} \partial_t n - \operatorname{div} J &= \nu\Delta n, \\ \partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n}\right) - \nabla(Tn) + n\nabla V + \frac{\varepsilon^2}{6} n\nabla\frac{\Delta\sqrt{n}}{\sqrt{n}} &= \nu\Delta J - \frac{J}{\tau} + \mu\nabla n, \\ \partial_t(ne) - \operatorname{div}\left(\frac{J}{n}(ne+P)\right) + J\cdot\nabla V &= -\frac{2}{\tau}\left(ne - \frac{d}{2}n\right) + \nu\Delta(ne) + \mu\operatorname{div} J, \\ P &= Tn\,\mathrm{id}_{\mathbb{R}^d} - \frac{\varepsilon^2}{12} n\,(\nabla\otimes\nabla)\ln(n), \\ ne &= \frac{|J|^2}{2n} + \frac{d}{2}Tn - \frac{\varepsilon^2}{24} n\Delta\ln(n), \\ \lambda^2\Delta V &= n - \mathcal{C}, \end{cases}$$

which is given by the stationary one-dimensional viscous quantum hydrodynamic model with a generic pressure term p and an additional barrier potential V_B

$$\begin{cases} J' &= -\nu n'', \\ 2\varepsilon^2 n\left(\frac{\sqrt{n}''}{\sqrt{n}}\right)' - \nu J'' - (p(n))' + \frac{1}{\tau}J &= \left(\frac{J^2}{n}\right)' - n(V+V_B)', \\ \lambda^2 V'' &= n - \mathcal{C}. \end{cases}$$

Here, $\mathcal{C}$ is the doping profile of the semiconductor. The unknown functions are the electron density n, the electric potential V and the electric current J. This system of equations describes a viscous flow of electrons and the viscosity is denoted by the constant ν. We may interpret these equations as a generalisation of the stationary Euler-Poisson system which has been augmented with additional pressure terms. Quantum effects are introduced by the Bohm potential term $\frac{\sqrt{n}''}{\sqrt{n}}$ and the corresponding pressure term bears the quantum parameter ε, which is the scaled Planck constant $\hbar$. The second model under consideration in this thesis is a variant of the stationary bipolar quantum drift-diffusion model

$$\begin{cases} F &= V + h_n(n) - \varepsilon^2\frac{\Delta\sqrt{n}}{\sqrt{n}}, \\ G &= -V + h_p(p) - \xi\varepsilon^2\frac{\Delta\sqrt{p}}{\sqrt{p}}, \\ \operatorname{div}(\mu_n n\nabla F) &= R_0(n,p)R_1(F,G), \\ \operatorname{div}(-\mu_p p\nabla G) &= -R_0(n,p)R_1(F,G), \\ -\lambda^2\Delta V &= n - p - \mathcal{C} \end{cases}$$

for the enthalpies

$$h_n(n) = T_n \ln(n) \quad \text{and} \quad h_p(p) = T_p \ln(p),$$

which is given by the isothermal quasi 1D approximation

$$\text{(1)} \qquad \begin{cases} F &= V + T_n \ln(n) - \varepsilon^2 \frac{\sqrt{n}''}{\sqrt{n}}, \\ -\lambda^2 V'' &= n - \exp(V/T_p) - \mathcal{C}, \end{cases}$$

proposed in [CUA] and [BCD]. The so-called Fermi level F is a given constant and $\mathcal{C}$ again denotes the doping profile of the semiconductor. The system describes an inviscid flow of electrons and positive particles by means of the unknown electron density n and the density of holes $p = \exp(V/T_p)$, where the electric potential V is also an unknown function. In Chapter 2, we will see that the stationary one-dimensional viscous quantum hydrodynamic model is actually equivalent to the similar system of equations

$$\text{(2)} \qquad \begin{cases} F &= -(V + V_B) + h(n) + \frac{\nu}{\tau} \ln(n) - 2(\varepsilon^2 + \nu^2) \frac{\sqrt{n}''}{\sqrt{n}}, \\ nF' &= -\left(\frac{J_0^2}{n}\right)' + 2J_0\nu \left(2\frac{\sqrt{n}''}{\sqrt{n}} - \frac{(n')^2}{2n^2}\right) + \frac{J_0}{\tau}, \\ \lambda^2 V'' &= n - \mathcal{C}, \end{cases}$$

where J_0 is a constant and the enthalpy h fulfills $sh'(s) = p'(s)$ for $s > 0$. Both systems of equations possess characteristic parameters which are given by the coefficients ε^2 and $\kappa := \varepsilon^2 + \nu^2$ of the highest order derivative, respectively. The main objective of this thesis is to analyse the qualitative behavior of solutions of the respective models with respect to these characteristic parameters.

Rewriting the quasi 1D approximation (1) of the stationary bipolar quantum drift-diffusion model in terms of the function $\varrho = \sqrt{n}$, we see that the square root of the eletron density fulfills the differential equation

$$\varepsilon^2 \varrho'' = \left(V - F + T_n \ln(\varrho^2)\right) \varrho.$$

Since the quantity ε^2 is the coefficient of the highest order derivative, the solutions $\varrho = \varrho_\varepsilon$ potentially depend significantly on ε. We want to illustrate the arising phenomena in a simple example. Consider the boundary value problem

$$\begin{cases} \varepsilon^2 f_\varepsilon'' &= f_\varepsilon - 1, \text{ in } (0,1), \\ f_\varepsilon(0) &= 0, \\ f_\varepsilon(1) &= 1, \end{cases}$$

with corresponding solutions f_ε. Formally letting $\varepsilon = 0$ in the differential equation, we expect $f_0 \equiv 1$ to be the limiting function of f_ε in some sense as ε tends to zero. However, since all functions admit the boundary value $f_\varepsilon(0) = 0$, it is impossible that convergence is given in spaces with strong topologies, like $L^\infty(0,1)$. And even if f_ε converges pointwise to f_0, we already deduce that the slope of the functions must become large in a vicinity of 0 when ε tends to zero. The existence of a regime where our solutions change their behavior drastically is typical for fluid-dynamical equations and this area is named to be a boundary layer. Usually, it has a certain width which is proportional to a power of the characteristic parameter ε. All presumptions on the behavior of f_ε, as ε tends to zero, are easily verified with the explicit representations

$$f_\varepsilon(x) = \frac{\exp(\frac{x-2}{\varepsilon}) - \exp(-\frac{x}{\varepsilon})}{1 - \exp(-\frac{2}{\varepsilon})} + 1$$

and considering the term $\exp(-\frac{x}{\varepsilon})$ in this expression, we also presume that the width of the boundary layer is proportional to ε. To understand the behavior of the solutions inside the boundary layer, we introduce the scaling $g_\varepsilon(x) = f_\varepsilon(\varepsilon x)$ and conclude that g_ε fulfills the differential equation

$$\begin{cases} g_\varepsilon'' &= g_\varepsilon - 1, \text{ in } (0, \varepsilon^{-1}), \\ g_\varepsilon(0) &= 0, \\ g_\varepsilon(\varepsilon^{-1}) &= 1. \end{cases}$$

This differential equation only depends on the parameter ε at the right boundary value and it is reasonable to expect that the original solutions f_ε approximately coincide with the scaled functions $g\left(\frac{\cdot}{\varepsilon}\right)$ near $x = 0$, where $g(y) = -\exp(-y) + 1$ is the solution to

$$\begin{cases} g'' &= g - 1, \text{ in } (0, \infty), \\ g(0) &= 0, \\ \lim_{x\to\infty} g(x) &= 1. \end{cases}$$

Assuming that f_0 has a bounded derivative (which is trivial in our example), the so-called asymptotic expansion of zeroth order

$$f_\varepsilon(x) = \left(g\left(\tfrac{x}{\varepsilon}\right) - 1\right) f_0(0) + f_0(x) + \mathcal{O}(\varepsilon)$$

is expected to hold. We call $\left(g\left(\frac{x}{\varepsilon}\right) - 1\right) f_0(0)$ the inner function and see that it solely has a significant influence on the solution in the boundary layer $[0, \varepsilon]$. For $x > \varepsilon$, the contribution of the inner function vanishes and the behavior is dominated by the so-called outer function f_0. In fact, it is easily seen that even the approximation $f_\varepsilon(x) = -\exp\left(-\frac{x}{\varepsilon}\right) + 1 + \mathcal{O}(\exp(-\varepsilon^{-1}))$ holds in our example.
The objective of this thesis is to perform a boundary layer analysis for the systems of equations under consideration. As indicated in our example, the formation of boundary layers is not mandatory, but a consequence of the choice of boundary values. In [BCD], S. Bian, L. Chen and M. Dreher have shown that solutions to the quasi 1D approximation (1) of the bipolar quantum drift-diffusion equations exist for the boundary values

$$n(0) = 0, \quad n(1) = n_B, \quad V'(0) = \beta(V(0) - V_{GS}), \quad V(1) = V_B, \quad F = V_B + T_n \ln(n_B).$$

The boundary value $n(0) = 0$ leads to a singularity in the differential equations, which yields the formation of a boundary layer near $x = 0$. In [BCD] it has been shown that a solution n_* to the formal limiting equations exists, which describes the zeroth order asymptotic expansion of $\varrho_\varepsilon = \sqrt{n_\varepsilon}$ by means of

$$\varrho_\varepsilon = \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + R_\varepsilon$$

for $\varrho_0 = \sqrt{n_*}$ and a certain function Z_0 admitting $Z_0(0) = 0$ and $\lim_{y\to\infty} Z_0(y) = 1$ exponentially fast. It has been shown that the remainder R_ε actually decays with rate ε^1 in the norm of $L^2(0,1)$. Due to the great technical difficulties, only an estimate $\|R_\varepsilon\|_{L^\infty(0,1)} \le C\varepsilon^{3/4}$ was established for the L^∞-norm at this point. By extending the results of [BCD] to a first order asymptotic expansion

$$\varrho_\varepsilon = \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon \varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right) + \mathcal{O}(\varepsilon^{3/2})$$

with certain functions ϱ_1 and Z_1, we rigorously prove the optimality of the rate ε^1 for the remainder terms R_ε for both the L^2- and the L^∞-norm. The derivation of differential equations describing ϱ_1 and Z_1 and the corresponding existence results are carried out in Chapter 4. The

main results on the first order asymptotic expansion are summarized in Corollary 4.12.
The reformulation (2) gives opportunity to prove the solvability of our variant of the viscous quantum hydrodynamic model for Dirichlet boundary conditions (Lemma 2.9), homogeneous Neumann boundary conditions (Lemma 2.13) and periodic boundary conditions (Lemma 2.14) for the electron densities n and constant Fermi levels F. For periodic boundary conditions and homogeneous Neumann boundary conditions, we also consider the case, when the total mass of electrons $\int_0^1 n(x)\,dx$ in the device is a prescribed quantity (Lemma 2.17 and Lemma 2.18). By means of fixed point arguments, we extend the results for periodic boundary conditions and prescribed masses to arbitrary large, non-constant Fermi levels (Lemma 2.21). An analogous result for homogeneous Neumann boundary conditions was derived under a smallness condition on the Fermi levels (Lemma 2.29).
We perform a boundary layer analysis for the electron densities $n = n_\kappa$ in the case of constant Fermi levels F. For the electron densities, we consider periodic boundary conditions and homogeneous Neumann boundary conditions. In contrast to the situation of the quasi 1D approximation of the bipolar quantum drift-diffusion model, boundary layers do not result from the choice of zero boundary values at the endpoints of the interval. We consider the case of piecewise constant barrier potentials V_B and show that boundary layers emerge at any point s_0 of jump discontinuity of V_B. In terms of the characteristic parameter $\kappa = \varepsilon^2 + \nu^2$, we establish uniform upper and lower bounds to the electron densities $n = n_\kappa$ for a large class of pressure terms p. Considering the roots $u_\kappa = \sqrt{n_\kappa}$, pointwise convergence of u_κ to a limiting function u_0 and strong convergence of the electric potentials V_κ are established in Lemma 3.8 and Lemma 3.6, respectively. A subsequent discussion elaborates the details of the boundary layer analysis. An intermediate result then locally reads as

$$u_\kappa(s_0 + \cdot) = \frac{u_0(s_0 + \cdot)}{u_0(s_0+)} w\left(\frac{\cdot}{\kappa^{1/2}} + c_\kappa\right) + \mathcal{O}(\kappa^{1/8})$$

for a certain function $w : (0, \infty) \longrightarrow \mathbb{R}$ and uniquely given positive constants c_κ. A unified representation results in the zeroth order asymptotic expansion

$$u_\kappa = \frac{u_0}{c_0} W_\kappa + R_\kappa$$

with a remainder term fulfilling $\|R_\kappa\|_{L^2(0,1)} \leq C\kappa^{1/2}$ and $\|R_\kappa\|_{L^\infty(0,1)} \leq C\kappa^{1/4}$ (Lemma 3.20).
This thesis is structured as follows:
The derivation and motivation of the semiconductor models under consideration are carried out in **Chapter 1**. The existence results on the stationary one-dimensional viscous quantum hydrodynamic model are discussed in **Chapter 2**. We give the definition of a solution to our model and introduce conditions on the given data and the pressure term. A reformulation of the system of equations in terms of a viscosity-adjusted Fermi level is the starting point for the solvability results presented. We consider the cases of constant Fermi levels with periodic boundary conditions, homogeneous Neumann boundary conditions and Dirichlet boundary conditions for the electron densities, respectively. The existence of solutions for arbitrary large non-constant Fermi levels is proven by fixed point arguments for periodic boundary conditions and prescribed total masses for the electron densities n. An analogous result for small non-constant Fermi levels is also elaborated for homogeneous Neumann boundary conditions. In all cases, the electric potential V admits prescribed Dirchlet boundary values. In **Chapter 3**, the dependency of solutions on the characteristic parameter $\kappa = \varepsilon^2 + \nu^2$ is investigated. We establish uniform estimates for the electron densities, which render it possible to construct the zeroth order asymptotic expansion of these functions. A rigorous analysis proves the convergence of the potentials V_κ to a

limiting function V_0 and examines the rates of the remainders of the zeroth order approximations in different norms. In **Chapter 4**, the stationary bipolar quantum drift-diffusion model is considered. We will present the main results of the paper [BCD] in which the zeroth order asymptotic expansion of the electron densities was established. Differential equations describing the first order approximations are derived and a subsequent discussion verifies that their solutions actually extend the asymptotic expansion. We also provide numerical results which indicate that the first order asymptotic approximations are optimal.
The presentation of this thesis follows the usual notations and conventions. A summary of the appearing spaces and utilised theorems is given in the **Appendix**. Throughout this thesis, the symbol C denotes a generic positive constant, i.e. C stands for a positive constant whose value may change from line to line but which is independent from the relevant objects. To present certain calculations in a more traceable way, we will sometimes introduce further constants $C_0, C_1, \dots$ (or similar). They stand for the same value at each appearance and may be incorporated into the symbol C at a later point in time. Unless otherwise specified, the Landau notation $\mathcal{O}(\cdot)$ refers to the L^∞-norm on the relevant domain.

Chapter 1

Derivation of Two semiconductor models

A fundamental approach to describe the electron flow in electronic devices is given by the many-particle Schrödinger equation

$$\begin{cases} i\hbar\partial_t\psi(t,x) &= -\frac{\hbar^2}{2m}\sum_{j=1}^M \Delta_{x_j}\psi(t,x) - qV(t,x)\psi(t,x), \quad (t,x)\in\mathbb{R}\times\Omega^M, \\ \psi(0,x) &= \psi_0(x), \quad x\in\Omega^M \end{cases}$$

in a domain $\Omega \subset \mathbb{R}^d$ with a given electric potential $V : \mathbb{R}\times\Omega^M \longrightarrow \mathbb{R}$ and inital state $\psi_0 : \Omega^M \longrightarrow \mathbb{C}$. The constants $\hbar, m$ and q stand for the Planck constant, the mass and the charge of a single particle, respectively. A solution $\psi : \mathbb{R}\times\Omega^M \longrightarrow \mathbb{C}$ is called the wave function to the ensemble of M particles.

A universal problem of many-particle systems is that they are inapplicable in many situations. In particular, this applies to numerics, since the number of particles M is usually very large. Therefore, several macroscopic reformulations, approximations and generalisations of the Schrödinger equation have been recently considered, involving quantum mechanical, kinetic, and fluid-dynamical viewpoints. In this thesis, we will discuss two models for the distribution of charged particles in semiconductor devices arising from fluid-dynamical approaches. This chapter gives a brief and rather formal derivation of these models. We follow the textbook [Ju] of A. Jüngel and the review paper [CD] of L. Chen and M. Dreher, where a comprehensive presentation of the hierarchy of fluid-dynamical quantum semiconductor models was given. For the results of the subsequent section, we also refer to the Chapters 1.4 and 1.5 of the textbook [MRS] by P.A. Markowich, C.A. Ringhofer and C. Schmeiser.

1.1 From the Schrödinger equation to a macroscopic description

By a scaling of the variables in the Schrödinger equation, we may assume $m = 1$, $q = 1$ and replace $\hbar$ by some scaled constant ε. A reformulation of the Schrödinger equation by means of the propability density matrix

$$\varrho(t,r,s) = \overline{\psi(t,r)}\psi(t,s), \quad (t,r,s)\in\mathbb{R}\times\mathbb{R}^{dM}\times\mathbb{R}^{dM},$$

is then given by the Heisenberg equation

$$\begin{cases} i\varepsilon\partial_t\varrho(t,r,s) &= (H_s - H_r)\varrho(t,r,s), \quad (t,r,s)\in\mathbb{R}\times\mathbb{R}^{dM}\times\mathbb{R}^{dM}, \\ \varrho(0,r,s) &= \overline{\psi_0(r)}\psi_0(s), \quad (r,s)\in\mathbb{R}^{dM}\times\mathbb{R}^{dM}, \end{cases}$$

where H denotes the Hamilton operator defined by

$$H_x = -\frac{\varepsilon^2}{2}\sum_{j=1}^{M}(\Delta_{x_j} - V(t,x)), \quad (t,x) \in \mathbb{R} \times \mathbb{R}^{dM}.$$

The objective of the following discussion is to transform the Heisenberg equation into the phase space by considering the Wigner transform

$$w(t,x,v) = \frac{1}{(2\pi)^{dM}} \int_{\mathbb{R}^{dM}} e^{i\eta v} \varrho\left(t, x + \tfrac{\varepsilon}{2}\eta, x - \tfrac{\varepsilon}{2}\eta\right)\, d\eta, \quad (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^{dM} \times \mathbb{R}^{dM}.$$

At this point, we will also make use of certain physical assumptions and approximations which are appropriate in the situation of electron flow through semiconductor devices. The main assumption is, that the material under consideration has a periodic structure so that the potential V is essentially given as a periodic function as well. It is a characteristic property of semiconductor materials that the range of energies E, which fulfill the eigenvalue equations

$$H\psi = E\psi$$

for some wave function ψ, exhibits so-called energy gaps, so that the set of all admissible energies of the system consists of energy bands E_n which are disjoint intervals in $\mathbb{R}$. Considering a fixed energy gap, the first energy band above this gap is called the conduction band, whereas the first energy band below the gap is refered to as the valance band. We now consider wave vectors k in a vicinity of a local minimum of a conduction band. After shifting, we may assume that the minimum is attained at $k = 0$ and $E_n(0) = 0$. For small k, we may employ Taylor's formula to deduce

$$E_n(k) = E_n(0) + \nabla_k E_n(0) \cdot k + \frac{1}{2} k^t \left(\frac{d^2}{dk^2} E_n(0) \right) k + \mathcal{O}(|k|^3).$$

The matrix $m^* := \frac{d^2}{dk^2} E_n(0)$ represents an effective mass. Since it is positive definite, we may assume, after a change of coordinates, that it is diagonal. Supposing the isotropic situation, i.e. the entries of the matrix are equal, we may identify the effective mass with a scalar and deduce the parabolic band approximation

$$E_n(k) = \frac{\hbar^2}{2m^*}|k|^2,$$

which describes the dispersion relation of a free electron gas with the electron rest mass m replaced by the effective mass m^*. In this case, the mean velocity $\frac{1}{\hbar}\nabla_k E_n(k)$ simplifies to $\frac{\hbar}{m^*}k$. Multiplying the mean velocity by the effective mass then yields the crystal momentum $v = \hbar k$. It can be shown that the Wigner-function w is a solution to the quantum Liouville equation

$$\begin{cases} \partial_t w(t,x,v) + v \cdot \nabla_x w(t,x,v) + (\theta[V]w)(t,x,v) = 0, & (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^{dM} \times \mathbb{R}^{dM}, \\ w(0,x,v) = w_0(x,v), & (x,v) \in \mathbb{R}^{dM} \times \mathbb{R}^{dM}, \end{cases}$$

where $\theta[V]$ denotes the pseudodifferential operator

$$(\theta[V]w)(t,x,v) := \frac{1}{(2\pi)^{dM}} \int_{\mathbb{R}^{dM}} \int_{\mathbb{R}^{dM}} e^{i\eta(v-v')} \delta V(t,x,\eta) w(t,x,v')\, dv'\, d\eta,$$

$(t,x,\eta) \in \mathbb{R}_+ \times \mathbb{R}^{dM} \times \mathbb{R}^{dM}$, corresponding to the symbol δV

$$\delta V(t,x,\eta) := \frac{i}{\varepsilon}\left(V(t,x+\tfrac{\varepsilon}{2}\eta) - V(t,x-\tfrac{\varepsilon}{2}\eta)\right), \quad (t,x,\eta) \in \mathbb{R}_+ \times \mathbb{R}^{dM} \times \mathbb{R}^{dM}.$$

We mention that this symbol converges, at least formally, to $i\nabla_x V \cdot \eta$ as ε approaches zero. Then the quantum Liouville equation formally passes to the classical Liouville equation, where the expression $\theta[V]w$ turns into $\nabla_x V \cdot \nabla_v w$. We refer to [Ju, Chapt. 11.1] for some further references. The quantum Liouville equation is still a many-particle system. In order to obtain a macroscopic description, several additional assumptions are imposed:

(i) The potential decomposes into an external potential V_{ext} and internal potentials V_{inter} describing the interactions between pairs of particles:

$$V(t,x_1,\ldots,x_M) = \sum_{j=1}^{M} V_{ext}(t,x_j) + \frac{1}{2}\sum_{i,j=1}^{M} V_{inter}(x_i,x_j), \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^{dM},$$

and $V_{inter}(x_i,x_j) = V_{inter}(x_j,x_i) = \mathcal{O}(1/M)$ for $i,j = 1,\ldots,M$.

(ii) The particles are indistinguishable, meaning that for all permutations $\pi \in S_M$ it holds

$$\psi(t,x_1,\ldots,x_M) = \operatorname{sgn}(\psi)\psi(t,x_{\pi(1)},\ldots x_{\pi(M)})$$

for $(t,x) \in \mathbb{R}_+ \times \mathbb{R}^{dM}$.

(iii) For $m = 1,\ldots,M-1$, the subensemble density matrices

$$\begin{aligned}&\varrho^{(m)}(t,r_1,\ldots r_m,s_1,\ldots,s_m)\\ := &\int_{\mathbb{R}^{d(M-m)}} \varrho(t,r_1,\ldots,r_m,z_{m+1},\ldots,z_M,s_1,\ldots,s_m,z_{m+1},\ldots,z_M)\,dz_{m+1}\,\ldots dz_M,\end{aligned}$$

$(t,r_1,\ldots,r_M,s_1,\ldots,s_M) \in \mathbb{R}_+ \times \mathbb{R}^{dm} \times \mathbb{R}^{dm}$, initially fulfill the Hartree ansatz, i.e. at time $t=0$ they can be factorised into

$$\varrho^{(m)}(0,r_1,\ldots,r_m,s_1,\ldots,s_m) = \prod_{j=1}^{m} R_0(r_j,s_j),$$

$(r_1,\ldots,r_m,s_1,\ldots,s_m) \in \mathbb{R}^{dm} \times \mathbb{R}^{dm}$.

It can be shown that the third condition is also fulfilled for $t > 0$, i.e. there exists a factorising function R such that

$$\varrho^{(m)}(t,r_1,\ldots,r_m,s_1,\ldots,s_m) = \prod_{j=1}^{m} R(t,r_j,s_j)$$

for $(t,r_1,\ldots,r_m,s_1,\ldots,s_m) \in [0,\infty) \times \mathbb{R}^{dm} \times \mathbb{R}^{dm}$. More precisely, R is determined by the equation

$$i\varepsilon\partial_t R(t,r,s) = -\frac{\varepsilon^2}{2}(\Delta_r - \Delta_s)R(t,r,s) - (V_{\text{eff}}(r,t) - V_{\text{eff}}(s,t))R(t,r,s),$$

$(t,r,s) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d$, where the effective potential V_{eff} is given by

$$V_{\text{eff}}(t,x) := V_{ext}(x) + \int_{\mathbb{R}^d} n(t,z) V_{inter}(x,z)\, dz, \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d,$$

with the quantum electron density $n(t,x) = MR(t,x,x)$, $(t,x) \in \mathbb{R}_+ \times \mathbb{R}^d$. Then,

$$W(t,x,v) := \frac{M}{(2\pi)^d} \int_{\mathbb{R}^d} e^{i\eta v} R\left(t, x + \tfrac{\varepsilon}{2}\eta, x - \tfrac{\varepsilon}{2}\eta\right)\, d\eta, \quad (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d,$$

is a solution to the quantum Vlasov equation

$$\begin{cases} \partial_t W(t,x,v) + v \cdot \nabla_x W(t,x,v) - \left(\theta[V_{\text{eff}}]W\right)(t,x,v) &= 0, \quad (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d, \\ W(0,x,v) &= W_0(x,v), \quad (x,v) \in \mathbb{R}^d \times \mathbb{R}^d, \end{cases}$$

for the pseudodifferential operator $\theta[V_{\text{eff}}]$,

$$\left(\theta[V_{\text{eff}}]w\right)(t,x,v) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} e^{i\eta(v-v')} \delta V_{\text{eff}}(t,x,\eta) w(t,x,v')\, dv'\, d\eta,$$

$(t,x,\eta) \in \mathbb{R}_+ \times \mathbb{R}^{dM} \times \mathbb{R}^{dM}$, with symbol

$$\delta V_{\text{eff}}(t,x,\eta) := \frac{i}{\varepsilon} \left(V_{\text{eff}}(t, x + \tfrac{\varepsilon}{2}\eta) - V_{\text{eff}}(t, x - \tfrac{\varepsilon}{2}\eta) \right), \quad (t,x,\eta) \in \mathbb{R}_+ \times \mathbb{R}^{dM} \times \mathbb{R}^{dM}.$$

Usually, the internal potential is given by Coulomb's law,

$$V_{inter}(x,y) = V_{Coulomb}(x,y) = -\frac{4}{\pi\varepsilon_s} \frac{1}{|x-y|}, \quad (x,y) \in \mathbb{R}^3 \times \mathbb{R}^3,$$

with a constant ε_s which depends on the electric permittivity of the semiconductor material. In this situation, the effective potential is a solution to the Poisson equation

$$\varepsilon_s \Delta V_{\text{eff}}(t,x) = n(t,x) - \mathcal{C}(x), \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^3,$$

where the function $\mathcal{C} = -\varepsilon_s \Delta V_{ext}$ specifies the doping profile of the semiconductor. We obtain the quantum Vlasov-Poisson system, which already represents a macroscopic model for the particle flow in the semiconductor and which also includes quantum effects and electrostatic interactions. We are now in the position to derive the two models which are considered in this thesis. We augment the quantum Vlasov-Poisson system with a nonlinear right hand side $Q(W)$, which describes short-range interactions between particles, like collisions, and obtain the quantum Boltzmann equation

$$\begin{cases} \partial_t W(t,x,v) + v \cdot \nabla_x W(t,x,v) - \left(\theta[V_{\text{eff}}]W\right)(t,x,v) &= Q(W), \quad (t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d, \\ W(0,x,v) &= W_0(x,v), \quad (x,v) \in \mathbb{R}^d \times \mathbb{R}^d, \end{cases}$$

coupled to the Poisson equation

$$\varepsilon_s \Delta V_{\text{eff}}(t,x) = n(t,x) - \mathcal{C}(x), \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d.$$

1.2 The viscous quantum hydrodynamic equations

The origin for the derivation of the viscous quantum hydrodynamic equations is given by the quantum Boltzmann equation supplied with the Fokker-Planck collision operator

$$Q(W) = \frac{1}{\tau_0} \operatorname{div}_v \left(c_1 \nabla_v W + vW \right) + \frac{1}{\tau_0} \operatorname{div}_x \left(c_2 \nabla_v W + c_3 \nabla_x W \right)$$

for certain physical constants $c_1, \dots, c_3 > 0$ and a relaxation time parameter $\tau_0 > 0$. The following argumentations are meant to be a brief and formal derivation of the model which is considered in Chapter 2 and Chapter 3. Therefore, some aspects of the physical motivation are disregarded. The main modification to the quantum Boltzmann equation is a reformulation by means of the moments

$$\begin{aligned} n(t,x) &= \int_{\mathbb{R}^d} W(t,x,v)\, dv, \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d, \\ J(t,x) &= -\int_{\mathbb{R}^d} vW(t,x,v)\, dv, \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d, \\ (ne)(t,x) &= \frac{1}{2} \int_{\mathbb{R}^d} |v|^2 W(t,x,v)\, dv, \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d. \end{aligned}$$

It should be mentioned that these functions can be interpreted as the particle density, the current density and the energy density, respectively. In the following discussion, the formal abbreviation

$$\langle f \rangle (t,x) := \int_{\mathbb{R}^d} f(v) W(t,x,v)\, dv, \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d$$

will be used. Integrating the quantum Boltzmann equation over $\mathbb{R}^d$ with respect to the variable v and assuming that W and it's derivatives decay sufficiently fast for $|v| \to \infty$, we obtain

$$\partial_t n(t,x) - \operatorname{div}_x J(t,x) + \int_{\mathbb{R}^d} \left(\theta[V] W \right)(t,x,v)\, dv = \nu_0 \Delta_x n(t,x), \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d,$$

where $\nu_0 = \frac{c_3}{\tau_0}$. Writing $\hat{W}$ for the Fourier transform of W with respect to the velocity variable v, the pseudodifferential operator calculus yields

$$\int_{\mathbb{R}^d} \left(\theta[V] W \right)(t,x,v)\, dv = (2\pi)^{d/2} \Big((\delta V)(t,x,\eta) \hat{W}(t,x,\eta) \Big) \Big|_{\eta=0} = 0$$

and we deduce the equation

$$\partial_t n - \operatorname{div} J = \nu_0 \Delta n.$$

Multiplying the quantum Boltzmann equation by v and integrating over $\mathbb{R}^d$ yields

$$-\partial_t J + \operatorname{div}_x \langle v \otimes v \rangle - n \nabla_x V = -\nu_0 \Delta_x J - \nu_2 \nabla_x n + \frac{J}{\tau_0},$$

where $\nu_2 = \frac{c_2}{\tau_0}$, and using $\frac{1}{2}|v|^2$ as a multiplicator, we obtain

$$\partial_t (ne) + \operatorname{div}_x \left\langle \frac{1}{2} v |v|^2 \right\rangle + \nabla V \cdot J = -\frac{2}{\tau_0} ne + \frac{d c_1}{\tau_0} n + \frac{c_2}{\tau_0} \operatorname{div} J + \nu_0 \Delta (ne).$$

At this point, it seems to be unachieveable to rewrite the expressions $\langle v \otimes v \rangle$ and $\left\langle \frac{1}{2} v |v|^2 \right\rangle$ in terms of the moments n, J and ne. As a consequence, we impose so-called closure conditions.

These additional physical assumptions render it possible to express the last two equations solely in terms of the potential V and the functions n, J and ne. We now demand W to coincide with the thermal equilibrium density W_{eq} up to a shift in the velocity variable v, so that

$$W(t,x,v) = W_{eq}(t,x,v-u(t,x)), \quad (t,x) \in \mathbb{R}_+ \times \mathbb{R}^d,$$

with an unknown function u. The thermal equilibrium density is the minimizer of the quantum entropy functional, which will be briefly introduced below. Let $\mathrm{Op}(k)$ be the linear operator defined by the convolution

$$(\mathrm{Op}(k)\varphi)(x) := \int_{\mathbb{R}^d} k(x,y)\varphi(y)\,dy, \quad x \in \mathbb{R}^d, \varphi \in \mathcal{S}(\mathbb{R}^d),$$

where $k : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow \mathbb{R}$ is a sufficiently regular function. The Schwartz kernel theorem (c.f. [Ho, Thm. 5.2.1]) states that Op is an isomorphism. Writing

$$(\mathcal{W}(\varrho))(x,v) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{i\eta v} \varrho\left(x + \tfrac{\varepsilon}{2}\eta, x - \tfrac{\varepsilon}{2}\eta\right) d\eta, \quad (x,v) \in \mathbb{R}^d \times \mathbb{R}^d, \tag{1.1}$$

for the Wigner transform of a sufficiently regular function ϱ it is seen that the inverse of $\mathcal{W}$ is given by

$$(\mathcal{W}^{-1}(\varrho))(x,y) = \int_{\mathbb{R}^d} e^{\frac{i}{\varepsilon}v(x-y)} w\left(\tfrac{x+y}{2}, v\right) dv.$$

The quantum logarithm and the quantum exponential are then defined via the spectral theorem by

$$\begin{aligned} \mathrm{LN}(w) &:= \mathcal{W}\left(\mathrm{Op}^{-1}(\ln \mathrm{Op}(\mathcal{W}^{-1}(w)))\right), \\ \mathrm{EXP}(w) &:= \mathcal{W}\left(\mathrm{Op}^{-1}(\exp \mathrm{Op}(\mathcal{W}^{-1}(w)))\right), \end{aligned}$$

for all w for which $\mathrm{Op}(\mathcal{W}^{-1}(w))$ is self-adjoint and positive definite. The quantum entropy functional is given by

$$H(w) := \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} w(x,v)\left((\mathrm{LN}(w))(x,v) - 1 + \tfrac{1}{2}|v|^2 - V(x)\right) dx\,dv.$$

Its minimizer admits the representation $W_{eq}(t,x,v) = \mathrm{EXP}\left(A(t,x) - \frac{|v|^2}{2T(t,x)} + \frac{V(t,x)}{T(t,x)}\right)$ for a certain function $A : \mathbb{R}_+ \times \mathbb{R}^d \longrightarrow \mathbb{R}$ and where $T : \mathbb{R}_+ \times \mathbb{R}^d \longrightarrow \mathbb{R}$ denotes the electron temperature. We wish to replace the quantum exponential by a more explicit representation. In [DMR] it has been proven with considerable technical effort that the approximation

$$W_{eq} = \exp\left(A - \frac{|v|^2}{2T} + \frac{V}{T}\right)\left(1 + \frac{\varepsilon^2}{8T}\Delta_x V + \frac{\varepsilon^2}{24T^3}|\nabla_x V|^2 - \frac{\varepsilon^2}{24T^3}\sum_{i,j=1}^d v_i v_j \partial_{x_i}\partial_{x_j} V + \mathcal{O}(\varepsilon^4)\right)$$

is satisfied. Assuming that A varies rather slowly and that T is positive, it is possible to compute the relations

$$\begin{aligned} n &= (2\pi T)^{d/2} A \exp\left(\frac{V}{T}\right)\left(1 + \frac{\varepsilon^2}{12T^2}\Delta V + \frac{\varepsilon^2}{24T^3}|\nabla V|^2\right) + \mathcal{O}(\varepsilon^4), \\ J &= -nu, \\ \langle v \otimes v \rangle &= nu \otimes u + nT\,\mathrm{id}_{\mathbb{R}^d} - \frac{\varepsilon^2}{12T} n \,(\nabla \otimes \nabla)\, V + \mathcal{O}(\varepsilon^4), \\ \left\langle v|v|^2 \right\rangle &= nu|u|^2 + \left(dT - \frac{\varepsilon^2}{12T}\Delta V\right) + 2\left(T\,\mathrm{id}_{\mathbb{R}^d} - \frac{\varepsilon^2}{12T}(\nabla \otimes \nabla)\, V\right) nu + \mathcal{O}(\varepsilon^4). \end{aligned}$$

From a physical point of view it is also desirable to drop the dependency on the second order derivatives of the potential V, which appear in the last two expressions. Taking the first equation into account, we formally approximate

$$\ln(n) = \ln\left((2\pi T)^{d/2} A\right) + \frac{V}{T} + \mathcal{O}(\varepsilon^2).$$

Assuming that A and T vary only very slowly, we expect

$$\partial_j \partial_k \ln(n) = \frac{1}{T}\partial_j \partial_k V + \mathcal{O}(\varepsilon^2).$$

Dropping the terms of order $\mathcal{O}(\varepsilon^2)$, we obtain, after rescaling, the full viscous quantum hydrodynamic system

$$\begin{cases} \partial_t n - \operatorname{div} J &= \nu \Delta n, \\ \partial_t J - \operatorname{div}\left(\frac{J\otimes J}{n}\right) - \nabla(Tn) + n\nabla V + \frac{\varepsilon^2}{6} n \nabla \frac{\Delta\sqrt{n}}{\sqrt{n}} &= \nu\Delta J - \frac{J}{\tau} + \mu \nabla n, \\ \partial_t(ne) - \operatorname{div}\left(\frac{J}{n}(ne + P)\right) + J\cdot\nabla V &= -\frac{2}{\tau}\left(ne - \frac{d}{2}n\right) + \nu\Delta(ne) + \mu \operatorname{div} J, \\ \lambda^2 \Delta V &= n - \mathcal{C} \end{cases}$$

with a constant $\mu > 0$ proportional to $\frac{\nu}{\varepsilon}$ (c.f. [JuMi] for the details of the scaling). Here, the pressure tensor P and the energy density ne are given by

$$P = Tn \operatorname{id}_{\mathbb{R}^d} - \frac{\varepsilon^2}{12} n \left(\nabla \otimes \nabla\right) \ln(n)$$

and

$$ne = \frac{|J|^2}{2n} + \frac{d}{2}Tn - \frac{\varepsilon^2}{24} n \Delta \ln(n).$$

The model was introduced by F. Castella, L. Erdös, F. Frommlet and P. A. Markowich in [CEFM]. It describes a viscous variant of the quantum hydrodynamic equations of C. L. Gardner [Ga]. We now assume the following situation:

(i) The underlying domain is the one-dimensional interval $[0, 1]$.

(ii) The stationary case is considered so that all time derivatives vanish from the equations.

(iii) The electron temperature T is assumed to depend on the electron density n only by means of a relation of the form $T = T_0 n^{\gamma-1}$ for a positive constant T_0 and some $\gamma \geq 1$.

(iv) An additional barrier potential V_B is introduced into the second equation.

The assumption that the electron temperature is given as a function of n now implies that the third equation decouples from the system and can be omitted. Additionally, we merge the pressure terms Tn and μn appearing in the second equation into a universal pressure term $p(n)$. Then the model, which is considered in Chapter 2 and Chapter 3, reads as

$$\begin{cases} J' &= -\nu n'', \\ 2\varepsilon^2 n \left(\frac{\sqrt{n}''}{\sqrt{n}}\right)' - \nu J'' - (p(n))' + \frac{1}{\tau} J &= \left(\frac{J^2}{n}\right)' - n(V + V_B)', \\ \lambda^2 V'' &= n - \mathcal{C}. \end{cases}$$

The motivation of the additional barrier potential V_B is the modeling of distinct materials in the semiconductor devices. Since in general the barrier potential will not be continuous at the interfaces between different materials, we have to consider the case of V_B being a non-smooth function. Then, the second equation has to be understood in a formal sense. A suitable weak definition of this equality will be introduced in Chapter 2.

1.3 The quantum drift-diffusion equations

The quantum drift-diffusion model principally focuses on the situation when many collisions between particles occur in the relevant time interval. We equip the quantum Boltzmann equation with the relaxation-type collision operator

$$Q(W) = M[W] - W,$$

where the quantum Maxwellian $M[W]$ will be introduced in the following.
As in the derivation of the viscous quantum hydrodynamic equations, let $\mathcal{W}$ denote the Wigner transform (1.1) and let the quantum logarithm and the quantum exponential be given by

$$\begin{aligned} \mathrm{LN}(w) &:= \mathcal{W}\left(\mathrm{Op}^{-1}(\ln \mathrm{Op}(\mathcal{W}^{-1}(w)))\right), \\ \mathrm{EXP}(w) &:= \mathcal{W}\left(\mathrm{Op}^{-1}(\exp \mathrm{Op}(\mathcal{W}^{-1}(w)))\right), \end{aligned}$$

for all w for which $\mathrm{Op}(\mathcal{W}^{-1}(w))$ is self-adjoint and positive definite. We recall the quantum entropy

$$H(w) = \int_{\mathbb{R}^d}\int_{\mathbb{R}^d} w(x)\left((\mathrm{LN}(w))(x) - 1 + \tfrac{1}{2}|v|^2 - V(x)\right)\, dx\, dv$$

and define $M[W]$ to be the unique minimizer (if it exists) of this functional with respect to the constraint

$$\int_{\mathbb{R}^d} M[W](x,v)\, dv = \int_{\mathbb{R}^d} W(x,v)\, dv, \quad x \in \mathbb{R}^d.$$

Considering the Euler-Lagrange equation of the functional, it is seen that $M[W]$ has the representation

$$M[W] = \mathrm{EXP}(A - \tfrac{1}{2}|v|^2)$$

for the function $A = V - \lambda^*$, where λ^* arises as the Lagrange multiplier due to the integral constraint given above. A rescaling of the quantum Boltzmann equation by substituting t by $\frac{t}{\delta}$ and $Q(W)$ by $\frac{Q(W)}{\delta}$ for a small parameter $\delta > 0$ yields the system

$$\left\{\begin{aligned} \delta\partial_t W_\delta(t,x,v) + v\cdot\nabla_x W_\delta(t,x,v) - (\theta[V_{\mathrm{eff}}]W_\delta)(t,x,v) &= \tfrac{1}{\delta}\left(M[W_\delta] - W_\delta\right), \\ \varepsilon_s \Delta V_{\mathrm{eff}}(t,x) &= n(t,x) - \mathcal{C}(x), \\ W_\delta(0,x,v) &= W_0(x,v) \end{aligned}\right.$$

for $(t,x,v) \in \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d$ and $n(t,x) = \int_{\mathbb{R}^d} W(t,x,v)\, dv$. The physical meaning of the rescaling is, that the collisions should have a significant impact on the behavior of the particle flow and that the corresponding time periods are large.
It is now possible to perform the limit $\delta \to 0$ at least formally and the resulting system reads as

$$\left\{\begin{aligned} \partial_t n - \operatorname{div} J &= 0, \\ J &= \operatorname{div} P - n\nabla V, \\ n &= \int_{\mathbb{R}^d} W_0(\cdot, v)\, dv, \\ P &= \int_{\mathbb{R}^d} v\otimes v W_0(\cdot,v)\, dv, \\ \lambda^2 \Delta V(t,x) &= n(t,x) - \mathcal{C}(x), \end{aligned}\right. \tag{1.2}$$

with

$$W_0(t,x,v) = \mathrm{EXP}(A(t,x) - \tfrac{1}{2}|v|^2)$$

and the renaming $\lambda^2 = \varepsilon_s$. The quantum drift-diffusion model is finally obtained by an approximation of the quantum exponential. We refer to [DMR] for the expansion

$$\mathrm{EXP}\left(A - \frac{1}{2}|v|^2\right) = \exp\left(A - \frac{1}{2}|v|^2\right)\left(1 + \frac{\varepsilon^2}{8}\left(\Delta A + \frac{1}{3}|\nabla A|^2 - \frac{1}{3}v^t D^2 A v\right)\right) + \mathcal{O}(\varepsilon^4)$$

and conclude the approximations

$$\begin{aligned} n &= (2\pi)^{d/2}\exp(A) + \mathcal{O}(\varepsilon^2), \\ \operatorname{div} P &= \nabla n - \frac{\varepsilon^2}{12} n \nabla\left(\Delta A + \frac{1}{2}|\nabla A|^2\right) + \mathcal{O}(\varepsilon^4), \\ \nabla A &= \frac{\nabla n}{n} + \mathcal{O}(\varepsilon^2). \end{aligned}$$

As a result, the quantum drift-diffusion model

$$\left\{ \begin{aligned} \partial_t n - \operatorname{div} J_0 &= 0, \\ J_0 &= \nabla n - n\nabla V - \tfrac{\varepsilon^2}{6} n \nabla\left(\tfrac{\Delta\sqrt{n}}{\sqrt{n}}\right), \\ \lambda^2 \Delta V(t,x) &= n(t,x) - \mathcal{C}(x) \end{aligned} \right. \tag{1.3}$$

is an approximation of the system (1.2), at least formally, in the following sense: If (n, J, V) is a solution of (1.2) and (n, J_0, V) is a solution of the quantum drift-diffusion model (1.3) for the same electron density n, then $J = J_0 + \mathcal{O}(\varepsilon^4)$. A higher universality is achieved by the bipolar quantum drift-diffusion model

$$\left\{ \begin{aligned} n_t &= \operatorname{div}\left(-\varepsilon^2 n \nabla \tfrac{\Delta\sqrt{n}}{\sqrt{n}} + \nabla P_n(n) - n\nabla V\right), \\ p_t &= \operatorname{div}\left(-\xi\varepsilon^2 p \nabla \tfrac{\Delta\sqrt{p}}{\sqrt{p}} + \nabla P_P(p) + p\nabla V\right), \\ \lambda^2 \Delta V &= n - p - \mathcal{C}, \end{aligned} \right.$$

where also the positive charges (holes) are modeled and more general pressure terms P_n, P_p are considered. We mention the most relevant choices $P_n(n) = T_n n^\alpha$, $P_p(p) = T_p p^\beta$ for $\alpha, \beta \geq 1$ with lattice temperatures $T_n, T_p > 0$. The case $\alpha, \beta = 1$ is called the isothermal case, whereas the choices $\alpha, \beta > 1$ are refered to as the isentropic cases. Here, ξ is the ratio of the effective masses of electrons and holes. We now focus on the stationary case, where all time derivatives in the equations vanish. The following stationary bipolar quantum drift-diffusion model

$$\left\{ \begin{aligned} F &= V + h_n(n) - \varepsilon^2 \tfrac{\Delta\sqrt{n}}{\sqrt{n}}, \\ G &= -V + h_p(p) - \xi\varepsilon^2 \tfrac{\Delta\sqrt{p}}{\sqrt{p}}, \\ \operatorname{div}(\mu_n n \nabla F) &= R_0(n,p) R_1(F,G), \\ \operatorname{div}(-\mu_p p \nabla G) &= -R_0(n,p) R_1(F,G), \\ -\lambda^2 \Delta V &= n - p - \mathcal{C}, \end{aligned} \right.$$

is also refered to as the density gradient model. It introduces generation/recombination effects by the coupling with the algebraic functions R_0, R_1. The system was originally introduced by

Ancona ([An], [AnTi]). Our presentation follows the paper [AbUn]. Here, μ_n and μ_p are characteristic constants describing the mobility of the negative and positive particles, respectively. The functions h_n and h_p are the enthalpy functions of the electrons and holes and admit the functional identities

$$h_n'(s) = \frac{P_n'(s)}{s} \quad \text{and} \quad h_p'(s) = \frac{P_p'(s)}{s}, \quad s > 0.$$

To obtain the quasi 1D approximation of the bipolar stationary quantum drift-diffusion model, which is discussed in Chapter 4, we now impose some additional assumptions. In [CUA], Cumberbatch, Uno and Abebe considered the domain $\Omega := (0,1) \times (0,1)$ and proposed the following:

(i) The quantum quasi Fermi level F is assumed to be constant in direction of the variable x and the other occuring functions are supposed to depend insignificantly on the variable y.

(ii) Generation/recombination effects are omitted, i.e. $R_0 R_1 \equiv 0$.

(iii) The isothermal case is considered, i.e. $h_n(n) = T_n \ln(n)$ for some $T_n > 0$.

The role of the holes, however, was ommited in [CUA]. The modeling of positive particles was reintroduced by S. Bian, L. Chen and M. Dreher in [BCD] by demanding

(iv) The quantum quasi Fermi level G of the holes is in thermal equilibrium, i.e. $G \equiv 0$.

(v) The ratio ξ of effective masses of electrons and holes is negligible small.

(vi) The isothermal case $h_p(p) = T_p \ln(p)$ for some $T_p > 0$ is assumed.

Assumptions (iv) to (vi) then imply $0 = -V + h_p(p)$ and we can write p as a function of V by $p = \exp(V/T_p)$. Dropping the dependency on the variable y in the notation, the system, which is considered in Chapter 4, now reads as

$$\begin{cases} F = V + T_n \ln(n) - \varepsilon^2 \frac{\sqrt{n}''}{\sqrt{n}}, \\ -\lambda^2 V'' = n - \exp(V/T_p) - \mathcal{C}. \end{cases}$$

Chapter 2

The viscous quantum Hydrodynamic equations

In the present chapter, we will prove the existence of stationary solutions to the one-dimensional viscous quantum hydrodynamic equations with non-smooth barrier potentials. As indicated in the derivation of the model, this non-smooth component of the equations implies that only a weak formulation of the problem is appropriate. We will propose the corresponding definition of a solution in the following section. Though being meaningful, the concept of weak solutions increases the difficulties in finding solutions. Therefore, we will introduce a reformulation of the original problem which turns the system of weak equalities into a system of strong equalities. More precisely, we will choose the L^2-based Sobolev spaces as the ambient environment for our analysis.

2.1 Reformulation of the stationary problem in the one-dimensional case

Definition 2.1 (**Weak solutions**).
Let $\varepsilon, \tau, \nu, \lambda > 0$ and $\mathcal{C}, V_B \in L^2(0,1)$. The tuple $(n, V, J) \in W^{2,2}(0,1) \times W^{2,2}(0,1) \times W^{1,2}(0,1)$ is called a weak solution to the equations

$$\left\{ \begin{array}{rcl} J' &=& -\nu n'', \\ 2\varepsilon^2 n \left(\frac{\sqrt{n}''}{\sqrt{n}} \right)' - \nu J'' - (p(n))' + \frac{1}{\tau} J &=& \left(\frac{J^2}{n} \right)' - n(V + V_B)', \\ \lambda^2 V'' &=& n - \mathcal{C}, \end{array} \right. \tag{2.1}$$

if and only if $n > 0$ in $[0,1]$, $J' = -\nu n''$, $\lambda^2 V'' = n - \mathcal{C}$ in $L^2(0,1)$ and

$$-2\varepsilon^2 \left\langle \frac{\sqrt{n}''}{\sqrt{n}}, (n\varphi)' \right\rangle + \nu \left\langle J', \varphi' \right\rangle - \left\langle (p(n))', \varphi \right\rangle + \frac{1}{\tau} \left\langle J, \varphi \right\rangle = \left\langle \left(\frac{J^2}{n} \right)', \varphi \right\rangle + \left\langle V + V_B, (n\varphi)' \right\rangle$$

for all $\varphi \in C_c^\infty(0,1)$.

Definition 2.2 (**Admissible pressure term**).
A smooth function $p : [0, \infty) \longrightarrow \mathbb{R}$ is called an admissible pressure term, if and only if $p'(s) > 0$ for $s > 0$ and if there exists an enthalpy function $h : (0, \infty) \longrightarrow \mathbb{R}$ fulfilling

(i) $sh'(s) = p'(s) \quad (s > 0)$,

(ii) $g := \frac{\ln}{h}$ *is continuous on* $(0, \infty)$,

(iii) For all positive $f \in W^{1,2}(0,1)$, *it holds* $g(f), h(f) \in W^{1,2}(0,1)$ *with the chain rule being valid,*

(iv) The mapping $s \mapsto \sqrt{s}h(s)$ *extends to a continuous function on* $[0, \infty)$.

Remark 2.3.
Note that assumption (ii) in Definition 2.2 only demands for an additive shift of the function h *in case that* h *has a zero in* $(0, \infty)$. *Adding this uniquely given constant to* h, *we may assume* $h(1) = 0$ *and then L'Hôpital's rule already yields the continuity of* g. *Since* $W^{1,2}(0,1)$ *embeds into* $C([0,1])$ *by Theorem A.6, any function* $n \in W^{1,2}(0,1)$, $n > 0$, *is actually bounded from above and away from zero. The availability of chain rules for Sobolev functions, c.f. Lemma A.4, shows that assumption (iii) on* g *and* h *is fulfilled for a large class of pressure terms* p. *The assumptions on* g *and* h, *especially assumption (iv), are motivated by the technical requirements which will arise in the subsequent analysis. We mention the choices* $p(s) = T_0 s^\gamma + \mu s$ *for* $T_0, \mu > 0$ *and* $\gamma \geq 1$ *as in the derivation of the viscous quantum hydrodynamic model. The enthalpy is then given by*

$$h(s) = \begin{cases} (T_0 + \mu)\ln(s), & \gamma = 1, \\ \frac{T_0\gamma}{\gamma-1}s^{\gamma-1} - \frac{T_0\gamma}{\gamma-1} + \mu\ln(s), & \gamma > 1. \end{cases}$$

The one-dimensional setting provides a big opportunity for the analysis of the stationary problem: The equation $J' = -\nu n''$ uniquely determines the electric current density J up to a constant J_0 of integration. We can therefore eliminate the first equation of the system (2.1) and we are in the position to derive a reformulation in terms of the viscosity-adjusted Fermi level

$$F := -(V + V_B) + h(n) + \frac{\nu}{\tau}\ln(n) - 2(\varepsilon^2 + \nu^2)\frac{\sqrt{n}''}{\sqrt{n}},$$

where h is the enthalpy to an admissible pressure term p. The following lemmas will elaborate the details of the transformations.

Lemma 2.4.
Let $\varepsilon, \tau, \nu, \lambda > 0$ *and assume* $\mathcal{C}, V_B \in L^2(0,1)$. *Let* p *be an admissible pressure term and* h *be a corresponding enthalpy. Let* (n, V, J) *be a weak solution to the system of equations* (2.1). *Then there exists* $J_0 \in \mathbb{R}$ *such that* (n, V) *is a solution to*

$$\begin{cases} F &= -(V + V_B) + h(n) + \frac{\nu}{\tau}\ln(n) - 2(\varepsilon^2 + \nu^2)\frac{\sqrt{n}''}{\sqrt{n}}, \\ nF' &= -\left(\frac{J_0^2}{n}\right)' + 2J_0\nu\left(2\frac{\sqrt{n}''}{\sqrt{n}} - \frac{(n')^2}{2n^2}\right) + \frac{J_0}{\tau}, \\ \lambda^2 V'' &= n - \mathcal{C}, \end{cases} \tag{2.2}$$

with equalities in $L^2(0,1)$ *and, in particular,* $F \in W^{1,2}(0,1)$.

Proof. We use the abbreviation $B(n) = \frac{\sqrt{n}''}{\sqrt{n}}$. The Sobolev embedding theorems A.6 yield $n, J, V \in C^1([0,1])$. By integrating the first equation in (2.1), we obtain

$$J = \nu n'(0) + J(0) - \nu n' =: J_0 - \nu n'.$$

We claim that the equality

$$-\left\langle F,(n\varphi)'\right\rangle = -\left\langle \left(\frac{J_0^2}{n}\right)',\varphi\right\rangle + 2J_0\nu\left\langle 2B(n)-\frac{(n')^2}{2n^2},\varphi\right\rangle + \frac{J_0}{\tau}\left\langle 1,\varphi\right\rangle \tag{2.3}$$

holds for all test functions $\varphi \in W_0^{1,2}(0,1)$.
Using the second equation of (2.1), we have

$$\begin{aligned}
-\left\langle F,(n\varphi)'\right\rangle &= \left\langle V+V_B,(n\varphi)'\right\rangle - \left\langle h(n)+\frac{\nu}{\tau}\ln(n),(n\varphi)'\right\rangle + 2(\varepsilon^2+\nu^2)\left\langle B(n),(n\varphi)'\right\rangle \\
&= \nu\left\langle J',\varphi'\right\rangle - \left\langle (p(n))',\varphi\right\rangle + \frac{1}{\tau}\left\langle J,\varphi\right\rangle - \left\langle \left(\frac{J^2}{n}\right)',\varphi\right\rangle + 2\nu^2\left\langle B(n),(n\varphi)'\right\rangle \\
&\quad - \left\langle h(n)+\frac{\nu}{\tau}\ln(n),(n\varphi)'\right\rangle \\
&= -\nu^2\left\langle n'',\varphi'\right\rangle + \left\langle p(n),\varphi'\right\rangle + \frac{1}{\tau}\left\langle J,\varphi\right\rangle - \left\langle \left(\frac{J^2}{n}\right)',\varphi\right\rangle + 2\nu^2\left\langle B(n),(n\varphi)'\right\rangle \\
&\quad - \left\langle h(n),(n\varphi)'\right\rangle + \left\langle \frac{\nu}{\tau}\ln(n)',n\varphi\right\rangle
\end{aligned}$$

for any $\varphi \in W_0^{1,2}(0,1)$.
Employing the functional identities for h and p, we also obtain

$$\begin{aligned}
&\left\langle p(n),\varphi'\right\rangle - \left\langle h(n),(n\varphi)'\right\rangle + \left\langle \frac{\nu}{\tau}\ln(n)',n\varphi\right\rangle \\
&= -\left\langle n'p'(n),\varphi\right\rangle + \left\langle n'nh'(n),\varphi\right\rangle + \left\langle \frac{\nu}{\tau}n\ln(n)',\varphi\right\rangle \\
&= \left\langle \frac{\nu}{\tau}n',\varphi\right\rangle.
\end{aligned}$$

Since $W^{1,2}(0,1)$ is a Banach algebra in the one-dimensional case (c.f. [Adams, Thm. 4.39]), we may use the representation $B(n)=\frac{n''}{2n}-\frac{(n')^2}{4n^2}$ and calculate

$$\begin{aligned}
&-\left\langle \left(\frac{J^2}{n}\right)',\varphi\right\rangle - \nu^2\left\langle n'',\varphi'\right\rangle + 2\nu^2\left\langle B(n),(n\varphi)'\right\rangle \\
&= \left\langle \frac{(J_0-\nu n')^2}{n},\varphi'\right\rangle - \nu^2\left\langle n'',\varphi'\right\rangle + 2\nu^2\left\langle B(n)n',\varphi\right\rangle + 2\nu^2\left\langle B(n)n,\varphi'\right\rangle \\
&= \left\langle \frac{J_0^2}{n},\varphi'\right\rangle - 2\nu J_0\left\langle \frac{n'}{n},\varphi'\right\rangle + \nu^2\left\langle \frac{(n')^2}{n},\varphi'\right\rangle - \nu^2\left\langle n'',\varphi'\right\rangle \\
&\quad + \nu^2\left\langle \frac{n''n'}{n}-\frac{(n')^3}{2n^2},\varphi\right\rangle + \nu^2\left\langle n''-\frac{(n')^2}{2n},\varphi'\right\rangle \\
&= -\left\langle \left(\frac{J_0^2}{n}\right)',\varphi\right\rangle + 2\nu J_0\left\langle \left(\frac{n'}{n}\right)',\varphi\right\rangle - \frac{\nu^2}{2}\left\langle \left(\frac{(n')^2}{n}\right)',\varphi\right\rangle \\
&\quad + \nu^2\left\langle \frac{n''n'}{n}-\frac{(n')^3}{2n^2},\varphi\right\rangle
\end{aligned}$$

$$
\begin{aligned}
&= - \left\langle \left(\frac{J_0^2}{n} \right)', \varphi \right\rangle + 2\nu J_0 \left\langle \frac{nn'' - (n')^2}{n^2}, \varphi \right\rangle - \frac{\nu^2}{2} \left\langle \frac{2nn'n'' - (n')^3}{n^2}, \varphi \right\rangle \\
&\quad + \nu^2 \left\langle \frac{n''n'}{n} - \frac{(n')^3}{2n^2}, \varphi \right\rangle \\
&= - \left\langle \left(\frac{J_0^2}{n} \right)', \varphi \right\rangle + 2\nu J_0 \left\langle \frac{nn'' - (n')^2}{n^2}, \varphi \right\rangle \\
&= - \left\langle \left(\frac{J_0^2}{n} \right)', \varphi \right\rangle + 2\nu J_0 \left\langle 2B(n) - \frac{(n')^2}{2n^2}, \varphi \right\rangle .
\end{aligned}
$$

As $J = J_0 - \nu n'$, we find

$$
\frac{1}{\tau} \langle J, \varphi \rangle + \frac{\nu}{\tau} \langle n', \varphi \rangle = \frac{J_0}{\tau} \langle 1, \varphi \rangle .
$$

Now the weak formulation (2.3) of the second equation of (2.2) follows when combining all appearing terms. Since n is continuous, we know that there exists a lower bound $C > 0$ such that $n \geq C > 0$. Therefore, the substitution $\varphi \mapsto n\varphi =: \psi \in W_0^{1,2}(0,1)$ is bijective. Thus,

$$
- \langle F, \psi' \rangle = - \left\langle \frac{1}{n} \left(\frac{J_0^2}{n} \right)', \psi \right\rangle + 2J_0\nu \left\langle 2\frac{B(n)}{n} - \frac{(n')^2}{2n^3}, \psi \right\rangle + \frac{J_0}{\tau} \left\langle \frac{1}{n}, \psi \right\rangle \quad (\psi \in W_0^{1,2}(0,1)).
$$

In particular, the distributional derivative F' is indeed an element of $L^2(0,1)$ and the second equation of (2.2) is actually an equality in $L^2(0,1)$. □

Lemma 2.5.
Let $\varepsilon, \tau, \nu, \lambda > 0$, assume $\mathcal{C}, V_B \in L^2(0,1)$ and assume that the function h arising in the equations (2.2) *is induced by an admissible pressure term p. Let $(n, F, V) \in W^{2,2}(0,1) \times W^{1,2}(0,1) \times W^{2,2}(0,1)$ be a solution to the system of equations* (2.2) *for some $J_0 \in \mathbb{R}$ which satisfies $n > 0$ in $[0,1]$. Then, for $J := J_0 - \nu n'$, it holds that (n, V, J) is a weak solution of the system* (2.1).

Proof. Plugging the first equation of (2.2) into the second one, the assertion follows from the same calculations as in Lemma 2.4. □

The reformulation of the viscous quantum hydrodynamic equations in terms of the Fermi level suggests to consider the special cases of constant Fermi levels F. In these situations, the second equation of (2.2) is trivially fulfilled for the choice $J_0 = 0$ and the system reduces to the equations

$$
\left\{ \begin{array}{rcl} F &=& -(V + V_B) + h(n) + \frac{\nu}{\tau} \ln(n) - 2(\varepsilon^2 + \nu^2) \frac{\sqrt{n}''}{\sqrt{n}}, \\ \lambda^2 V'' &=& n - \mathcal{C}, \end{array} \right. \tag{2.4}
$$

which are strongly related to the quantum drift-diffusion model. In the subsequent sections, we will follow the approach of N. Ben Abdallah and A. Unterreiter [AbUn] to prove the solvability of systems of equations of the form (2.4) with Fermi levels $F \in L^\infty(0,1)$. We consider the situations of (positive) Dirichlet boundary values (Lemma 2.10), homogeneous Neumann boundary conditions (Lemma 2.13) and periodic boundary conditions (Lemma 2.14). In the case of Dirichlet boundary conditions, we also allow Ω to be an arbitrary bounded C^2-domain in $\mathbb{R}^N$, $N \leq 3$, for the sake of generality.

A-priori estimates to solutions (n, V) and the continuous dependence of solutions on their Fermi levels (Lemma 2.12) will put us in a position, in which we can reconsider the full system (2.2) with the aid of fixed point arguments. However, the mutual dependencies of n, F and J_0 require some additional assumptions on the solutions. In particular, we face the problem of choosing meaningful and appropriate boundary conditions for the functions n and F. Since the second equation of (2.2) is an identity for F', it is tempting to choose the boundary operator

$$F_{1;0} := F(1) - F(0)$$

for the Fermi levels F. Indeed, if n, F and V are solutions to (2.2) with the regularities as given in Lemma 2.5, we can divide the second line of (2.2) by the positive function n and employ the identities

$$-\frac{1}{n}\left(\frac{J_0^2}{n}\right)' = -\left(\frac{J_0^2}{2n^2}\right)' \quad \text{and} \quad 2\frac{\sqrt{n}''}{\sqrt{n}} - \frac{(n')^2}{2n^2} = (\ln(n))'',$$

to obtain the equation

$$\begin{aligned} F' &= -\frac{1}{n}\left(\frac{J_0^2}{n}\right)' + \frac{2J_0\nu}{n}(\ln(n))'' + \frac{J_0}{\tau n} \\ &= -\left(\frac{J_0^2}{2n^2}\right)' + \frac{2\nu J_0}{n}(\ln(n))'' + \frac{J_0}{\tau n}. \end{aligned} \tag{2.5}$$

Since the Sobolev embedding theorem yields $F \in C([0,1])$ and $n \in C^1([0,1])$, integrations by parts result in

$$\begin{aligned} F(1) - F(0) &= \int_0^1 -\left(\frac{J_0^2}{2n(x)^2}\right)' + \frac{2\nu J_0}{n(x)}\ln(n(x))'' + \frac{J_0}{\tau n(x)}\, dx \\ &= -\frac{J_0^2}{2n(x)^2}\Bigg|_{x=0}^{x=1} + 2\nu J_0 \frac{\ln(n(x))'}{n(x)}\Bigg|_{x=0}^{x=1} \\ &\quad + 2\nu J_0 \int_0^1 \ln(n(x))' \frac{n'(x)}{n(x)^2}\, dx + \frac{J_0}{\tau}\int_0^1 \frac{1}{n(x)}\, dx \\ &= -\frac{J_0^2}{2n(x)^2}\Bigg|_{x=0}^{x=1} + 2\nu J_0 \frac{n'(x)}{n(x)^2}\Bigg|_{x=0}^{x=1} + J_0 \int_0^1 2\nu \frac{n'(x)^2}{n(x)^3} + \frac{1}{\tau n(x)}\, dx. \end{aligned}$$

If we consider periodic boundary conditions $n(0) = n(1)$ and $n'(0) = n'(1)$ for n, the relation

$$F_{1;0} = J_0 \int_0^1 2\nu \frac{n'(x)^2}{n(x)^3} + \frac{1}{\tau n(x)}\, dx \tag{2.6}$$

holds. Some important properties should be mentioned: The boundary value $F_{1;0}$ is zero if and only if J_0 is zero. And taking the representation (2.5) of F' into account, this is equivalent to $F' = 0$ or rather $F = \text{const}$. Moreover, this identity enables us to define the number J_0 as a function of $F_{1;0}$ and n. However, to do so, it is crucial to gain control over the integral expression in (2.6). More precisely, we are looking for a constraint to the electron densities n which yields a uniform lower bound to the integrals. We will see, that the natural assumption that the total mass of electrons $\int_0^1 n(x)\, dx$ is a fixed constant is a suitable choice. The necessary modifications to solve the partial problem (2.4) are provided in Lemma 2.17. The existence of solutions to the full system is the result of Theorem 2.21.

Concerning homogeneous Neumann boundary conditions, analogous results are derived in Lemma 2.18 and Theorem 2.29. However, since the relation between $F_{1;0}$, n and J_0 is now given by the quadratic equation

$$F_{1;0} = -\frac{J_0^2}{2}\left(\frac{1}{n(1)^2} - \frac{1}{n(0)^2}\right) + J_0 \int_0^1 2\nu \frac{n'(x)^2}{n(x)^3} + \frac{1}{\tau n(x)}\, dx,$$

an additional smallness assumption to $F_{1;0}$ has to be imposed.

2.2 Dirichlet boundary conditions

Throughout this section let Ω be a bounded C^2-domain in $\mathbb{R}^N$, $N \leq 3$.
Assuming positivity of the function u, we may formally substitute $n = u^2$ in the equations (2.4) and we wish to solve a system of the form

$$(2.7) \qquad \begin{cases} 2\kappa\Delta u &= -(V + L - k(u^2))u, & \text{in } \Omega, \\ \lambda^2 \Delta V &= u^2 - \mathcal{C}, & \text{in } \Omega, \\ \operatorname{Tr} u &= u_\Gamma, & \text{on } \partial\Omega, \\ \operatorname{Tr} V &= V_\Gamma, & \text{on } \partial\Omega \end{cases}$$

for $(u, V) \in W^{2,2}(\Omega) \times W^{2,2}(\Omega)$, where $\kappa, \lambda > 0$ and $L, \mathcal{C} \in L^\infty(\Omega)$, $u_\Gamma, V_\Gamma \in B^{3/2}_{2,2}(\partial\Omega)$, $u_\Gamma > 0$, are given. We can rewrite this system of differential equations to u and V as a sole functional equation for u via

$$(2.8) \qquad \begin{cases} 2\kappa\Delta u &= -(\Phi(u^2) + V_{inh} + L - k(u^2))u, & \text{in } \Omega, \\ \operatorname{Tr} u &= u_\Gamma, & \text{on } \partial\Omega, \end{cases}$$

by letting $\Phi : L^2(\Omega) \longrightarrow W^{2,2}(\Omega)$ be the continuous solution operator (c.f. [GiTr, Thm. 8.8, Thm. 8.9, Thm. 8.12]) to the equations

$$\lambda^2 \Delta V = u^2 \text{ in } \Omega, \quad \operatorname{Tr} V = 0 \text{ on } \partial\Omega$$

and choosing $V_{inh} \in W^{2,2}(\Omega)$ as the solution to the constant part of the Poisson equation to V:

$$\lambda^2 \Delta V_{inh} = -\mathcal{C} \text{ in } \Omega, \quad \operatorname{Tr} V = V_\Gamma \text{ on } \partial\Omega.$$

The objective is to define a functional $\mathcal{F} : W^{1,2}(\Omega) \longrightarrow \mathbb{R}$ whose Euler-Lagrange equation provides the first equation of (2.8) so that any minimizer of $\mathcal{F}$ in the set $\{u \in W^{1,2}(\Omega) : \operatorname{Tr} u = u_\Gamma\}$ is a solution to the system (2.8). A subsequent discussion will improve the regularity results and will show that the minimizers can actually be chosen as positive functions. The argumentations reveal that growth conditions on k play an important role for the characteristics of solutions. We mention that the choices $k = h + \frac{\nu}{\tau}\ln$ with h belonging to an admissible pressure term p (c.f. Definition 2.2) always comply with the assumptions of the forthcoming results.

Proposition 2.6 (Definition of the functional and existence of minimizers).
Let $\kappa, \lambda > 0$, $L, \mathcal{C} \in L^\infty(\Omega)$ and $u_\Gamma, V_\Gamma \in B^{3/2}_{2,2}(\partial\Omega)$ with $u_\Gamma > 0$. Let $k : (0,\infty) \longrightarrow \mathbb{R}$ be continuous and strictly increasing with $\lim_{s\to 0} k(s) = -\infty$, $\lim_{s\to\infty} k(s) = \infty$ and assume that $s \mapsto \sqrt{s}k(s)$ extends to a continuous function on $[0,\infty)$. Define the functional $\mathcal{F} = G + H$ by

$$G(u) := \int_\Omega 2\kappa|\nabla u(x)|^2 + K(u^2(x)) - (V_{inh}(x) + L(x))u^2(x)\, dx \quad (u \in W^{1,2}(\Omega))$$

and

$$H(u) := \frac{\lambda^2}{2} \int_\Omega |\nabla \Phi(u^2)(x)|^2 \, dx \quad (u \in W^{1,2}(\Omega)),$$

where

$$K(s) := \int_1^s k(t) \, dt + K_0$$

for some arbitrary $K_0 \in \mathbb{R}$*. Here,* $\Phi : L^2(\Omega) \longrightarrow W^{2,2}(\Omega)$ *is the solution operator to the equations*

$$\lambda^2 \Delta V = u^2 \text{ in } \Omega, \quad \operatorname{Tr} V = 0 \text{ on } \partial\Omega,$$

and $V_{inh} \in W^{2,2}(\Omega)$ *is the solution to*

$$\lambda^2 \Delta V_{inh} = -\mathcal{C} \text{ in } \Omega, \quad \operatorname{Tr} V = V_\Gamma \text{ on } \partial\Omega.$$

Then $\mathcal{F}$ *has a unique non-negative minimizer* u *on the set*

$$U := \left\{ u \in W^{1,2}(\Omega) \, : \, \operatorname{Tr} u = u_\Gamma \right\}.$$

Proof. We use Proposition A.13. By the Mazur lemma (c.f. [Alt, 6.14]) U is a weakly closed subset of $W^{1,2}(\Omega)$, since it is convex and closed. Concerning the coerciveness of $\mathcal{F}$, we claim that there exists $C_0 > 0$ such that

$$\mathcal{F}(u) \geq G(u) \geq 2\kappa \|\nabla u\|^2_{L^2(\Omega)} + \|u\|^2_{L^2(\Omega)} - C_0 \quad (u \in W^{1,2}(\Omega)). \tag{2.9}$$

The continuity of $s \mapsto \sqrt{s} k(s)$ on $[0, \infty)$ yields

$$|k(s)| \leq \frac{C}{\sqrt{s}}$$

for all s in some neighborhood of zero and we conclude that K is well-defined and differentiable on $[0, \infty)$. Moreover,

$$K(s) \geq K_{min} \quad (s \in [0, \infty)).$$

Because $k(s) \longrightarrow \infty$ as $s \longrightarrow \infty$, there exists $s_0 > 0$ such that

$$K(s) \geq \left(\|V_{inh} + L\|_{L^\infty(\Omega)} + 1 \right) s \quad (s \geq s_0). \tag{2.10}$$

Writing

$$\begin{aligned} G(u) &= \int_\Omega 2\kappa |\nabla u(x)|^2 + K(u^2(x)) - (V_{inh}(x) + L(x)) u^2(x) \, dx \\ &= \int_{\{u^2 \leq s_0\}} 2\kappa |\nabla u(x)|^2 + K(u^2(x)) - (V_{inh}(x) + L(x)) u^2(x) \, dx \\ &\quad + \int_{\{u^2 > s_0\}} 2\kappa |\nabla u(x)|^2 + K(u^2(x)) - (V_{inh}(x) + L(x)) u^2(x) \, dx \\ &=: I_1 + I_2 \end{aligned}$$

for $u \in W^{1,2}(\Omega)$, we estimate

$$\begin{aligned} I_1 &\geq 2\kappa \|\nabla u\|^2_{L^2(\{u^2 \leq s_0\})} - |K_{min}| \operatorname{vol}(\Omega) - s_0 \operatorname{vol}(\Omega) \|V_{inh} + L\|_{L^\infty(\Omega)} \\ &= 2\kappa \|\nabla u\|^2_{L^2(\{u^2 \leq s_0\})} - C. \end{aligned}$$

Using the estimate (2.10) for K, we also find

$$\begin{aligned} I_2 &\geq 2\kappa\|\nabla u\|^2_{L^2(\{u^2>s_0\})} + \int_{\{u^2>s_0\}} \big(\|V_{inh}+L\|_{L^\infty(\Omega)} + 1 - (V_{inh}(x)+L(x))\big)\, u^2(x) \\ &\geq 2\kappa\|\nabla u\|^2_{L^2(\{u^2>s_0\})} + \int_{\{u^2>s_0\}} u^2(x)\, dx \\ &= 2\kappa\|\nabla u\|^2_{L^2(\{u^2>s_0\})} + \|u\|^2_{L^2(\Omega)} - \int_{\{u^2\leq s_0\}} u^2(x)\, dx \\ &\geq 2\kappa\|\nabla u\|^2_{L^2(\{u^2>s_0\})} + \|u\|^2_{L^2(\Omega)} - s_0\,\mathrm{vol}(\Omega) \\ &= 2\kappa\|\nabla u\|^2_{L^2(\{u^2>s_0\})} + \|u\|^2_{L^2(\Omega)} - C. \end{aligned}$$

We obtain

$$G(u) = I_1 + I_2 \geq 2\kappa\|\nabla u\|^2_{L^2(\Omega)} + \|u\|^2_{L^2(\Omega)} - C_0,$$

with a positive constant C_0 depending on $\|V_{inh}+L\|_{L^\infty(0,1)}$, which implies the coerciveness of $\mathcal{F}$.

We show that G and H are weakly sequentially lower semi-continuous. Since the embedding $W^{1,2}(\Omega) \hookrightarrow L^4(\Omega)$ is compact (c.f. Theorem A.6), any weakly convergent sequence in $W^{1,2}(\Omega)$ converges strongly in $L^4(\Omega)$ (c.f. [Alt, Lem 8.2]). By continuity of $\Phi : L^2(\Omega) \longrightarrow W^{2,2}(\Omega)$, we conclude that $H : W^{1,2}(\Omega) \longrightarrow \mathbb{R}$ is weakly continuous.

Concerning G, we wish to use Proposition A.14 and define $J : \Omega \times \mathbb{R} \times \mathbb{R}^N \longrightarrow \mathbb{R}$ by

$$J(x,u,p) := 2\kappa|p|^2 + K(u^2) - (V_{inh}(x)+L(x))u^2.$$

Then

$$J(x,u,p) \geq K(u^2) - \|V_{inh}+L\|_{L^\infty(\Omega)} u^2.$$

Employing the estimate (2.10) for K once more, we obtain

$$J(x,u,p) \geq u^2 \geq s_0$$

whenever $u^2 \geq s_0$ and

$$J(x,u,p) \geq K_{min} - s_0\|V_{inh}+L\|_{L^\infty(\Omega)}$$

if $u^2 \leq s_0$. We now apply Proposition A.14 with the constant function

$$\Phi(x) := \min\big\{s_0, K_{min} - s_0\|V_{inh}+L\|_{L^\infty(\Omega)}\big\} \in L^1(\Omega).$$

Let $(u_n)_{n\in\mathbb{N}} \subset U$ be a sequence converging weakly in $W^{1,2}(\Omega)$ to some $u \in U$. Then, as the embedding $W^{1,2}(\Omega) \hookrightarrow L^1(\Omega)$ is compact and $W^{1,2}(\Omega)$ is reflexive, $u_n \longrightarrow u$ in $L^1(\Omega)$ (c.f. [Alt, Lem. 8.2]) and convergence is also given in $L^1(\Omega')$ for any subdomain $\Omega' \subset \Omega$. For all $\varphi \in (L^2(\Omega))'$, the mapping

$$u \mapsto \varphi(\nabla u) \quad (u \in W^{1,2}(\Omega))$$

defines an element of $(W^{1,2}(\Omega))'$. Hence, weak convergence of $(u_n)_{n\in\mathbb{N}}$ in $W^{1,2}(\Omega)$ to u implies weak convergence of $(\nabla u_n)_{n\in\mathbb{N}}$ in $L^2(\Omega)$ to ∇u. Fixing some $\varphi \in (L^1(\Omega))'$, the Hölder inequality yields

$$|\varphi(\nabla u - \nabla u_n)| \leq \|\varphi\|_{L(L^1(\Omega),\mathbb{R})}\|\nabla u - \nabla u_n\|_{L^1(\Omega)} \leq C\|\nabla u - \nabla u_n\|_{L^2(\Omega)} \quad (n \in \mathbb{N}),$$

since Ω is bounded. Therefore, ∇u_n converges weakly in $L^1(\Omega)$ and in $L^1(\Omega')$ for any subdomain $\Omega' \subset \Omega$ to ∇u.
By Proposition A.14, we conclude

$$G(u) \leq \liminf_{n\to\infty} G(u_n),$$

which is the weak sequential lower semi-continuity of G.
Proposition A.13 now ensures the existence of a minimizer $u \in U$ to $\mathcal{F}$. Since $\mathcal{F}(u) = \mathcal{F}(|u|)$, the minimizer can be chosen as a non-negative function. Uniqueness of the non-negative minimizer is an immediate consequence of the pseudo-convex inequality for $\mathcal{F}$ which will be shown in Lemma 2.8 below. □

Remark 2.7.
The minimizers of the functional introduced in Proposition 2.6 obviously do not depend on the choice of the constant $K_0 = K(1)$. *However, since we are mainly interested in the situation* $k = h + \frac{\nu}{\tau}\ln$, *with* h *being the enthalpy to an admissible pressure term* p, *it is convenient to choose* $K_0 := h(1) - p(1) - \frac{\nu}{\tau}$. *In this case, the equality*

$$K(s) = sk(s) - p(s) - \frac{\nu}{\tau}s \quad (s > 0)$$

holds, which is seen by differentiation. This identity will prove useful in the forthcoming analysis.

Lemma 2.8 (**Pseudo-convexity of the functional**).
Let the functional $\mathcal{F}$ *be defined as in Proposition 2.6. Then, for* $0 < t < 1$ *and* $u_1, u_2 \in W^{1,2}(\Omega)$, *there holds* $\sqrt{tu_1^2 + (1-t)u_2^2} \in W^{1,2}(\Omega)$ *and the pseudo-convex inequality*

$$\mathcal{F}\left(\sqrt{tu_1^2 + (1-t)u_2^2}\right) \leq t\mathcal{F}(u_1) + (1-t)\mathcal{F}(u_2)$$

is satisfied. If $u_1^2 \neq u_2^2$, *the inequality is strict.*

Proof. We abbreviate $u_t := \sqrt{tu_1^2 + (1-t)u_2^2}$. Then u_t clearly is an element of $L^2(\Omega)$. Since the square root function does not possess a bounded derivative towards zero, we define $u_t^\varepsilon := \sqrt{tu_1^2 + (1-t)u_2^2 + \varepsilon}$ for $\varepsilon > 0$ and apply the chain rule of Lemma A.4 with

$$f(x) := \begin{cases} \sqrt{x}\psi(x), & x \geq 0, \\ 0, & x < 0, \end{cases}$$

where $\psi \in C^\infty(\mathbb{R})$ is a smooth cut-off function satisfying $\psi(x) = 0$ $(x \leq \frac{1}{3}\sqrt{\varepsilon})$ and $\psi(x) = 1$ $(x \geq \frac{2}{3}\sqrt{\varepsilon})$. Note that the inner function $u := tu_1^2 + (1-t)u_2^2 + \varepsilon$ is an element of $W^{1,1}_{loc}(\Omega)$ by Lemma A.5. Now,

$$\partial_i u_t^\varepsilon = \frac{tu_1\partial_i u_1 + (1-t)u_2\partial_i u_2}{\sqrt{tu_1^2 + (1-t)u_2^2 + \varepsilon}} \quad (i = 1, \dots, n).$$

Since

$$\begin{aligned} &\left|\sqrt{tu_1^2(x) + (1-t)u_2^2(x) + \varepsilon} - \sqrt{tu_1^2(x) + (1-t)u_2^2(x)}\right| \\ &= \frac{\varepsilon}{\sqrt{tu_1^2(x) + (1-t)u_2^2(x) + \varepsilon} + \sqrt{tu_1^2(x) + (1-t)u_2^2(x)}} \\ &\leq \sqrt{\varepsilon} \end{aligned}$$

uniformly for $x \in \Omega$, it follows that $u_t^\varepsilon \longrightarrow u_t$ in $L^\infty(\Omega)$ as $\varepsilon \longrightarrow 0$. Therefore, for $i = 1, \ldots, n$ and $\varphi \in C_c^\infty(\Omega)$, we may calculate

$$\begin{aligned}
\int_\Omega u_t(x)\partial_i\varphi(x)\,dx &= \lim_{\varepsilon\to 0}\int_\Omega u_t^\varepsilon(x)\partial_i\varphi(x)\,dx \\
&= -\lim_{\varepsilon\to 0}\int_\Omega \frac{tu_1(x)\partial_i u_1(x) + (1-t)u_2(x)\partial_i u_2(x)}{\sqrt{tu_1^2(x) + (1-t)u_2^2(x) + \varepsilon}}\varphi(x)\,dx \\
&= -\int_\Omega \frac{tu_1(x)\partial_i u_1(x) + (1-t)u_2(x)\partial_i u_2(x)}{\sqrt{tu_1^2(x) + (1-t)u_2^2(x)}}\varphi(x)\,dx,
\end{aligned}$$

where we have used Lebesgue's monotone convergence theorem to obtain the last equality. The fracture on the right hand side should be read as zero if both the nominator and denominator are zero. In other words, we have

$$\partial_i u_t(x) = \begin{cases} \frac{tu_1(x)\partial_i u_1(x)+(1-t)u_2(x)\partial_i u_2(x)}{\sqrt{tu_1^2(x)+(1-t)u_2^2(x)}}, & u_1(x) \neq 0 \text{ or } u_2(x) \neq 0, \\ 0, & u_1(x) = u_2(x) = 0 \end{cases}$$

and for $x \in \Omega$ with $u_1(x) \neq 0$ or $u_2(x) \neq 0$, there holds

$$\begin{aligned}
(\partial_i u_t(x))^2 &= (\partial_i u_1(x))^2 \frac{t^2 u_1^2(x)}{tu_1^2(x) + (1-t)u_2^2(x)} \\
&\quad + \partial_i u_1(x)\partial_i u_2(x)\frac{2t(1-t)u_1(x)u_2(x)}{tu_1^2(x) + (1-t)u_2^2(x)} \\
&\quad + (\partial_i u_2(x))^2 \frac{(1-t)^2 u_2^2(x)}{tu_1^2(x) + (1-t)u_2^2(x)} \quad (i = 1, \ldots, n).
\end{aligned}$$

Since all occuring fractions are bounded and $\partial_i u_1, \partial_i u_2 \in L^2(\Omega)$, we conclude $\nabla u_t \in L^2(\Omega)$ and $u_t \in W^{1,2}(\Omega)$.

We prove the claimed pseudo-convexity. Remember $\mathcal{F}(u) = G(u) + H(u)$, where

$$\begin{aligned}
G(u) &= \int_\Omega 2\kappa|\nabla u(x)|^2\,dx + \int_\Omega K(u^2(x))\,dx - \int_\Omega (V_{inh}(x) + L(x))u^2(x)\,dx \\
&=: I_1(\nabla u) + I_2(u) + I_3(u)
\end{aligned}$$

and

$$H(u) = \frac{\lambda^2}{2}\int_\Omega \left|\left(\nabla\Phi(u^2)\right)(x)\right|^2\,dx$$

for $u \in W^{1,2}(\Omega)$.

Concerning $I_1(\nabla u_t)$, we note that for $i = 1, \ldots, n$ the inequalities

$$(t(u_1\partial_i u_1) + (1-t)(u_2\partial_i u_2))^2 \leq \left(t(\partial_i u_1)^2 + (1-t)(\partial_i u_2)^2\right)\left(tu_1^2 + (1-t)u_2^2\right)$$

follow through a direct calculation. Summing up, one obtains

$$\sum_{i=1}^n (tu_1\partial_i u_1 + (1-t)u_2\partial_i u_2)^2 \leq \left(t\sum_{i=1}^n(\partial_i u_1)^2 + (1-t)\sum_{i=1}^n(\partial_i u_2)^2\right)\left(tu_1^2 + (1-t)u_2^2\right)$$

so that

$$\begin{aligned} 2\kappa|\nabla u_t|^2 &= 2\kappa\frac{\sum_{i=1}^n (tu_1\partial_i u_1 + (1-t)u_2\partial_i u_2)^2}{tu_1^2 + (1-t)u_2^2} \leq 2\kappa t\sum_{i=1}^n(\partial_i u_1)^2 + 2\kappa(1-t)\sum_{i=1}^n(\partial_i u_2)^2 \\ &= 2\kappa t|\nabla u_1|^2 + 2\kappa(1-t)|\nabla u_2|^2 \end{aligned}$$

and therefore

$$I_1(\nabla u_t) \leq tI_1(\nabla u_1) + (1-t)I_1(\nabla u_2).$$

Turning to I_2, convexity of $s \mapsto K(s)$ follows by the monotonicity of $K' = k$. Then

$$K(u_t^2) = K(tu_1^2 + (1-t)u_2^2) \leq tK(u_1^2) + (1-t)K(u_2^2)$$

and

$$I_2(u_t) \leq tI_2(u_1) + (1-t)I_2(u_2).$$

The equality

$$I_3(u_t) = tI_3(u_1) + (1-t)I_3(u_2)$$

is obvious. Furthermore, we have

$$\begin{aligned} \left|\nabla\Phi(u_t^2)\right|^2 &= \left|t\nabla\Phi(u_1^2) + (1-t)\nabla\Phi(u_2^2)\right|^2 \\ &\leq t|\nabla\Phi(u_1^2)|^2 + (1-t)|\nabla\Phi(u_2^2)|^2. \end{aligned}$$

Since the mapping $v \mapsto |v|^2$, $\mathbb{R}^n \to \mathbb{R}$, is strictly convex and $\nabla\Phi$ is injective, equality can solely hold almost everywhere if $u_1^2 = u_2^2$. Therefore,

$$H(u_t) \leq tH(u_1) + (1-t)H(u_2).$$

This inequality is strict, provided that $u_1^2 \neq u_2^2$. Summing up all inequalities, the pseudo-convexity of $\mathcal{F}$ follows.

□

As $K' = k$ is not bounded at zero, well-known differentiability results like Theorem A.17 do not directly apply. Therefore, we need to introduce a regularisation of the functional to derive the Euler-Lagrange equation. We consider a clamped version k_γ of k with corresponding functionals $\mathcal{F}_\gamma$ defined analogously to $\mathcal{F}$, where $0 < \gamma < \gamma_0$ is a parameter.

Lemma 2.9 (Differentiability of the regularised functional and the Euler-Lagrange equation).
Let $\mathcal{F}$ be given as in Proposition 2.6 and define $\mathcal{F}_\gamma = G_\gamma + H$ analogously to $\mathcal{F}$ when k and K are replaced by

$$k_\gamma(s) := \begin{cases} k(\gamma), & 0 \leq s \leq \gamma, \\ k(s), & \gamma \leq s \leq \frac{1}{\gamma}, \\ k(\frac{1}{\gamma}), & \frac{1}{\gamma} \leq s, \end{cases}$$

and

$$K_\gamma(s) := \int_1^s k_\gamma(t)\, dt + K_0 \quad (0 < \gamma < 1),$$

respectively. Then, for some $\gamma_0 > 0$ *and all* $0 < \gamma < \gamma_0$*, the functionals* $\mathcal{F}_\gamma$ *possess unique non-negative minimizers* $u_\gamma \in U$*. The functionals* $\mathcal{F}_\gamma$ *are Fréchet-differentiable in* $W^{1,2}(\Omega)$ *with*

$$\begin{aligned} \mathcal{F}'_\gamma(u_\gamma)h &= 2\int_\Omega 2\kappa \langle \nabla u_\gamma(x), \nabla h(x)\rangle + k_\gamma(u_\gamma^2(x))u_\gamma(x)h(x)\,dx \\ &\quad -2\int_\Omega (V_{inh}(x) + \Phi(u_\gamma^2)(x) + L(x))u_\gamma(x)h(x)\,dx \end{aligned}$$

for $u_\gamma, h \in W^{1,2}(\Omega)$*. In particular, the Euler-Lagrange equation*

$$2\kappa\Delta u_\gamma = -(V_\gamma + L - k(u_\gamma^2))u_\gamma,$$

where $V_\gamma = \Phi(u_\gamma^2) + V_{inh}$*, holds.*

Proof. Existence and uniqueness of non-negative minimizers for $\mathcal{F}_\gamma$ follow by the same argumentations as used in Proposition 2.6 and Lemma 2.8. It should be mentioned that K_γ is uniformly bounded with respect to $0 < \gamma < \gamma_0$ from below, since

$$K_\gamma(s) \geq K_{\min} \quad (s \in [0,\infty),\ 0 < \gamma < \gamma_0).$$

Therefore, the constant C_0 in the coerciveness inequality (2.9) is also independent of $0 < \gamma < \gamma_0$. As k_γ is bounded, K_γ grows only linearly and Theorem A.17 yields that G_γ is continuously Fréchet-differentiable with

$$G'_\gamma(u_\gamma)h = 2\int_0^1 2\kappa\langle \nabla u_\gamma(x), \nabla h(x)\rangle + k_\gamma(u_\gamma^2(x))u_\gamma(x)h(x) - (V_{inh}(x) + L(x))u_\gamma(x)h(x)\,dx$$

for $u_\gamma, h \in W^{1,2}(\Omega)$. We claim that H is also Fréchet-differentiable and

$$H'(u_\gamma)h = -2\int_\Omega u_\gamma(x)h(x)\Phi(u_\gamma^2)(x)\,dx \quad (u_\gamma, h \in W^{1,2}(\Omega)).$$

The divergence theorem implies

$$H(u_\gamma) = \frac{\lambda^2}{2}\int_\Omega \left|\left(\nabla\Phi(u_\gamma^2)\right)(x)\right|^2\,dx = -\frac{1}{2}\int_\Omega \Phi(u_\gamma^2)(x)u_\gamma^2(x)\,dx$$

and we find

$$\begin{aligned} H(u_\gamma + h) - H(u_\gamma) - H'(u_\gamma)h &= -\frac{1}{2}\int_\Omega h^2(x)\Phi(u_\gamma^2 + 2u_\gamma h + (u_\gamma + h)^2)(x)\,dx \\ &\quad -\frac{1}{2}\int_\Omega 2u_\gamma(x)h(x)\Phi(2u_\gamma h)(x)\,dx \\ &=: I_1 + I_2. \end{aligned}$$

Then, for small $\|h\|_{W^{1,2}(\Omega)}$, we conclude that $u_\gamma^2 + 2u_\gamma h + (u_\gamma + h)^2$ is uniformly bounded in $L^2(\Omega)$ with respect to h, since any appearing factor in the products of this term consists of elements of $L^4(\Omega)$ due to the Sobolev embedding $W^{1,2}(\Omega) \hookrightarrow L^4(\Omega)$. By continuity of $\Phi : L^2(\Omega) \longrightarrow W^{2,2}(\Omega) \hookrightarrow L^\infty(\Omega)$, we conclude $|I_1| \leq C\|h\|^2_{L^2(\Omega)} \leq C\|h\|^2_{W^{1,2}(\Omega)}$. The Hölder inequality shows

$$|I_2| \leq 2\|u_\gamma h\|_{L^2(\Omega)}\|\Phi(u_\gamma h)\|_{L^2(\Omega)} \leq C\|u_\gamma h\|^2_{L^2(\Omega)} \leq C\|u_\gamma\|^2_{L^4(\Omega)}\|h\|^2_{L^4(\Omega)} \leq C\|h\|^2_{W^{1,2}(\Omega)}$$

so that
$$\frac{|H(u_\gamma + h) - H(u_\gamma) - H'(u_\gamma)h|}{\|h\|_{W^{1,2}(\Omega)}} \leq C\|h\|_{W^{1,2}(\Omega)} \longrightarrow 0$$

as $\|h\|_{W^{1,2}(\Omega)} \longrightarrow 0$.
Since u_γ is a local minimizer to $\mathcal{F}_\gamma$, we conclude $0 = \mathcal{F}'_\gamma(u_\gamma)\varphi$ for any test function $\varphi \in C_c^\infty(\Omega)$, which means that the Euler-Lagrange equation holds. □

Lemma 2.10 (**The Euler-Lagrange equation to the original functional**).
Let u_γ be the non-negative minimizers to $\mathcal{F}_\gamma$ for $0 < \gamma < \gamma_0$ introduced in Lemma 2.9 and let $V_\gamma := \Phi(u_\gamma^2) + V_{inh}$. Then there exist $C_0, C_1 > 0$ such that the estimates

$$\|u_\gamma\|_{W^{2,2}(\Omega)} + \|V_\gamma\|_{W^{2,2}(\Omega)} \leq C_0,$$

$$\|u_\gamma\|_{L^\infty(\Omega)} + \|V_\gamma\|_{L^\infty(\Omega)} \leq C_0$$

and

$$u_\gamma \geq C_1 > 0$$

hold uniformly with respect to $0 < \gamma < \gamma_0$. Uniform estimates of the same form are also valid if the parameter function L in the definition of $\mathcal{F}_\gamma$ varies in a bounded subset of $L^\infty(\Omega)$.
For sufficiently small $0 < \gamma < \gamma_0$, the minimizers $u = u_\gamma$ coincide and they are the unique positive minimizer to the original functional $\mathcal{F}$. The Euler-Lagrange equation

$$2\kappa\Delta u = -(V + L - k(u^2))u$$

holds, where $V = \Phi(u^2) + V_{inh}$.

Proof. By continuity of $\Phi : L^2(\Omega) \longrightarrow W^{2,2}(\Omega)$ and the Sobolev embedding theorems, there holds

$$\begin{aligned} \|V_\gamma\|_{L^\infty(\Omega)} \leq C\|V_\gamma\|_{W^{2,2}(\Omega)} &\leq C\left(\|u_\gamma^2\|_{L^2(\Omega)} + \|V_{inh}\|_{W^{2,2}(\Omega)}\right) \\ &= C\left(\|u_\gamma\|^2_{L^4(\Omega)} + \|V_{inh}\|_{W^{2,2}(\Omega)}\right) \\ &\leq C\left(\|u_\gamma\|^2_{W^{1,2}(\Omega)} + 1\right). \end{aligned}$$

The claimed uniform estimates to V_γ will therefore directly follow from a uniform estimate $\|u_\gamma\|_{W^{1,2}(\Omega)} \leq C$. As the constant in the coerciveness inequality (2.9) for $\mathcal{F}_\gamma$ is independent of $0 < \gamma < \gamma_0$ and only depends on $\|L\|_{L^\infty(\Omega)}$ but not on the particular choice of L, we infer

$$\|u_\gamma\|_{L^2(\Omega)} + 2\kappa\|\nabla u_\gamma\|_{L^2(\Omega)} \leq \mathcal{F}_\gamma(u_\gamma) + C \leq \mathcal{F}_\gamma(u^*) + C \leq C$$

with some arbitrary bounded function $u^* \in U$. We conclude

$$\|u_\gamma\|_{W^{1,2}(\Omega)} \leq C,$$

where the constant on the right hand side, however, depends on κ.
Concerning the L^∞-estimate to u_γ, we consider

$$\varphi(x) := \begin{cases} \frac{\max(u_\gamma(x) - C_2, 0)}{u_\gamma(x)}, & u_\gamma(x) \neq 0, \\ 0, & u_\gamma(x) = 0, \end{cases}$$

for some $C_2 > \| \operatorname{Tr} u_\gamma \|_{L^\infty(\partial\Omega)}$ to be determined later on. By Lemma A.3 this defines an element of $W_0^{1,2}(\Omega)$. Using φ as a test function, we arrive at

$$\begin{aligned} 0 &= \int_\Omega 2\kappa \langle \nabla u_\gamma(x), \nabla \varphi(x) \rangle \; dx + \int_\Omega \big(k_\gamma(u_\gamma(x)^2) - (V_\gamma(x) + L(x)) \big) \, u_\gamma(x) \varphi(x) \; dx \\ &= C_2 2\kappa \int_\Omega \frac{|\nabla \max(u_\gamma(x) - C_2, 0)|^2}{u_\gamma(x)^2} \; dx \\ &\quad + \int_\Omega \big(k_\gamma(u_\gamma(x)^2) - (V_\gamma(x) + L(x)) \big) \max(u_\gamma(x) - C_2, 0) \; dx. \end{aligned}$$

As k_γ is monotonically increasing with $\lim_{s\to\infty} k(s) = \infty$ and V_γ is uniformly bounded in $L^\infty(\Omega)$, we can choose C_2 large enough such that

$$\big(k_\gamma(u_\gamma(x)^2) - (V_\gamma(x) + L(x)) \big) > 0,$$

whenever $u_\gamma(x) > C_2$ and $0 < \gamma < \gamma_0$ for sufficiently small γ_0. Since in this case both appearing integrands are positive, we conclude that the sets $\{x \in \Omega \, : \, u_\gamma(x) > C_2\}$, $0 < \gamma < \gamma_0$, have Lebesgue measure zero, which shows

$$\|u_\gamma\|_{L^\infty(\Omega)} \le C \quad (0 < \gamma < \gamma_0).$$

Therefore, $k_\gamma(u_\gamma^2) - (V_\gamma + L)$ is uniformly bounded in L^∞ and $(k_\gamma(u_\gamma^2) - (V_\gamma + L))u_\gamma$ is uniformly bounded in $L^2(\Omega)$. The elliptic equation $2\kappa \Delta u_\gamma = -(V_\gamma + L - k_\gamma(u_\gamma^2))u_\gamma$ now implies, by continuity of $\Phi : L^2(\Omega) \longrightarrow W^{2,2}(\Omega)$ in concern with $u_\Gamma \in B^{3/2}_{2,2}(\Gamma)$, that

$$\|u_\gamma\|_{W^{2,2}(\Omega)} \le C \quad (0 < \gamma < \gamma_0).$$

We will show that the minimizers u_γ, $0 < \gamma < \gamma_0$, are uniformly bounded away from zero, provided that $k(0) = -\infty$. Possibly reducing γ_0 once more, there exists $C_1 > 0$, $\|u_\Gamma\|_{L^\infty(\partial\Omega)} > C_1$, such that

$$\|V_\gamma + L\|_{L^\infty(0,1)} - k(u^2) > 0 \quad (0 < \gamma < \gamma_0)$$

whenever $u \le C_1$. By continuity of u_γ, the sets

$$M_\gamma := \left\{ x \in \Omega \, : \, u_\gamma(x) = \min_{y\in\Omega} u_\gamma(y) \right\} \quad (0 < \gamma < \gamma_0)$$

are closed. Assuming $\min\limits_{y\in\Omega} u_\gamma(y) \le C_1$, we conclude by continuity of u_γ that

$$2\kappa \Delta u_\gamma(z) = -(V(z) + L(z) - k(u(z)^2))u(z) \le 0 \quad (z \in U_{x_0})$$

for any $x_0 \in M_\gamma$ and some neighborhood U_{x_0} of x_0. The maximum principle A.10 shows that u_γ is constant in U_{x_0} and we infer that the sets M_γ, $0 < \gamma < \gamma_0$, are open. Since Ω is connected, either $M_\gamma = \Omega$ or $M_\gamma = \emptyset$. Both options, however, yield a contradiction.
Because all minimizers are uniformly bounded from above and away from zero, we conclude

$$\mathcal{F}_\gamma(u_\gamma) = \mathcal{F}_{\tilde{\gamma}}(u_\gamma)$$

for $0 < \gamma, \tilde{\gamma} < \gamma_0$ and since the non-negative minimizers are unique, we see that all functions $u := u_\gamma$, $0 < \gamma < \gamma_0$, coincide. In fact, since the non-negative minimizer u_0 of $\mathcal{F}$ is unique and

$$\mathcal{F}(u) = \lim_{\gamma \searrow 0} \mathcal{F}_\gamma(u) = \lim_{\gamma \searrow 0} \mathcal{F}_\gamma(u_\gamma) \le \lim_{\gamma \searrow 0} \mathcal{F}_\gamma(u_0) = \mathcal{F}(u_0),$$

we find $u = u_0$. □

Remark 2.11.
Note that without any additional analysis it remains unclear, whether $\mathcal{F}$ is Fréchet-differentiable at the positive minimizer u, since in the higher-dimensional case there is no neighborhood $V \subset W^{1,2}(\Omega)$ of u such that $v \geq C_1 > 0$ for all $v \in V$. Differentiability at some positive u, however, is given in the one-dimensional case, since the embedding $W^{1,2}(\Omega) \hookrightarrow L^\infty(\Omega)$ then shows that positivity is preserved in some neighborhood of u.
In the case of Dirichlet boundary data, the assumption $k(0) = -\infty$ is not necessary. If $k(0) \in \mathbb{R}$, we may use the Harnack inequality A.11 instead of the maximum principle to prove positivity of minimizers in a similar fashion.

Lemma 2.12 (Continuous dependence of minimizers on F).
For $L \in L^\infty(0,1)$, let the functional $\mathcal{F} = \mathcal{F}^L$ be defined as in Proposition 2.6. The mapping $\mathcal{M} : L^\infty \longrightarrow W^{2,2}(\Omega)$, which maps L to the unique non-negative minimizer u of $\mathcal{F}$ is well-defined and continuous. More general, for all $1 \leq p \leq \infty$ and any sequence $(L_n)_{n\in\mathbb{N}} \subset L^\infty(0,1)$ which is bounded in $L^\infty(0,1)$ and converges in $L^p(0,1)$ to some $L \in L^\infty(0,1)$, it holds that $\mathcal{M}(L_n) \longrightarrow \mathcal{M}(L)$ in $W^{2,2}(0,1)$ as $n \longrightarrow \infty$.

Proof. Taking the pseudo-convex inequality of Lemma 2.8 into account, we see that $\mathcal{F} = \mathcal{F}^L$ has a unique non-negative minimizer $u \in W^{2,2}(\Omega)$ for any $L \in L^\infty(\Omega)$, which yields that $\mathcal{M}$ is well-defined. We first show that $\mathcal{M}$ is continuous from $L^\infty(\Omega)$ to $W^{2-\varepsilon,2}(\Omega)$, where $0 < \varepsilon < 1$ is chosen so small, that $W^{2-\varepsilon,2}(\Omega)$ still embeds continuously in $L^\infty(\Omega)$ (c.f. Theorem A.6). For $(L_n)_{n\in\mathbb{N}} \subset L^\infty(\Omega)$, $L_n \longrightarrow L \in L^\infty(\Omega)$ let $u_n := \mathcal{M}(L_n)$ and $u := \mathcal{M}(L)$. Since $(L_n)_{n\in\mathbb{N}}$ is contained in a bounded subset of $L^\infty(\Omega)$ we gain boundedness of $(u_n)_{n\in\mathbb{N}}$ in $W^{2,2}(\Omega)$ by using the a-priori estimates of Lemma 2.10. Assuming that $\mathcal{M}$ is not continuous, we may extract a subsequence $(u_{n_k})_{k\in\mathbb{N}}$ of $(u_n)_{n\in\mathbb{N}}$ such that $\|u_{n_k} - u\|_{W^{2-\varepsilon,2}(\Omega)} \geq \delta$ for some $\delta > 0$ and $k \in \mathbb{N}$. The compact embedding $W^{2,2}(\Omega) \hookrightarrow W^{2-\varepsilon,2}(\Omega)$ yields that some subsequence $(u_{n_l})_{l\in\mathbb{N}}$ of $(u_{n_k})_{k\in\mathbb{N}}$ converges in $W^{2-\varepsilon,2}(\Omega)$ and therefore in $W^{1,2}(\Omega)$ to some non-negative limit $\widetilde{u} \in W^{1,2}(\Omega)$. Since the mapping $v \mapsto \mathcal{F}^L(v)$ is weakly lower semi-continuous from $W^{1,2}(\Omega)$ to $\mathbb{R}$, we find

$$\begin{aligned}
\mathcal{F}^L(\widetilde{u}) \leq \liminf_{l\longrightarrow\infty} \mathcal{F}^L(u_{n_l}) &= \liminf_{l\longrightarrow\infty} \left(\mathcal{F}^{L_{n_l}}(u_{n_l}) + \int_\Omega (L_{n_l}(x) - L(x)) u_{n_l}^2(x)\, dx \right) \\
&\leq \liminf_{l\longrightarrow\infty} \left(\mathcal{F}^{L_{n_l}}(u) + C\|L_{n_l} - L\|_{L^1(\Omega)} \right) \\
&\leq \liminf_{l\longrightarrow\infty} \left(\mathcal{F}^{L_{n_l}}(u) + C\|L_{n_l} - L\|_{L^p(\Omega)} \right) \\
&= \mathcal{F}^L(u).
\end{aligned}$$

Since the non-negative minimizer of $\mathcal{F}^L$ is unique, we conclude $u = \widetilde{u}$, which is a contradition to the fact that $\|u_{n_l} - u\|_{W^{2-\varepsilon,2}(\Omega)} \geq \delta$ for all $l \in \mathbb{N}$. Continuity of $\mathcal{M} : L^\infty(\Omega) \longrightarrow W^{2,2}(\Omega)$ follows from the Euler-Lagrange equation for u by continuity of $\Phi : L^2(\Omega) \longrightarrow W^{2,2}(\Omega)$. □

2.3 Homogeneous Neumann boundary conditions

We now consider the one-dimensional case $\Omega = (0,1)$ and provide the necessary modifications to replace the Dirichlet boundary conditions for u by homogeneous Neumann boundary conditions.

Lemma 2.13 (Homogeneous Neumann boundary conditions).
Let $\mathcal{C} \in L^2(0,1)$, $L \in L^\infty(0,1)$ and $V_0, V_1 \in \mathbb{R}$. Assume $\lambda, \kappa > 0$ and let $k : (0,\infty) \longrightarrow \mathbb{R}$ be continuous and strictly increasing with $\lim_{s\to 0} k(s) = -\infty$, $\lim_{s\to\infty} k(s) = \infty$ and assume that

$s \mapsto \sqrt{s}k(s)$ extends to a continuous function on $[0,\infty)$. Then there exists a unique positive minimizer u of the functional $\mathcal{F}$ defined as in Proposition 2.6 in the minimizing set $W^{1,2}(0,1)$. The tuple $(u,V) \in (W^{2,2}(0,1))^2$, where $V = \Phi(u^2) + V_{inh}$ as in Lemma 2.10, is a solution to the problem

$$\begin{cases} 2\kappa u'' &= -(V + L - k(u^2))u, \quad \text{in } [0,1], \\ \lambda^2 V'' &= u^2 - \mathcal{C}, \quad \text{in } [0,1], \\ V(0) &= V_0, \\ V(1) &= V_1, \\ u'(0) &= 0, \\ u'(1) &= 0. \end{cases}$$

The mapping $\mathcal{M} : L^\infty(0,1) \longrightarrow W^{2,2}(\Omega)$ which maps L to the unique positive minimizer u of $\mathcal{F}$ is continuous. If L varies in a bounded subset of $L^\infty(0,1)$, the uniform estimates

$$\|u\|_{W^{2,2}(0,1)} + \|V\|_{W^{2,2}(0,1)} \le C_0,$$

$$\|u\|_{L^\infty(0,1)} + \|V\|_{L^\infty(0,1)} \le C_0,$$

$$u \ge C_1 > 0,$$

hold for certain constants $C_0, C_1 > 0$.

Proof. We define the clamped functionals $\mathcal{F}_\gamma$ as in Lemma 2.9 and we find for the unique non-negative minimizer u_γ to $\mathcal{F}_\gamma$

$$0 = (\mathcal{F}_\gamma)'(u_\gamma)\varphi = \int_0^1 2\kappa u_\gamma(x)'\varphi(x)'\,dx + \int_0^1 \left(k_\gamma(u_\gamma(x)^2) - (V_\gamma(x) + L(x)\right) u_\gamma(x)\varphi(x)\,dx$$

for all $\varphi \in W^{1,2}(0,1)$. Choosing $\varphi \in C_c^\infty(0,1)$ as an arbitrary test function we conclude

$$2\kappa u_\gamma'' = -(V + L - k(u_\gamma^2))u_\gamma \quad (0 < \gamma < \gamma_0),$$

so that actually $u_\gamma \in W^{2,2}(0,1)$. Since

$$\int_0^1 u_\gamma(x)'\varphi(x)'\,dx = -\int_0^1 u_\gamma''(x)\varphi(x)\,dx \quad (\varphi \in W^{1,2}(0,1))$$

implies $u'(0) = u'(1) = 0$ (choose the particular test functions $\varphi(x) = x$ and $\varphi(x) = 1 - x$, respectively), we know that the boundary conditions are fulfilled.
To establish the claimed a-priori estimates, which will also remove the regularisation from the functional, some modifications are in order. Uniform boundedness of $\|u_\gamma\|_{W^{1,2}(0,1)}$, $\|V_\gamma\|_{W^{2,2}(0,1)}$ and $\|V_\gamma\|_{L^\infty(0,1)}$ follow by the same arguments as before. As it is not known in advance, that the Dirichlet boundary values $u_\gamma(0)$ and $u_\gamma(1)$ are uniformly bounded from above, the maximum principle does not directly apply. Therefore, we exploit the embedding $W^{1,2}(0,1) \hookrightarrow C([0,1])$ to conclude the uniform boundedness of $\|u_\gamma\|_{L^\infty(0,1)}$. This in combination with the uniform boundedness of $u_\gamma'' = -(V + L - k_\gamma(u_\gamma^2))u_\gamma$ in $L^2(0,1)$ yields the remaining estimate

$$\|u_\gamma\|_{W^{2,2}(0,1)} \le C \quad (0 < \gamma < \gamma_0).$$

Uniform estimates from below to the minimizers u_γ require additional arguments. Since all functions u_γ, $0 < \gamma < \gamma_0$, have a vanishing derivative at 0 and 1, they can be extended by constants to a differentiable function on $\mathbb{R}$. Using the maximum principle as in Lemma 2.10, we conclude that the continuated solution is a constant if its minimum underruns a certain constant. Then u_γ is of course also constant in $(0, 1)$. This, however, is not a direct contradiction, since we do not have a lower bound on the traces $u_\gamma(0)$ and $u_\gamma(1)$. For this reason, we need to show that small constant functions cannot be minimizers of $\mathcal{F}_\gamma$ for $0 < \gamma < \gamma_0$.
We claim that there exists $\bar{u} > 0$ such that $\mathcal{F}_\gamma(0) > \mathcal{F}_\gamma(\bar{u})$ holds uniformly in $0 < \gamma < \gamma_0$. Considering

$$\begin{aligned}\mathcal{F}_\gamma(0) - \mathcal{F}_\gamma(\bar{u}) &= K_\gamma(0) - K_\gamma(\bar{u}^2) + \bar{u}^2 \left(\int_0^1 V_{inh}(x) + L(x)\, dx \right) - \frac{\lambda^2}{2} \|\Phi(\bar{u}^2)'\|^2_{L^2(0,1)} \\ &= I_1 + I_2 + I_3,\end{aligned}$$

we obviously have

$$|I_2| \leq \bar{u}^2 \|V_{inh} + L\|_{L^\infty(0,1)} \leq C\bar{u}^2 \quad (0 < \gamma < \gamma_0).$$

This estimate is also uniform in L if L varies in a bounded subset of $L^\infty(0, 1)$. Imposing the condition $|\bar{u}| \leq 1$, we conclude that $\|\Phi(\bar{u}^2)'\|_{L^2(0,1)}$ is bounded for any choice of $\bar{u}$. By linearity and continuity of Φ, we obtain

$$\|\Phi(\bar{u}^2)'\|^2_{L^2(0,1)} \leq C\bar{u}^4 \|\Phi(1)\|^2_{W^{1,2}(0,1)} \leq C\bar{u}^4$$

so that

$$|I_3| \leq C\bar{u}^2 \quad (0 < \gamma < \gamma_0).$$

We estimate

$$I_1 = K_\gamma(0) - K_\gamma(\bar{u}^2) = -\int_0^{\bar{u}^2} k_\gamma(t)\, dt \geq -\bar{u}^2 k_\gamma(\bar{u}^2)$$

and therefore, for sufficiently small $\bar{u}$,

$$I_1 \geq |k_\gamma(\bar{u}^2)|\bar{u}^2.$$

Since $|k(s)| \longrightarrow \infty$ as $s \to 0$, we can achieve that the coefficient $|k_\gamma(\bar{u}^2)|$ is arbitrary large for some small fixed $\bar{u} > 0$ by restricting the range $0 < \gamma < \gamma_0$ once more. We conclude

$$I_1 + I_2 + I_3 \geq C > 0$$

or rather

$$\mathcal{F}_\gamma(0) > \mathcal{F}_\gamma(\bar{u}) + C.$$

Because $|k_\gamma(\bar{u})^2|$ is monotonically increasing as $\gamma \searrow 0$ for fixed $\bar{u}$, these estimates are even uniform in $0 < \gamma < \gamma_0$. Therefore, the zero function is not a minimizer of $\mathcal{F}_\gamma$ for $0 < \gamma < \gamma_0$. By continuity of $c \mapsto \mathcal{F}_\gamma(c)$, $\mathbb{R} \longrightarrow \mathbb{R}$, we conclude that there exists $C_1 > 0$ such that any constant function c with $0 < c < C_1$ is not a minimizer to $\mathcal{F}_\gamma$ for $0 < \gamma < \gamma_0$. □

2.4 Periodic boundary conditions

We now investigate periodic boundary conditions in the interval $(0,1)$. The corresponding minimizing set is naturally given by $U := \{u \in W^{1,2}(0,1) \,:\, u(0) = u(1)\}$. However, it is impossible to impose the additional periodic boundary conditions $u'(0) = u'(1)$ without losing the weak closedness of U in $W^{1,2}(0,1)$. Fortunately, a closer consideration of the minimizers of the functional in the set U will reveal that the periodicity of the derivatives is automatically given.

Lemma 2.14 (**Periodic boundary conditions**).
Let $\mathcal{C} \in L^2(0,1)$, $L \in L^\infty(0,1)$ and $V_0, V_1 \in \mathbb{R}$. Assume $\lambda, \kappa > 0$ and let $k : (0,\infty) \longrightarrow \mathbb{R}$ be continuous and strictly increasing with $\lim_{s\to 0} k(s) = -\infty$, $\lim_{s\to\infty} k(s) = \infty$ and assume that $s \mapsto \sqrt{s}k(s)$ extends to a continuous function on $[0,\infty)$. Then there exists a unique positive minimizer u of the functional $\mathcal{F}$ defined as in Proposition 2.6 in the minimizing set

$$U := \{u \in W^{1,2}(0,1) \,:\, u(0) = u(1)\}\,.$$

The tuple $(u,V) \in (W^{2,2}(0,1))^2$, where $V = \Phi(u^2) + V_{inh}$ as in Lemma 2.10, is a solution to the problem

$$\begin{cases} 2\kappa u'' &= -(V + L - k(u^2))u, \quad \text{in } [0,1], \\ \lambda^2 V'' &= u^2 - \mathcal{C}, \quad \text{in } [0,1], \\ V(0) &= V_0, \\ V(1) &= V_1, \\ u(0) &= u(1), \\ u'(0) &= u'(1). \end{cases}$$

The mapping $\mathcal{M} : L^\infty(0,1) \longrightarrow W^{2,2}(\Omega)$ which maps L to the unique positive minimizer u of $\mathcal{F}$ is continuous. If L varies in a bounded subset of $L^\infty(0,1)$, the uniform estimates

$$\|u\|_{W^{2,2}(0,1)} + \|V\|_{W^{2,2}(0,1)} \le C_0,$$

$$\|u\|_{L^\infty(0,1)} + \|V\|_{L^\infty(0,1)} \le C_0,$$

$$u \ge C_1 > 0,$$

hold for certain constants $C_0, C_1 > 0$.

Proof. U is a convex and closed subset of $W^{1,2}(0,1)$ by the embedding $W^{1,2}(0,1) \hookrightarrow C([0,1])$. Therefore, U is weakly closed. Although it is not apparent at the moment, the choice of the minimizing set will be sufficient to guarantee the desired properties of the solution. Defining the clamped functionals $\mathcal{F}_\gamma$ as in Lemma 2.9, one can find non-negative minimizers u_γ, $0 < \gamma < \gamma_0$, satisfying

$$\begin{aligned} 0 = (\mathcal{F}_\gamma^\varphi)'(0) &= \int_0^1 2\kappa u_\gamma(x)'\varphi(x)'\,dx \\ &\quad + \int_0^1 \big(k_\gamma(u_\gamma(x)^2) - (V_\gamma(x) + L(x)\big)\, u_\gamma(x)\varphi(x)\,dx \end{aligned}$$

for any test function $\varphi \in C_c^\infty(0,1)$. It follows

$$2\kappa u_\gamma'' = -(V + L - k(u_\gamma^2))u_\gamma \quad (0 < \gamma < \gamma_0)$$

in the sense of distributions and therefore $u_\gamma \in W^{2,2}(0,1)$. On the other hand, since $1 \in U$, we may choose $\varphi \equiv 1$ in the integral equation above and obtain

$$2\kappa \int_0^1 u_\gamma''(x) = -\int_0^1 (V(x) + L(x) - k(u_\gamma^2(x)))u_\gamma(x)\, dx = 0.$$

This shows $u_\gamma'(0) = u_\gamma'(1)$ since the fundamental theorem of calculus is valid for Sobolev functions.

The claimed a-priori estimates follow from the same arguments as in the proof of Lemma 2.13 with a minor modification: The solutions u_γ are now considered to be extended periodically to $\mathbb{R}$ when using the maximum principle. □

Remark 2.15.
Remember that the choice $k(n) = h(n) + \frac{\nu}{\tau}\ln(n)$ depends on the original pressure term p through the relation $sh'(s) = p'(s)$. If h is the enthalpy belonging to an admissible pressure term p (c.f. Definition 2.2), we actually have $k(0) = -\infty$ and $\lim_{s\to\infty} k(s) = \infty$ thanks to the contribution of $\frac{\nu}{\tau}\ln(n)$. The assumption that $s \mapsto \sqrt{s}k(s)$ extends to a continuous function on $[0,\infty)$ is also satisfied in this situation. We mention that the enthalpies h, which fulfill $h(0) = -\infty$ and $\lim_{s\to\infty} h(s) = \infty$ are of particular interest, since in this case pointwise estimates from above and away from zero can be found that are even uniform in the parameter κ. This property is given for the pressure terms $p(n) = T_0 n^\gamma + \mu n$ for fixed $T_0, \mu > 0$ and $\gamma \geq 1$, c.f. Remark 2.3.

Corollary 2.16.
Let $F, V_B \in L^\infty(0,1)$, $\mathcal{C} \in L^2(0,1)$ and $V_0, V_1 \in \mathbb{R}$. Assume that h is the enthalpy to an admissible pressure term p. Then there exists a solution $(n,V) \in W^{2,2}(0,1) \times W^{2,2}(0,1)$ to the equations

$$\left\{ \begin{array}{rcl} F &=& -(V+V_B) + h(n) + \frac{\nu}{\tau}\ln(n) - 2(\varepsilon^2+\nu^2)\frac{\sqrt{n}''}{\sqrt{n}}, \quad in\ [0,1], \\ \lambda^2 V'' &=& n - \mathcal{C}, \quad in\ [0,1], \end{array} \right. \tag{2.11}$$

satisfying $V(0) = V_0$, $V(1) = V_1$, $n > 0$ in $[0,1]$, and fulfilling periodic boundary conditions

$$n(0) = n(1) \quad and \quad n'(0) = n'(1),$$

or homogeneous Neumann boundary conditions

$$n'(0) = n'(1) = 0,$$

or Dirichlet boundary conditions

$$n(0) = n_0 \quad and \quad n(1) = n_1$$

for given positive boundary values $n_0, n_1 > 0$.

Proof. Choosing $k(s) = h(s) + \frac{\nu}{\tau}\ln(s)$, $\kappa = \varepsilon^2 + \nu^2$ and $L = F + V_{inh} + V_B$, where $\lambda^2 V_{inh}'' = -\mathcal{C}$, $V_{inh}(0) = V_{inh}(1)$, we may use Lemma 2.14, Lemma 2.13 and Lemma 2.10 to obtain $n := u^2$ and V as a solution. Note that n' satisfies the respective boundary conditions by the chain rule. Moreover, $n = u^2 \in W^{2,2}(0,1)$, since $W^{2,2}(0,1)$ is a Banach algebra in the one-dimensional case (c.f. [Adams, Thm. 4.39]). □

2.5 Constrained solutions: The balance of mass

From a physical point of view, it is meaningful to demand that the total amount of charge $\int_0^1 n(x)\,dx$ in the device is a fixed quantity $C^* > 0$. A constraint of this form will be very useful for our anlysis, as it fixes the L^2-norms of the minimizers u, which have led to the solutions $n = u^2$. On the other hand, any positive solution n has a positive integral $\int_0^1 n(x)\,dx$ so that we do not have to assume that the set of solutions is reduced significantly, if C^* can be chosen arbitrarily. Imposing additional constraints to a minimizing set, however, has an effect on the Euler-Lagrange equation of the functional $\mathcal{F}$. We will see that the Euler-Lagrange equation shifts by an additive constant β, namely the Lagrange multiplier due to the integral constraint. The following results will present the cases of periodic boundary conditions and homogeneous Neumann boundary conditions. We will see that a similar result cannot hold for arbitrary charges in the case of Dirichlet boundary values.

Lemma 2.17 (**Periodic boundary conditions with balance of mass**).
Let $\mathcal{C} \in L^2(0,1)$, $L \in L^\infty(0,1)$ and $V_0, V_1 \in \mathbb{R}$. Assume $\lambda, \kappa > 0$ and let $k : (0,\infty) \longrightarrow \mathbb{R}$ be continuous and strictly increasing with $\lim_{s\to 0} k(s) = -\infty$, $\lim_{s\to\infty} k(s) = \infty$ and assume that $s \mapsto \sqrt{s}k(s)$ extends to a continuous function on $[0,\infty)$. Then there exist $B_0, B_1 > 0$ which only depend on the respective norms of the given data such that the unique positive minimizer u of the functional $\mathcal{F}$ as defined in Proposition 2.6 in the minimizing set

$$U := \Big\{ u \in W^{1,2}(0,1) \,:\, u(0) = u(1),\ u \geq B_0,\ \|u\|^2_{L^2(0,1)} = C^*,\ \|u'\|^2_{L^2(0,1)} \leq B_1 \Big\}$$

is a solution to the problem

$$\begin{cases} 2\kappa u'' &=& -(V + L + \beta - k(u^2))u, & \text{in } [0,1], \\ \lambda^2 V'' &=& u^2 - \mathcal{C}, & \text{in } [0,1], \\ V(0) &=& V_0, \\ V(1) &=& V_1, \\ u(0) &=& u(1), \\ u'(0) &=& u'(1), \\ \int_0^1 u^2(x)\,dx &=& C^*, \end{cases}$$

where $V = \Phi(u^2) + V_{inh}$ as in Lemma 2.10 and $\beta \in \mathbb{R}$ is a Lagrange multiplier due to the constraint $\int_0^1 u^2 = C^*$. The mapping $\mathcal{M} : L^\infty(0,1) \longrightarrow W^{2,2}(\Omega)$ which maps L to the unique positive minimizer u of $\mathcal{F}$ is continuous. If L varies in a bounded subset of $L^\infty(0,1)$, the uniform estimates

$$\|u\|_{W^{2,2}(0,1)} + \|V\|_{W^{2,2}(0,1)} \leq C_0,$$

$$\|u\|_{L^\infty(0,1)} + \|V\|_{L^\infty(0,1)} \leq C_0,$$

$$u \geq C_1 > 0,$$

hold for certain constants $C_0, C_1 > 0$.

Proof. For any choice of B_0 and B_1, we may write $U = U_1 \cap U_2$, where

$$U_1 := \big\{ u \in W^{1,2}(0,1) \,:\, u(0) = u(1),\ u \geq B_0 \big\}$$

and

$$U_2 = \left\{ u \in W^{1,2}(0,1) \,:\, \|u\|^2_{L^2(0,1)} = C^*,\ \|u'\|^2_{L^2(0,1)} \leq B_1 \right\}.$$

By the Mazur lemma U_1 is weakly closed. Any sequence $(u_n)_{n\in\mathbb{N}} \subset U_2$ which converges weakly to some $u \in W^{1,2}(0,1)$ converges strongly in $L^2(0,1)$, since the embedding $W^{1,2}(0,1) \hookrightarrow L^2(0,1)$ is compact. Then $\|u\|^2_{L^2(0,1)} = C^*$ and $\|u'\|^2_{L^2(0,1)} \leq \liminf_{n\to\infty} \|u'_n\|^2_{L^2(0,1)} \leq B_1$ so that $u \in U_2$. Therefore, U is weakly closed for any $B_1 > 0$ and $B_0 \geq 0$. To obtain intermediate results, we set B_0 equal to zero. Exploiting the coerciveness of $\mathcal{F}_\gamma$, we now fix $B_1 > 0$ by requiring that all minimizers u_γ to $\mathcal{F}_\gamma$ fulfill

$$\|u'_\gamma\|^2_{L^2(0,1)} \leq \frac{1}{2\kappa}(\mathcal{F}_\gamma(u_\gamma) + C) \leq \frac{1}{2\kappa}(\mathcal{F}_\gamma(\sqrt{C^*}) + C) < B_1 \quad (0 < \gamma < \gamma_0).$$

The non-negative minimizers to the functionals $\mathcal{F}_\gamma$ are unique, since the pseudo-convexity of $\mathcal{F}_\gamma$ still holds in the pseudo-convex set U. By the Lagrange multiplier rule (c.f. [Tro, Ch. 6.1.2]), we conclude that the Euler-Lagrange equation

$$2\kappa u''_\gamma = -(L+V)u_\gamma + k_\gamma(u^2_\gamma)u_\gamma - \beta u_\gamma$$

is fulfilled, where $V = \Phi(u^2_\gamma) + V_{inh}$ as in Lemma 2.10 and $\beta \in \mathbb{R}$ is a Lagrange multiplier. We can remove the γ-regularisation of the minimizers and deduce the claimed estimates to u in the same way as before, as soon as we have shown that the set of Lagrange multipliers β_γ, $0 < \gamma < \gamma_0$, is bounded. Multiplying the Euler-Lagrange equation by u_γ and integrating over $(0,1)$, we find

$$\beta_\gamma C^* = -\int_0^1 2\kappa u''_\gamma(x)u_\gamma(x) + (L(x) + V(x))u^2_\gamma(x)\,dx + \int_0^1 k_\gamma(u^2_\gamma(x))u^2_\gamma(x)\,dx$$

and therefore

$$|\beta_\gamma C^*| \leq 2\kappa\|u'\|^2_{L^2(0,1)} + \|L+V\|_{L^\infty(0,1)}C^* + \|k_\gamma(u^2_\gamma)u_\gamma\|_{L^2(0,1)}\|u_\gamma\|_{L^2(0,1)}.$$

Since Φ is continuous from $L^1(0,1)$ to $L^\infty(0,1)$, we conclude that $V = \Phi(u^2_\gamma) + V_{inh}$ is uniformly bounded in $L^\infty(0,1)$ for all u_γ with $\|u_\gamma\|^2_{L^2(0,1)} = C^*$. Due to the Sobolev embedding $W^{1,2}(0,1) \hookrightarrow L^\infty(0,1)$, we know $\|u_\gamma\|_{L^\infty(0,1)} \leq CB_1$. This in combination with the fact that $s \mapsto \sqrt{s}k_\gamma(s)$ is continuous and uniformly bounded for $0 < \gamma < \gamma_0$ in a neighbourhood of zero shows that $\|k_\gamma(u^2_\gamma)u_\gamma\|_{L^2(0,1)}$ is uniformly bounded for $0 < \gamma < \gamma_0$. We find

$$|\beta_\gamma C^*| \leq 2\kappa B_1 + C^*C.$$

Boundedness from below follows once more by the maximum principle. It should be mentioned that the only non-negative constant function in U is $\sqrt{C^*}$. As in Lemma 2.10, we conclude that the functionals $\mathcal{F}_\gamma$ and the corresponding minimizers u_γ as well as the Lagrange multipliers β_γ coincide for small γ, so that the regularisation vanishes. Finally, since the minimizers to $\mathcal{F}$ are uniformly bounded from below, we may replace $B_0 = 0$ by a positive constant without affecting the minimizers. □

The same argumentation yields a similar result for homogeneous Neumann boundary conditions:

Lemma 2.18 (**Homogeneous Neumann boundary conditions with balance of mass**).
Let $\mathcal{C} \in L^2(0,1)$, $L \in L^\infty(0,1)$ and $V_0, V_1 \in \mathbb{R}$. Assume $\lambda, \kappa > 0$ and let $k : (0,\infty) \longrightarrow \mathbb{R}$ be continuous and strictly increasing with $\lim_{s\to 0} k(s) = -\infty$, $\lim_{s\to\infty} k(s) = \infty$ and assume that $s \mapsto \sqrt{s}k(s)$ extends to a continuous function on $[0,\infty)$. Then there exist $B_0, B_1 > 0$ which only depend on the respective norms of the given data such that the unique positive minimizer u of the functional $\mathcal{F}$ as defined in Proposition 2.6 in the minimizing set

$$U := \left\{ u \in W^{1,2}(0,1) \;:\; u \geq B_0,\ \|u\|^2_{L^2(0,1)} = C^*,\ \|u'\|^2_{L^2(0,1)} \leq B_1 \right\}$$

is a solution to the problem

$$\begin{cases} 2\kappa u'' &= -(V + L + \beta - k(u^2))u, \quad \text{in } [0,1], \\ \lambda^2 V'' &= u^2 - \mathcal{C}, \quad \text{in } [0,1], \\ V(0) &= V_0, \\ V(1) &= V_1, \\ u'(0) &= 0, \\ u'(1) &= 0, \\ \int_0^1 u^2(x)\,dx &= C^*, \end{cases}$$

where $V = \Phi(u^2) + V_{inh}$ as in Lemma 2.10 and $\beta \in \mathbb{R}$ is a Lagrange multiplier due to the constraint $\int_0^1 u^2 = C^*$. The mapping $\mathcal{M} : L^\infty(0,1) \longrightarrow W^{2,2}(\Omega)$ which maps L to the unique positive minimizer u of $\mathcal{F}$ is continuous. If L varies in a bounded subset of $L^\infty(0,1)$, the uniform estimates

$$\|u\|_{W^{2,2}(0,1)} + \|V\|_{W^{2,2}(0,1)} \leq C_0,$$
$$\|u\|_{L^\infty(0,1)} + \|V\|_{L^\infty(0,1)} \leq C_0,$$
$$u \geq C_1 > 0,$$

hold for certain constants $C_0, C_1 > 0$.

Remark 2.19.
An analogous result does not hold for arbitrary masses $C^* > 0$ and Dirichlet boundary values $u(0) = u_0$, $u(1) = u_1$, since the coerciveness inequality (2.9) *demands*

$$(\max\{|u_0|, |u_1|\})^2 \leq C\|u\|^2_{W^{1,2}(0,1)} \leq C(\mathcal{F}(u) + C_0) \leq C(\mathcal{F}(\sqrt{C^*} + C_0).$$

But this inequality is void for fixed C^* and large boundary values u_0, u_1.

Remark 2.20 (**Representations for the Lagrange multiplier**).
In the situation of both Lemma 2.17 and Lemma 2.18 the following representations of the Lagrange multiplier β hold:

$$\beta = \frac{1}{C^*}\left(\int_0^1 2\kappa u'(x)^2 - (L(x) + V(x) - k(u^2(x)))u^2(x)\,dx\right), \tag{2.12}$$

$$\beta = \frac{1}{C^*}\left(\mathcal{F}(u) + \int_0^1 k(u^2(x))u^2(x) - K(u^2(x)) - \Phi(u^2)(x)u^2(x) - \frac{\lambda^2}{2}\Phi(u^2)'(x)\,dx\right)$$

$$= \frac{1}{C^*}\left(\mathcal{F}(u) + \int_0^1 k(u^2(x))u^2(x) - K(u^2(x)) - \frac{1}{2}\Phi(u^2)(x)u^2(x)\,dx\right), \tag{2.13}$$

$$\beta = -\left(\int_0^1 \left(L(x) + V(x) - k(u^2(x))\right)u(x)\,dx\right)\left(\int_0^1 u(x)\,dx\right)^{-1}. \tag{2.14}$$

Proof. Equality (2.12) is obtained by multiplying the Euler-Lagrange equation by u and integrating over $(0,1)$ by parts. Representation (2.13) now follows by comparing (2.12) with the functional. Finally, (2.14) follows by directly integrating the Euler-Lagrange equation, since the integral over u'' vanishes due to $u'(0) = u'(1)$. $\square$

Using the preparative results of the last sections, we are now able to solve the original problem, that is we are able to find solutions n and V to the system of equations (2.2).

2.6 Existence of stationary solutions for periodic boundary conditions with balance of mass

We now consider the case when the additional integral constraint $\int_0^1 n(x)\,dx = C^*$ is imposed on the original equations

$$\begin{cases} F &= -(V+V_B) + h(n) + \frac{\nu}{\tau}\ln(n) - 2(\varepsilon^2+\nu^2)\frac{\sqrt{n}''}{\sqrt{n}}, \quad \text{in } [0,1], \\ F' &= J_0\left(\frac{1}{\tau n} + 2\nu\frac{n'^2}{n^3}\right) - \left(\frac{J_0^2 - 4\nu J_0 n'}{2n^2}\right)', \quad \text{in } [0,1], \\ \lambda^2 V'' &= n - \mathcal{C}, \quad \text{in } [0,1]. \end{cases}$$

As seen in Lemma 2.17, such a constraint gives rise to an additional term in the Euler-Lagrange equation to the functional, namely some Lagrange multiplier β, which fortunately vanishes after differentiating the first line of the system. Therefore, it is still meaningful to consider solutions of the shifted problem

$$\begin{cases} F+\beta &= -(V+V_B) + h(n) + \frac{\nu}{\tau}\ln(n) - 2(\varepsilon^2+\nu^2)\frac{\sqrt{n}''}{\sqrt{n}}, \quad \text{in } [0,1], \\ F' &= J_0\left(\frac{1}{\tau n} + 2\nu\frac{n'^2}{n^3}\right) - \left(\frac{J_0^2 - 4\nu J_0 n'}{2n^2}\right)', \quad \text{in } [0,1], \\ \lambda^2 V'' &= n - \mathcal{C}, \quad \text{in } [0,1]. \end{cases} \tag{2.15}$$

The main theorem reads as follows.

Theorem 2.21 (Existence result for periodic boundary conditions with balance of mass).
Let $V_B \in L^\infty(0,1)$, $\mathcal{C} \in L^2(0,1)$, $\varepsilon, \lambda, \nu, \tau > 0$ and $F_{1;0}, V_0, V_1 \in \mathbb{R}$. Assume that h is the enthalpy to an admissible pressure term p and let

$$k := h + \frac{\nu}{\tau}\ln \quad \textit{and} \quad K(s) := \int_1^s k(t)\,dt \quad (s \geq 0).$$

Let $V_{inh} \in W^{2,2}(0,1)$ be the solution to $-\lambda^2 V_{inh}'' = \mathcal{C}$ in $(0,1)$, $V_{inh}(0) = V_0$, $V_{inh}(1) = V_1$. Define the continuous and linear operator $\Phi : L^2(0,1) \longrightarrow W^{2,2}(0,1)$, $f \mapsto V$, as the solution operator to the equations

$$\lambda^2 V'' = f \ \textit{in } (0,1), \quad V(0) = V(1) = 0.$$

Define the functional $\mathcal{F} : W^{1,2}(0,1) \longrightarrow \mathbb{R}$ by

$$\mathcal{F}(u) := \int_0^1 2(\varepsilon^2+\nu^2)u'(x)^2 - (F + V_B + V_{inh})\,u^2(x) + K(u^2(x)) + \frac{\lambda^2}{2}|\Phi(u^2)'(x)|^2\,dx.$$

For any $F \in L^\infty(0,1)$ there exists a unique positive minimizer $u \in U \cap W^{2,2}(0,1)$ of $\mathcal{F}$ in the minimizing set

$$U = \left\{ u \in W^{1,2}(0,1) \;:\; u(0) = u(1),\; u \geq B_0,\; \|u\|^2_{L^2(0,1)} = C^*,\; \|u'\|^2_{L^2(0,1)} \leq B_1 \right\}.$$

The corresponding maps $\mathcal{M} : L^\infty(0,1) \longrightarrow W^{1,2}_{pos}(0,1)$, $F \mapsto u$, and $\mathcal{L} : W^{1,2}_{pos}(0,1) \longrightarrow L^\infty(0,1)$, $u \mapsto F$, defined by

$$(\mathcal{L}u)(x) := J_0 \int_0^x \frac{1}{\tau u^2(y)} + 8\nu \frac{u'(y)^2}{u^4(y)}\, dy - \frac{J_0^2 - 8\nu J_0 u(x) u'(x)}{2u(x)^4} \qquad (u \in W^{1,2}_{pos}(0,1)),$$

where

$$J_0 := F_{1;0} \left(\int_0^1 \frac{1}{\tau u_0^2(y)} + 8\nu \frac{u_0'(y)^2}{u_0^4(y)}\, dy \right)^{-1},$$

are continuous. The bounds in the definition of U can be chosen in such a way that $\mathbb{F} := \mathcal{M} \circ \mathcal{L} : U \longrightarrow U$ is well-defined, continuous and compact. $\mathbb{F}$ has at least one fixed point in U and any fixed point u solves the Euler-Lagrange equation

$$2(\varepsilon^2 + \nu^2)u'' = -(F + V + V_B)u + (h(u^2) + \frac{\nu}{\tau}\ln(u^2))u - \beta u$$

for some $\beta \in \mathbb{R}$, where $F = \mathcal{L}(u)$. In this situation, the function $n := u^2$ is a solution to the entire system (2.15) and fulfills the periodic boundary conditions $n(0) = n(1)$, $n'(0) = n'(1)$ as well as the integral constraint $\int_0^1 u^2(x)\, dx = C^*$.

In order to prove the theorem, we need to introduce several regularisations for the functional $\mathcal{F}$. The main difficulty in finding suitable choices of B_0 and B_1 is that we need to take care of the fact that the minimizer, which will surely exist for any B_0, B_1, might not be an interior point of $\left\{ u \in W^{1,2}(0,1) \;:\; u(0) = u(1),\; u \geq B_0,\; \|u'\|^2_{L^2(0,1)} \leq B_1 \right\}$. In this situation, the Euler-Lagrange equation might not hold. This equation, however, is essential to prove higher order regularity estimates. We introduce the fully regularised functional under consideration.

Definition 2.22 (Fully regularised functional).
Let $\psi_\delta \in C^\infty(\mathbb{R})$ be a chosen function satisfying $\psi_\delta \geq \delta$, $|\psi_\delta'(s)| \leq 2$, $\psi_\delta(s) \geq \frac{|s|}{2}$ and

$$\psi_\delta(s) = \begin{cases} |s|, & |s| \geq 2\delta, \\ \delta, & 0 \leq |s| \leq \delta. \end{cases}$$

For $A \geq 0$ define

$$\xi_A(s) := \begin{cases} -A, & s \leq -A, \\ s, & -A < s < A, \\ A, & A \leq s. \end{cases}$$

Let $u_0 \in W^{1,2}(0,1)$ satisfy $u_0(0) = u_0(1)$, $\min\limits_{x \in [0,1]} u_0(x) > 0$ and $\|u_0\|^2_{L^2(0,1)} = C^*$.
Let $F_{\delta,A} = F_{\delta,A,u_0} \in W^{1,2}(0,1)$ be given by

$$F_{\delta,A}(x) := J_0 \int_0^x \frac{1}{\tau u_0^2(y)} + 8\nu \frac{u_0'(y)^2}{u_0^4(y)}\, dy - \frac{J_0^2}{2u_0^4(x)} + \frac{4\nu J_0 u_0(x) \xi_A(u_0'(x))}{\psi_\delta^2(u_0^2(x))},$$

where

$$J_0 := F_{1;0} \left(\int_0^1 \frac{1}{\tau u_0^2(y)} + 8\nu \frac{u_0'(y)^2}{u_0^4(y)} \, dy \right)^{-1}.$$

The fully regularised functional $\mathcal{F}_{\delta,A} = \mathcal{F}_{\delta,A,u_0} : W^{1,2}(0,1) \longrightarrow \mathbb{R}$ *is defined by*

$$\begin{aligned} \mathcal{F}_{\delta,A}(u) \quad := \quad & \int_0^1 2(\varepsilon^2 + \nu^2) u'(x)^2 - (F_{\delta,A}(x) + V_B(x) + V_{inh}(x))\, u^2(x) + K(u^2(x)) \\ & + \frac{\lambda^2}{2} |\Phi(u^2)'(x)|^2 \, dx \quad (u \in W^{1,2}(0,1)). \end{aligned}$$

We gather some a-priori estimates to minimizers of $\mathcal{F}_{\delta,A}$ and to $F_{\delta,A}$.

Lemma 2.23.
Let $u \in W^{1,2}(0,1)$ *be a positive function and let* $n = u^2$. *Define*

$$I(u) := \int_0^1 \frac{1}{\tau u^2(x)} + 8\nu \frac{u'(x)^2}{u^4(x)} \, dx = \int_0^1 \frac{1}{\tau n(x)} + 2\nu \frac{n'(x)^2}{n^3(x)} \, dx.$$

Then

$$\|u^{-1}\|_{L^2(0,1)} \leq (\tau I(u))^{1/2}, \tag{2.16}$$

$$\|(u^{-1})'\|_{L^2(0,1)} \leq C I(u)^{1/2} \nu^{-1/2}, \tag{2.17}$$

$$\|u^{-1}\|_{W^{1,2}(0,1)} \leq C I(u)^{1/2} (\tau^{1/2} + \nu^{-1/2}), \tag{2.18}$$

and for $\nu \leq \tau$

$$\|u^{-1}\|_{L^\infty(0,1)} \leq C I(u)^{1/2} \tau^{1/4} \nu^{-1/4}, \tag{2.19}$$

$$\|u^{-2}\|_{L^2(0,1)} \leq C I(u) \tau^{3/4} \nu^{-1/4}. \tag{2.20}$$

For $C^* = \int_0^1 u^2(x)\, dx$ *and* $J_0 = F_{1;0} I(u)^{-1}$, *there holds*

$$|J_0| \leq C\tau |F_{1;0}| C^*, \tag{2.21}$$

$$\left\| \frac{J_0}{u^2} \right\|_{L^\infty(0,1)} \leq C |F_{1;0}| \tau^{1/2} \nu^{-1/2}, \tag{2.22}$$

$$\left\| \frac{J_0}{u^2} \right\|_{L^2(0,1)} \leq C |F_{1;0}| \tau^{3/4} \nu^{-1/4}. \tag{2.23}$$

There exists a constant $C_{\delta,A} > 0$, *possibly depending on* $F_{1;0}, \nu$ *and* τ, *such that for any* $F_{\delta,A}$ *as in Definition 2.22*

$$\|F_{\delta,A}\|_{L^\infty(0,1)} \leq C_{\delta,A}. \tag{2.24}$$

Proof. Inequalities (2.16) to (2.18) directly follow from the definition of $I(u)$. Inequalities (2.19) and (2.20) are obtained by interpolation of (2.16) with (2.18) and (2.16) with (2.19), respectively. The Cauchy-Schwarz inequality shows

$$1 = \int_0^1 u(x) \frac{1}{u(x)} \, dx \leq \|u\|_{L^2(0,1)}^2 \|u^{-1}\|_{L^2(0,1)}^2 = C^* \int_0^1 \frac{1}{u^2(x)} \, dx,$$

which yields inequality (2.21). Combining this estimate with the inequalities (2.19) and (2.20), the remaining estimates (2.22) and (2.23) follow. Inequality (2.24) is valid by definition of J_0 and inequality (2.22) is satisfied, because

$$\begin{aligned}\|F_{\delta,A}\|_{L^\infty(0,1)} &\leq |F_{1;0}| + \left\|\frac{J_0^2}{2u_0^4}\right\|_{L^\infty(0,1)} + \left\|\frac{4\nu J_0 u_0 \xi_A(u_0')}{\psi_\delta^2(u_0^2)}\right\|_{L^\infty(0,1)} \\ &\leq |F_{1;0}| + CF_{1;0}^2\tau\nu^{-1} + 4\nu|J_0|A\delta^{-3/2} = C_{\delta,A}.\end{aligned}$$

□

Proposition 2.24.
Let $\mathcal{M} : L^\infty(0,1) \longrightarrow W^{1,2}(0,1)$ be the operator which maps $F_{\delta,A}$ to the unique positive minimizer of $\mathcal{F}_{\delta,A}$ and define $\mathcal{L}_{\delta,A}$ by

$$(\mathcal{L}_{\delta,A}u)(x) := J_0 \int_0^x \frac{1}{\tau u^2(y)} + 8\nu\frac{u'(y)^2}{u^4(y)}\, dy - \frac{J_0^2}{2u^4(x)} + \frac{4\nu J_0 u(x)\xi_A(u'(x))}{\psi_\delta^2(u^2(x))},$$

where

$$J_0 := F_{1;0}\left(\int_0^1 \frac{1}{\tau u^2(y)} + 8\nu\frac{u'(y)^2}{u^4(y)}\, dy\right)^{-1}. \tag{2.25}$$

There exist $B_{0,\delta,A}, B_{1,\delta,A} > 0$ such that $\mathbb{F}_{\delta,A} := \mathcal{M} \circ \mathcal{L}_{\delta,A} : U_{\delta,A} \longrightarrow U_{\delta,A}$ is well-defined, continuous and compact on the set

$$U_{\delta,A} := \left\{u \in W^{1,2}(0,1) \,:\, u(0) = u(1),\ u \geq B_{0,\delta,A},\ \|u\|_{L^2(0,1)}^2 = C^*,\ \|u'\|_{L^2(0,1)}^2 \leq B_{1,\delta,A}\right\}.$$

$\mathbb{F}_{\delta,A}$ has at least one fixed point $u \in U$ and the equations

$$\left\{\begin{aligned} F_{\delta,A} &= -(V+V_B) + k(u_{\delta,A}^2) - 2(\varepsilon^2+\nu^2)\tfrac{u_{\delta,A}''}{u_{\delta,A}} - \beta, \quad \text{in } [0,1], \\ F_{\delta,A}' &= J_0\left(\tfrac{1}{\tau u_{\delta,A}^2} + 8\nu\tfrac{u_{\delta,A}'^2}{u_{\delta,A}^4}\right) - \left(\tfrac{J_0^2}{2u_{\delta,A}^4} + \tfrac{4\nu J_0 u\xi_A(u_{\delta,A}')}{\psi_\delta^2(u_{\delta,A}^2)}\right)', \quad \text{in } [0,1], \\ \lambda^2 V'' &= u_{\delta,A}^2 - \mathcal{C}, \quad \text{in } [0,1], \end{aligned}\right. \tag{2.26}$$

hold.

Proof. The entirety of all positive minimizers $u_{\delta,A}$ of the respective functionals $\mathcal{F}_{\delta,A} = \mathcal{F}_{\delta,A,u_0}$ for all $u_0 \in U_1 := \left\{u \in W^{1,2}(0,1) \,:\, u_0 > 0,\ u(0) = u(1),\ \|u\|_{L^2(0,1)}^2 = C^*\right\}$ is uniformly bounded in $W^{1,2}(0,1)$ and away from zero according to Lemma 2.17, because the corresponding functions $F_{\delta,A} = F_{\delta,A,u_0} = \mathcal{L}_{\delta,A}(u_0)$ are uniformly bounded in $L^\infty(0,1)$ by inequality (2.24). We choose $B_{0,\delta,A}$ and $B_{1,\delta,A}$ equal to the constants B_0 and B_1 which were introduced in Lemma 2.17. Then, $\mathbb{F}_{\delta,A} = \mathcal{M} \circ \mathcal{L}_{\delta,A}$ maps the set $U_{\delta,A}$ into itself.
To prove continuity of $\mathbb{F}_{\delta,A}$, let $(u_n)_{n\in\mathbb{N}} \subset U_{\delta,A}$ be a sequence converging in $W^{1,2}(0,1)$ to some $u \in U_{\delta,A}$. By Lemma 2.12, it holds that $\mathcal{M}(\mathcal{L}_{\delta,A}(u_n)) \longrightarrow \mathcal{M}(\mathcal{L}_{\delta,A}(u))$ whenever $(\mathcal{L}_{\delta,A}(u_n))_{n\in\mathbb{N}}$ is bounded in $L^\infty(0,1)$ and $\mathcal{L}_{\delta,A}(u_n) \longrightarrow \mathcal{L}_{\delta,A}(u)$ in $L^2(0,1)$. Boundedness follows by inequality (2.24). For $u, v \in W^{1,2}(0,1)$ with $u, v > 0$, it follows from a short calculation that

$$\left|\int_0^x \left(\frac{1}{\tau u^2(y)} + 8\nu\frac{u'(y)^2}{u^4(y)}\right) - \left(\frac{1}{\tau v^2(y)} + 8\nu\frac{v'(y)^2}{v^4(y)}\right)\, dy\right| \leq C(u)(\|u-v\|_{W^{1,2}(0,1)})$$

uniformly for $x \in [0,1]$, where $C(u)$ is a constant which does not depend on v, if $\|u-v\|_{W^{1,2}(0,1)}$ is small. This shows that J_0 continuously depends on u. Taking the supremum over $x \in [0,1]$ in the inequality above, we see that $u \mapsto \int_0^x \frac{1}{\tau u^2(y)} + 8\nu \frac{u'(y)^2}{u^4(y)}\, dy$ is continuous from $W^{1,2}(0,1)$ to $L^\infty(0,1)$. Therefore, it is also continuous from $W^{1,2}(0,1)$ to $L^2(0,1)$. Another calculation yields that $u \mapsto -\frac{J_0^2}{2u^4} + \frac{4\nu J_0 u \xi_A(u')}{\psi_\delta^2(u^2)}$ is continuous from $W^{1,2}(0,1)$ to $L^2(0,1)$. We have shown that $\mathbb{F}_{\delta,A}$ is continuous. As the set of all minimizers $u_{\delta,A}$ is uniformly bounded in $W^{2,2}(0,1)$ by Lemma 2.17, compactness of $\mathbb{F}_{\delta,A}$ follows from the compactness of the embedding $W^{2,2}(0,1) \hookrightarrow W^{1,2}(0,1)$. Since all elements of $U_{\delta,A}$ have a common lower bound, we know that $u \mapsto u^2$ is a $W^{1,2}(0,1)$-homeomorphism between $U_{\delta,A}$ and the bounded, closed, convex set $\{u^2 \,:\, u \in U_{\delta,A}\}$. The Schauder fixed point theorem A.12 applies and each fixed point $u_{\delta,A}$ to $\mathbb{F}_{\delta,A}$ solves the system of equations (2.26). ☐

We now derive further estimates to fixed points of $\mathbb{F}_{\delta,A}$, which will show that the bounds in the definition of $U_{\delta,A}$ can be chosen independently of δ and A. Then, all regularisations of the original problem vanish.

Lemma 2.25.
There exist constants $C_0, C_1 > 0$ which do not depend on δ, ε, ν and A such that any fixed point $u_{\delta,A}$ of $\mathbb{F}_{\delta,A}$ from Proposition 2.24 fulfills

$$\int_0^1 \left|F_{\delta,A}(x) u_{\delta,A}^2(x)\right| \, dx \le C\left(1 + \nu \|u'_{\delta,A}\|_{L^2(0,1)}\right) \tag{2.27}$$

and

$$(\varepsilon^2 + \nu^2)\|u'_{\delta,A}\|^2_{L^2(0,1)} \le C_1(1 + \delta^{-1}\nu^{-1/2}). \tag{2.28}$$

In particular, the constant $B_{1,\delta,A}$ introduced in the definition of $U_{\delta,A}$ can be chosen independently of A. Moreover, the set of Lagrange multipliers $\beta_{\delta,A}$ belonging to fixed points $u_{\delta,A}$ is bounded independently of A.

Proof. Let $u_{\delta,A}$ be a fixed point of $\mathbb{F}_{\delta,A}$. Then $u_{\delta,A}$ is a minimizer of $\mathcal{F}_{\delta,A}$ with corresponding $F_{\delta,A}$,

$$F_{\delta,A} = G_{\delta,A} - \frac{J_0^2}{2u_{\delta,A}^4} + \frac{4\nu J_0 u_{\delta,A} \xi_A(u'_{\delta,A})}{\psi_\delta^2(u_{\delta,A}^2)},$$

where

$$G_{\delta,A}(x) = J_0 \int_0^x \frac{1}{\tau u_{\delta,A}^2(y)} + 8\nu \frac{u'_{\delta,A}(y)^2}{u_{\delta,A}^4(y)}\, dy \quad (x \in [0,1])$$

and

$$J_0 = F_{1;0}\left(\int_0^1 \frac{1}{\tau u_{\delta,A}^2(y)} + 8\nu \frac{u'_{\delta,A}(y)^2}{u_{\delta,A}^4(y)}\, dy\right)^{-1}.$$

Since $\mathcal{F}_{\delta,A}(u_{\delta,A}) \leq \mathcal{F}_{\delta,A}(\sqrt{C^*})$ and K is bounded from below, we find

$$
\begin{aligned}
2(\varepsilon^2+\nu^2)\|u'_{\delta,A}\|^2_{L^2(0,1)} \leq & \int_0^1 (F_{\delta,A}(x)+V_B(x)+V_{inh}(x))(u^2_{\delta,A}(x)-C^*)\,dx \\
& + \int_0^1 K(C^*)-K(u^2_{\delta,A}(x))\,dx \\
& + \frac{\lambda^2}{2}\left(\|\Phi(C^*)'\|^2_{L^2(0,1)} - \|\Phi(u^2_{\delta,A})'\|^2_{L^2(0,1)}\right) \\
\leq & \left|\int_0^1 F_{\delta,A}(x)u^2_{\delta,A}(x)\,dx\right| + \left|\int_0^1 F_{\delta,A}(x)C^*\,dx\right| + C,
\end{aligned}
$$

where C only depends on $A, C^*, \|V_B\|_{L^\infty(0,1)}$ and $\|V_{inh}\|_{L^\infty(0,1)}$. The estimate

$$
\|G_{\delta,A}\|_{L^\infty(0,1)} \leq |F_{1;0}|
$$

holds by definition of J_0. Using inequality (2.16), it follows

$$
\begin{aligned}
\int_0^1 \left|F_{\delta,A}(x)u^2_{\delta,A}(x)\right|\,dx \leq & \int_0^1 |G_{\delta,A}(x)|u^2_{\delta,A}(x)\,dx + \int_0^1 \frac{J_0^2}{2u^2_{\delta,A}(x)}\,dx \\
& + 4\nu\sqrt{|J_0|}\int_0^1 \frac{u^3_{\delta,A}(x)}{\psi_\delta^{3/2}(u^2_{\delta,A}(x))}\cdot\frac{\sqrt{|J_0|}}{\psi_\delta^{1/2}(u^2_{\delta,A}(x))}\cdot|\xi_A(u'_{\delta,A}(x)|\,dx \\
\leq & |F_{1;0}|C^* + \frac{|J_0|}{2}\tau|F_{1;0}| \\
& + C\nu\sqrt{|J_0|}\left\|\frac{u^3_{\delta,A}}{\psi_\delta^{3/2}(u^2_{\delta,A})}\right\|_{L^\infty(0,1)}\cdot\left\|\frac{\sqrt{|J_0|}}{\psi_\delta^{1/2}(u^2_{\delta,A})}\right\|_{L^2(0,1)}\cdot\left\|u'_{\delta,A}\right\|_{L^2(0,1)} \\
\leq & |F_{1;0}|C^* + \frac{1}{2}F^2_{1;0}\tau^2C^* + C\nu(\tau|F_{1;0}|C^*)^{1/2}(\tau|F_{1;0}|)^{1/2}\|u'_{\delta,A}\|_{L^2(0,1)} \\
\leq & C(1+\nu\|u'_{\delta,A}\|_{L^2(0,1)}),
\end{aligned}
$$

where the constant on the right hand side only depends on $|F_{1;0}|, \tau$ and C^*. Applying Young's inequality, we deduce

$$
\int_0^1 \left|F_{\delta,A}(x)u^2_{\delta,A}(x)\right|\,dx \leq C + \frac{\nu^2}{2}\|u'_{\delta,A}\|^2_{L^2(0,1)}.
$$

Using inequality (2.23), we estimate

$$\begin{aligned}
\int_0^1 |F_{\delta,A}(x)C^*|\ dx &\le \int_0^1 |G_{\delta,A}(x)|C^*\ dx + \int_0^1 \frac{J_0^2}{2u_{\delta,A}^4(x)}C^*\ dx \\
&\quad +4\nu \int_0^1 \frac{u_{\delta,A}(x)}{\psi_\delta^{1/2}(u_{\delta,A}^2(x))} \cdot \frac{|J_0|}{\psi_\delta(u_{\delta,A}^2(x))} \cdot \frac{C^*}{\psi_\delta^{1/2}(u_{\delta,A}^2(x))}|\xi_A(u'_{\delta,A}(x))|\ dx \\
&\le |F_{1;0}|C^* + \frac{C^*}{2}(|F_{1;0}|\tau^{3/4}\nu^{-1/4})^2 \\
&\quad +4\nu \left\| \frac{u_{\delta,A}}{\psi_\delta^{1/2}(u_{\delta,A}^2)} \right\|_{L^\infty(0,1)} \left\| \frac{J_0}{\psi_\delta(u_{\delta,A}^2)} \right\|_{L^2(0,1)} C^*\delta^{-1/2} \left\| u'_{\delta,A} \right\|_{L^2(0,1)} \\
&\le |F_{1;0}|C^* + \frac{C^*}{2}(|F_{1;0}|\tau^{3/4}\nu^{-1/4})^2 + \nu C|F_{1;0}|\tau^{3/4}\nu^{-1/4}C^*\delta^{-1/2} \left\| u'_{\delta,A} \right\|_{L^2(0,1)} \\
&\le C\left(1+\nu^{-1/2}+\nu^{3/4}\delta^{-1/2}\left\| u'_{\delta,A} \right\|_{L^2(0,1)}\right) \\
&\le C(1+\nu^{-1/2}+\delta^{-1}\nu^{-1/2}) + \frac{\nu^2}{2}\|u'_{\delta,A}\|^2_{L^2(0,1)},
\end{aligned}$$

where we have also used Young's inequality in the final step. Combining all inequalities and assuming $\delta, \nu < 1$, we obtain

$$(\varepsilon^2+\nu^2)\|u'_{\delta,A}\|^2_{L^2(0,1)} \le C(1+\delta^{-1}\nu^{-1/2}).$$

Thus, the inequality

$$\int_0^1 F_{\delta,A}(x)u_{\delta,A}^2(x)\ dx \le C + \frac{\nu^2}{2}\|u'_{\delta,A}\|^2_{L^2(0,1)} \le C(1+\delta^{-1}\nu^{-1/2})$$

is satisfied as well. We can now replace $B_{1,\delta,A}$ by a number $B_{1,\delta}$ which is larger than $C(1+\delta^{-1}\nu^{-1/2})$ and independent of A. Reconsidering the representation (2.12) for the Lagrange multipliers, we conclude that the set of Lagrange multipliers is bounded independently of A. □

Lemma 2.26.
There exists a constant $B_{0,\delta} > 0$ which does not depend on A such that

$$B_{0,\delta} < u_{\delta,A}$$

for any fixed point $u_{\delta,A}$ of the mapping $\mathbb{F}_{\delta,A}$ introduced in Proposition 2.24. In particular, the lower bound $B_{0,\delta,A}$ in the definition of $U_{\delta,A}$ can be chosen independently of A.

Proof. By Lemma 2.25 we know that the set of fixed points $u_{\delta,A}$ to $\mathbb{F}_{\delta,A}$ is bounded in $W^{1,2}(0,1)$ independently of A. Then $F_{\delta,A}u_{\delta,A}$ is also uniformly bounded in $L^2(0,1)$ with respect to A. Because the set of Lagrange multipliers $\beta_{\delta,A}$ is also bounded independently of A, we may employ the Euler-Lagrange equation

$$2(\varepsilon^2+\nu^2)u''_{\delta,A} = -(F_{\delta,A}+V_B+V+\beta-k(u_{\delta,A}^2))u_{\delta,A}$$

to deduce that $2(\varepsilon^2+\nu^2)\|u''_{\delta,A}\|_{L^2(0,1)}$ is actually bounded independently of A. The Sobolev embedding Theorem A.6 now implies

$$\|u'_{\delta,A}\|_{L^\infty(0,1)} \le C\|u_{\delta,A}\|_{W^{2,2}(0,1)} \le C_\delta.$$

The corresponding functions $F_{\delta,A} = F_{\delta,A,u_{\delta,A}}$ are therefore bounded independently of A in $L^\infty(0,1)$. Applying the maximum principle as in Lemma 2.10, we find a lower bound to the fixed points $u_{\delta,A}$, which does not depend on A. □

We now replace the set $U_{\delta,A}$ in Proposition 2.24 by

$$U_\delta := \left\{ u \in W^{1,2}(0,1) \,:\, u(0) = u(1),\ u \geq B_{0,\delta},\ \|u\|^2_{L^2(0,1)} = C^*,\ \|u'\|^2_{L^2(0,1)} \leq B_{1,\delta} \right\},$$

where the constants $B_{0,\delta}$ and $B_{1,\delta}$ are given by Lemma 2.25 and Lemma 2.26. In the following, we will drop the index A and the regularisation function ξ_A.

Lemma 2.27.
There exists a constant $B_0 > 0$ which does not depend on δ such that for any fixed point u_δ of $\mathbb{F}_\delta$ it holds

$$B_0 < u_\delta.$$

In particular, for small $0 < \delta < \delta_0$, it follows that $\psi^2_\delta(u^2_\delta) = u^4_\delta$ for the function ψ_δ introduced in Definition 2.22. The constants $B_{0,\delta}$ and $B_{1,\delta}$ in the definition of U_δ can be replaced by positive constants B_0 and B_1 which do not depend on δ.

Proof. We show that the Lagrange multipliers β_δ belonging to the fixed points u_δ are bounded from below independently of δ. Multiplying the Euler-Lagrange equation

$$2(\varepsilon^2 + \nu^2)u''_\delta = -(F_\delta + V_B + V + \beta - k(u^2_\delta))u_\delta$$

by u_δ and integrating over $(0,1)$, we obtain as in (2.12)

$$\begin{aligned}
\beta C^* &= 2(\varepsilon^2+\nu^2)\|u'_\delta\|^2_{L^2(0,1)} - \int_0^1 (F_\delta(x) + V_B(x) + V_{inh}(x))\, u^2_\delta(x)\, dx \\
&\quad - \int_0^1 \Phi(u^2_\delta)(x) u^2_\delta(x)\, dx + \int_0^1 k(u^2_\delta(x)) u^2_\delta(x)\, dx \\
&\geq 2(\varepsilon^2+\nu^2)\|u'_\delta\|^2_{L^2(0,1)} - \left| \int_0^1 F_\delta(x) u^2_\delta(x)\, dx \right| - \|V_B + V_{inh}\|_{L^\infty(0,1)} C^* \\
&\quad + \int_0^1 |\Phi(u^2_\delta)'(x)|^2\, dx + \int_0^1 k(u^2_\delta(x)) u_\delta(x) \cdot u_\delta(x)\, dx.
\end{aligned}$$

Since $s \mapsto \sqrt{s}k(s)$ is continuous on $[0,\infty)$ and $k(s) \to \infty$ for $s \to \infty$, it follows that the term $k(u^2_\delta(x))u_\delta(x)$ is bounded from below and it can only be negative on a set of the form $\{x \in [0,1] \,:\, u_\delta(x) \leq C\}$. Therefore,

$$\int_0^1 k(u^2_\delta(x)) u_\delta(x) \cdot u_\delta(x)\, dx \geq -C.$$

Using the estimate $\left|\int_0^1 F_\delta(x) u_\delta(x)^2\, dx\right| \leq C\left(1 + \nu\|u'_\delta\|_{L^2(0,1)}\right)$ (c.f. inequality (2.27)), we deduce

$$\beta_\delta C^* \geq 2(\varepsilon^2+\nu^2)\|u'_\delta\|^2_{L^2(0,1)} - \nu\|u'_\delta\|_{L^2(0,1)} - C.$$

Boundedness of β_δ from below then follows from

$$\beta_\delta C^* \geq (2\varepsilon^2 + \nu^2)\|u'_\delta\|^2_{L^2(0,1)} - C.$$

We reconsider the Euler-Lagrange equation

$$2(\varepsilon^2+\nu^2)u_\delta'' = -\left(F_\delta + V_B + V_{inh} + \Phi(u_\delta^2) - k(u_\delta^2) + \beta_\delta\right) u_\delta,$$

where

$$\begin{aligned} F_\delta &= G_\delta - \frac{J_0^2}{2u_\delta^4} + \frac{4\nu J_0 u_\delta u_\delta'}{\psi_\delta^2(u_\delta^2)}, \\ J_0 &= F_{1;0}\left(\int_0^1 \frac{1}{\tau u_\delta^2(x)} + 8\nu \frac{u_\delta'^2(x)}{u_\delta^4(x)}\, dx\right)^{-1}, \\ G_\delta(x) &= J_0 \int_0^x \frac{1}{\tau u_\delta^2(y)} + 8\nu \frac{u_\delta'^2(y)}{u_\delta^4(y)}\, dy \quad (x \in [0,1]). \end{aligned}$$

Since Φ is a continuous operator from $L^1(0,1)$ to $L^\infty(0,1)$, we deduce that the functions $\Phi(u_\delta^2)$ are bounded in $L^\infty(0,1)$ independently of δ. We have $\|G_\delta\|_{L^\infty(0,1)} \le F_{1;0}$ and by inequality (2.22), we know $\left\|\frac{J_0^2}{2u_\delta^4}\right\|_{L^\infty(0,1)} \le CF_{1;0}^2\tau\nu^{-1}$. Since the Lagrange multipliers β_δ are bounded from below independently of δ and $k(0)=-\infty$, we find a constant $0 < c_0 < \sqrt{C^*}$, which does not depend on δ, such that

$$G_\delta - \frac{J_0^2}{2u_\delta^4} + V_B + V_{inh} + \Phi(u_\delta^2) - k(c_0) + \beta_\delta > 0. \tag{2.29}$$

Assume $\min_{x\in[0,1]} u_\delta(x) \le c_0$. For any minimizer

$$x_0 \in \left\{ x \in [0,1] \,:\, u_\delta(x) = \min_{y\in[0,1]} u_\delta(y) \right\},$$

we know that $u_\delta'(x_0)=0$ and therefore $\frac{4\nu J_0 u_\delta(x_0) u_\delta'(x_0)}{\psi_\delta^2(u_\delta^2(x_0))} = 0$. By continuity of u_δ and u_δ' and by inequality (2.29), we see that

$$2(\varepsilon^2+\nu^2)u_\delta'' \le 0$$

in some neighborhood $B(x_0,r_0)$ of x_0. The maximum principle A.10 yields that u_δ must be a constant function in $B(x_0,r_0)$. This shows that the set of minimizers of u_δ is open. Since it is also closed, we deduce that u_δ is a constant function in $[0,1]$. This, however, leads to

$$C^* = \|u_\delta\|_{L^2(0,1)}^2 \le c_0^2 < C^*,$$

which is a contradiction. Thus, we have shown that c_0 is a lower bound to fixed points u_δ, which does not depend on δ. □

2.7 Existence of stationary solutions for homogeneous Neumann boundary conditions with balance of mass

We discuss some modifications of the last section in order to treat homogeneous Neumann boundary conditions. The relationship between J_0, u and $F_{1;0}$ is obtained by integration (by parts) of the identity (2.5) and reads as

$$\begin{aligned} F_{1;0} &= -\frac{J_0^2}{2}\left(\frac{1}{u^4(1)} - \frac{1}{u^4(0)}\right) + J_0 \int_0^1 \frac{1}{\tau u^2(y)} + 8\nu \frac{u'(y)^2}{u^4(y)}\, dy \\ &=: -\frac{J_0^2}{2} H(u) + J_0 I(u). \end{aligned} \tag{2.30}$$

We want to define J_0 as a function of u in such a way, that this equality holds at least in the fixed point of $\mathcal{F} = \mathcal{M} \circ \mathcal{L}$ and at least for sufficiently small $|F_{1;0}|$. In the case of $H(u) \neq 0$, the solutions

$$J_0 = \frac{I(u) \pm \sqrt{I(u)^2 - 2H(u)F_{1;0}}}{H(u)}$$

exist. However, since we are only interested in small, real-valued J_0, the rigorous definition

$$J_0 = J_0(u) := \begin{cases} F_{1;0} I(u)^{-1}, & H(u) = 0, \\ \mathrm{Re}\left(\frac{I(u) - \sqrt{I(u)^2 - 2H(u)F_{1;0}}}{H(u)}\right), & H(u) \neq 0, \end{cases} \tag{2.31}$$

is a promising choice. To prove an analogous result to Theorem 2.21, the estimates (2.16) to (2.24) have to be verified. Surely, inequalities (2.16) to (2.20) are still given. We claim that by definition (2.31) of J_0, inequalities (2.21) to (2.24) remain valid:

Lemma 2.28.
Let $C^* > 0$. For any positive $u \in W^{1,2}(0,1)$ with $\int_0^1 u^2(x)\,dx = C^*$ and corresponding J_0, defined by (2.31), there holds

$$|I(u)J_0| \leq 2|F_{1;0}|.$$

Thus, the estimates (2.21) to (2.24) are satisfied.
The assignment $u \mapsto J_0(u)$, $W^{1,2}_{pos}(0,1) \to \mathbb{R}$, is continuous.

Proof. We distinguish three cases:
If $H(u) = 0$, then $|I(u)J_0| \leq |F_{1;0}|$ obviously holds.
If $I(u)^2 - 2H(u)F_{1;0} \leq 0$, then $J_0 = \frac{I(u)}{H(u)}$ and $0 \leq I(u)^2 \leq 2H(u)F_{1;0} = 2|H(u)||F_{1;0}|$ yields $|I(u)J_0| \leq 2|F_{1;0}|$.
In the third case $I(u)^2 - 2H(u)F_{1;0} > 0$, we have $J_0 = \frac{I(u) - \sqrt{I(u)^2 - 2H(u)F_{1;0}}}{H(u)}$ and then, because $I(u) > 0$,

$$\begin{aligned} |I(u)J_0| &= \left| \mathrm{sgn}(H(u)) \left| \frac{I(u)^2}{H(u)} \right| - \mathrm{sgn}(H(u)) \left| \frac{I(u)}{H(u)} \right| \sqrt{I(u)^2 - 2H(u)F_{1;0}} \right| \\ &= \left| \left| \frac{I(u)^2}{H(u)} \right| - \sqrt{ \left| \frac{I(u)^2}{H(u)} \right|^2 - 2F_{1;0}\,\mathrm{sgn}(H(u)) \left| \frac{I(u)^2}{H(u)} \right| } \right|. \end{aligned}$$

The desired estimate now follows, since for any $\alpha \geq 0$ the functions

$$f : (0,\infty) \longrightarrow \mathbb{R}, \quad z \mapsto z - \sqrt{z^2 + \alpha z}$$

and

$$g : (\alpha,\infty) \longrightarrow \mathbb{R}, \quad z \mapsto z - \sqrt{z^2 - \alpha z}$$

fulfill $0 \geq f(z) > -\frac{\alpha}{2}$ for $z > 0$ and $\frac{\alpha}{2} < g(z) \leq \alpha$ for $z \geq \alpha$. Note that $\left|\frac{I(u)^2}{H(u)}\right| > 2\,\mathrm{sgn}(H(u))F_{1;0}$ is given in the third case, because $I(u)^2 > 2H(u)F_{1;0} = 2F_{1;0}\,\mathrm{sgn}(H(u))|H(u)|$. We mention that both functions are monotonically decreasing with $\lim_{z\to\infty} f(z) = -\dfrac{\alpha}{2}$ and $\lim_{z\to\infty} g(z) = \dfrac{\alpha}{2}$.
It remains to prove that $u \mapsto J_0(u)$ is continuous from $W^{1,2}(0,1)$ to $\mathbb{R}$. We already know that $u \mapsto I(u)$, $W^{1,2}_{pos}(0,1) \to \mathbb{R}$, is continuous. Exploiting the embedding $W^{1,2}(0,1) \hookrightarrow C([0,1])$, we

also know that $u \mapsto H(u)$, $W^{1,2}_{pos}(0,1) \to \mathbb{R}$, is continuous. Therefore, the only critical points for the continuity of $u \mapsto J_0(u)$ are the zeros of H. Let $v \in W^{1,2}(0,1)$ with $H(v) = 0$. Since $I(u) > \frac{1}{\tau C^*}$, we know $I(u)^2 - 2H(u)F_{1;0} > 0$ for small $H(u)$ and then

$$\begin{aligned} |I(u)J_0(u) - I(v)J_0(v)| &= \left| \frac{I(u)^2}{H(u)} - \frac{I(u)}{H(u)}\sqrt{I(u)^2 - 2H(u)F_{1;0}} - F_{1;0} \right| \\ &= \left| \left|\frac{I(u)^2}{H(u)}\right| - \sqrt{\left|\frac{I(u)^2}{H(u)}\right|^2 - 2F_{1;0}\operatorname{sgn}(H(u))\left|\frac{I(u)^2}{H(u)}\right|} - \operatorname{sgn}(H(u))F_{1;0} \right|. \end{aligned}$$

Taking the asymptotics of the functions f and g into account, we see that $I(u)J_0(u)$ tends to $I(v)J_0(v)$ when $u \to v$. This shows that $u \mapsto I(u)J_0(u)$ is continuous in v. Since $I(u) \geq \frac{1}{\tau C^*} > 0$, we deduce that $u \mapsto J_0(u)$ is also continuous in v.

□

Theorem 2.29 (Existence result for homogeneous Neumann boundary conditions with balance of mass).
Let $V_B \in L^\infty(0,1)$, $\mathcal{C} \in L^2(0,1)$, $\varepsilon, \lambda, \nu, \tau > 0$ and $F_{1;0}, V_0, V_1 \in \mathbb{R}$. Assume that h is the enthalpy to an admissible pressure term p and let

$$k := h + \frac{\nu}{\tau}\ln \quad \text{and} \quad K(s) := \int_1^s k(t)\, dt \quad (s \geq 0).$$

Let $V_{inh} \in W^{2,2}(0,1)$ be the solution to $-\lambda^2 V''_{inh} = \mathcal{C}$ in $(0,1)$, $V_{inh}(0) = V_0$, $V_{inh}(1) = V_1$. Define the continuous and linear operator $\Phi : L^2(0,1) \longrightarrow W^{2,2}(0,1)$, $f \mapsto V$, as the solution operator to the equations

$$\lambda^2 V'' = f \text{ in } (0,1), \quad V(0) = V(1) = 0.$$

Define the functional $\mathcal{F} : W^{1,2}(0,1) \longrightarrow \mathbb{R}$ by

$$\mathcal{F}(u) := \int_0^1 2(\varepsilon^2 + \nu^2)u'(x)^2 - (F + V_B + V_{inh})\,u^2(x) + K(u^2(x)) + \frac{\lambda^2}{2}|\Phi(u^2)'(x)|^2\, dx.$$

For any $F \in L^\infty(0,1)$, there exists a unique positive minimizer $u \in U \cap W^{2,2}(0,1)$ of $\mathcal{F}$ in the set

$$U = \left\{ u \in W^{1,2}(0,1) \;:\; u \geq B_0,\ \|u\|^2_{L^2(0,1)} = C^*,\ \|u'\|^2_{L^2(0,1)} \leq B_1 \right\}.$$

The corresponding maps $\mathcal{M} : L^\infty(0,1) \longrightarrow W^{1,2}_{pos}(0,1)$, $F \mapsto u$, and $\mathcal{L} : W^{1,2}_{pos}(0,1) \longrightarrow L^\infty(0,1)$, $u \mapsto F$, defined by

$$(\mathcal{L}u)(x) := J_0 \int_0^x \frac{1}{\tau u^2(y)} + 8\nu\frac{u'(y)^2}{u^4(y)}\, dy - \frac{J_0^2 - 8\nu J_0 u(x)u'(x)}{2u(x)^4} \quad (u \in W^{1,2}_{pos}(0,1)),$$

where

$$J_0 := \begin{cases} F_{1;0} I(u)^{-1}, & H(u) = 0, \\ \operatorname{Re}\left(\frac{I(u) - \sqrt{I(u)^2 - 2H(u)F_{1;0}}}{H(u)} \right), & H(u) \neq 0, \end{cases}$$

with

$$I(u) = \int_0^1 \frac{1}{\tau u^2(y)} + 8\nu\frac{u'(y)^2}{u^4(y)}\, dy \quad \text{and} \quad H(u) = \frac{1}{u^4(1)} - \frac{1}{u^4(0)}$$

are continuous. The bounds in the definition of U *can be chosen in such a way, that* $\mathbb{F} := \mathcal{M} \circ \mathcal{L} : U \longrightarrow U$ *is well-defined, continuous and compact.* $\mathbb{F}$ *has at least one fixed point in* U *and any fixed point* u *solves the Euler-Lagrange equation*

$$2(\varepsilon^2 + \nu^2)u'' = -(F + V + V_B)u + (h(u^2) + \frac{\nu}{\tau}\ln(u^2))u - \beta u$$

for some $\beta \in \mathbb{R}$*, where* $F = \mathcal{L}(u)$*.*
There exists $F_{\max} > 0$ *such that the function* $n := u^2$ *is a solution to the system of equations* (2.15) *and fulfills both the homogeneous Neumann boundary condition and the integral constraint* $\int_0^1 u^2(x)\,dx = C^*$*, if* $|F_{1;0}| \leq F_{\max}$*.*

Proof. In Lemma 2.28 it has been shown that the estimates (2.16) to (2.24) hold for the choice of J_0. We can now proceed as in the proof of Theorem 2.21. Note that the homogeneous Neumann boundary conditions also allow for the integration by parts as applied in Lemma 2.27. Moreover, the appearing function G_δ should now be estimated against $2|F_{1;0}|$ in the L^∞-norm. We then obtain a solution u with corresponding F as a fixed point to $\mathcal{M} \circ \mathcal{L}$ as before. To conclude that the boundary condition $F_{1;0} = F(1) - F(0)$ actually holds, we have to ensure that J_0 fulfills the identity (2.30). By definition (2.31) of J_0, this is the case if $I(u)^2 - 2H(u)F_{1;0} > 0$. This situation is given for sufficiently small values of $|F_{1;0}|$: Restricting the set of admissible $F_{1;0}$ to some arbitrary bounded set, inequality (2.24) becomes independent of the particular choice of $F_{1;0}$ and the set of all possibly appearing functions F is uniformly bounded in $L^\infty(0,1)$ by a constant not depending on $F_{1;0}$. By Lemma 2.18, we know that uniform lower bounds to all possibly appearing functions u exist and we deduce that the corresponding numbers $H(u)$ are uniformly bounded with respect to $F_{1;0}$. Since for any u with $\int_0^1 u^2(x)\,dx = C^*$ it holds $I(u) \geq \frac{1}{\tau C^*}$, we conclude that actually $I(u)^2 - 2H(u)F_{1;0} > 0$ if $|F_{1;0}|$ is sufficiently small. □

Chapter 3

The combined viscous semi-classical limit

In this chapter, the behavior of solutions $n_\kappa = u_\kappa^2$ to the stationary viscous quantum hydrodynamic system, where $\kappa = \varepsilon^2 + \nu^2$, is investigated when κ approaches zero. We will mainly focus on the special case in which the Fermi level is a constant function. We will see that even in this case no uniform bounds to u_κ may exist in the usual Sobolev norms. Formally letting $\kappa = 0$, we expect to find pointwise limiting functions u_0 and V_0 which fulfill

$$\begin{cases} 0 &= -\left(F + V_B + V_0 - h(u_0^2)\right) u_0, \quad \text{in } [0,1], \\ \lambda^2 V_0'' &= u_0^2 - \mathcal{C}, \quad \text{in } [0,1]. \end{cases}$$

The system of equations is degenerated and any positive solution u_0 must be discontinuous at any point of discontinuity of the barrier potential V_B. The most relevant choices of V_B are, however, piecewise constant functions and therefore we expect the solutions u_κ to behave characteristically different in a vicinity of any point of jump discontinuity of the barrier potential. The main result of this chapter is the analysis of fluid-dynamical boundary layers which form up in this situation. We will focus on both the case of periodic boundary conditions and the case of homogeneous Neumann boundary conditions for u_κ.
In a prelimininary step, a-priori estimates to the solutions u_κ and V_κ will be established in Lemmas 3.1 and 3.4 as well as in Corollary 3.5. We are then in a position to prove convergence in $W^{1,2}(0,1)$ of the potentials V_κ to a limiting function V_0 in Lemma 3.6. This, in turn, yields convergence of u_κ to a limit u_0 in $L^p(0,1)$ for $1 \leq p < \infty$ and locally in $L^\infty(0,1)$ as will be shown in Lemma 3.8. In Lemma 3.13, a differential equation describing the interior layer of u_κ in a vicinity of points of jump discontinuities of V_B is derived. The corresponding solution of this differential equation is then combined with the pointwise limiting function u_0 in order to obtain the zeroth order summand of the asymptoptic expansion of the electron densities u_κ. Corollary 3.17 and Lemma **??** present the local results at a single point of jump discontinuity of the barrier potential. A joint representation for the whole interval $(0,1)$ is given in Corollary 3.19. The chapter concludes with refined remainder estimates in Lemma 3.20.

3.1 Basic interior estimates in the parameter $\kappa = \varepsilon^2 + \nu^2$

Lemma 3.1 (**Uniform pointwise estimates in κ for constant Fermi levels**).
Let $\varepsilon, \lambda, \nu, \tau > 0$, $\mathcal{C} \in L^2(0,1)$, $V_B \in L^\infty(0,1)$ and assume that the Fermi level is a constant

function $F \in \mathbb{R}$. Let h be the enthalpy to an admissible pressure term p which additionally fulfills

$$\lim_{s\to 0} h(s) = -\infty \quad \textit{and} \quad \lim_{s\to\infty} h(s) = \infty.$$

For $\kappa := \varepsilon^2 + \nu^2$, let u_κ be the solution of

$$\begin{cases} 2\kappa u_\kappa'' &= -\left(F + V_B + V_\kappa - h(u_\kappa^2) - \frac{\nu}{\tau}\ln(u_\kappa^2)\right) u_\kappa, \quad \textit{in } [0,1], \\ \lambda^2 V_\kappa'' &= u_\kappa^2 - \mathcal{C}, \quad \textit{in } [0,1], \\ V_\kappa(0) &= V_0, \\ V_\kappa(1) &= V_1, \end{cases}$$

which is obtained from Lemma 2.10 for Dirichlet boundary conditions, from Lemma 2.13 for homogeneous Neumann boundary conditions, and from Lemma 2.14 for periodic boundary conditions, respectively. Let V_κ be the corresponding potential functions. There exist constants $C_0, C_1, C_2 > 0$ such that

$$C_0 \le u_\kappa \le C_1$$

and

$$\|V_\kappa\|_{C^1(0,1)} \le C_2$$

for $0 < \kappa < \kappa_0$. For given $C^* > 0$, the estimates are also valid for the solutions u_κ, V_κ of the equations

$$\begin{cases} 2\kappa u_\kappa'' &= -\left(F + \beta_\kappa + V_B + V_\kappa - h(u_\kappa^2) - \frac{\nu}{\tau}\ln(u_\kappa^2)\right) u_\kappa, \quad \textit{in } [0,1], \\ \lambda^2 V_\kappa'' &= u_\kappa^2 - \mathcal{C}, \quad \textit{in } [0,1], \\ \int_0^1 u_\kappa^2(x)\,dx &= C^*, \\ V_\kappa(0) &= V_0, \\ V_\kappa(1) &= V_1, \end{cases}$$

which are obtained from Lemma 2.18 for homogeneous Neumann boundary conditions and from Lemma 2.17 for periodic boundary conditions, respectively.

Proof. We begin with the solutions u_κ for which the balance of mass is not demanded. The coerciveness inequality (2.9) shows, in particular,

$$\|u_\kappa\|^2_{L^2(0,1)} \le \mathcal{F}(u_\kappa) + C_0 \le \mathcal{F}(\widetilde{u}) + C_0 = C$$

for a chosen function $\widetilde{u}$ fulfilling the respective boundary conditions. We therefore have a uniform bound in $L^2(0,1)$ for the solutions u_κ. By continuity of $\Phi : L^1(0,1) \longrightarrow C^1([0,1])$ (c.f. Lemma A.18), this yields a uniform upper bound to $\|V_\kappa\|_{C^1([0,1])}$. In particular, we have a uniform L^∞-bound for the functions V_κ. Applying the maximum principle as in the proofs of the respective lemmas, we obtain the desired uniform pointwise estimates to u_κ and then the claimed estimate to V_κ also follows. Note, however, that we need to exploit the asymptotics of the enthalpy h, since the magnitude of the term $\frac{\nu}{\tau}\ln(u_\kappa)$ depends on ν.
If the balance of mass is demanded, we obviously have the boundedness of $\|u_\kappa\|^2_{L^2(0,1)} = C^*$ and a uniform estimate to $\|V_\kappa\|_{C^1([0,1])}$ follows. To proceed as in the first part of the proof, we

need to find uniform estimates to the Lagrange multipliers β_κ. Multiplying the Euler-Lagrange equation by u_κ and integrating over $(0,1)$, we find for $k = h + \frac{\nu}{\tau}\ln$,

$$\begin{aligned} C^*(F+\beta_\kappa) &= 2\kappa\|u'\|^2_{L^2(0,1)} - \int (V_B + V_{inh} + \Phi(u_\kappa^2))u_\kappa^2 + \int k(u_\kappa^2)u_\kappa^2 \\ &\geq -\|V_B + V_{inh} + \Phi(u_\kappa^2)\|_{L^\infty(0,1)}C^* - C \\ &\geq -C, \end{aligned}$$

where the constant on the right hand side does not depend ond κ. Applying the maximum principle as before, we find a lower bound to u_κ which does not depend on κ.
Multiplying the Euler-Lagrange equation by $\frac{1}{u\max(1,k(u^2))}$ and integrating over $(0,1)$, we obtain

$$\begin{aligned} &\int_0^1 \frac{F+\beta_\kappa}{\max(1,k(u_\kappa^2(x)))}\,dx \\ = \quad & -\int_0^1 \frac{V_\kappa(x)+V_B(x)}{\max(1,k(u^2(x)))}\,dx + \int_0^1 \frac{k(u_\kappa^2(x))}{\max(1,k(u_\kappa^2(x)))} - 2\kappa\int_0^1 \frac{u_\kappa''(x)}{u_\kappa(x)\max(1,k(u_\kappa^2(x)))}\,dx \\ =: \quad & I_1 + I_2 + I_3. \end{aligned}$$

We already know that I_1 is uniformly bounded in absolute value. Furthermore, I_2 is bounded from above independently of κ. Concerning I_3, an integration by parts shows

$$\begin{aligned} I_3 &= 2\kappa\int_0^1 u_\kappa'(x)\left(\frac{1}{u_\kappa\max(1,k(u_\kappa^2))}\right)'(x)\,dx \\ &= -2\kappa\int_0^1 u_\kappa'(x)\frac{u_\kappa'(x)\max(1,k(u_\kappa(x))) + u_\kappa(x)(k(u_\kappa^2))'(x)\chi_{\{k(u_\kappa^2)\geq 1\}}(x)}{u_\kappa^2(x)\max(1,k(u_\kappa^2(x)))^2}\,dx \\ &= -2\kappa\int_0^1 \frac{u_\kappa'(x)^2}{u_\kappa(x)^2}\frac{\max(1,k(u_\kappa^2(x))) + 2u_\kappa^2(x)k'(u_\kappa^2(x))\chi_{\{k(u_\kappa^2)\geq 1\}}(x)}{\max(1,k(u_\kappa^2(x)))^2}\,dx \\ &\leq 0 \end{aligned}$$

because of $k' > 0$. Therefore,

$$F + \beta_\kappa \leq C\left(\int_0^1 \frac{1}{\max(1,k(u_\kappa^2(x)))}\,dx\right)^{-1}$$

and an upper bound to $F+\beta_\kappa$ follows if $\int_0^1 \frac{1}{\max(1,k(u_\kappa^2(x)))}\,dx$ is uniformly bounded away from zero. By monotonicity of k, the equality

$$\Omega := \left\{x \in (0,1)\ :\ u_\kappa^2(x) \leq 2C^*\right\} = \left\{x \in (0,1)\ :\ k(u_\kappa^2(x)) \leq k(2C^*)\right\}$$

holds and the integral constraint $\int_0^1 u_\kappa^2(x)\,dx = C^*$ implies $\mathrm{vol}(\Omega) \geq \frac{1}{2}$. Then

$$\int_0^1 \frac{1}{\max(1,k(u_\kappa^2(x)))}\,dx \geq \int_\Omega \frac{1}{\max(1,k(u_\kappa^2(x)))}\,dx \geq \frac{1}{2}\frac{1}{\max(1,k(2C^*))}.$$

Since $F+\beta_\kappa$ is uniformly bounded from above, the maximum principle can now be applied to gain a pointwise upper bound for u_κ which does not depend on κ.

□

Remark 3.2.
Note that the bounds for $F+\beta_\kappa$ do not depend on the choice of $F \in \mathbb{R}$ if the integral condition is assumed to hold. In this case, the estimates of Lemma 3.1 are still given if we allow the constants $F = F_\kappa$ to vary in κ. We also cover the case in which the integral condition is not assumed to hold if we assume that $(F_\kappa)_{0<\kappa<\kappa_0}$ is uniformly bounded in $L^\infty(0,1)$ so that the coerciveness inequality yields a uniform upper bound to $\|u_\kappa\|_{L^2(0,1)}$ as required in the proof of the previous lemma. We also recall that the pressure terms $p(s) = T_0 s^\gamma + \mu s$, where $T_0, \mu > 0$ and $\gamma \geq 1$ are fixed, yield enthalpies h which fulfill the growth conditions of Lemma 3.1.

In Lemma 3.1, we have seen that solutions to the one-dimensional stationary viscous quantum hydrodynamic equations exist for various choices of boundary values and for the most relevant pressure terms. As the existence of such solutions with corresponding uniform estimates in κ is ensured and since the forthcoming analysis will not rely on the construction of these solutions, we will now formulate a general assumption on the properties of the solutions under consideration.

Assumption 3.3 (Solutions under consideration).
Let $\lambda, \tau, C^* > 0$, $\mathcal{C} \in L^2(0,1)$, $V_B \in L^\infty(0,1)$, an enthalpy h to an admissible pressure term p, a constant Fermi level $F \in \mathbb{R}$ and Dirichlet boundary values $V_0, V_1 \in \mathbb{R}$ be fixed. For varying $\varepsilon, \nu > 0$, abbreviate $\kappa = \varepsilon^2 + \nu^2$ and let $u_\kappa \in W^{2,2}_{pos}(0,1)$ and $V_\kappa \in W^{2,2}(0,1)$ be solutions of

$$\begin{cases} 2\kappa u_\kappa'' &= -\left(F + \beta_\kappa + V_B + V_\kappa - h(u_\kappa^2) - \frac{\nu}{\tau}\ln(u_\kappa^2)\right) u_\kappa, \quad \text{in } [0,1], \\ \lambda^2 V_\kappa'' &= u_\kappa^2 - \mathcal{C}, \quad \text{in } [0,1], \\ V_\kappa(0) &= V_0, \\ V_\kappa(1) &= V_1, \end{cases}$$

for some $\beta_\kappa \in \mathbb{R}$ if the constraint $\int_0^1 u_\kappa^2(x)\,dx = C^*$ is imposed and for $\beta_\kappa = 0$, otherwise. u_κ is supposed to admit homogeneous Neumann boundary conditions $u_\kappa'(0) = u_\kappa'(1) = 0$ or periodic boundary conditions $u_\kappa(0) = u_\kappa(1)$, $u_\kappa'(0) = u_\kappa'(1)$. It is assumed that the uniform estimates

$$0 < C_0 \leq u_\kappa \leq C_1 \quad \text{and} \quad \|V_\kappa\|_{W^{2,2}(0,1)} \leq C_2$$

and consequently

$$|\beta_\kappa| \leq C_3$$

hold for $0 < \kappa < \kappa_0$.

We will now provide some basic exterior estimates to the solutions. By Definition 2.1, the second line of the original equations (2.1) holds in the weak sense if and only if for any test function $\varphi \in C_0^\infty(0,1)$

$$-2\varepsilon^2 \left\langle \frac{\sqrt{n}''}{\sqrt{n}}, (n\varphi)' \right\rangle + \nu \left\langle J', \varphi' \right\rangle - \left\langle (p(n))', \varphi \right\rangle + \frac{1}{\tau}\left\langle J, \varphi \right\rangle = \left\langle \left(\frac{J^2}{n}\right)', \varphi \right\rangle + \left\langle V + V_B, (n\varphi)' \right\rangle,$$

where J_0 is determined by the relation $J = -\nu n' + J_0$. Using the representation $\frac{\sqrt{n}''}{\sqrt{n}} = \frac{n''}{2n} - \frac{n'^2}{4n^2}$ as well as the following integrations by parts

$$2\varepsilon^2 \int_0^1 \frac{n'^2(x)}{4n^2(x)} (n\varphi)'(x)\,dx = -2\varepsilon^2 \int_0^1 \left(\frac{n'^2}{4n^2}\right)'(x) n(x)\varphi(x)\,dx$$

and

$$\int_0^1 V(x)\,(n\varphi)'(x)\,dx = -\int_0^1 V'(x)n(x)\varphi(x)\,dx,$$

we can rearrange the equation to see that the equivalent weak formulation

$$\begin{aligned}&\int_0^1 \left(2J_0\nu\left(\frac{n'(x)}{n(x)}\right)' - \left(p'(n(x)) + \frac{\nu}{\tau} - \frac{J_0^2}{n^2(x)}\right)n'(x)\right)\varphi(x)\,dx\\ &-(\varepsilon^2+\nu^2)\int_0^1\left(\frac{n'(x)^2}{n(x)}\right)'\varphi(x)\,dx + \int_0^1\left(n(x)V'(x)+\frac{J_0}{\tau}\right)\varphi(x)\,dx\\ &-\int_0^1 V_B(x)(n(x)\varphi(x))'\,dx - (\varepsilon^2+\nu^2)\int_0^1 n''(x)\varphi'(x)\,dx = 0 \end{aligned} \tag{3.1}$$

$(\varphi \in C_0^\infty(0,1))$ can be used.

Lemma 3.4 (**Basic exterior estimates to solutions**).
Let $\varepsilon, \nu, \tau, \lambda > 0$, $\mathcal{C} \in L^2(\Omega)$ and let $V_0, V_1 \in \mathbb{R}$. Assume that V_B is constant in some non-trivial interval $[x_0, x_1] \subset (0,1)$. Let $n \in W^{2,2}(0,1)$ be a positive function which fulfills homogeneous Neumann boundary conditions or periodic boundary conditions and which solves the weak formulation (3.1) coupled to the potential equation $\lambda^2 V'' = n - \mathcal{C}$, $V(0) = V_0$, $V(1) = V_1$. Assume that the subsonic-type conditions

$$p'(n) - \frac{J_0^2}{n^2} \geq C_0$$

and

$$\frac{|J_0|}{n} \leq C_1$$

are fulfilled in $[x_0, x_1]$ for some constants $C_0, C_1 > 0$. Then, for $C^* = \int_0^1 n(x)\,dx$ and $u = \sqrt{n}$, the estimates

$$\begin{aligned}&\left(C_0 + 4\frac{\nu}{\tau}\right)\int_{x_0+\sigma L}^{x_1-\sigma L} u'(x)^2\,dx + (\varepsilon^2+\nu^2)\int_{x_0+\sigma L}^{x_1-\sigma L} u''(x)^2 + \frac{10}{96}\frac{u'(x)^4}{u^2(x)}\,dx + \frac{1}{\lambda^2}\int_{x_0+\sigma L}^{x_1-\sigma L} u^4(x)\,dx\\ \leq\ & \frac{4(\varepsilon^2+\nu^2)CC^*}{\sigma^4L^4} + \frac{|J_0|CC_1}{\sigma^2L^2} + \frac{CC^*}{\lambda^2} + \frac{4(C+C^*)C^*}{\lambda^2\sigma L} + \frac{C_1|J_0|}{3C_0\tau^2}\end{aligned} \tag{3.2}$$

and

$$\begin{aligned}&\left(C_0 + 4\frac{\nu}{\tau}\right)\int_{x_0+\sigma L}^{x_1-\sigma L} u'(x)^2\,dx + (\varepsilon^2+\nu^2)\int_{x_0+\sigma L}^{x_1-\sigma L} u''(x)^2 + \frac{10}{96}\frac{u'(x)^4}{u^2(x)}\,dx\\ \leq\ & \frac{4(\varepsilon^2+\nu^2)CC^*}{\sigma^4L^4} + \frac{|J_0|CC_1}{\sigma^2L^2} + \frac{CC^*}{C_0\lambda^4} + \frac{2C_1|J_0|}{3C_0\tau^2},\end{aligned} \tag{3.3}$$

where C only depends on $\|\mathcal{C}\|_{L^\infty(0,1)}$, V_0 and V_1 and where $L := x_1 - x_0$ is the length of the interval $[x_0, x_1]$, hold for small σ.

Proof. Let $a_0 := \frac{1}{\sigma^4 L^4}$ and define $\psi \in W_0^{1,2}(0,1)$ by

$$\psi(x) := \begin{cases} a_0(x-x_0)^4, & x_0 \leq x \leq x_0 + \sigma L,\\ 1, & x_0 + \sigma L \leq x \leq x_1 - \sigma L,\\ a_0(x_1 - x)^4, & x_1 - \sigma L \leq x \leq x_1,\\ 0, & x \notin [x_0, x_1].\end{cases}$$

Surely,

$$\psi'(x) = \begin{cases} \frac{4}{\sigma L}\psi^{3/4}, & x \in [x_0, x_0+\sigma L], \\ 0, & x \in (x_0+\sigma L, x_1-\sigma L), \\ -\frac{4}{\sigma L}\psi^{3/4}, & x \in [x_1-\sigma L, x_1]. \end{cases}$$

Using $\varphi := \frac{n'}{n}\psi$ as a test function in the weak formulation (3.1), we obtain in terms of $u = \sqrt{n}$

$$\begin{aligned} & 4\int_0^1 \left(p'(u^2(x)) + \frac{\nu}{\tau} - \frac{J_0^2}{u^4(x)}\right) u'(x)^2\psi(x)\,dx \\ & +4(\varepsilon^2+\nu^2)\int_0^1 2(u'^2)'(x)\frac{u'(x)}{u(x)}\psi(x) + (u''(x)u(x)+u'(x)^2)\left(\frac{u'}{u}\psi\right)'(x)\,dx \\ = {} & 8J_0\nu\int_0^1 \frac{u'(x)}{u(x)}\left(\frac{u'}{u}\right)'(x)\psi(x)\,dx + 2\int_0^1 u(x)u'(x)V'(x)\psi(x)\,dx + \frac{2J_0}{\tau}\int_0^1 \frac{u'(x)}{u(x)}\psi(x)\,dx, \end{aligned}$$

because $\int_0^1 V_B(x)(n'\psi)'(x)\,dx = 0$ as V_B is constant on $\operatorname{supp}\psi$. We abbreviate the equality by

$$I_1 + 4(\varepsilon^2+\nu^2)I_2 = J_1 + J_2 + J_3.$$

Then

$$4\left(C_0 + \frac{\nu}{\tau}\right)\int_0^1 u'(x)^2\psi(x)\,dx \le I_1$$

and integrations by parts show

$$\begin{aligned} I_2 &= \int_0^1 -2u'(x)^2\left(\frac{u'}{u}\psi\right)'(x) + (u''(x)u(x)+u'(x)^2)\left(\frac{u'}{u}\psi\right)'(x)\,dx \\ &= \int_0^1 (u''(x)u(x)-u'(x)^2)\left(\frac{u(x)u''(x)-u'(x)^2}{u^2(x)}\psi(x) + \frac{u'(x)}{u(x)}\psi'(x)\right)\,dx \\ &= \int_0^1 \left(u''(x)^2 - 2\frac{u''(x)u'(x)^2}{u(x)} + \frac{u'(x)^4}{u^2(x)}\right)\psi(x) + \left(u''(x)u'(x) - \frac{u'(x)^3}{u(x)}\right)\psi'(x)\,dx. \end{aligned}$$

Since

$$\begin{aligned} \int_0^1 \frac{u''(x)u'(x)^2}{u(x)}\psi(x)\,dx &= -\int_0^1 u'(x)\left(\frac{u'^2}{u}\psi\right)'(x)\,dx \\ &= -\int_0^1 2\frac{u''(x)u'(x)^2}{u(x)}\psi(x) - \frac{u'(x)^4}{u^2(x)}\psi(x) + \frac{u'(x)^3}{u(x)}\psi'(x)\,dx, \end{aligned}$$

it follows that

$$\int_0^1 \frac{u''(x)u'(x)^2}{u(x)}\psi(x)\,dx = \frac{1}{3}\int_0^1 \frac{u'(x)^4}{u^2(x)}\psi(x) - \frac{u'(x)^3}{u(x)}\psi'(x)\,dx$$

and therefore,

$$\begin{aligned} I_2 &= \int_0^1 \left(u''(x)^2 + \frac{1}{3}\frac{u'(x)^4}{u^2(x)}\right)\psi(x) + u''(x)u'(x)\psi'(x) - \frac{1}{3}\frac{u'(x)^3}{u(x)}\psi'(x)\,dx \\ &=: \int_0^1 \left(u''(x)^2 + \frac{1}{3}\frac{u'(x)^4}{u^2(x)}\right)\psi(x)\,dx + I_{2,1} + I_{2,2}. \end{aligned}$$

Using $|\psi'| \leq \frac{4}{\sigma L}\psi^{3/4}$, we get

$$
\begin{aligned}
|I_{2,1}| &\leq \int_0^1 \left|u''(x)\psi^{1/2}(x)\right| \cdot \left|\frac{u'(x)\psi^{1/4}(x)}{2u^{1/2}(x)}\right| \cdot \frac{8u^{1/2}(x)}{\sigma L}\, dx \\
&\leq \int_0^1 \frac{1}{2}u''(x)^2\psi(x)\, dx + \int_0^1 \frac{u'(x)^2\psi^{1/2}(x)}{4u(x)} \cdot \frac{32u(x)}{\sigma^2 L^2}\, dx \\
&\leq \int_0^1 \frac{1}{2}u''(x)^2\psi(x)\, dx + \int_0^1 \frac{u'(x)^4}{32u^2(x)}\psi(x) + \int_0^1 \frac{512u^2(x)}{\sigma^4 L^4}\chi_{[x_0,x_1]}\, dx
\end{aligned}
$$

by Young's inequality. Using Young's inequality with the exponents $\frac{4}{3}$ and 4 we further obtain

$$
\begin{aligned}
|I_{2,2}| &\leq \frac{1}{3}\int_0^1 \frac{(u'(x)^4\psi(x))^{3/4}}{u^{3/2}(x)} \cdot \frac{4u^{1/2}(x)}{\sigma L}\, dx \\
&\leq \frac{1}{3}\int_0^1 \frac{3}{4}\frac{u'(x)^4}{u^2(x)}\psi(x)\, dx + \frac{1}{4}\frac{256u^2(x)}{\sigma^4 L^4}\chi_{[x_0,x_1]}(x)\, dx \\
&= \int_0^1 \frac{u'(x)^4}{4u^2(x)}\psi(x) + \frac{64u^2(x)}{3\sigma^4 L^4}\chi_{[x_0,x_1]}(x)\, dx.
\end{aligned}
$$

Since $\int_0^1 u^2(x)\, dx = C^*$, we infer

$$
\int_0^1 \frac{1}{2}u''(x)^2\psi(x)\, dx + \left(\frac{1}{3} - \frac{1}{32} - \frac{1}{4}\right)\int_0^1 \frac{u'(x)^4}{u^2(x)}\psi(x)\, dx \leq I_2 + \frac{512C^*}{\sigma^4 L^4} + \frac{64C^*}{3\sigma^4 L^4}.
$$

Thus,

$$
2(\varepsilon^2 + \nu^2)\int_0^1 \left(u''(x)^2 + \frac{10}{96}\frac{u'(x)^4}{u^2(x)}\right)\psi(x)\, dx \leq 4(\varepsilon^2 + \nu^2)I_2 + \frac{4(\varepsilon^2 + \nu^2)CC^*}{\sigma^4 L^4}.
$$

Integrating J_1 by parts, we estimate

$$
\begin{aligned}
|J_1| &= 4\left|J_0\nu\int_0^1 \left(\frac{u'(x)}{u(x)}\right)^2 \psi'(x)\, dx\right| \\
&\leq 4\int_0^1 \nu\sqrt{\frac{5}{96}}\frac{u'(x)^2}{u(x)}\psi^{1/2}(x) \cdot \sqrt{\frac{96}{5}}\frac{4}{\sigma L}\frac{|J_0|}{u(x)}\psi^{1/4}(x)\, dx \\
&\leq \frac{10}{96}\nu^2\int_0^1 \frac{u'(x)^4}{u^2(x)}\psi(x)\, dx + \int_0^1 \frac{3072}{5\sigma^2 L^2}\frac{J_0^2}{u^2(x)}\psi^{1/2}(x)\, dx \\
&\leq \frac{10}{96}\nu^2\int_0^1 \frac{u'(x)^4}{u^2(x)}\psi(x)\, dx + \frac{3072}{5\sigma^2 L^2}|J_0|C_1.
\end{aligned}
$$

Concerning J_2, we find

$$\begin{aligned}
J_2 &= \int_0^1 {u^2}'(x)V'(x)\psi(x)\,dx \\
&= -\int_0^1 u^2(x)\left(V''(x)\psi(x)+V'(x)\psi'(x)\right)\,dx \\
&= -\int_0^1 u^2(x)\lambda^{-2}(u^2(x)-\mathcal{C}(x))\psi(x)+u^2(x)V'(x)\psi'(x)\,dx \\
&\leq -\frac{1}{\lambda^2}\int_0^1 u^4(x)\psi(x)\,dx+\frac{1}{\lambda^2}\int_0^1 u^2(x)\mathcal{C}(x)\psi(x)\,dx+\|V'\psi'\|_{L^\infty(0,1)}\int_0^1 u^2(x)\,dx \\
&\leq -\frac{1}{\lambda^2}\int_0^1 u^4(x)\psi(x)\,dx+\frac{\|\mathcal{C}\|_{L^\infty(0,1)}C^*}{\lambda^2}+\frac{4(C+C^*)C^*}{\lambda^2\sigma L},
\end{aligned}$$

where we have used that V can be written as $V=V_{inh}+\Phi(u^2)$ with V_{inh} solving $\lambda^2 V_{inh}=-\mathcal{C}$, $V_{inh}(0)=V_0$, $V_{inh}(1)=V_1$ and $\Phi: L^1(0,1)\longrightarrow C^1(0,1)$ being the solution operator to $\lambda^2V''=f$, $V(0)=V(1)=0$, whose operator norm is bounded by $\frac{C}{\lambda^2}$.
We also estimate

$$\begin{aligned}
|J_3| &= 2\left|\int_0^1 \frac{1}{\sqrt{3C_0}\tau}\frac{J_0}{u(x)}\psi^{1/2}(x)\cdot\sqrt{3C_0}u'(x)\psi^{1/2}(x)\,dx\right| \\
&\leq \int_0^1 \frac{1}{3C_0\tau^2}\frac{J_0^2}{u^2(x)}\psi(x)\,dx+3C_0\int_0^1 u'(x)^2\psi(x)\,dx \\
&\leq \frac{C_1|J_0|}{3C_0\tau^2}+3C_0\int_0^1 u'(x)^2\psi(x)\,dx.
\end{aligned}$$

Combining the previous estimates yields

$$\begin{aligned}
&\left(C_0+4\frac{\nu}{\tau}\right)\int_0^1 u'(x)^2\psi(x)\,dx+(2\varepsilon^2+\nu^2)\int_0^1\left(u''(x)^2+\frac{10}{96}\frac{u'(x)^4}{u^2(x)}\right)\psi(x)\,dx \\
\leq\ & \frac{4(\varepsilon^2+\nu^2)CC^*}{\sigma^4L^4}+\frac{|J_0|CC_1}{\sigma^2L^2}+\frac{CC^*}{\lambda^2}+\frac{4(C+C^*)C^*}{\lambda^2\sigma L}+\frac{C_1|J_0|}{3C_0\tau^2}
\end{aligned}$$

and because $\psi=1$ on $[x_0+\sigma L, x_1-\sigma L]$, the first assertion is proven. Concerning the second inequality, we alternatively estimate J_2 by

$$\begin{aligned}
|J_2| &\leq 2\int_0^1\sqrt{\frac{3}{2}C_0}\,|u'(x)|\,\psi^{1/2}(x)\cdot\frac{\sqrt{2}}{\sqrt{3C_0}}u(x)\,|V'(x)|\,\psi^{1/2}(x)\,dx \\
&\leq \frac{3}{2}C_0\int_0^1 u'(x)^2\psi(x)\,dx+\frac{2}{3C_0}\int_0^1 u^2(x)V'(x)^2\psi(x)\,dx \\
&\leq \frac{3}{2}C_0\int_0^1 u'(x)^2\psi(x)\,dx+\frac{C\|V'\|^2_{L^\infty(0,1)}C^*}{C_0} \\
&\leq \frac{3}{2}C_0\int_0^1 u'(x)^2\psi(x)\,dx+\frac{CC^*}{\lambda^4C_0}.
\end{aligned}$$

Repeating the estimate for J_3 with the constant $3C_0$ replaced by $\frac{3}{2}C_0$ everything follows. □

Provided that u_κ and V_κ fulfill Assumption 3.3, we obtain the following corollary:

Corollary 3.5 (**Uniform estimates in κ for the solutions under consideration**). *Let $u_\kappa \in W^{2,2}_{pos}(0,1)$ and $V_\kappa \in W^{2,2}(0,1)$ satisfy Assumption 3.3 and assume that V_B is constant in some non-trivial interval $[x_0, x_1] \subset (0,1)$. Let $L := x_1 - x_0$ and $I_\kappa := [x_0 + \kappa^{1/4}L, x_1 - \kappa^{1/4}L]$. Then*

$$\|u_\kappa'\|_{L^2(I_\kappa)} \leq C, \tag{3.4}$$

$$\|\kappa u_\kappa''\|_{L^2(I_\kappa)} \leq C\kappa^{1/2}, \tag{3.5}$$

$$\|u_\kappa'\|_{L^\infty(I_\kappa)} \leq C\kappa^{-1/4}, \tag{3.6}$$

$$\left\|2\kappa \frac{u_\kappa''}{u_\kappa}\right\|_{L^\infty(I_\kappa)} \leq C\kappa^{1/4}, \tag{3.7}$$

with some constant C which does not depend on $0 < \kappa < \kappa_0$.

Proof. Since F is a constant, the system of equations (2.2) is fulfilled for $J_0 = 0$ and the functions u_κ are uniformly bounded from above and away from zero for $0 < \kappa < \kappa_0$ by assumption. Then, $p'(u_\kappa^2)$ is uniformly bounded away from zero and $(u_\kappa)_{0<\kappa<\kappa_0}$ is also uniformly bounded in $L^2(0,1)$. We make use of Lemma 3.4 and choose $\sigma = \kappa^{1/4}$ in estimate (3.3) to obtain

$$\left(C_0 + 4\frac{\nu}{\tau}\right) \int_{x_0+\kappa^{1/4}L}^{x_1-\kappa^{1/4}L} u'(x)^2 \, dx + \kappa \int_{x_0+\kappa^{1/4}L}^{x_1-\kappa^{1/4}L} u''(x)^2 \leq C,$$

with some constant C which does not depend on $0 < \kappa < \kappa_0$. Inequalities (3.4) and (3.5) follow. These estimates can now be used in the interpolation inequalities A.8 to derive inequality (3.6). As $\frac{u_\kappa''}{u_\kappa}$ is smooth in I_κ, we find

$$\begin{aligned} 2\kappa \left(\frac{u_\kappa''}{u_\kappa}\right)' &= -\left(F + V_B + V_\kappa + \beta_\kappa - h(u_\kappa^2) - \frac{\nu}{\tau}\ln(u_\kappa^2)\right)' = -V_\kappa' + 2u_\kappa u_\kappa' h'(u_\kappa^2) + 2\frac{\nu}{\tau}\frac{u_\kappa'}{u_\kappa} \\ &= -V_\kappa' + 2\left(p'(u_\kappa^2) + \frac{\nu}{\tau}\right)\frac{u_\kappa'}{u_\kappa} \end{aligned}$$

as an equality in I_κ. The right hand side is uniformly bounded in $L^2(I_\kappa)$ by inequality (3.4), the pointwise upper and lower bounds to u_κ and the uniform boundedness of $\|V_\kappa\|_{W^{2,2}(0,1)}$. Joining this bound with inequality (3.5), we obtain

$$\left\|2\kappa \frac{u_\kappa''}{u_\kappa}\right\|_{W^{1,2}(I_\kappa)} \leq C.$$

This inequality can be combined with estimate (3.5) in the interpolation inequalities A.8 to gain inequality (3.7). □

3.2 Basic convergence results for constant Fermi levels as κ tends to zero

Using the basic exterior estimates from the last section, we are now in a position to prove the convergence of V_κ and u_κ as κ tends to zero. We start our analysis by considering the potentials V_κ, for which convergence is even given in higher order Sobolev norms.

Lemma 3.6 (Convergence of V_κ as κ tends to zero).
Let $(u_\kappa)_{0<\kappa<\kappa_0}$ and $(V_\kappa)_{0<\kappa<\kappa_0}$ fulfill Assumption 3.3. Let either all u_κ fulfill the integral constraint $\int_0^1 u_\kappa^2(x)\,dx = C^*$ for a fixed $C^* > 0$ or assume otherwise that $\beta_\kappa = 0$ for $0 < \kappa < \kappa_0$. Let the Fermi level F be a constant function and assume that the barrier potential V_B is a piecewise constant function. Then

$$\|V_{\kappa_1} - V_{\kappa_2}\|^2_{W^{1,2}(0,1)} + |\beta_{\kappa_1} - \beta_{\kappa_2}|^2 \leq C\kappa_1^{1/2} \quad (0 < \kappa_2 \leq \kappa_1 < \kappa_0).$$

In particular, $(V_\kappa)_{0<\kappa<\kappa_0}$ converges in $W^{1,2}(0,1)$ to some V_0 and $(\beta_\kappa)_{0<\kappa<\kappa_0}$ converges to some $\beta_0 \in \mathbb{R}$ with

$$\begin{aligned} \|V_0 - V_\kappa\|_{W^{1,2}(0,1)} &\leq C\kappa^{1/4}, \\ |\beta_0 - \beta_\kappa| &\leq C\kappa^{1/4} \quad (0 < \kappa < \kappa_0). \end{aligned}$$

Proof. Let $I^1, \dots, I^N$ be the maximal intervals in which V_B is constant with corresponding subintervals $I^1_\kappa, \dots, I^N_\kappa$ introduced in Corollary 3.5. Consider the identity

$$h(u_\kappa^2) = F + V_B + V_\kappa + \beta_\kappa + 2\kappa\frac{u_\kappa''}{u_\kappa} - \frac{\nu}{\tau}\ln(u_\kappa^2).$$

Due to the strict monotonicity of $h : (0,\infty) \to \mathbb{R}$ and the pointwise estimates $0 < C_0^2 \leq u_\kappa^2 \leq C_1^2$, we conclude

$$R\left(h \circ u_\kappa^2\right) \subset h\left(\left[C_0^2, C_1^2\right]\right) \subsetneq h\left(\left[\tfrac{1}{2}C_0^2, 2C_1^2\right]\right),$$

where the second inclusion is a proper inclusion of closed intervals. For sufficiently small κ, we conclude that $F + V_B + V_\kappa + \beta_\kappa$ is still in the range of h. Write

$$u_\kappa^2 = h^{-1}(F + V_B + V_\kappa + \beta_\kappa) + r_\kappa$$

with

$$r_\kappa := h^{-1}\left(F + V_B + V_\kappa + \beta_\kappa + 2\kappa\frac{u_\kappa''}{u_\kappa} - \frac{\nu}{\tau}\ln(u_\kappa^2)\right) - h^{-1}(F + V_B + V_\kappa + \beta_\kappa).$$

As h' is positive and continuous on $\left[\frac{1}{2}C_0^2, 2C_1^2\right]$, we know that h' is bounded away from zero. Consequently, $(h^{-1})'$ is bounded from above on the relevant range and h^{-1} is Lipschitz continuous on $h\left(\left[C_0^2, C_1^2\right]\right)$ with some Lipschitz constant $C_L > 0$. We find

$$\begin{aligned} |r_\kappa(x)| &\leq C_L\left|2\kappa\frac{u_\kappa''(x)}{u_\kappa(x)} - \frac{\nu}{\tau}\ln(u_\kappa^2(x))\right| \\ &\leq C\left(\left|2\kappa\frac{u_\kappa''(x)}{u_\kappa(x)}\right| + \kappa^{1/2}\right) \quad (x \in (0,1)), \end{aligned}$$

which implies together with inequalities (3.5) and (3.7)

$$\|r_\kappa\|_{L^2(I_\kappa)} \leq C\kappa^{1/2} \tag{3.8}$$

and

$$\|r_\kappa\|_{L^\infty(I_\kappa)} \leq C\kappa^{1/4} \tag{3.9}$$

for $0 < \kappa < \kappa_0$. Let $0 < \kappa_2 \le \kappa_1 < \kappa_0$, abbreviate $u_i := u_{\kappa_i}$, $V_i := V_{\kappa_i}$, $\beta_i := \beta_{\kappa_i}$, $r_i := r_{\kappa_i}$ and define $\widetilde{V}_i := V_i + \beta_i$ for $i = 1, 2$. Obviously $\widetilde{V}_i' = V_i'$ for $i = 1, 2$ so that an integration by parts yields

$$\lambda^2 \int_0^1 \left(V_1'(x) - V_2'(x)\right)^2 \, dx = -\int_0^1 \left(u_1^2(x) - u_2^2(x)\right)\left(\widetilde{V}_1(x) - \widetilde{V}_2(x)\right) \, dx.$$

In this equality the boundary terms actually vanish, since

$$\begin{aligned}
\lambda^2 \left(\widetilde{V}_1 - \widetilde{V}_2\right)\left(\widetilde{V}_1' - \widetilde{V}_2'\right)\Big|_0^1 &= \lambda^2(\beta_1 - \beta_2)\left(\widetilde{V}_1'(1) - \widetilde{V}_1'(0) - \widetilde{V}_2'(1) + \widetilde{V}_2'(0)\right) \\
&= (\beta_1 - \beta_2)\left(\lambda^2 \int_0^1 \widetilde{V}_1''(x) \, dx - \lambda^2 \int_0^1 \widetilde{V}_2''(x) \, dx\right) \\
&= (\beta_1 - \beta_2)\left(\int_0^1 u_1^2(x) - \mathcal{C}(x) \, dx - \int_0^1 u_2^2(x) - \mathcal{C}(x) \, dx\right) \\
&= 0
\end{aligned}$$

in both cases if $\int_0^1 u_\kappa^2(x) \, dx = C^*$ or $\beta_\kappa = 0$ for $0 < \kappa < \kappa_0$. We split the integral into

$$\begin{aligned}
\lambda^2 \int_0^1 \left(V_1'(x) - V_2'(x)\right)^2 \, dx &= -\sum_{i=1}^N \int_{I^i \setminus I^i_{\kappa_1}} \left(u_1^2(x) - u_2^2(x)\right)\left(\widetilde{V}_1(x) - \widetilde{V}_2(x)\right) \, dx \\
&\quad - \sum_{i=1}^N \int_{I^i_{\kappa_1}} \left(u_1^2(x) - u_2^2(x)\right)\left(\widetilde{V}_1(x) - \widetilde{V}_2(x)\right) \, dx \\
&=: S_1 + S_2.
\end{aligned}$$

Using the uniform pointwise boundedness of u_κ^2 for $0 < \kappa < \kappa_0$, Young's inequality, the Sobolev embedding $W^{1,2}(0,1) \hookrightarrow L^\infty(0,1)$ and Poincaré's inequality, we find

$$\begin{aligned}
S_1 &\le C \sum_{i=1}^N \|\widetilde{V}_1 - \widetilde{V}_2\|_{L^\infty(I^i \setminus I^i_{\kappa_1})} \kappa_1^{1/4} \\
&\le C \left(\sum_{i=1}^N \gamma^2 \|\widetilde{V}_1 - \widetilde{V}_2\|^2_{L^\infty(I^i \setminus I^i_{\kappa_1})} + \gamma^{-2} \kappa_1^{1/2}\right) \\
&\le C \left(\sum_{i=1}^N \gamma^2 \|\widetilde{V}_1 - \widetilde{V}_2\|^2_{W^{1,2}(0,1)} + \gamma^{-2} \kappa_1^{1/2}\right) \\
&\le C \left(\sum_{i=1}^N \gamma^2 \left(2\|V_1 - V_2\|^2_{W^{1,2}(0,1)} + 2\|\beta_1 - \beta_2\|^2_{W^{1,2}(0,1)}\right) + \gamma^{-2} \kappa_1^{1/2}\right) \\
&\le K_1 \left(\gamma^2 \|V_1' - V_2'\|^2_{L^2(0,1)} + \gamma^2 |\beta_1 - \beta_2|^2 + \gamma^{-2} \kappa_1^{1/2}\right)
\end{aligned}$$

where $K_1 > 0$ is a constant und $\gamma > 0$ is a free parameter which will be chosen later on.

Concerning S_2, we calculate

$$\begin{aligned}
& -\sum_{i=1}^{N}\int_{I^i_{\kappa_1}} \left(u_1^2(x)-u_2^2(x)\right)\left(\widetilde{V}_1(x)-\widetilde{V}_2(x)\right)\,dx \\
= & -\sum_{i=1}^{N}\int_{I^i_{\kappa_1}} \left(h^{-1}(F+V_B+\widetilde{V}_1(x))-h^{-1}(F+V_B+\widetilde{V}_2(x))\right)\left(\widetilde{V}_1(x)-\widetilde{V}_2(x)\right)\,dx \\
& -\sum_{i=1}^{N}\int_{I^i_{\kappa_1}} \left(r_1(x)-r_2(x)\right)\left(\widetilde{V}_1(x)-\widetilde{V}_2(x)\right)\,dx.
\end{aligned}$$

By the mean value theorem, we know that for certain $\xi_i(x)$ belonging to some compact set K it follows

$$\begin{aligned}
& -\sum_{i=1}^{N}\int_{I^i_{\kappa_1}} \left(h^{-1}(F+V_B+\widetilde{V}_1(x))-h^{-1}(F+V_B+\widetilde{V}_2(x))\right)\left(\widetilde{V}_1(x)-\widetilde{V}_2(x)\right)\,dx \\
= & -\sum_{i=1}^{N}\int_{I^i_{\kappa_1}} (h^{-1})'(\xi_i(x))\left(\widetilde{V}_1(x)-\widetilde{V}_2(x)\right)^2\,dx \\
\leq & -\min_{z\in K}(h^{-1})'(z)\sum_{i=1}^{N}\int_{I^i_{\kappa_1}}\left(\widetilde{V}_1(x)-\widetilde{V}_2(x)\right)^2\,dx \\
= & -K_2\sum_{i=1}^{N}\|\widetilde{V}_1-\widetilde{V}_2\|^2_{L^2(I^i_{\kappa_1})}.
\end{aligned}$$

The Cauchy-Schwarz inequality in combination with both the uniform boundedness of $(\widetilde{V}_\kappa)_{0<\kappa<\kappa_0}$ in $L^2(0,1)$ and the estimate (3.8) implies

$$\begin{aligned}
-\sum_{i=1}^{N}\int_{I^i_{\kappa_1}} \left(r_1(x)-r_2(x)\right)\left(\widetilde{V}_1(x)-\widetilde{V}_2(x)\right)\,dx \;&\leq\; \sum_{i=1}^{N}\|r_1-r_2\|_{L^2(I^i_{\kappa_1})}\|\widetilde{V}_1-\widetilde{V}_2\|_{L^2(I^i_{\kappa_1})} \\
&\leq\; K_3\kappa_1^{1/2}
\end{aligned}$$

and we conclude

$$S_2 \leq -K_2\sum_{i=1}^{N}\|\widetilde{V}_1-\widetilde{V}_2\|^2_{L^2(I^i_{\kappa_1})}+K_3\kappa_1^{1/2}.$$

Combining all estimates, we obtain

$$\begin{aligned}
&\left(\lambda^2-K_1\gamma^2\right)\|V_1'-V_2'\|^2_{L^2(0,1)} \\
\leq\; & K_1\gamma^2|\beta_1-\beta_2|^2-K_2\sum_{i=1}^{N}\|\widetilde{V}_1-\widetilde{V}_2\|^2_{L^2(I^i_{\kappa_1})}+K_1\gamma^{-2}\kappa_1^{1/2}+K_3\kappa_1^{1/2}.
\end{aligned}\tag{3.10}$$

Let $\delta > 0$ be a parameter to be determined later on. We estimate

$$\begin{aligned}\delta|\beta_1-\beta_2|^2(1-2\kappa_1^{1/4}) &= \delta\sum_{i=1}^N \|\beta_1-\beta_2\|^2_{L^2(I^i_{\kappa_1})}\\ &= \delta\sum_{i=1}^N \|(\widetilde{V}_1-\widetilde{V}_2)-(V_1-V_2)\|^2_{L^2(I^i_{\kappa_1})}\\ &\leq 2\delta\sum_{i=1}^N \|\widetilde{V}_1-\widetilde{V}_2\|^2_{L^2(I^i_{\kappa_1})} + 2\delta N\|V_1-V_2\|^2_{L^2(0,1)}\\ &\leq 2\delta\sum_{i=1}^N \|\widetilde{V}_1-\widetilde{V}_2\|^2_{L^2(I^i_{\kappa_1})} + 2\delta N K_4\|V_1'-V_2'\|^2_{L^2(0,1)}\end{aligned}$$

with some constant $K_4 > 0$ arising from the Poincaré inequality. We may assume $\kappa_1^{1/4} \leq \frac{1}{4}$ so that

$$\frac{\delta}{2}|\beta_1-\beta_2|^2 \leq 2\delta\sum_{i=1}^N \|\widetilde{V}_1-\widetilde{V}_2\|^2_{L^2(I^i_{\kappa_1})} + 2\delta N K_4\|V_1'-V_2'\|^2_{L^2(0,1)}. \tag{3.11}$$

Adding estimates (3.10) and (3.11), the inequality

$$\begin{aligned}&\left(\lambda^2-K_1\gamma^2-2\delta N K_4\right)\|V_1'-V_2'\|^2_{L^2(0,1)} + \left(\frac{\delta}{2}-K_1\gamma^2\right)|\beta_1-\beta_2|^2\\ &\leq (2\delta-K_2)\sum_{i=1}^N \|\widetilde{V}_1-\widetilde{V}_2\|^2_{L^2(I^i_{\kappa_1})} + K_1\gamma^{-2}\kappa_1^{1/2} + K_3\kappa_1^{1/2}\end{aligned}$$

follows. After choosing $\delta > 0$ and $\gamma > 0$ subject to the conditions

$$\lambda^2-K_1\gamma^2-2\delta N K_4 > 0, \quad \frac{\delta}{2}-K_1\gamma^2 > 0 \quad \text{and} \quad 2\delta-K_2 \leq 0,$$

we infer

$$\|V_1'-V_2'\|^2_{L^2(0,1)} + |\beta_1-\beta_2|^2 \leq C\kappa_1^{1/2}.$$

Finally, the Poincaré inequality implies the assertion. □

Remark 3.7.
Note that all estimates which follow from the Sobolev embedding theorem have to be used with care, as the domain depends on a parameter. However, since $(I_\kappa)_{0<\kappa<\kappa_0}$ is an ascending sequence of intervals as κ tends to zero, a uniform constant for the Sobolev embeddings exists, c.f. Theorem A.6.

Lemma 3.8 (Exterior convergence of u_κ as κ tends to zero).
In the situation of Lemma 3.6 let $I^1,\dots,I^N$ be the maximal intervals where V_B is constant and let $I^1_\kappa,\dots,I^N_\kappa$ be the corresponding subintervals introduced in Corollary 3.5. Then

$$\|u_0^2-u_\kappa^2\|_{L^\infty(I^i_\kappa)} \leq C\kappa^{1/4} \quad (i=1,\dots,N)$$

and

$$\|u_0^2-u_\kappa^2\|_{L^p(0,1)} \leq C\kappa^{1/4p} \quad (1 \leq p < \infty),$$

where

$$u_0^2 := h^{-1}(F + V_B + V_0 + \beta_0) \in L^\infty(0,1)$$

with the limits V_0 *and* β_0 *derived in Lemma 3.6.*

Proof. First, it should be mentioned that u_0^2 is well-defined. A pointwise examination shows that the expression $F+V_B+V_0+\beta_0$ is in the range of h, since V_κ converges in $L^\infty(0,1)$ to V_0 and β_κ converges to β_0. Moreover, $2\kappa\frac{u_\kappa''}{u_\kappa}$ converges to zero in $L^\infty(I_\kappa^i)$ for $i=1,\ldots,N$. The definition of u_0 by $u_0=\sqrt{u_0^2}$ is meaningful, i.e. a positive, real-valued function, because a subsequence of $u_\kappa>0$ converges pointwise to u_0. We abbreviate $k_\nu := h+\frac{\nu}{\tau}\ln$ and $B(u_\kappa^2)=\frac{u_\kappa''}{u_\kappa}$. Since V_κ, β_κ and $2\kappa\frac{u_\kappa''}{u_\kappa}$ are uniformly bounded in $L^\infty(I_\kappa^i)$ for $0<\kappa<\kappa_0$ and $i=1,\ldots,N$, the local Lipschitz continuity of k_ν^{-1}, Lemma A.19 and inequality (3.7) imply

$$\begin{aligned}
\|u_0^2-u_\kappa^2\|_{L^\infty(I_\kappa)} &= \|h^{-1}(F+V_B+V_0+\beta_0)-k_\nu^{-1}(F+V_B+V_\kappa+\beta_\kappa+2\kappa B(u_\kappa^2)\|_{L^\infty(I_\kappa^i)}\\
&\le \|h^{-1}(F+V_B+V_0+\beta_0)-k_\nu^{-1}(F+V_B+V_0+\beta_0)\|_{L^\infty(I_\kappa^i)}\\
&\quad +\|k_\nu^{-1}(F+V_B+V_0+\beta_0)-k_\nu^{-1}(F+V_B+V_\kappa+\beta_\kappa+2\kappa B(u_\kappa^2)\|_{L^\infty(I_\kappa^i)}\\
&\le C\nu+\|V_0-V_\kappa+\beta_0-\beta_\kappa-2\kappa B(u_\kappa^2)\|_{L^\infty(I_\kappa^i)}\\
&\le C\kappa^{1/2}+\|V_0-V_\kappa\|_{L^\infty(I_\kappa)}+|\beta_0-\beta_\kappa|+\|2\kappa B(u_\kappa^2)\|_{L^\infty(I_\kappa^i)}\\
&\le C\kappa^{1/4}.
\end{aligned}$$

The second inequality is obtained by

$$\|u_0^2-u_\kappa^2\|_{L^p((0,1)\setminus\cup_{i=1}^N I_\kappa^i)} \le \|u_0^2-u_\kappa^2\|_{L^\infty(0,1)}\|\chi_{(0,1)\setminus\cup_{i=1}^N I_\kappa^i)}\|_{L^p(0,1)} \le C(\kappa^{1/4})^{1/p},$$

so that

$$\|u_0^2-u_\kappa^2\|_{L^p(0,1)} \le \|u_0^2-u_\kappa^2\|_{L^p((0,1)\setminus\cup_{i=1}^N I_\kappa^i)} + \sum_{i=1}^N \|u_0^2-u_\kappa^2\|_{L^p(I_\kappa^i)} \le C\kappa^{1/4p}.$$

□

Remark 3.9 (Convergence of V_κ revisited, Remarks on the convergence of u_κ). *Considering the potential equation to* V_κ*, Lemma 3.8 yields convergence of* V_κ *to* V_0 *in* $W^{2,2}(0,1)$ *with rate* $\kappa^{1/8}$*. Choosing* $p=1$*, we also see that* C^1*-convergence and* $W^{2,1}$*-convergence with rate* $\kappa^{1/4}$ *is given. The rates of convergence will be improved in a following section.*
Since the limiting function u_0 *is discontinuous at any point of discontinuity of* V_B*, convergence is neither possible in* $L^\infty(0,1)$ *nor in* $W^{1,p}(0,1)$*,* $1\le p\le\infty$*. Moreover, we lack boundedness of* u_κ *in* $W^{1,p}(0,1)$ *for* $p>1$*, since this would also imply* $L^\infty(0,1)$*-convergence through the interpolation inequalities A.8. In the next section, we will give some detailed information about the slope of* u_κ *at any point of jump discontinuity of* V_B*.*

3.3 Behavior of solutions at points of jump discontinuity in the barrier potential

Throughout this section we suppose that the barrier potential V_B is a piecewise constant function and that the solutions $(u_\kappa)_{0<\kappa<\kappa_0}$ and $(V_\kappa)_{0<\kappa<\kappa_0}$ satisfy Assumption 3.3 with corresponding constants $(\beta_\kappa)_{0<\kappa<\kappa_0}$, where β_κ is zero in case that the integral condition for u_κ is not supposed to hold. As introduced in Lemma 3.6 and Lemma 3.8, let u_0 and V_0 denote the limiting functions of $(u_\kappa)_{0<\kappa<\kappa_0}$ and $(V_\kappa)_{0<\kappa<\kappa_0}$. Since

$$u_0^2 = h^{-1}(F + V_B + V_0 + \beta_0),$$

we see that u_0 has a jump discontinuity at any point s_0, where V_B has a jump discontinuity. By the mean value theorem we then already know that the derivatives of u_κ must become rather large in a neighborhood of s_0 as κ tends to zero. Applying the scaling $x \mapsto \frac{x}{\kappa^{1/2}}$ to the differential equation for u_κ, we will obtain a more precise description of the situation. First, we prove that the magnitude of the derivatives $u_\kappa'(s_0)$ is of order $\kappa^{-1/2}$.

Lemma 3.10 (L^∞**-estimate to the derivatives of the solutions).**
The derivatives of the solutions u_κ enjoy the estimate

$$\|u_\kappa'\|_{L^\infty(0,1)} \le C\kappa^{-1/2}.$$

Proof. Let $I^1 = [s_1, s_2], \dots, I^N = [s_N, s_{N+1}]$ be the maximal intervals in which V_B is constant and consider $\xi, x \in [0,1]$ with $[\xi, x] \subset [s_i, s_{i+1}]$ for an $i \in \{1, \dots N\}$. Let K be a primitive of $k = h + \frac{\nu}{\tau}\ln$. Multiplying the differential equation for u_κ by u_κ' and integrating over (ξ, x), we obtain

$$\begin{aligned}
\kappa u_\kappa'(x)^2 - \kappa u_\kappa'(\xi)^2 &= -\frac{1}{2}(F + V_B + \beta_\kappa)(u_\kappa^2(x) - u_\kappa^2(\xi)) + \frac{1}{2}\int_\xi^x (k(u_\kappa^2(s)) - V_\kappa(s))(u_\kappa^2)'(s)\,ds \\
&= -\frac{1}{2}\Big((F + V_B + \beta_\kappa)(u_\kappa^2(x) - u_\kappa^2(\xi)) - (K(u_\kappa^2(x)) - K(u_\kappa^2(\xi))) \\
&\quad + (V_\kappa(x)u_\kappa^2(x) - V_\kappa(\xi)u_\kappa^2(\xi)) - \frac{1}{2}\int_\xi^x V_\kappa'(s)u_\kappa^2(s)\,ds\Big) \\
&=: r_\kappa(x,\xi).
\end{aligned}$$

As implied by Assumption 3.3, $r_\kappa(x,\xi)$ is uniformly bounded for $0 < \kappa < \kappa_0$ and $x, \xi \in [0,1]$. By integration, it follows that

$$\kappa u_\kappa'(\xi)^2|s_{i+1} - s_i| = \kappa\int_{s_i}^{s_{i+1}} u_\kappa'(\xi)^2\,dx = \kappa\int_{s_i}^{s_{i+1}} u_\kappa'(x)^2\,dx - \int_{s_i}^{s_{i+1}} r_\kappa(x,\xi)\,dx.$$

The coerciveness inequality (2.9) now implies $\kappa u_\kappa'(\xi)^2 \le \frac{C}{|s_{i+1}-s_i|}$ for all $\xi \in [s_i, s_{i+1}]$. Therefore,

$$\|u_\kappa'\|_{L^\infty(0,1)} \le C\kappa^{-1/2}.$$

□

Lemma 3.11 (Lower estimates to $u_\kappa'^2$ at points of jump discontinuity of V_B)**.**
Let s_0 be a point of jump discontinuity of V_B. Then there exists $C_0 > 0$ such that

$$\kappa u_\kappa'^2(s_0) \ge C_0 > 0$$

for $0 < \kappa < \kappa_0$.

Proof. Some technical preparations are in order. Let h be the enthalpy to the pressure term p and let K be the primitive of $k = h + \frac{\nu}{\tau}\ln$ which fulfills

$$K(z) = zk(z) - p(z) - \frac{\nu}{\tau}z \quad (z > 0), \tag{3.12}$$

c.f. Remark 2.7. Accordingly, let

$$H(z) := zh(z) - p(z) \quad (z > 0) \tag{3.13}$$

be the canonical primitive of h. We adopt the notations

$$V_B(s_0+) := \lim_{h\searrow 0} V_B(s_0 + h) \quad \text{and} \quad u_0(s_0+) := \lim_{h\searrow 0} u_0(s_0 + h).$$

Multiplying the differential equation for u_κ by u_κ' and integrating over an interval $[s_0, s_0 + x]$ where V_B is constant, we obtain

$$\begin{aligned}
2\kappa \int_{s_0}^{s_0+x} u_\kappa''(s)u_\kappa'(s)\,ds &= -\int_{s_0}^{s_0+x} \left(F + V_B(s_0+) + V_\kappa(s) + \beta_\kappa - k(u_\kappa^2(s))\right) u_\kappa(s)u_\kappa'(s)\,ds \\
&= -\frac{1}{2}\left(F + V_B(s_0+) + \beta_\kappa\right)\left(u_\kappa^2(s_0 + x) - u_\kappa^2(s_0)\right) \\
&\quad +\frac{1}{2}\left(K(u_\kappa^2(s_0 + x)) - K(u_\kappa^2(s_0))\right) \\
&\quad -\frac{1}{2}\left(V_\kappa u_\kappa^2\right)\Big|_{s_0}^{s_0+x} + \frac{1}{2}\int_{s_0}^{s_0+x} V_\kappa'(s)u_\kappa^2(s)\,ds.
\end{aligned}$$

Introducing the additional term $-k(u_\kappa^2(s_0 + x))u_\kappa^2(s_0 + x)$ into the equation and evaluating the integral on the left hand side, we can rearrange this equality to get

$$\begin{aligned}
&\kappa u_\kappa'^2(s_0) + \frac{1}{2}\left(F + V_B(s_0+) + V_\kappa(s_0) + \beta_\kappa\right) u_\kappa^2(s_0) - \frac{1}{2}K(u_\kappa^2(s_0)) \\
&\quad +\frac{1}{2}K(u_\kappa^2(s_0 + x)) - \frac{1}{2}k(u_\kappa^2(s_0 + x))u_\kappa^2(s_0 + x) \\
&= \kappa u_\kappa'^2(s_0 + x) + \frac{1}{2}\left(F + V_B(s_0+) + V_\kappa(s_0 + x) + \beta_\kappa - k(u_\kappa^2(s_0 + x))\right) u_\kappa^2(s_0 + x) \\
&\quad -\frac{1}{2}\int_{s_0}^{s_0+x} V_\kappa'(s)u_\kappa^2(s)\,ds.
\end{aligned} \tag{3.14}$$

We try to give a more detailed description of the slope $u_\kappa'(s_0)$ at the point of jump discontinuity by estimating the terms on the right hand side. In particular, we are interested in the L^2-norms on the subintervals $J_\kappa := [\kappa^{1/4}L, 2\kappa^{1/4}L]$, where L again denotes the length of the maximal interval $[s_0, s_0 + L]$ in which V_B is constant. Assuming that $0 < \kappa < \kappa_0$ is sufficiently small, we have $s_0 + J_\kappa \subset I_\kappa$ in the notation of Corollary 3.5. Employing the interpolation inequalities A.8 with the estimates (3.4) and (3.6), we obtain

$$\begin{aligned}
\kappa\left\|u_\kappa'(s_0 + \cdot)^2\right\|_{L^2(J_\kappa)} &= \kappa\left\|u_\kappa'(s_0 + \cdot)\right\|_{L^4(J_\kappa)}^2 \\
&\le \kappa\left\|u_\kappa'(s_0 + \cdot)\right\|_{L^2(J_\kappa)}\left\|u_\kappa'(s_0 + \cdot)\right\|_{L^\infty(J_\kappa)} \\
&\le C\kappa^{3/4}.
\end{aligned}$$

Inequality (3.5) in concern with the uniform boundedness of u_κ yields

$$\begin{aligned}
&\frac{1}{2}\left\|\left(F + V_B(s_0+) + V_\kappa(s_0+\cdot) + \beta_\kappa - k(u_\kappa^2(s_0+\cdot))\right) u_\kappa^2(s_0+\cdot)\right\|_{L^2(J_\kappa)} \\
&= \left\|\kappa u_\kappa''(s_0+\cdot) u_\kappa(s_0+\cdot)\right\|_{L^2(J_\kappa)} \\
&\leq C\kappa^{1/2}.
\end{aligned}$$

Thanks to the uniform estimates to $\|V_\kappa'\|_{L^\infty(0,1)}$ and $\|u_\kappa\|_{L^\infty(0,1)}$, there holds

$$\left\|\int_{s_0}^{s_0+(\cdot)} V_\kappa'(s) u_\kappa^2(s)\, ds\right\|_{L^2(J_\kappa)} \leq \left(\int_{\kappa^{1/4}L}^{2\kappa^{1/4}L} (Cx)^2\, dx\right)^{1/2} \leq C\kappa^{3/8}.$$

We employ the identity (3.12) to simplify the left hand side of equation (3.14). An intermediate result then reads

$$\begin{aligned}
\text{(3.15)}\quad &\Big\|\kappa u_\kappa'^2(s_0) + \frac{1}{2}\Big((F + V_B(s_0+) + V_\kappa(s_0) + \beta_\kappa)\, u_\kappa^2(s_0) \\
&\qquad - K(u_\kappa^2(s_0)) - p(u_\kappa^2(s_0+\cdot)) - \frac{\nu}{\tau} u_\kappa^2(s_0+\cdot)\Big)\Big\|_{L^2(J_\kappa)} \leq C\kappa^{3/8}.
\end{aligned}$$

The objective is to replace the function $p(u_\kappa^2(s_0+\cdot))$ by it's one-sided limit and to drop the contributions of all terms which are small in κ so that we can compare $u_\kappa'(s_0)$ to a constant rather than to a function. We therefore investigate the expression

$$\begin{aligned}
\text{(3.16)}\quad & \frac{1}{2}\left((F + V_B(s_0+) + V_0(s_0) + \beta_0)\, u_\kappa^2(s_0) - H(u_\kappa^2(s_0)) - p(u_0^2(s_0+))\right) \\
= \quad & \frac{1}{2}\Big((F + V_B(s_0+) + V_\kappa(s_0) + \beta_\kappa)\, u_\kappa^2(s_0) - K(u_\kappa^2(s_0)) - p(u_\kappa^2(s_0+\cdot)) - \frac{\nu}{\tau} u_\kappa^2(s_0+\cdot)\Big) \\
& + \frac{1}{2} p(u_\kappa^2(s_0+\cdot) - \frac{1}{2} p(u_0^2(s_0+\cdot) \\
& + \frac{1}{2} p(u_0^2(s_0+\cdot)) - \frac{1}{2} p(u_0^2(s_0+)) \\
& + \mathcal{O}(\kappa^{3/8}),
\end{aligned}$$

where $\mathcal{O}(\kappa^{3/8})$ refers to the norm in $L^2(J_\kappa)$ and arises due to the replacement of V_κ, β_κ, k and K by their limiting functions. By Lipschitz continuity of p on compact subsets of $(0,\infty)$, we find

$$\|p(u_\kappa^2(s_0+\cdot)) - p(u_0^2(s_0+\cdot))\|_{L^2(J_\kappa)} \leq C\|u_\kappa^2(s_0+\cdot) - u_0^2(s_0+\cdot)\|_{L^\infty(J_\kappa)}\|1\|_{L^2(J_\kappa)} \leq C\kappa^{3/8}$$

thanks to Lemma 3.8. Because $u_0^2 = h^{-1}(F + V_B(s_0+) + V_0 + \beta_0)$ on $[s_0, s_0+L]$, we conclude by local Lipschitz continuity of $p \circ h^{-1}$ that

$$\begin{aligned}
\|p(u_0^2(s_0+\cdot)) - p(u_0^2(s_0+))\|_{L^2(J_\kappa)} &\leq C\|V_0(s_0+\cdot) - V_0(s_0)\|_{L^2(J_\kappa)} \\
&\leq C\left(\int_{\kappa^{1/4}L}^{2\kappa^{1/4}L} (\|V_0'\|_{L^\infty(0,1)}\, x)^2\, dx\right)^{1/2} \\
&\leq C\kappa^{3/8}.
\end{aligned}$$

We obtain

$$\|\kappa u_\kappa'^2(s_0) - C_\kappa^+\|_{L^2(J_\kappa)} \le C\kappa^{3/8}$$

and consequently

$$|\kappa u_\kappa'^2(s_0) - C_\kappa^+| \le C\kappa^{1/4}, \tag{3.17}$$

where the constant

$$C_\kappa^+ = -\frac{1}{2}\left((F + V_B(s_0+) + V_0(s_0) + \beta_0)\, u_\kappa^2(s_0) - H(u_\kappa^2(s_0)) - p(u_0^2(s_0+))\right)$$

only depends on κ via $u_\kappa(s_0)$.
Repeating the argumentation in the area left to s_0, we also obtain $|\kappa u_\kappa'^2(s_0) - C_\kappa^-| \le C\kappa^{1/4}$ for an analogously defined constant C_κ^- and therefore,

$$|2\kappa u_\kappa'^2(s_0) - (C_\kappa^+ + C_\kappa^-)| \le C\kappa^{1/4}.$$

We now establish a uniform lower bound $C_\kappa^+ + C_\kappa^- \ge 2C_0 > 0$, as this implies $\kappa u_\kappa'^2(s_0) \ge C_0 > 0$ for $0 < \kappa < \kappa_0$. By definition of H, we can reshape C_κ^+ and C_κ^-

$$\begin{aligned}
C_\kappa^\pm &= -\frac{1}{2}\left(\left(F + V_B(s_0+) + V_0(s_0) + \beta_0 - h(u_\kappa^2(s_0))\right) u_\kappa^2(s_0) + p(u_\kappa^2(s_0)) - p(u_0^2(s_0\pm))\right)\\
&= -\frac{1}{2}\left(F + V_B(s_0+) + V_0(s_0) + \beta_0 - h(u_0^2(s_0\pm))\right) u_\kappa^2(s_0)\\
&\quad -\frac{1}{2}\left(\left(h(u_0^2(s_0\pm)) - h(u_\kappa^2(s_0))\right) u_\kappa^2(s_0) + p(u_\kappa^2(s_0)) - p(u_0^2(s_0\pm))\right)\\
&= \frac{1}{2}\left(h(u_\kappa^2(s_0)) - h(u_0^2(s_0\pm))\right) u_\kappa^2(s_0) + \frac{1}{2}\left(p(u_0^2(s_0\pm)) - p(u_\kappa^2(s_0))\right),
\end{aligned}$$

where the last equality holds by definition of u_0. Let the functions $g^\pm : [0,\infty) \longrightarrow \mathbb{R}$ be defined by

$$g^\pm(z) := \frac{1}{2}\left(h(z) - h(u_0^2(s_0\pm))\right) z + \frac{1}{2}\left(p(u_0^2(s_0\pm)) - p(z)\right) \quad (z \ge 0). \tag{3.18}$$

Then

$$g^{\pm\prime}(z) = \frac{1}{2}\left(h(z) - h(u_0^2(s_0\pm))\right) \quad (z \ge 0)$$

due to $h'(z) = \frac{p'(z)}{z}$. Thanks to the monotonicity assumptions on the admissible pressure term p, we find

$$g^+(0) = \frac{1}{2}\left(p(u_0^2(s_0+)) - p(0)\right) > 0 = g^+(u_0^2(s_0+))$$

and observing that $g^{+\prime}(z)$ is positive for $z > u_0^2(s_0+)$, we conclude that g^+ attains its minimum in $(0,\infty)$. Therefore,

$$0 = g^{+\prime}(z_0^+) = \frac{1}{2}\left(h(z_0^+) - h(u_0^2(s_0+))\right)$$

at any point $z_0^+ \in (0,\infty)$ where the minimum is attained. Since h is injective, we know that z_0^+ is uniquely determined by $z_0^+ = u_0^2(s_0+)$. By the same reasoning, the unique minimizer of g^- is found to be $z_0^- = u_0^2(s_0-)$. We conclude that the lower bound $2C_0$ to $(C_\kappa^+ + C_\kappa^-)$ exists if

$$|u_\kappa^2(s_0) - u_0^2(s_0+)| + |u_\kappa^2(s_0) - u_0^2(s_0-)| \ge C > 0$$

for some $C > 0$ not depending on $0 < \kappa < \kappa_0$. However, since u_0 has a jump discontinuity at s_0, this inequality is immediate thanks to

$$0 \neq |u_0^2(s_0+) - u_0^2(s_0-)| \leq |u_\kappa^2(s_0) - u_0^2(s_0+)| + |u_\kappa^2(s_0) - u_0^2(s_0-)|.$$

□

Corollary 3.12.
To summarize, we have shown that there exist $C_0, C_1 > 0$ such that

$$C_0\kappa^{-1/2} \leq |u_\kappa'(s_0)| \leq C_1\kappa^{-1/2} \tag{3.19}$$

and

$$C_0\kappa^{-1/2} \leq \|u_\kappa'\|_{L^\infty(0,1)} \leq C_1\kappa^{-1/2} \tag{3.20}$$

for $0 < \kappa < \kappa_0$ and for any point $s_0 \in [0,1]$, where V_B has a jump discontinuity.

We now derive an ordinary differential equation describing the boundary layer. Roughly speaking, we will extract the fast component of the solution u_κ, which is dominant in a vicinity of a point s_0 of jump discontinuity of V_B. Without loss of generality, we focus on a regime right to s_0. The assertions can easily be transfered to the domain left to it.

Lemma 3.13.
As before, let s_0 be a point of jump discontinuity of V_B and assume that $[s_0, s_0+L]$ is the maximal interval where V_B is constant. There exist $C_2 > 0$ and functions $w_\kappa : [0, C_2] \longrightarrow \mathbb{R}$ such that

$$\left\| u_\kappa(s_0 + \cdot) - w_\kappa\left(\frac{\cdot}{\kappa^{1/2}}\right)\right\|_{L^\infty([0,C_2\kappa^{1/2}])} \leq C\kappa^{1/4}. \tag{3.21}$$

Proof. We approximate and rescale the differential equation (3.14) for u_κ in a small intervall $[0, \kappa^{1/4}L]$. We rearrange this equality and use both the convergence results of Lemma 3.6 and the uniform estimates for u_κ, V_κ and β_κ from Assumption 3.3 in order to obtain

$$\begin{aligned}
\kappa u_\kappa'^2(s_0+x) &= \kappa u_\kappa'^2(s_0) + \frac{1}{2}\left(F + V_B(s_0+) + V_\kappa(s_0) + \beta_\kappa\right)u_\kappa^2(s_0) - \frac{1}{2}K(u_\kappa^2(s_0)) \\
&\quad -\frac{1}{2}\left(F + V_B(s_0+) + V_\kappa(s_0+x) + \beta_\kappa\right)u_\kappa^2(s_0+x) \\
&\quad +\frac{1}{2}K(u_\kappa^2(s_0+x)) + \frac{1}{2}\int_{s_0}^{s_0+x} V_\kappa'(s)u_\kappa^2(s)\,ds \\
&= \kappa u_\kappa'^2(s_0) + \frac{1}{2}\left(F + V_B(s_0+) + V_0(s_0) + \beta_0\right)u_\kappa^2(s_0) - \frac{1}{2}H(u_\kappa^2(s_0)) \\
&\quad -\frac{1}{2}\left(F + V_B(s_0+) + V_0(s_0+x) + \beta_0\right)u_\kappa^2(s_0+x) \\
&\quad +\frac{1}{2}H(u_\kappa^2(s_0+x)) + \mathcal{O}(\kappa^{1/4}) \\
&= \kappa u_\kappa'^2(s_0) - C_\kappa^+ + \frac{1}{2}h(u_\kappa^2(s_0))u_\kappa^2(s_0) - \frac{1}{2}p(u_\kappa^2(s_0)) + \frac{1}{2}p(u_0^2(s_0+)) \\
&\quad -\frac{1}{2}H(u_\kappa^2(s_0)) - \frac{1}{2}\left(F + V_B(s_0+) + V_0(s_0+x) + \beta_0\right)u_\kappa^2(s_0+x) \\
&\quad +\frac{1}{2}H(u_\kappa^2(s_0+x)) + \mathcal{O}(\kappa^{1/4})
\end{aligned}$$

for $x \in [0, \kappa^{1/4}L]$, where $\mathcal{O}(\kappa^{1/4})$ refers to the L^∞-norm on $[0, \kappa^{1/4}L]$. By introducing the terms $\pm h(u_0^2(s_0+x))$ and using the identity (3.13) and estimate (3.17), we obtain

$$\begin{aligned}
\kappa u_\kappa'^2(s_0+x) &= -\frac{1}{2}\left(F + V_B(s_0+) + V_0(s_0+x) + \beta_0 - h(u_0^2(s_0+x))\right) u_\kappa^2(s_0+x) \\
&\quad -\frac{1}{2} h(u_0^2(s_0+x)) u_\kappa^2(s_0+x) \\
&\quad +\frac{1}{2} p(u_0^2(s_0+)) + \frac{1}{2} H(u_\kappa^2(s_0+x)) + \mathcal{O}(\kappa^{1/4}) \\
&= \frac{1}{2}\left(H(u_\kappa^2(s_0+x)) - h(u_0^2(s_0+x)) u_\kappa^2(s_0+x) + p(u_0^2(s_0+))\right) + \mathcal{O}(\kappa^{1/4}) \\
&= \frac{1}{2}\left(h(u_\kappa^2(s_0+x)) - h(u_0^2(s_0+x))) u_\kappa^2(s_0+x)\right) \\
&\quad +\frac{1}{2}\left(p(u_0^2(s_0)) - p(u_\kappa^2(s_0+x))\right) + \mathcal{O}(\kappa^{1/4}).
\end{aligned}$$

In the last equality, the expression $h(u_0^2(s_0+x))$ can also be approximated by $h(u_0^2(s_0+))$ on $[0, \kappa^{1/4}L]$, because $h(u_0^2)' = V_0'$ is actually a bounded function. We now show that the solutions u_κ stay away from the limiting function u_0 at the point s_0. More precisely, there exists a constant $C > 0$ and $\kappa_0 > 0$, such that

$$|u_\kappa(s_0) - u_0(s_0+)| \geq C \quad (0 < \kappa < \kappa_0). \tag{3.22}$$

Otherwise, there exists a sequence $(\kappa_n)_{n\in\mathbb{N}}$ converging to zero such that $|u_{\kappa_n}(s_0) - u_0(s_0+)|$ converges to zero as well. Then, the right hand side of

$$\kappa u_\kappa'^2(s_0) = \frac{1}{2}\left(h(u_\kappa^2(s_0)) - h(u_0^2(s_0+))) u_\kappa^2(s_0)\right) + \frac{1}{2}\left(p(u_0^2(s_0+)) - p(u_\kappa^2(s_0))\right) + \mathcal{O}(\kappa^{1/4})$$

tends to zero, whereas the left hand side of the equation is uniformly bounded from below by estimate (3.19), which yields a contradiction.
Introducing the variable transformation $y = \frac{x}{\kappa^{1/2}}$, we define the scaled functions

$$v_\kappa : [0, \kappa^{-1/2}L] \longrightarrow \mathbb{R}, \quad v_\kappa(y) := u_\kappa(s_0 + \kappa^{1/2}y) = u_\kappa(s_0+x)$$

and

$$v_0 : [0, \kappa^{-1/2}L] \longrightarrow \mathbb{R}, \quad v_0(y) := u_0(s_0 + \kappa^{1/2}y) = u_0(s_0+x)$$

with the convention $v_0(0) := u_0(s_0+)$.
For $y \in [0, \kappa^{-1/4}L]$, the scaled differential equation now reads

$$\begin{aligned}
v_\kappa'(y)^2 &= \frac{1}{2}\left(H(v_\kappa^2(y)) - h(v_0^2(0)) v_\kappa^2(y) + p(v_0^2(0))\right) + \mathcal{O}(\kappa^{1/4}) \\
&= \frac{1}{2}\left(h(v_\kappa^2(y)) - h(v_0^2(0))\right) v^2(y) + \frac{1}{2}\left(p(v_0^2(0)) - p(v_\kappa^2(y))\right) + \mathcal{O}(\kappa^{1/4}),
\end{aligned}$$

supplied with the initial value $v_\kappa(0) = u_\kappa(s_0)$. Note that the rate in the remainder term $\mathcal{O}(\kappa^{1/4})$ does not change in the L^∞-norm. We also mention that estimate (3.22) guarantees that the right hand side of the equation is bounded away from zero in a vicinity of $v_\kappa(0)$. We now consider the explicit formulation

$$\left\{\begin{aligned}
v_\kappa'(y) &= \pm\sqrt{\tfrac{1}{2}\left(h(v_\kappa^2(y)) - h(v_0^2(0))\right) v_\kappa^2(y) + \tfrac{1}{2}\left(p(v_0^2(0)) - p(v_\kappa^2(y))\right) + \mathcal{O}(\kappa^{1/4})}, \\
v_\kappa(0) &= u_\kappa(s_0),
\end{aligned}\right. \tag{3.23}$$

where the sign of the root is chosen equal to the sign of $u'_\kappa(s_0)$. The classical theory of ordinary differential equations yields existence and uniqueness of solutions as long as the radicand stays away from zero. A regime not depending on κ, in which this is the case, actually exists: Since $|u_\kappa(s_0) - u_0(s_0+)| \geq C$ for $0 < \kappa < \kappa_0$ by inequality (3.22) and since v'_κ is uniformly bounded for $0 < \kappa < \kappa_0$ on some fixed interval, we conclude $|v_\kappa(y) - v_0(0)| = |u_\kappa(s_0 + x) - u_0(s_0+)| \geq C$ uniformly for $y \in [0, C_2]$, or in terms of the original variable, for $x \in [s_0, s_0 + C_2\kappa^{1/2}]$ for some constant $C_2 > 0$.
We now drop the term of order $\mathcal{O}(\kappa^{1/4})$ in the differential equation. Using the same arguments as given above, the solution w_κ to

$$\left\{ \begin{array}{rcl} w'_\kappa(y) & = & \pm\sqrt{\frac{1}{2}\left(h(w_\kappa^2(y)) - h(v_0^2(0))\right) w_\kappa^2(y) + \frac{1}{2}\left(p(v_0^2(0)) - p(w_\kappa^2(y))\right)}, \\ w_\kappa(0) & = & u_\kappa(s_0) \end{array} \right. \tag{3.24}$$

exists in an interval $[0, C_2]$, where C_2 does not depend on $0 < \kappa < \kappa_0$. Note that the differential equations in (3.23) and (3.24) can be written as

$$v'_\kappa = \sqrt{g^+(v_\kappa^2) + \mathcal{O}(\kappa^{1/4})} \quad \text{and} \quad w'_\kappa = \sqrt{g^+(w_\kappa^2)}$$

with the function g^+ defined in (3.18). Classical perturbation results (c.f. [Wa, III §12 Thm. VI]) now yield

$$\|v_\kappa - w_\kappa\|_{L^\infty([0,C_2])} \leq C\kappa^{1/4}$$

with a constant $C > 0$ not depending on $0 < \kappa < \kappa_0$. In terms of the original variable, this result simply reads as

$$\left\| u_\kappa(s_0 + \cdot) - w_\kappa\left(\frac{\cdot}{\kappa^{1/2}}\right)\right\|_{L^\infty([0,C_2\kappa^{1/2}])} \leq C\kappa^{1/4}.$$

□

Remark 3.14.
In addition to the points of jump discontinuity of V_B, the solutions u_κ may potentially form a further boundary layer at the endpoints of the interval $[0,1]$ if u_κ satisfies periodic boundary conditions. Since V_κ converges in $W^{1,2}(0,1)$ to V_0, the Dirichlet boundary values of V_0 are preserved and we see that the periodic extension of $u_0^2 = h^{-1}(F + V_B + V_0 + \beta_0)$ to $\mathbb{R}$ has jump discontinuities at 0 and 1 if $V_B(0) + V_0(0) \neq V_B(1) + V_1(1)$. In either case, the results of Corollary 3.12 and Lemma 3.13 also hold for $s_0 = 0$ and $s_0 = 1$ when constructing w_κ in the same manner. Note, however, that one should choose w_κ as the constant function $u_0(0)$ if, by coincidence, $u_\kappa(0) = u_0(0)$. Analogously, w_κ should be chosen as $u_0(1)$ if $u_\kappa(1) = u_0(1)$.

We now gather further information on the functions w_κ. An important property of w_κ is that it depends on the parameter κ in a simple manner, as the ordinary differential equations belonging to w_κ are autonomous.

Lemma 3.15.
Let s_0 be a point of jump discontinuity of V_B. There exist constants $c_\kappa > 0$ for $0 < \kappa < \kappa_0$ such that the unique solutions w_κ of the initial value problems (3.24) are given by

$$w_\kappa(y) = w(y + c_\kappa) \quad (0 < \kappa < \kappa_0)$$

for a certain function $w \in C^1((0,\infty),\mathbb{R})$*. Moreover,*

$$|w(y) - u_0(s_0+)| \leq C\exp(-\sqrt{C_1}y), \tag{3.25}$$
$$|w'(y)| \leq C\exp(-\sqrt{C_1}y), \tag{3.26}$$
$$|w''(y))| \leq C\exp(-\sqrt{C_1}y), \tag{3.27}$$

and

$$\left\| w\left(\frac{\cdot}{\kappa^{1/2}}\right) - u_0(s_0+)\right\|_{L^1(0,\infty)} \leq \frac{C}{\sqrt{C_1}}\kappa^{1/2}, \tag{3.28}$$

where $C_1 = p'(u_0^2(s_0+))$*.*

Proof. We have already shown that the unique solutions exist in a common interval $[0, C_2]$ because $|u_\kappa(s_0) - u_0(s_0+)| \geq C$ by inequality (3.22). For the sake of simplicity, we assume that the sign of the root in the equations (3.24) is positive and we choose w as the unique solution with initial value $w(0) = w_0 := \inf_{0<\kappa<\kappa_0} u_\kappa(s_0) < u_0(s_0+)$. It is well-known that solutions to first-order autonomous ordinary differential equations are monotone. In our case, w is monotonically increasing. Employing the differential equation, it is easy to see that w cannot converge to a constant smaller than $u_0(s_0+)$. Then, for any $0 < \kappa < \kappa_0$ there exists a constant $c_\kappa > 0$ such that $w(c_\kappa) = u_\kappa(s_0)$. By uniqueness of the solutions to the initial value problem (3.24), the claimed identity is valid.
In the following, we will show that w indeed converges rather fast to the limit $u_0(s_0+)$. We temporarily abbreviate $c_0 := u_0(s_0+)$, introduce the variable transform $z = c_0 - w$ and write $\widetilde{h}(y) := h(y^2)$ and $\widetilde{p}(y) := p(y^2)$ for $y > 0$. Employing a Taylor expansion with respect to z in the radicand on the right hand side of (3.24), we obtain

$$\begin{aligned}
g^+(w^2) &= \frac{1}{2}\left(h(w^2) - h(c_0^2)\right)w^2 + \left(p(c_0^2) - p(w^2)\right) \\
&= \frac{1}{2}\left(\widetilde{h}(c_0 - z) - \widetilde{h}(c_0)\right)(c_0 - z)^2 + \frac{1}{2}\left(\widetilde{p}(c_0) - \widetilde{p}(c_0 - z)\right) \\
&= \frac{1}{2}\left(\widetilde{h}'(c_0)(-z) + \widetilde{h}''(c_0)\frac{(-z)^2}{2} + \widetilde{h}'''(\xi_1)\frac{(-z)^3}{6}\right)\left(c_0^2 - 2c_0 z + z^2\right) \\
&\quad -\frac{1}{2}\left(\widetilde{p}'(c_0)(-z) + \widetilde{p}''(c_0)\frac{(-z)^2}{2} + \widetilde{p}'''(\xi_2)\frac{(-z)^3}{3}\right) \\
&=: z^2\left(C_1 + zr(z,\xi_1,\xi_2)\right)
\end{aligned}$$

with certain $\xi_1, \xi_2 \in (c_0 - |z|, c_0 + |z|)$, a constant C_1 not depending on z and the remainder term r being uniformly bounded for sufficiently small $|z|$. Note that the coefficient of the power z^1 actually vanishes thanks to the identity $h'(y) = \frac{p'(y)}{y}$. Moreover, a short calculation yields

$$C_1 = \frac{c_0^2}{4}\widetilde{h}''(c_0) + c_0\widetilde{h}'(c_0) - \frac{1}{4}\widetilde{p}''(c_0) = p'(c_0^2) > 0.$$

It is easily seen that

$$w \mapsto \frac{1}{\sqrt{g^+(w^2)}} - \frac{1}{\sqrt{C_1}}\frac{1}{(c_0 - w)} = \frac{1}{c_0 - w}\left(\frac{1}{\sqrt{C_1 + (c_0 - w)r(c_0 - w, \xi_1, \xi_2)}} - \frac{1}{\sqrt{C_1}}\right)$$

extends to a continuous function on $[w_0, c_0]$. Using the separation of variables formula, the solution w is implicitely given by

$$\begin{aligned} y &= \int_{w_0}^{w(y)} \frac{1}{\sqrt{g^+(\omega^2)}}\, d\omega \\ &= \int_{w_0}^{w(y)} \frac{1}{\sqrt{g^+(\omega^2)}} - \frac{1}{\sqrt{C_1}} \frac{1}{c_0-\omega}\, d\omega + \frac{1}{\sqrt{C_1}} \int_{w_0}^{w(y)} \frac{1}{c_0-\omega}\, d\omega \\ &=: I(w(y)) - \frac{1}{\sqrt{C_1}} \left(\ln(c_0 - w(y)) - \ln(c_0 - w_0)\right) \end{aligned}$$

and $I(w)$ is bounded for all $w \in [w_0, c_0]$. Now,

$$|c_0 - w(y)| = \left|\exp(\sqrt{C_1} I(w(y)) + \ln(c_0 - w_0) - \sqrt{C_1} y)\right| \le C \exp(-\sqrt{C_1} y)$$

proves inequality (3.25) and we observe that the first equality also implies $|w(y) - c_0| \ge C > 0$ on any bounded interval of existence of w. By a continuation argument, w is defined on the whole half-line $(0, \infty)$.
Next, we consider w''. Observe that by definition of g^+ (c.f. (3.18)) and the differential equation for w, there holds

$$w'' = \sqrt{g^+(w^2)}' = \frac{{g^+}'(w^2) 2ww'}{2w'} = {g^+}'(w^2) w = \frac{1}{2}(h(w^2) - h(c_0^2))w. \tag{3.29}$$

The estimate to w'' now follows by boundedness of w, the local Lipschitz continuity of h and inequality (3.25). Writing

$$|w'(z) - w'(y)| = \left|\int_y^z w''(s)\, ds\right| \le \int_y^z C e^{-\sqrt{C_1} s}\, ds = C\left(e^{-\sqrt{C_1} y} - e^{-\sqrt{C_1} z}\right)$$

for $z \ge y$, we obtain the estimate to w' by sending z to infinity. Trivially, estimate (3.28) follows by

$$\int_0^\infty \left| w\left(\frac{x}{\kappa^{1/2}}\right) - u_0(s_0+)\right|\, dx \le \int_0^\infty C \exp\left(-\sqrt{C_1} \frac{x}{\kappa^{1/2}}\right)\, dx = \frac{C}{\sqrt{C_1}} \kappa^{1/2}.$$

□

Remark 3.16.
Note that the assertions of Lemma 3.15 also hold at the endpoints $s_0 = 0$ and $s_0 = 1$, even if the solutions u_κ do not form a boundary layer. The function w is obtained as before, and in case that $u_\kappa(0) = u_0(0)$ or $u_\kappa(1) = u_0(1)$, we formally set $c_\kappa = \infty$ and $w_\kappa(y) = w(\infty) = u_0(0)$ and $w_\kappa(y) = u_0(1)$, respectively. We treat the endpoints of the interval in the same way as the points of jump discontinuity of V_B in order to obtain a unified and meaningful representation. The remainder terms $R_{u_\kappa} = u_\kappa(s_0 + \cdot) - u_0(s_0 + \cdot)\frac{w\left(\frac{\cdot}{\kappa^{1/2}} + c_\kappa\right)}{u_0(s_0+)}$ will be considered in subsequent discussions. As future computations require $R_{u_\kappa}(0) = R_{u_\kappa}(1) = 0$, the procedure is justified and w merely acts as a cut-off function near the endpoints of $(0,1)$.

Corollary 3.17.
Let s_0 be a point of jump discontinuity of V_B and let $[s_0, s_0+L]$ be the maximal interval where V_B is constant. In a layer of characteristic length $C_2\kappa^{1/2}$, it holds

$$\left\| u_\kappa(s_0+\cdot) - u_0(s_0+\cdot)\frac{w\left(\frac{\cdot}{\kappa^{1/2}}+c_\kappa\right)}{u_0(s_0+)} \right\|_{L^\infty(0,C_2\kappa^{1/2})} \leq C\kappa^{1/4}$$

and inside the interval $[s_0, s_0+L]$, we also have

$$\left\| u_\kappa(s_0+\cdot) - u_0(s_0+\cdot)\frac{w\left(\frac{\cdot}{\kappa^{1/2}}+c_\kappa\right)}{u_0(s_0+)} \right\|_{L^\infty(\kappa^{1/4}L,(1-\kappa^{1/4})L)} \leq C\kappa^{1/4}$$

for the function w and the constants c_κ introduced in Lemma 3.15.

Proof. Write $u_0(s_0+x) = u_0(s_0+) + u_0'(\xi)x$. Then

$$\begin{aligned}
&\left| u_\kappa(s_0+x) - u_0(s_0+x)\frac{w\left(\frac{x}{\kappa^{1/2}}+c_\kappa\right)}{u_0(s_0+)} \right| \\
\leq\ & \left| u_\kappa(s_0+x) - w\left(\frac{x}{\kappa^{1/2}}+c_\kappa\right)\right| + \left| x\frac{u_0'(\xi)}{u_0(s_0+)} w\left(\frac{x}{\kappa^{1/2}}+c_\kappa\right)\right| \\
\leq\ & C\kappa^{1/4} + C\kappa^{1/2} \\
\leq\ & C\kappa^{1/4}
\end{aligned}$$

for $x \in [0, C_2\kappa^{1/2}]$ by inequality (3.21) and by a trivial estimate to $x\frac{u_0'(\xi)}{u_0(s_0)}w\left(\frac{x}{\kappa^{1/2}}+c_\kappa\right)$. For $x \in [\kappa^{1/4}L, (1-\kappa^{1/4})L]$, we estimate

$$\begin{aligned}
&\left| u_\kappa(s_0+x) - u_0(s_0+x)\frac{w\left(\frac{x}{\kappa^{1/2}}+c_\kappa\right)}{u_0(s_0+)} \right| \\
\leq\ & |u_\kappa(s_0+x) - u_0(s_0+x)| + \left| \frac{u_0(s_0+x)}{u_0(s_0+)}\left(u_0(s_0+) - w\left(\frac{x}{\kappa^{1/2}}+c_\kappa\right)\right)\right| \\
\leq\ & C\kappa^{1/4} + C\left| u_0(s_0+) - w\left(\frac{x}{\kappa^{1/2}}+c_\kappa\right)\right| \\
\leq\ & C\kappa^{1/4} + C\left| u_0(s_0+) - w\left(\frac{L}{\kappa^{1/4}}+c_\kappa\right)\right| \\
\leq\ & C\kappa^{1/4} + C\exp(-\sqrt{C_1}(L\kappa^{-1/4}+c_\kappa)) \\
\leq\ & C\kappa^{1/4}
\end{aligned}$$

by the exterior convergence result of Lemma 3.8 and inequality (3.25). □

Lemma 3.18.
Let s_0 be a point of jump discontinuity of V_B and let $[s_0, s_0+L]$ be the maximal interval where V_B is constant. In the remaining subinterval $[C_2\kappa^{1/2}, \kappa^{1/4}L]$, the estimate

$$\left\| u_\kappa(s_0+\cdot) - u_0(s_0+\cdot)\frac{w\left(\frac{\cdot}{\kappa^{1/2}}+c_\kappa\right)}{u_0(s_0+)} \right\|_{L^\infty(C_2\kappa^{1/2},\kappa^{1/4}L)} \leq C\kappa^{1/8}$$

holds for the function w and the constants c_κ from Lemma 3.15.

Proof. We first consider the L^∞-norm of

$$d(x) := u_\kappa(s_0 + x) - w\left(\frac{x}{\kappa^{1/2}} + c_\kappa\right) \quad (x \in [C_2\kappa^{1/2}, \kappa^{1/4}L]).$$

There exists $x^* \in [C_2\kappa^{1/2}, \kappa^{1/4}L]$ such that $\|d\|_{L^\infty(C_2\kappa^{1/2},\kappa^{1/4}L)} = \pm d(x^*)$. If $x^* = C_2\kappa^{1/2}$ or $x^* = \kappa^{1/4}L$, then $\|d\|_{L^\infty(C_2\kappa^{1/2},\kappa^{1/4}L)} \leq C\kappa^{1/4}$ is readily shown with the aid of Corollary 3.17. Otherwise, $d(x^*)$ is a local extremum so that

$$0 = d'(x^*) = u_\kappa'(s_0 + x^*) - \kappa^{-1/2}w'\left(\frac{x}{\kappa^{1/2}} + c_\kappa\right).$$

The differential equations for u_κ and w (c.f. Lemma 3.13) now imply for $u^* := u_\kappa(s_0 + x^*)$ and $w^* := w\left(\frac{x^*}{\kappa^{1/2}} + c_\kappa\right)$ that

$$g^+(u^{*2}) + \mathcal{O}(\kappa^{1/4}) = g^+(w^{*2}). \tag{3.30}$$

We recall that w is a monotone function. Without loss of generality, we still assume that w is monotonically increasing so that $w^* \leq c_0 = u_0(s_0+)$. We distinguish the cases $u^* \leq c_0$ and $u^* > c_0$.

Assume $u^* \leq c_0$. Without loss of generality, we also assume $w^* \leq u^*$ so that $g^+(w^{*2}) \geq g^+(u^{*2})$ because g^+ is monotonically decreasing due to

$$g^{+'}(z) = \frac{1}{2}\left(h(z) - h(c_0^2)\right) \leq 0 \quad (0 < z \leq c_0^2).$$

Since $g^{+''}(z) = \frac{1}{2}h'(z) = \frac{1}{2}\frac{p'(z)}{z} > 0$ for $z > 0$, we also know that $g^{+'}$ is monotonically increasing and deduce

$$\begin{aligned}
\mathcal{O}(\kappa^{1/4}) &= g^+(w^{*2}) - g^+(u^{*2}) \\
&\geq g^+(w^{*2} - u^{*2} + c_0^2) - g^+(c_0^2) \\
&= g^+(w^{*2} - u^{*2} + c_0^2).
\end{aligned}$$

Now,

$$\begin{aligned}
g^+(w^{*2} - u^{*2} + c_0^2) &= g^+(c_0^2) + g^{+'}(c_0^2)(w^{*2} - u^{*2}) + \frac{1}{2}g^{+''}(\xi)(w^{*2} - u^{*2})^2 \\
&= \frac{1}{2}g^{+''}(\xi)(w^{*2} - u^{*2})^2
\end{aligned}$$

for some $\xi \in (w^{*2} - u^{*2} + c_0^2, c_0^2)$. In particular, $\xi \in (w^{*2}, c_0^2) \subset (w^2(0), c_0^2)$ because $w^* \geq w_0 > 0$. Since

$$\inf_{\xi \in [w^2(0), c_0^2]} g^{+''}(\xi) = \inf_{\xi \in [w^2(0), c_0^2]} \frac{1}{2}h'(\xi) = \inf_{\xi \in [w^2(0), c_0^2]} \frac{p'(\xi)}{\xi} > 0,$$

we conclude

$$(w^{*2} - u^{*2})^2 \leq C\kappa^{1/4}$$

and then

$$|w^{*2} - u^{*2}| \leq C\kappa^{1/8} \quad \text{as well as} \quad |w^* - u^*| \leq C\kappa^{1/8}.$$

Concerning the case $u^* > c_0$, let

$$x_0 := \min\{x \, : \, u_\kappa(s_0 + x) = c_0\}.$$

Since $u_\kappa(s_0) < c_0$ by inequality (3.22) and $u^* > c_0$, we conclude by continuity that x^* is greater or equal than x_0 and therefore,

$$|u^* - c_0| \leq \|u_\kappa(s_0 + \cdot) - c_0\|_{L^\infty(x_0, \kappa^{1/4}L)}.$$

We estimate the norm on the right hand side. At the left endpoint x_0 of the interval, we have $|u_\kappa(s_0 + x_0) - c_0| = 0$ by definition. Considering the right endpoint $\kappa^{1/4}L$, we find by the mean value theorem and Lemma 3.8

$$\begin{aligned} |u_\kappa(s_0 + \kappa^{1/4}L) - u_0(s_0+)| &\leq |u_\kappa(s_0 + \kappa^{1/4}L) - u_0(s_0 + \kappa^{1/4}L)| + |u_0'(\xi)\kappa^{1/4}L| \\ &\leq C\kappa^{1/4}. \end{aligned}$$

If the norm is attained at an interior point $\widetilde{x}$ of $[x_0, \kappa^{1/4}L]$, we have

$$0 = u_\kappa'(s_0 + \widetilde{x}) = \kappa^{-1/2}\sqrt{g^+(u_\kappa^2(s_0 + \widetilde{x})) + \mathcal{O}(\kappa^{1/4})}$$

so that

$$\begin{aligned} \mathcal{O}(\kappa^{1/4}) &= g^+(u_\kappa^2(s_0 + \widetilde{x})) \\ &= g^+(c_0^2) + g^{+'}(c_0^2)(u_\kappa^2(s_0 + \widetilde{x}) - c_0^2) + \frac{1}{2}g^{+''}(\xi)(u_\kappa^2(s_0 + \widetilde{x}) - c_0^2)^2 \\ &= \frac{1}{2}g^{+''}(\xi)(u_\kappa^2(s_0 + \widetilde{x}) - c_0^2)^2 \\ &\geq C(u_\kappa^2(s_0 + \widetilde{x}) - c_0^2)^2. \end{aligned}$$

Therefore,

$$|u_\kappa^2(s_0 + \widetilde{x}) - c_0^2| \leq C\kappa^{1/8} \quad \text{as well as} \quad |u_\kappa(s_0 + \widetilde{x}) - c_0| \leq C\kappa^{1/8}$$

and altogether

$$\|u_\kappa(s_0 + \cdot) - c_0\|_{L^\infty(x_0, \kappa^{1/4}L)} \leq C\kappa^{1/8},$$

which implies

$$|u^* - c_0| \leq C\kappa^{1/8}.$$

Rewriting the identity (3.30), we obtain

$$\begin{aligned} \mathcal{O}(\kappa^{1/4}) &= g^+(w^{*2}) - g^+(c_0^2) + g^+(c_0^2) - g^+(u^{*2}) \\ &= g^{+'}(c_0^2)(w^{*2} - c_0^2) + \frac{1}{2}g^{+''}(\xi_1)(w^{*2} - c_0^2)^2 \\ &\quad - g^{+'}(c_0^2)(u^{*2} - c_0^2) - \frac{1}{2}g^{+''}(\xi_2)(u^{*2} - c_0^2)^2 \\ &= \frac{1}{2}g^{+''}(\xi_1)(w^{*2} - c_0^2)^2 - \frac{1}{2}g^{+''}(\xi_2)(u^{*2} - c_0^2)^2 \end{aligned}$$

for certain $\xi_1 \in (w^{*2}, c_0^2)$ and $\xi_2 \in (c_0^2, u^{*2})$. It follows

$$(w^{*2} - c_0^2)^2 \leq C(\kappa^{1/4} + (u^{*2} - c_0^2)^2) \leq C\kappa^{1/4}$$

and we conclude

$$|w^{*2} - c_0^2| \leq C\kappa^{1/8} \quad \text{as well as} \quad |w^* - c_0| \leq C\kappa^{1/8}.$$

Trivially, the triangle inequality now yields $|w^* - u^*| \leq C\kappa^{1/8}$. To summarize, we have shown

$$\left\| u_\kappa(s_0 + \cdot) - w\left(\frac{\cdot}{\kappa^{1/2}} + c_\kappa\right) \right\|_{L^\infty(C_2\kappa^{1/2}, \kappa^{1/4}L)} \leq C\kappa^{1/8}.$$

Like in the beginning of the proof of Corollary 3.17, we then obtain

$$\left\| u_\kappa(s_0 + \cdot) - u_0(s_0 + \cdot) \frac{w\left(\frac{\cdot}{\kappa^{1/2}} + c_\kappa\right)}{u_0(s_0+)} \right\|_{L^\infty(C_2\kappa^{1/2}, \kappa^{1/4}L)} \leq C\kappa^{1/8}.$$

□

Corollary 3.19.
Let s_0 be a point of jump discontinuity of V_B and assume that V_B is constant in the intervals $[s_0 - R, s_0)$ and $(s_0, s_0 + R]$ left and right to s_0 for some $R > 0$. Then there exist $\widetilde{w}_\kappa : \mathbb{R} \longrightarrow \mathbb{R}$ such that

$$\left\| u_\kappa(s_0 + \cdot) - u_0(s_0 + \cdot) \frac{\widetilde{w}_\kappa\left(\frac{x}{\kappa^{1/2}}\right)}{\widetilde{c}_0(x)} \right\|_{L^\infty(-R,R)} \leq C\kappa^{1/8},$$

where $\widetilde{c}_0 = \chi_{\{x \leq 0\}} u_0(s_0-) + \chi_{\{x>0\}} u_0(s_0+)$.
Let $s_1 = 0$, $s_{N+1} = 1$ and let $s_2, \ldots, s_N$ be the points of jump discontinuity of V_B. There are functions $W_\kappa : [0,1] \longrightarrow \mathbb{R}$ such that

$$\left\| u_\kappa - u_0 \frac{W_\kappa}{c_0} \right\|_{L^\infty(0,1)} \leq C\kappa^{1/8},$$

where $c_0 : [0,1] \longrightarrow (0,\infty)$ is a positive function which fulfills (if appropriate)

$$c_0(s_i\pm) = u_0(s_i\pm) \quad (i = 1, \ldots, N+1).$$

It holds

$$\left\| \frac{W_\kappa}{c_0} - 1 \right\|_{L^1(0,1)} \leq C\kappa^{1/2}. \tag{3.31}$$

Proof. Fix a point of jump discontinuity s_0 of V_B and let

$$\widetilde{w}_\kappa(y) = \begin{cases} w^+(y + c_\kappa^+), & y \geq 0, \\ w^-(y + c_\kappa^-), & y \leq 0, \end{cases}$$

where w^+ and c_κ^+ coincide with w and c_κ from Lemma 3.15 and w^- and $c_\kappa-$ are constructed analogously in the regime left to s_0 with $u_0(s_0+)$ replaced by $u_0(s_0-)$. For $s_1 = 0$ and $s_{N+1} = 1$, we point to Remark 3.16. Employing Corollary 3.17 and Lemma 3.18, the first inequality follows. Let $(\varphi_i)_{i=1,\ldots,N+1} \subset C^\infty(\mathbb{R}, [0,1])$ be a family of functions satisfying $\sum_{i=1}^{N+1} \varphi_i(x) = 1$, $x \in [0,1]$,

$$\operatorname{supp} \varphi_1 \subset \left[0, \tfrac{2}{3}s_2\right], \quad \varphi_1 = 1 \text{ in } \left[0, \tfrac{1}{3}s_2\right],$$

$\operatorname{supp}\varphi_i \subset \left[s_i - \frac{2}{3}(s_i - s_{i-1}), s_i + \frac{2}{3}(s_{i+1} - s_i)\right], \quad \varphi_i = 1$ in $\left[s_i - \frac{1}{3}(s_i - s_{i-1}), s_i + \frac{1}{3}(s_{i+1} - s_i)\right]$ for $i = 2, \dots, N$ and

$$\operatorname{supp}\varphi_{N+1} \subset \left[1 - \tfrac{2}{3}(1 - s_N), 1\right], \quad \varphi_{N+1} = 1 \text{ on } [1 - \frac{1}{3}(1 - s_N), 1].$$

For $i = 1, \dots, N+1$, let $\widetilde{w}_\kappa^i$ be the functions constructed in the first part of the proof with corresponding $\widetilde{c}_0^i$ and the conventions $\widetilde{c}_0^1 = u_0(0+)$ and $\widetilde{c}_0^{N+1} = u_0(1-)$. The function

$$\widetilde{W}_\kappa(x) := \sum_{i=1}^{N+1} \frac{\widetilde{w}_\kappa^i\left(\frac{x - s_i}{\kappa^{1/2}}\right)}{\widetilde{c}_0^i(x - s_i)}\varphi_i(x)$$

now fulfills $\left\| u_\kappa - u_0 \widetilde{W}_\kappa \right\|_{L^\infty(0,1)} \le C\kappa^{1/8}$ and since $\widetilde{W}_\kappa$ has no zeros, there exists a positive function c_0 such that

$$W_\kappa(x) := \sum_{i=1}^{N+1} \widetilde{w}_\kappa^i\left(\frac{x - s_i}{\kappa^{1/2}}\right)\varphi_i(x) \quad (x \in \mathbb{R})$$

admits $\frac{W_\kappa}{c_0} = \widetilde{W}_\kappa$.

Since $\frac{W_\kappa}{c_0} - 1 = \sum_{i=1}^{N+1}\left(\frac{\widetilde{w}_\kappa^i\left(\frac{x - s_i}{\kappa^{1/2}}\right)}{\widetilde{c}_0^i(x - s_i)} - 1\right)\varphi_i(x)$, estimate (3.31) easily follows from inequality (3.28). □

3.4 Refined remainder estimates

Throughout this section let u_κ, u_0, V_κ, $V_0, \beta_\kappa, \beta_0$ be given as before and let W_κ, c_0 be given as in Corollary 3.19. Moreover, let $s_1 = 0$, $s_{N+1} = 1$ and let $s_2, \dots, s_N$ be the points of jump discontinuity of V_B. We will now derive differential equations for the remainders

$$\begin{aligned} R_{u_\kappa} &:= u_\kappa - \frac{u_0}{c_0} W_\kappa, \\ R_{V_\kappa} &:= V_\kappa - V_0, \\ R_{\beta_\kappa} &:= \beta_\kappa - \beta_0, \\ R_{V_\kappa,\beta_\kappa} &:= R_{V_\kappa} + R_{\beta_\kappa}, \end{aligned}$$

in order to derive improved estimates. Differentiating R_{u_κ} twice, we find

$$\begin{aligned} 2\kappa R_{u_\kappa}'' &= 2\kappa u_\kappa'' - 2\kappa\left(\frac{u_0}{c_0} W_\kappa'' + \frac{1}{W_\kappa}\left(W_\kappa^2\left(\frac{u_0}{c_0}\right)'\right)'\right) \\ &= -\left(F + V_B + V_0 + \beta_0 - h(u_0^2) + (V_\kappa - V_0) + (\beta_\kappa - \beta_0) + (h(u_0^2) - k(u_\kappa^2))\right) u_\kappa \\ &\quad -2\kappa\left(\frac{u_0}{c_0} W_\kappa'' + \frac{1}{W_\kappa}\left(W_\kappa^2\left(\frac{u_0}{c_0}\right)'\right)'\right) \\ &= -R_{V_\kappa,\beta_\kappa} u_\kappa - \left(h(u_0^2) - k(u_\kappa^2)\right) u_\kappa - 2\kappa\frac{u_0}{c_0} W_\kappa'' - 2\kappa\frac{1}{W_\kappa}\left(W_\kappa^2\left(\frac{u_0}{c_0}\right)'\right)'. \end{aligned}$$

Using

$$R''_{u_\kappa} = \frac{1}{W_\kappa}\left(W_\kappa^2\left(\frac{R_{u_\kappa}}{W_\kappa}\right)'\right)' + \frac{R_{u_\kappa}}{W_\kappa}W''_\kappa$$

and

$$-2\kappa W''_\kappa\left(\frac{R_{u_\kappa}}{W_\kappa}+\frac{u_0}{c_0}\right) = -2\kappa W''_\kappa\frac{u_\kappa}{W_\kappa},$$

we can rearrange the equation to

$$\begin{aligned}(3.32)\qquad & \frac{2\kappa}{W_\kappa}\left(W_\kappa^2\left(\frac{R_{u_\kappa}}{W_\kappa}\right)'\right)' \\ = \quad & -R_{V_\kappa,\beta_\kappa}u_\kappa - \left(h(u_0^2)-k(u_\kappa^2)\right)u_\kappa - 2\kappa W''_\kappa\frac{u_\kappa}{W_\kappa} - 2\kappa\frac{1}{W_\kappa}\left(W_\kappa^2\left(\frac{u_0}{c_0}\right)'\right)',\end{aligned}$$

which will be the starting point of the following refined remainder estimates.

Lemma 3.20 (**Refined estimates to the remainders**).
The remainders fulfill

$$(3.33)\qquad \kappa\int_0^1 W_\kappa^2(x)\left(\frac{R_{u_\kappa}}{W_\kappa}\right)'^2(x)\,dx + \frac{\lambda^2}{4}\int_0^1 R'^2_{V_\kappa}(x)\,dx + \int_0^1 R^2_{u_\kappa}(x)\,dx \le C\kappa.$$

In particular,

$$(3.34)\qquad \left\|u_\kappa - \frac{u_0}{c_0}W_\kappa\right\|_{L^2(0,1)} \le C\kappa^{1/2},$$

$$(3.35)\qquad \left\|u_\kappa - \frac{u_0}{c_0}W_\kappa\right\|_{L^\infty(0,1)} \le C\kappa^{1/4}$$

and, by Poincaré's inequality,

$$(3.36)\qquad \|V_\kappa - V_0\|_{H^1(0,1)} \le C\kappa^{1/2}.$$

Proof. Multiplying equation (3.32) by R_{u_κ} and integrating by parts we obtain, thanks to $R_{u_\kappa}(0) = R_{u_\kappa}(1) = 0$,

$$\begin{aligned}& 2\kappa\int_0^1 W_\kappa^2(x)\left(\frac{R_{u_\kappa}}{W_\kappa}\right)'^2(x)\,dx \\ = & \int_0^1 R_{V_\kappa,\beta_\kappa}(x)R_{u_\kappa}(x)u_\kappa(x)\,dx + \int_0^1\left(h(u_0^2(x))-k(u_\kappa^2(x))\right)u_\kappa(x)R_{u_\kappa}(x)\,dx \\ & +2\kappa\int_0^1 W''_\kappa(x)\frac{u_\kappa(x)}{W_\kappa(x)}R_{u_\kappa}(x)\,dx - 2\kappa\int_0^1 W_\kappa(x)\left(\frac{R_{u_\kappa}}{W_\kappa}\right)'(x)\cdot W_\kappa(x)\left(\frac{u_0}{c_0}\right)'(x)\,dx.\end{aligned}$$

Applying Young's inequality in the third integral on the right hand side, the estimate

$$\begin{aligned}
&\kappa \int_0^1 W_\kappa^2(x) \left(\frac{R_{u_\kappa}}{W_\kappa}\right)'^2 (x)\, dx \\
\leq\ & \int_0^1 R_{V_\kappa,\beta_\kappa}(x) R_{u_\kappa}(x) u_\kappa(x)\, dx + \int_0^1 \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\, dx \\
&+2\kappa \int_0^1 W_\kappa''(x) \frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\, dx + \kappa \int_0^1 W_\kappa^2(x) \left(\frac{u_0}{c_0}\right)'^2 (x)\, dx \\
\leq\ & \int_0^1 R_{V_\kappa,\beta_\kappa}(x) R_{u_\kappa}(x) u_\kappa(x)\, dx + \int_0^1 \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\, dx \\
&+2\kappa \int_0^1 W_\kappa''(x) \frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa(x)}\, dx + C\kappa \qquad (3.37)
\end{aligned}$$

follows. We derive an estimate to R_{β_κ}. Write

$$\begin{aligned}
\beta_\kappa - \beta_0 &= -F - V_B - V_\kappa + k(u_\kappa^2) - 2\kappa \frac{u_\kappa''}{u_\kappa} - \left(-F - V_B - V_0 + h(u_0^2)\right) \\
&= -R_{V_\kappa} - \left(h(u_0^2) - k(u_\kappa^2)\right) - 2\kappa \frac{u_\kappa''}{u_\kappa}.
\end{aligned}$$

Let $I = [s_1, s_2]$. We use the notation $I_\kappa := [s_1 + \kappa^{1/4}(s_2 - s_1), s_2 - \kappa^{1/4}(s_2 - s_1)]$ as in Corollary 3.5. For $0 < \kappa < \kappa_0$, we then have

$$\begin{aligned}
|\beta_\kappa - \beta_0| &\leq \frac{2}{s_2 - s_1} \|\beta_\kappa - \beta_0\|_{L^1(I_\kappa)} \\
&\leq C\|R_{V_\kappa}\|_{L^1(I_\kappa)} + C\left\|h(u_\kappa^2) - h(u_0^2)\right\|_{L^1(I_\kappa)} + C\frac{\nu}{\tau}\left\|\ln(u_\kappa^2)\right\|_{L^1(I_\kappa)} + C2\kappa \left\|\frac{u_\kappa''}{u_\kappa}\right\|_{L^1(I_\kappa)} \\
&\leq C\|R_{V_\kappa}\|_{L^2(0,1)} + C\|u_\kappa - u_0\|_{L^1(I_\kappa)} + C\kappa^{1/2} + C2\kappa\|u_\kappa''\|_{L^2(I_\kappa)} \\
&\leq C\|R_{V_\kappa}\|_{L^2(0,1)} + C\left\|R_{u_\kappa} - u_0\left(1 - \frac{W_\kappa}{c_0}\right)\right\|_{L^1(I_\kappa)} + C\kappa^{1/2} \\
&\leq C\|R_{V_\kappa}\|_{L^2(0,1)} + C\|R_{u_\kappa}\|_{L^2(0,1)} + C\left\|1 - \frac{W_\kappa}{c_0}\right\|_{L^1(0,1)} + C\kappa^{1/2} \\
&\leq C\|R_{V_\kappa}\|_{L^2(0,1)} + C\|R_{u_\kappa}\|_{L^2(0,1)} + C\kappa^{1/2},
\end{aligned}$$

where we have used the local Lipschitz continuity of $s \mapsto h(s^2)$ and the uniform boundedness of u_κ for the third inequality, estimate (3.5) for the forth line and (3.31) for the last inequality. Using the Sobolev embedding $H^1(0,1) \hookrightarrow L^\infty(0,1)$ and Poincaré's inequality, we deduce the intermediate result

$$\begin{aligned}
\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)} &\leq \|R_{V_\kappa}\|_{L^\infty(0,1)} + |\beta_\kappa - \beta_0| \\
&\leq C\|R_{V_\kappa}\|_{H^1(0,1)} + C\|R_{V_\kappa}\|_{L^2(0,1)} + C\|R_{u_\kappa}\|_{L^2(0,1)} + C\kappa^{1/2} \\
&\leq C\|R'_{V_\kappa}\|_{L^2(0,1)} + C\|R_{u_\kappa}\|_{L^2(0,1)} + C\kappa^{1/2} \qquad (3.38)
\end{aligned}$$

which will be useful to achieve an estimate for R'_{V_κ}: Integration by parts and the differential equations for V_κ and V_0 yield

$$\begin{aligned}
\frac{\lambda^2}{2}\int_0^1 R'^2_{V_\kappa,\beta_\kappa}(x)\,dx &= \frac{\lambda^2}{2}\int_0^1 R'_{V_\kappa,\beta_\kappa}(x)R'_{V_\kappa}(x)\,dx \\
&= -\frac{1}{2}\int_0^1 R_{V_\kappa,\beta_\kappa}(x)\left(u_\kappa^2(x)-u_0^2(x)\right)\,dx \\
&= -\int_0^1 R_{V_\kappa,\beta_\kappa}(x)R_{u_\kappa}(x)u_\kappa(x)\,dx + \frac{1}{2}\int_0^1 R^2_{u_\kappa}(x)R_{V_\kappa,\beta_\kappa}(x)\,dx \\
&\quad -\frac{1}{2}\int_0^1 u_0^2(x)\left(\frac{W_\kappa^2(x)}{c_0^2(x)}-1\right)R_{V_\kappa,\beta_\kappa}(x)\,dx,
\end{aligned}$$

so that

$$\begin{aligned}
&\frac{\lambda^2}{2}\int_0^1 R'^2_{V_\kappa,\beta_\kappa}(x)\,dx \\
\leq\ & -\int_0^1 R_{V_\kappa,\beta_\kappa}(x)R_{u_\kappa}(x)u_\kappa(x)\,dx + \frac{1}{2}\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)}\int_0^1 R^2_{u_\kappa}(x)\,dx \\
& +C\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)}\left\|\frac{W_\kappa}{c_0}-1\right\|_{L^1(0,1)} \\
\leq\ & -\int_0^1 R_{V_\kappa,\beta_\kappa}(x)R_{u_\kappa}(x)u_\kappa(x)\,dx + \frac{1}{2}\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)}\int_0^1 R^2_{u_\kappa}(x)\,dx \\
& +\frac{\lambda^2}{4}\|R'_{V_\kappa}\|^2_{L^2(0,1)} + \frac{C}{\lambda^2}\left\|\frac{W_\kappa}{c_0}-1\right\|^2_{L^1(0,1)} \\
& +\gamma\|R_{u_\kappa}\|^2_{L^2(0,1)} + \frac{C}{\gamma}\left\|\frac{W_\kappa}{c_0}-1\right\|^2_{L^1(0,1)} + C\kappa^{1/2}\left\|\frac{W_\kappa}{c_0}-1\right\|_{L^1(0,1)} \\
\leq\ & -\int_0^1 R_{V_\kappa,\beta_\kappa}(x)R_{u_\kappa}(x)u_\kappa(x)\,dx + \left(\frac{1}{2}\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)}+\gamma\right)\int_0^1 R^2_{u_\kappa}(x)\,dx \\
& +\frac{\lambda^2}{4}\|R'_{V_\kappa}\|^2_{L^2(0,1)} + C\left(\frac{C}{\lambda^2}+\frac{C}{\gamma}+1\right)\kappa,
\end{aligned}$$

where we have used inequality (3.38) and Young's inequality twice (with some parameter $\gamma > 0$ to be determined later on) for the second inequality. Estimate (3.31) has been used in the last line. Since $R'_{V_\kappa} = R'_{V_\kappa,\beta_\kappa}$, we conclude

$$\begin{aligned}
\frac{\lambda^2}{4}\int_0^1 R'^2_{V_\kappa}(x)\,dx &\leq -\int_0^1 R_{V_\kappa,\beta_\kappa}(x)R_{u_\kappa}(x)u_\kappa(x)\,dx \\
&\quad +\left(\frac{1}{2}\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)}+\gamma\right)\int_0^1 R^2_{u_\kappa}(x)\,dx \\
&\quad +C\left(\frac{C}{\lambda^2}+\frac{C}{\gamma}+1\right)\kappa. \qquad (3.39)
\end{aligned}$$

Combining inequalities (3.37) and (3.39), we find

$$\kappa \int_0^1 W_\kappa^2(x) \left(\frac{R_{u_\kappa}}{W_\kappa}\right)'^2 (x)\, dx + \frac{\lambda^2}{4} \int_0^1 R_{V_\kappa}'^2(x)\, dx - \left(\frac{1}{2}\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)} + \gamma\right) \int_0^1 R_{u_\kappa}^2(x)\, dx$$
$$\leq \int_0^1 \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x) + 2\kappa W_\kappa''(x) \frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\, dx + C\left(\frac{C}{\lambda^2} + \frac{C}{\gamma} + 1\right)\kappa,$$

where we can choose $\gamma > 0$ arbitrarily small and already know $\|R_{V_\kappa,\beta_\kappa}\|_{L^\infty(0,1)} \longrightarrow 0$ as $\kappa \longrightarrow 0$. Therefore, it only remains to show

$$\text{(3.40)} \qquad C_0 \int_0^1 R_{u_\kappa}^2(x)\, dx$$
$$\leq \; - \int_0^1 \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x) + 2\kappa W_\kappa''(x) \frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\, dx + C\kappa$$

for some $C_0 > 0$. We recall that $k(u_\kappa^2) = h(u_\kappa^2) + \frac{\nu}{\tau}\ln(u_\kappa^2) = h(u_\kappa^2) + \mathcal{O}(\kappa^{1/2})$ and that $W_\kappa(x) = w_\kappa^i\left(\frac{x-s_i}{\kappa^{1/2}}\right)$ for $i = 1, \ldots, N$ in $[s_i, s_i + \frac{1}{3}(s_{i+1} - s_i)]$ holds by construction of W_κ in Corollary 3.19. To enhance the readability of the following argumentations, we will formally abbreviate

$$L = s_{i+1} - s_i \quad \text{and} \quad w = w_\kappa^i\left(\frac{\cdot - s_i}{\kappa^{1/2}}\right).$$

With the representation $w_\kappa^{i\,\prime\prime} = \frac{1}{2}\left(h({w_\kappa^i}^2) - h(u_0(s_i+)^2\right) w_\kappa^i$ (c.f. (3.29)), we now calculate

$$- \int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x) + 2\kappa W_\kappa''(x) \frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\, dx$$
$$= \; - \int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_0^2(x)) - h(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x) + 2\kappa w''(x) \frac{u_\kappa(x)}{w(x)} R_{u_\kappa}(x)\, dx$$
$$+ \int_{s_i}^{s_i+\kappa^{1/4}L} \frac{\nu}{\tau} \ln(u_\kappa^2(x)) u_\kappa(x) R_{u_\kappa}(x)\, dx$$
$$= \; - \int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_0^2(x)) - h(u_\kappa^2(x)) + h(w^2(x)) - h(u_0(s_i+)^2)\right) u_\kappa(x) R_{u_\kappa}(x)\, dx$$
$$+ \int_{s_i}^{s_i+\kappa^{1/4}L} \frac{\nu}{\tau} \ln(u_\kappa^2(x)) u_\kappa(x) R_{u_\kappa}(x)\, dx$$

and conclude by Young's inequality, for some parameter $C_1 > 0$ to be determined later, that

$$- \int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x) + 2\kappa W_\kappa''(x) \frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\, dx + \frac{C}{C_1}\kappa$$
$$\geq \; - \int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_0^2(x)) - h(u_\kappa^2(x)) + h(w^2(x)) - h(u_0(s_i+)^2)\right) u_\kappa(x) R_{u_\kappa}(x)\, dx$$
$$- C_1 \int_0^1 R_{u_\kappa}^2(x)\, dx.$$

We estimate the first integral on the right hand side and write

$$
\begin{aligned}
&-\int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_0^2(x)) - h(u_\kappa^2(x)) + h(w^2(x)) - h(u_0(s_i+)^2)\right) u_\kappa(x) R_{u_\kappa}(x)\,dx \\
= &\int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_\kappa^2(x)) - h\left(\frac{u_0^2(x)w^2(x)}{u_0(s_i+)^2}\right)\right) u_\kappa(x) R_{u_\kappa}(x)\,dx \\
&+\int_{s_i}^{s_i+\kappa^{1/4}L} \left(h\left(\frac{u_0^2(x)w^2(x)}{u_0(s_i+)^2}\right) - h(u_0^2(x)) - h(w^2(x)) + h(u_0(s_i+)^2)\right) u_\kappa(x) R_{u_\kappa}(x)\,dx \\
=: &\ I_1 + I_2.
\end{aligned}
$$

As the derivative of $s \mapsto h(s^2)$ is bounded away from zero in the relevant range, the mean value theorem and the uniform lower bound of u_κ imply

$$
I_1 \geq K \int_{s_i}^{s_i+\kappa^{1/4}L} R_{u_\kappa}^2(x)\,dx
$$

for some $K > 0$. Young's inequality and the uniform boundedness of u_κ yield

$$
\begin{aligned}
|I_2| \leq &\ \frac{C}{C_2}\int_{s_i}^{s_i+\kappa^{1/4}L} \left(h\left(\frac{u_0^2(x)w^2(x)}{u_0(s_i+)^2}\right) - h(u_0^2(x)) - h(w^2(x)) + h(u_0(s_i+)^2)\right)^2 dx \\
&+C_2\int_{s_i}^{s_i+\kappa^{1/4}L} R_{u_\kappa}^2(x)\,dx
\end{aligned}
$$

for a parameter $C_2 > 0$ to be chosen later on. We consider the first integral on the right hand side and estimate

$$
\begin{aligned}
&\left|h\left(\frac{u_0^2(x)w^2(x)}{u_0(s_i+)^2}\right) - h(u_0^2(x)) - h(w^2(x)) + h(u_0(s_i+)^2)\right| \\
= &\left|\int_{w^2(x)}^{u_0(s_i+)^2} h'(s)\,ds - \int_{\frac{u_0^2(x)w^2(x)}{u_0(s_i+)^2}}^{u_0^2(x)} h'(s)\,ds\right| \\
= &\left|\int_{w^2(x)}^{u_0(s_i+)^2} \frac{p'(s)}{s}\,ds - \int_{w^2(x)}^{u_0(s_i+)^2} \frac{p'\left(\frac{u_0^2(x)}{u_0(s_i+)^2}s\right)}{s}\,ds\right| \\
\leq &\ C\int_{w^2(x)}^{u_0(s_i+)^2} \left|1 - \frac{u_0^2(x)}{u_0(s_i+)^2}\right| ds \\
\leq &\ C\kappa^{1/4}|u_0(s_i+)^2 - w^2(x)|
\end{aligned}
$$

for $x \in [s_i, s_i + \kappa^{1/4}L]$, because $u_0^2 = u_0(s_i+)^2 + \mathcal{O}(\kappa^{1/4})$ in $[s_i, s_i + \kappa^{1/4}L]$. Therefore,

$$
\begin{aligned}
|I_2| \leq &\ \frac{C}{C_2}\int_{s_i}^{s_i+\kappa^{1/4}L} \kappa^{1/2}|u_0(s_i+)^2 - w^2(x)|^2\,dx + C_2\int_{s_i}^{s_{i+1}+\kappa^{1/4}L} R_{u_\kappa}^2(x)\,dx \\
\leq &\ \frac{C}{C_2}\kappa^{1/2}\|u_0(s_i+)^2 - w^2\|_{L^\infty(s_i,s_i+\kappa^{1/4}L)}\|u_0(s_i+)^2 - w^2\|_{L^1(s_i,s_i+\kappa^{1/4}L)} \\
&+C_2\int_{s_i}^{s_{i+1}+\kappa^{1/4}L} R_{u_\kappa}^2(x)\,dx \\
\leq &\ \frac{C}{C_2}\kappa + C_2\int_{s_i}^{s_{i+1}+\kappa^{1/4}L} R_{u_\kappa}^2(x)\,dx
\end{aligned}
$$

by inequality (3.28). Choosing $C_1, C_2 > 0$ by the condition $C_1 + C_2 \leq \frac{K}{2}$, we obtain the intermediate result

$$\begin{aligned} \frac{K}{2}\int_{s_i}^{s_i+\kappa^{1/4}L} R_{u_\kappa}^2(x)\,dx \ \ &\leq\ \ -\int_{s_i}^{s_i+\kappa^{1/4}L} \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x) \\ &\quad +2\kappa\int_{s_i}^{s_i+\kappa^{1/4}L} W_\kappa''(x)\frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\,dx + C\kappa \end{aligned} \tag{3.41}$$

and similar calculations show

$$\begin{aligned} \frac{K}{2}\int_{s_{i+1}-\kappa^{1/4}L}^{s_{i+1}} R_{u_\kappa}^2(x)\,dx \ \ &\leq\ \ -\int_{s_{i+1}-\kappa^{1/4}L}^{s_{i+1}} \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\,dx \\ &\quad +2\kappa\int_{s_{i+1}-\kappa^{1/4}L}^{s_{i+1}} W_\kappa''(x)\frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\,dx + C\kappa \end{aligned} \tag{3.42}$$

for $i = 1, \ldots, N$. We provide the final estimate for the interior parts of the intervals $[s_i, s_{i+1}]$. For $x \in [s_i + \kappa^{1/4}L, s_{i+1} - \kappa^{1/4}L]$, we know that

$$W_\kappa''(x) = \left(\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 \left(\widetilde{w}_\kappa^i\left(\frac{x-s_i}{\kappa^{1/2}}\right)\varphi_i(x) + \widetilde{w}_\kappa^{i+1}\left(\frac{x-s_{i+1}}{\kappa^{1/2}}\right)\varphi_{i+1}(x)\right)$$

is actually uniformly bounded for $0 < \kappa < \kappa_0$, as the derivatives of $\widetilde{w}_\kappa^i$ and $\widetilde{w}_\kappa^{i+1}$ converge exponentially fast to zero according to inequalities (3.26) and (3.27). Therefore,

$$\left|\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} 2\kappa W_\kappa''(x)\frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\,dx\right| \leq C\kappa.$$

Furthermore, we have

$$\begin{aligned} &-\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\,dx \\ =\ &-\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \left(h(u_0^2(x)) - h(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\,dx \\ &+\frac{\nu}{\tau}\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \ln(u_\kappa^2(x)) u_\kappa(x) R_{u_\kappa}(x)\,dx \end{aligned}$$

and Young's inequality yields

$$\begin{aligned} &-\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\,dx + \frac{C}{C_3}\kappa \\ \geq\ &-\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \left(h(u_0^2(x)) - h(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\,dx - C_3\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} R_{u_\kappa}^2(x)\,dx. \end{aligned}$$

We rewrite the first integral on the right hand side to

$$\begin{aligned}
&-\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \left(h(u_0^2(x)) - h(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\, dx \\
= &\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \left(h(u_\kappa^2(x)) - h\left(u_0^2(x)\frac{W_\kappa^2(x)}{c_0^2(x)}\right)\right) u_\kappa(x) R_{u_\kappa}(x)\, dx \\
&+\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} h'(\xi(x)) \left(u_0^2(x)\frac{W_\kappa^2(x)}{c_0^2(x)} - u_0^2(x)\right) u_\kappa(x) R_{u_\kappa}(x)\, dx \\
=: &\ I_1 + I_2
\end{aligned}$$

with some $\xi(x)$ between $u_0^2(x)$ and $u_0^2(x)\frac{W_\kappa^2(x)}{c_0^2(x)}$ for $x \in [s_i + \kappa^{1/4}L, s_{i+1} - \kappa^{1/4}L]$. Using the mean value theorem and the uniform lower bound of u_κ, we obtain

$$I_1 \geq K \int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} R_{u_\kappa}^2(x)\, dx.$$

For $x \in [s_i + \kappa^{1/4}L, s_{i+1} - \kappa^{1/4}L]$, it holds

$$\begin{aligned}
\left|\frac{W_\kappa(x)}{c_0(x)} - 1\right| &= \left|\left(\frac{\widetilde{w}_\kappa^i\left(\frac{x-s_i}{\kappa^{1/2}}\right)}{\widetilde{c}_0^i(x-s_i)} - 1\right)\varphi_i(x) + \left(\frac{\widetilde{w}_\kappa^{i+1}\left(\frac{x-s_{i+1}}{\kappa^{1/2}}\right)}{\widetilde{c}_0^{i+1}(x-s_{i+1})} - 1\right)\varphi_{i+1}(x)\right| \\
&\leq C\exp\left(-\frac{C}{\kappa^{1/4}}\right)(\varphi_i(x) + \varphi_{i+1}(x)) \\
&\leq C\kappa
\end{aligned}$$

by inequality (3.25). Therefore,

$$|I_2| \leq C\kappa.$$

Choosing $C_3 > 0$ with $C_3 < \frac{K}{2}$ and combining the estimates, we find

$$\begin{aligned}
\frac{K}{2}\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} R_{u_\kappa}^2(x)\, dx \leq &-\int_{s_i+\kappa^{1/4}L}^{s_{i+1}-\kappa^{1/4}L} \left(h(u_0^2(x)) - k(u_\kappa^2(x))\right) u_\kappa(x) R_{u_\kappa}(x)\, dx \\
&+2\kappa \int W_\kappa''(x)\frac{u_\kappa(x)}{W_\kappa(x)} R_{u_\kappa}(x)\, dx + C\kappa.
\end{aligned} \tag{3.43}$$

Summing up inequalities (3.41), (3.42) and (3.43) for $i = 1, \ldots, N$, we obtain inequality (3.40) with $C_0 = \frac{K}{2}$. This completes the proof of estimate (3.33) and we immediately obtain estimates (3.34) and (3.36). Since W_κ is uniformly bounded from above and away from zero, we also derive

$$\left\|\left(\frac{R_{u_\kappa}}{W_\kappa}\right)'\right\|_{L^2(0,1)} \leq C \quad \text{and} \quad \left\|\frac{R_{u_\kappa}}{W_\kappa}\right\|_{L^2(0,1)} \leq C\kappa^{1/2} \quad (0 < \kappa < \kappa_0)$$

from inequality (3.33). The interpolation inequalities A.8 yield $\left\|\frac{R_{u_\kappa}}{W_\kappa}\right\|_{L^\infty(0,1)} \leq C\kappa^{1/4}$. Then we also have $\|R_{u_\kappa}\|_{L^\infty(0,1)} \leq C\kappa^{1/4}$, which corresponds to inequality (3.35). □

Remark 3.21.
It is expected that the rate of convergence $\kappa^{1/2}$ for the asymptotic expansion of u_κ also holds with respect to the L^∞-norm and that this rate is optimal for the zeroth order approximations $\frac{u_0}{c_0}W_\kappa$ and V_0. A rigorous proof of this assertion follows from extending the asymptotic expansions with uniformly bounded functions $u_{1,\kappa}, V_{1,\kappa} \in L^\infty(0,1)$ such that

$$u_\kappa = \frac{u_0}{c_0}W_\kappa + \kappa^{1/2}u_{1,\kappa} + o(\kappa^{1/2}) \quad \textit{and} \quad V_\kappa = V_0 + \kappa^{1/2}V_{1,\kappa} + o(\kappa^{1/2}) \quad (0 < \kappa < \kappa_0).$$

It is supposed that $V_{1,\kappa}$ coincides with a common function V_1 for all $0 < \kappa < \kappa_0$. For any point of jump discontinuity s_0 of V_B, the local representation

$$u_{1,\kappa}(s_0 \pm \cdot) = u_1(s_0 \pm \cdot)Z_{s_0,\pm}\left(\frac{\cdot}{\kappa^{1/2}}\right) \quad (0 < \kappa < \kappa_0)$$

is presumed, where $u_1 \in L^\infty(0,1)$ and $Z_{s_0,+}, Z_{s_1,-}$ are certain functions fulfilling $Z_{s_0,\pm}(0) = 0$ and $Z_{s_0,\pm}(y) \to 1$ exponentially fast for $y \to \pm\infty$.

Chapter 4

Results on the quantum drift-diffusion model of Bian, Chen and Dreher

The last chapter is a direct continuation of the boundary layer analysis for the quasi 1D approximation of the bipolar quantum drift-diffusion model derived in Chapter 1. We present the results of S. Bian, L. Chen and M. Dreher on the zeroth order approximations of the solutions to this model and derive differential equations which yield the first order summands complementing the asymptotic expansions.

4.1 Statement of the problem and known results

In [BCD], the quasi 1D approximation

$$F = V(x) + T_n \ln(n(x)) - \varepsilon^2 \frac{\sqrt{n}''(x)}{\sqrt{n(x)}} \quad (0 < x \leq 1), \tag{4.1}$$

$$-\lambda^2 V''(x) = n(x) - \exp(V(x)/T_p) - C(x) \quad (0 \leq x \leq 1), \tag{4.2}$$

of the stationary bipolar quantum drift-diffusion model is considered for the boundary values

$$n(0) = 0, \quad n(1) = n_B, \quad V'(0) = \beta(V(0) - V_{GS}), \quad V(1) = V_B. \tag{4.3}$$

The quantum quasi Fermi level F is assumed to be a constant function which fulfills

$$F = V_B + T_n \ln(n_B). \tag{4.4}$$

The latter is to express that the solution does not depend on quantum effects at the right boundary of the interval $[0, 1]$. V_B and V_{GS} are real constants, $n_B > 0$ and $\beta \geq 0$. The choice of the boundary value $n(0) = 0$ leads to a singularity in the quantum mechanical Bohm term $\varepsilon^2 \frac{\sqrt{n}''}{\sqrt{n}}$, which yields the formation of a boundary layer depending on the scaled Planck constant $\varepsilon > 0$. The known results on both the solvability and the relationships between n, V and the functions n_*, V_*, which solve the limiting equations

$$F = V_*(x) + T_n \ln(n_*(x)) \quad (0 \leq x \leq 1), \tag{4.5}$$

$$-\lambda^2 V_*''(x) = n_*(x) - \exp(V_*(x)/T_p) - C(x) \quad (0 \leq x \leq 1), \tag{4.6}$$

with boundary values

(4.7) $\quad n_*(0) = \exp((F - V_*(0))/T_n), \quad n_*(1) = n_B, \quad V_*'(0) = \beta(V_*(0) - V_{GS}), \quad V_*(1) = V_B$

are as follows:

Theorem 4.1 (**Zeroth order asymptotic expansion**).
The system of equations (4.1) - (4.4) *has a solution* $(n, V) = (n_\varepsilon, V_\varepsilon) \in C^2([0,1])$ *for any* $\varepsilon > 0$*, which satisfies* $n > 0$ *in* $(0, 1]$ *and enjoys the uniform estimate*

$$\varepsilon^2 \|(\sqrt{n})'\|^2_{L^2(0,1)} + \|V'\|^2_{L^2(0,1)} \le C_0.$$

The system of equations (4.5) - (4.7) *admits a unique solution* $(n_*, V_*) \in C^2([0,1])$*. There exists a unique function* $Z \in C^2([0,\infty))$ *solving the problem*

$$Z''(y) = Z(y)\ln(Z(y)) \ (y > 0), \quad Z(0) = 0, \quad \lim_{y\to\infty} Z(y) = 1,$$

which converges exponentially fast to 1 *and whose derivatives also decay exponentially. The approximations* $n_{(0)}(x) := n_*(x) Z^2\left(\sqrt{2T_n}\frac{x}{\varepsilon}\right)$ *and* $V_{(0)}(x) := V_*(x)$ $(x \in [0,1])$ *fulfill*

$$\|n - n_{(0)}\|_{L^2(0,1)} + \|V - V_{(0)}\|_{W^{1,2}(0,1)} \le C\varepsilon, \tag{4.8}$$

$$\|n - n_{(0)}\|_{L^\infty(0,1)} \le C\varepsilon^{3/4} \tag{4.9}$$

and

$$|n(x) - n_{(0)}(x)| \le C\varepsilon^{3/4} \cdot \frac{x}{\varepsilon} \quad (0 \le x \le \varepsilon) \tag{4.10}$$

for sufficiently small $\varepsilon > 0$.

Proof. We refer to [BCD], Theorem 2.1, Theorem 2.2 and Theorem 2.3. For the properties of Z see [CUA, 3.38 - 3.40]. □

Remark 4.2 (**Notations in the forthcoming analysis**).
The results of Theorem 4.1 were obtained by considering the roots

$$\varrho_\varepsilon := \sqrt{n} = \sqrt{n_\varepsilon}.$$

We introduce the scaling

$$Z_0(y) := Z\left(\sqrt{2T_n} y\right) \quad (y \ge 0)$$

and the additional notations

$$\varrho_0 := \sqrt{n_*}, \quad V_0 := V_*, \quad R_{0,\varrho} := \varrho_\varepsilon - \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right), \quad R_{0,V} := V_\varepsilon - V_0.$$

As seen in the respective proofs, the given estimates also hold with n *replaced by* ϱ_ε *and* $n_{(0)}$ *replaced by* $\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)$*, respectively. Combining inequalities* (4.9) *and* (4.10)*, the useful estimate*

$$\left\| \frac{R_{0,\varrho}}{Z_0\left(\frac{\cdot}{\varepsilon}\right)} \right\|_{L^\infty(0,1)} \le C\varepsilon^{3/4}$$

follows.

4.2 Formal derivation of the first order asymptotic expansion

We now discuss the ansatz

$$\begin{aligned} V_\varepsilon(x) &= V_0(x) + \varepsilon V_1(x) + \mathcal{O}(\varepsilon^{1+\gamma}), \\ \varrho_\varepsilon(x) &= \varrho_0(x) Z_0\left(\tfrac{x}{\varepsilon}\right) + \varepsilon \varrho_{1,\varepsilon}(x) + \mathcal{O}(\varepsilon^{1+\gamma}), \end{aligned}$$

where the zeroth order approximations $V_0(x)$ and $\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)$ are already known from Theorem 4.1. In the following, we will assume that the claimed expansion for ϱ_ε holds for some $\gamma \in (0,1]$ with respect to the L^∞-norm and that $\varrho_{1,\varepsilon}$ has the same form as the zeroth order approximation, that is $\varrho_{1,\varepsilon}(x) = \varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right)$ for some function Z_1 fulfilling $Z_1(0) = 0$ and $Z_1 \longrightarrow 1$ exponentially. We suppose that $\frac{Z_1}{Z_0}$ is continuous on $[0,\infty)$. The remainder term $R_{1,\varrho} := \varrho_\varepsilon - \varrho_{0,\varepsilon} - \varepsilon\varrho_{1,\varepsilon}$ will be neglected frequently in the formal calculations. Based on these assumptions, we will now formally derive relations between ϱ_1, $\varrho_{1,\varepsilon}$ and V_1 which render it possible to determine these functions explicitly. A subsequent discussion confirms that this choice actually complements the asymptotic expansions of ϱ_ε and V_ε.
Let $V_{1,\varepsilon}(x)$ be defined by the identity $V_\varepsilon = V_0 + \varepsilon V_{1,\varepsilon}$. The estimates (4.8) to the zeroth order expansion of V_ε imply that $V_{1,\varepsilon}$ is uniformly bounded both in $W^{1,2}(0,1)$ and $L^\infty(0,1)$. Employing the differential equations (4.2) for V_ε and (4.6) for V_0, we find

$$\begin{aligned} -\lambda^2 \varepsilon V''_{1,\varepsilon}(x) &= \varrho_\varepsilon^2(x) - \varrho_0(x)^2 - \exp\left(\frac{V_\varepsilon(x)}{T_p}\right) + \exp\left(\frac{V_0(x)}{T_p}\right) \\ &= \left(\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right) + \varepsilon\varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right) + R_{1,\varrho}(x)\right)^2 - \varrho_0^2(x) \\ &\quad - \left(\exp\left(\frac{V_0(x) + \varepsilon V_{1,\varepsilon}(x)}{T_p}\right) - \exp\left(\frac{V_0(x)}{T_p}\right)\right) \\ &= \varrho_0^2(x)\left(Z_0^2\left(\frac{x}{\varepsilon}\right) - 1\right) + 2\varepsilon\varrho_0(x)\varrho_1(x) Z_0\left(\frac{x}{\varepsilon}\right) Z_1\left(\frac{x}{\varepsilon}\right) \\ &\quad - \varepsilon \frac{V_{1,\varepsilon}(x)}{T_p} \exp\left(\frac{V_0(x)}{T_p}\right) + \mathcal{O}(\varepsilon^{1+\gamma}). \end{aligned}$$

Therefore, $V_{1,\varepsilon}$ is a solution of the elliptic system

$$(4.11)\qquad \left\{ \begin{aligned} -\left(\lambda^2\partial_x^2 - \tfrac{1}{T_p}\exp\left(\tfrac{V_0}{T_p}\right)\right) V_{1,\varepsilon} &= \tfrac{1}{\varepsilon}\varrho_0^2\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right) - 1\right) \\ &\quad + 2\varrho_0\varrho_1 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) Z_1\left(\tfrac{\cdot}{\varepsilon}\right) + \mathcal{O}(\varepsilon^\gamma), \\ R_1 V_{1,\varepsilon} &= 0, \\ R_2 V_{1,\varepsilon} &= 0 \end{aligned}\right.$$

with the boundary operators

$$R_1 V_{1,\varepsilon} := \beta V_{1,\varepsilon}(0) - V'_{1,\varepsilon}(0) \quad \text{and} \quad R_2 V_{1,\varepsilon} := V_{1,\varepsilon}(1).$$

The boundary value problem is uniquely solvable, because an integration by parts shows

$$\lambda^2 \beta W(0)^2 + \lambda^2 \int_0^1 W'(x)^2\,dx + \frac{1}{T_p}\int_0^1 \exp\left(\frac{V_0(x)}{T_P}\right) W^2(x)\,dx = 0$$

for any solution $W \in W^{1,2}(0,1)$ of the homogeneous equation. This implies $W \equiv 0$ and uniqueness follows from the linearity of the boundary value problem.

We can now show that $V_{1,\varepsilon}$ converges to a limiting function V_1 and that convergence is even given in $L^\infty(0,1)$. To this end, let $G : [0,1] \times [0,1] \longrightarrow \mathbb{R}$ be the Green function to the boundary value problem (4.11), so that

$$V_{1,\varepsilon}(x) = \int_0^1 G(x,s)\frac{\varrho_0^2(s)}{\varepsilon}\left(Z_0^2\left(\frac{s}{\varepsilon}\right) - 1\right)\,ds + 2\int_0^1 G(x,s)\varrho_0(s)\varrho_1(s)Z_0\left(\frac{s}{\varepsilon}\right)Z_1\left(\frac{s}{\varepsilon}\right)\,ds + \mathcal{O}(\varepsilon^\gamma).$$

The derivative of G is bounded on the respective closed triangles $\{(x,y) \in [0,1]^2 \,:\, x \le y\}$ and $\{(x,y) \in [0,1]^2 \,:\, x \ge y\}$. Therefore, G is Lipschitz continuous on $[0,1]^2$ and the constant continuation $\widetilde{G} : [0,1] \times [0,\infty) \longrightarrow \mathbb{R}$ of G is Lipschitz continuous, as well. Because $\widetilde{G}$, ϱ_0 and ϱ_0' are bounded functions, it follows that $(x,y) \mapsto \widetilde{G}(x,y)\varrho_0(y)$, $[0,1] \times [0,\infty) \to \mathbb{R}$, is also Lipschitz continuous with some Lipschitz constant C_L.The uniform convergence of the first integral in the representation of $V_{1,\varepsilon}$ now follows from

$$\begin{aligned}
&\left|\int_0^1 G(x,s)\frac{\varrho_0^2(s)}{\varepsilon}\left(Z_0^2\left(\frac{s}{\varepsilon}\right) - 1\right)\,ds - G(x,0)\varrho_0^2(0)\int_0^\infty Z_0^2(t) - 1\,dt\right| \\
= \;& \left|\int_0^{1/\varepsilon}\left(G(x,t\varepsilon)\varrho_0^2(t\varepsilon) - G(x,0)\varrho_0^2(0)\right)\left(Z_0^2(t) - 1\right)\,dt\right| + \mathcal{O}(e^{-c/\varepsilon}) \\
\le \;& \int_0^\infty \left|\left(\widetilde{G}(x,t\varepsilon)\varrho_0^2(t\varepsilon) - \widetilde{G}(x,0)\varrho_0^2(0)\right)\left(Z_0^2(t) - 1\right)\right| dt + \mathcal{O}(e^{-c/\varepsilon}) \\
\le \;& \varepsilon C_L \int_0^\infty t\left|Z_0^2(t) - 1\right|\,dt + \mathcal{O}(e^{-c/\varepsilon}) \\
\le \;& C\varepsilon,
\end{aligned}$$

where we have used that Z_0 converges exponentially fast to 1.
Concerning the second integral, we find

$$\begin{aligned}
&\left|2\int_0^1 G(x,s)\varrho_0(s)\varrho_1(s)\left(Z_0\left(\frac{s}{\varepsilon}\right)Z_1\left(\frac{s}{\varepsilon}\right) - 1\right)\,ds\right| \\
\le \;& 2\|G\|_{L^\infty((0,1)\times(0,1))}\|\varrho_0\varrho_1\|_{L^\infty(0,1)}\left\|Z_0\left(\frac{\cdot}{\varepsilon}\right)Z_1\left(\frac{\cdot}{\varepsilon}\right) - 1\right\|_{L^1(0,1)} \\
\le \;& C\varepsilon
\end{aligned}$$

thanks to the exponential convergence of Z_0Z_1.
To summarize, we have shown $\|V_{1,\varepsilon} - V_1\|_{L^\infty(0,1)} \le C\varepsilon^\gamma$, where

$$V_1(x) := G(x,0)\varrho_0^2(0)\int_0^\infty \left(Z_0^2(t) - 1\right)\,dt + 2\int_0^1 G(x,s)\varrho_0(s)\varrho_1(s)\,ds \quad (x \in [0,1]). \tag{4.12}$$

Since $G(\cdot,0)$ is a solution of the homogeneous version of the system of equations (4.11),

$$-\lambda^2 V_1'' = -\frac{V_1}{T_p}\exp\left(\frac{V_0}{T_p}\right) + 2\varrho_0\varrho_1 \tag{4.13}$$

holds and V_1 fulfills the second boundary condition $R_2V_1 = 0$. Let φ and ψ be functions solving the homogeneous version of (4.11) satisfying $R_1\varphi = 0$, $R_2\varphi \ne 0$, $R_2\psi = 0$ and $R_1\psi \ne 0$. By Liouville's formula, the corresponding Wronksi determinant $W = \varphi\psi' - \psi\varphi'$ is a constant function. Due to $R_1\varphi = 0$, we find $W = W(0) = -\varphi(0)\left(\beta\psi(0) - \psi'(0)\right)$ and therefore

$$G(x,0) = \frac{\psi(x)}{\lambda^2\left(\beta\psi(0) - \psi'(0)\right)},$$

c.f. [Wa, VI §26 VI] for the representation of the Green function in terms of φ and ψ. This shows $R_1 G(\cdot,0) = \frac{1}{\lambda^2}$ so that

$$R_1 V_1 = \frac{\varrho_0^2(0) \int_0^\infty Z_0^2(t) - 1 \, dt}{\lambda^2}. \tag{4.14}$$

We now consider the differential equation for ϱ_ε to derive equations describing ϱ_1 and Z_1. Using the assumed asymptotic expansions for ϱ_ε and V_ε, the left hand side of the differential equation $\varepsilon^2 \varrho_\varepsilon'' = \left(V_\varepsilon + T_n \ln(\varrho_\varepsilon^2) - F\right) \varrho_\varepsilon$ now reads

$$\begin{aligned}
& \varepsilon^2 \varrho_\varepsilon''(x) \\
= \; & \varepsilon^2 \left(\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right) + \varepsilon \varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right) + R_{1,\varrho}(x)\right)'' \\
= \; & \varepsilon^2 \left(\varrho_0''(x) Z_0\left(\frac{x}{\varepsilon}\right) + \frac{2}{\varepsilon}\varrho_0'(x) Z_0'\left(\frac{x}{\varepsilon}\right) + \frac{1}{\varepsilon^2}\varrho_0(x) Z_0''\left(\frac{x}{\varepsilon}\right)\right) \\
& + \varepsilon^2 \left(\varepsilon \varrho_1''(x) Z_1\left(\frac{x}{\varepsilon}\right) + 2\varrho_1'(x) Z_1'\left(\frac{x}{\varepsilon}\right) + \frac{1}{\varepsilon}\varrho_1(x) Z_1''\left(\frac{x}{\varepsilon}\right)\right) + \varepsilon^2 R_{1,\varrho}''(x),
\end{aligned}$$

whereas the identity $F = V_0 + T_n \ln(\varrho_0^2)$ shows that the right hand side is given by

$$\begin{aligned}
& \left(V_\varepsilon(x) + T_n \ln(\varrho_\varepsilon^2(x)) - F\right) \varrho_\varepsilon(x) \\
= \; & \left(\varepsilon V_{1,\varepsilon}(x) + 2T_n \ln\left(\frac{\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right) + \varepsilon \varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right) + R_{1,\varrho}(x)}{\varrho_0(x)}\right)\right) \\
& \times \left(\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right) + \varepsilon \varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right) + R_{1,\varrho}(x)\right) \\
= \; & \left(\varepsilon V_{1,\varepsilon}(x) + 2T_n \ln\left(Z_0\left(\frac{x}{\varepsilon}\right)\right) + 2T_n \ln\left(1 + \varepsilon \frac{\varrho_1(x)}{\varrho_0(x)} \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} + \frac{R_{1,\varrho}(x)}{\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right)}\right)\right) \\
& \times \left(\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right) + \varepsilon \varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right) + R_{1,\varrho}(x)\right).
\end{aligned}$$

To derive differential equations for ϱ_1 and Z_1 from these identities, we formally extract the summands of order $o(\varepsilon)$ (neglecting $R_{1,\varrho}$ and it's derivatives) and find

$$\varepsilon^2 \varrho_\varepsilon''(x) = \varrho_0(x) Z_0''\left(\frac{x}{\varepsilon}\right) + \varepsilon\left(2\varrho_0'(x) Z_0'\left(\frac{x}{\varepsilon}\right) + \varrho_1(x) Z_1''\left(\frac{x}{\varepsilon}\right)\right) + o(\varepsilon). \tag{4.15}$$

For those $x \in [0,1]$, which admit $\frac{R_{1,\varrho}(x)}{\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right)} = o(\varepsilon)$, a Taylor expansion yields

$$\ln\left(1 + \varepsilon \frac{\varrho_1(x)}{\varrho_0(x)} \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} + \frac{R_{1,\varrho}(x)}{\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right)}\right) = \varepsilon \frac{\varrho_1(x)}{\varrho_0(x)} \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} + o(\varepsilon).$$

In this situation, we have

$$\begin{aligned}
& \left(V_\varepsilon(x) + T_n \ln(\varrho_\varepsilon^2(x)) - F\right) \varrho_\varepsilon(x) \\
= \; & 2T_n \varrho_0(x) \ln\left(Z_0\left(\frac{x}{\varepsilon}\right)\right) Z_0\left(\frac{x}{\varepsilon}\right) \\
& + \varepsilon\left(V_{1,\varepsilon}(x) \varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right) + 2T_n \varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right) + 2T_n \varrho_1(x) \ln\left(Z_0\left(\frac{x}{\varepsilon}\right)\right) Z_1\left(\frac{x}{\varepsilon}\right)\right) \\
& + o(\varepsilon).
\end{aligned}$$

Comparing the terms bearing the power ε^1 with the corresponding terms in equation (4.15), we are led to the discussion of the differential equation

$$\begin{aligned} \varrho_1(x)Z_1''\left(\tfrac{x}{\varepsilon}\right) &= -2\varrho_0'(x)Z_0'\left(\tfrac{x}{\varepsilon}\right)+V_{1,\varepsilon}(x)\varrho_0(x)Z_0\left(\tfrac{x}{\varepsilon}\right)+2T_n\varrho_1(x)Z_1\left(\tfrac{x}{\varepsilon}\right) \\ &\quad +2T_n\varrho_1(x)\ln\left(Z_0\left(\tfrac{x}{\varepsilon}\right)\right)Z_1\left(\tfrac{x}{\varepsilon}\right). \end{aligned} \tag{4.16}$$

Let $x\in[\varepsilon^{1/2},1]$ be fixed. The pointwise limit of equation (4.16) yields the identity

$$\varrho_1(x) = -\frac{V_1(x)\varrho_0(x)}{2T_n} \tag{4.17}$$

as ε tends to zero. Plugging this representation of ϱ_1 into equation (4.13), we finally obtain the elliptic system

$$\begin{cases} -\left(\lambda^2\partial_x^2-\left(\frac{1}{T_p}\exp\left(\frac{V_0}{T_p}\right)+\frac{\varrho_0^2}{T_n}\right)\right)V_1 &= 0, \\ R_1V_1 &= \frac{\varrho_0^2(0)\int_0^\infty Z_0^2(t)-1\,dt}{\lambda^2}, \\ R_2V_1 &= 0. \end{cases} \tag{4.18}$$

It should be mentioned that $V_1(0)\neq 0$, because by the unique solvability of (4.18) equipped with homogeneous Dirichlet boundary values, it follows $V_1\equiv 0$, otherwise. It remains to determine Z_1. Rewriting equation (4.16) in the variable $y=\frac{x}{\varepsilon}\in[0,1]$ and approximating all functions which only depend on x by their value at zero, we find

$$\frac{1}{2T_n}Z_1''(y)=\frac{2\varrho_0'(0)}{V_1(0)\varrho_0(0)}Z_0'(y)-Z_0(y)+Z_1(y)\left(\ln(Z_0(y))+1\right)+\mathcal{O}(\varepsilon^\gamma),$$

where we have also made use of identity (4.17) and $\|V_1-V_{1,\varepsilon}\|_{L^\infty(0,1)}\le C\varepsilon^\gamma$. Dropping the remainder $\mathcal{O}(\varepsilon^\gamma)$, a differential equation for Z_1 is obtained. In the following, we provide the necessary tools for the construction of Z_1.

Lemma 4.3 (A trace theorem for certain weighted Sobolev spaces).
Let $T>0$, $w\in C^1(0,T)$ and assume that $Z:[0,T)\longrightarrow[0,\infty)$ is a continuous and monotonically increasing function with the sole zero $Z(0)=0$. If $\int_0^T|w'(x)Z(x)|\,dx<\infty$, then

$$\lim_{t\searrow 0} w(t)Z(t)=0.$$

Proof. Essentially, the conclusion has been given in [Adams, Lemma 4.57]. Let $\varepsilon>0$ and choose $s\in(0,T/2)$ by the condition $\int_0^s|w'(x)Z(x)|\,dx<\frac{\varepsilon}{3}$. By the assumptions on Z, there exists $\delta\in(0,s)$ such that $Z(\delta)|w(T/2)|<\frac{\varepsilon}{3}$ as well as $\frac{Z(\delta)}{Z(s)}\int_s^{T/2}|w'(x)Z(x)|\,dx<\frac{\varepsilon}{3}$. By the fundamental theorem of calculus, it holds $|w(t)|\le|w(T/2)|+\int_t^{T/2}|w'(x)|\,dx$ for $0<t<\delta$. For t in this range, we conclude by monotonicity of Z that

$$\begin{aligned} Z(t)|w(t)| &\le Z(\delta)|w(T/2)|+Z(t)\int_t^s|w'(x)|\,dx+\frac{Z(\delta)}{Z(s)}Z(s)\int_s^{T/2}|w'(x)|\,dx \\ &\le Z(\delta)|w(T/2)|+\int_t^s|w'(x)Z(x)|\,dx+\frac{Z(\delta)}{Z(s)}\int_s^{T/2}|w'(x)Z(x)|\,dx \\ &< \varepsilon. \end{aligned}$$

□

Lemma 4.4 (**Existence and uniqueness for a singular boundary value problem**). *Let* $Z_0 : [0,\infty) \longrightarrow [0,1)$ *be the solution of the boundary value problem* $\frac{1}{2T_n}Z_0'' = Z_0 \ln(Z_0)$, $Z(0) = 0$, $\lim_{y\to\infty} Z(y) = 1$. *For any* $C_0 \in \mathbb{R}$, *there exists a unique solution* Z_1 *to the singular boundary value problem*

$$\begin{cases} \frac{1}{2T_n}Z_1'' &=& C_0 Z_0' - Z_0 + Z_1(\ln(Z_0)+1), \\ Z_1(0) &=& 0, \\ \lim\limits_{y\to\infty} Z_1(y) &=& 1. \end{cases}$$

More precisely, for certain constants $C, \beta > 0$, *the estimates*

$$|Z_1(y) - 1| \quad \leq \quad Ce^{-\beta y} \tag{4.19}$$

and

$$\left|Z_1'(y)\right| \quad \leq \quad Ce^{-\beta y} \tag{4.20}$$

hold for $y \geq 0$. *In particular,* Z_1 *and* Z_1' *are bounded functions.*

Proof. By a scaling argument we may assume $\frac{1}{2T_n} = 1$. It is meaningful to assume that Z_1 has about the same growth behavior as Z_0 so that the appearing term $Z_1 \ln(Z_0)$ is actually continuous up to zero. We make the ansatz $Z_1 = Z_0(1+w)$ for some bounded, sufficiently smooth function w. Plugging this into the differential equation, we obtain

$$\begin{aligned} Z_0''(1+w) + 2Z_0'w' + Z_0 w'' &= C_0 Z_0' - Z_0 + Z_0(1+w)(\ln(Z_0)+1) \\ &= C_0 Z_0' + Z_0'' + Z_0'' w + Z_0 w \end{aligned}$$

on $(0,\infty)$ thanks to the differential equation for Z_0. This leads to the equation

$$2Z_0'w' + Z_0 w'' = C_0 Z_0' + Z_0 w, \tag{4.21}$$

which can be reshaped to

$$-\left(Z_0^2 w'\right)' + Z_0^2 w = -C_0 Z_0' Z_0. \tag{4.22}$$

In the following, we will introduce a weighted Sobolev space to find a solution w to this equation. Another discussion will show that in fact $w \in W^{2,2}_{loc}(0,\infty)$ so that the formal calculations can be done in reverse order, yielding that $Z_1 = Z_0(1+w)$ is actually a solution. Let

$$L^2_{Z_0^2} := \left\{ u \in L^1_{loc}(0,\infty) \ : \ \|u\|_{L^2_{Z_0^2}} := \left(\int_0^\infty u(x)^2 Z_0^2(x)\, dx \right)^{1/2} < \infty \right\}$$

and

$$H^1_{Z_0^2} := \left\{ u \in L^2_{Z_0^2} \ : \ u' \in L^2_{Z_0^2} \right\}, \quad \|u\|_{H^1_{Z_0^2}} := \|u\|_{L^2_{Z_0^2}} + \|u'\|_{L^2_{Z_0^2}}.$$

Obviously, $L^2_{Z_0^2} = L^2((0,\infty), d\mu)$ for the measure $d\mu = Z_0^2 d\lambda$. Therefore, $H^1_{Z_0^2}$ is a Hilbert space with respect to the scalar product

$$\langle u, v \rangle_{Z_0^2} := \langle u Z_0, v Z_0 \rangle_{L^2(0,\infty)} + \left\langle u' Z_0, v' Z_0 \right\rangle_{L^2(0,\infty)}.$$

By monotonicity of Z_0 and the pointwise bounds $0 \le Z_0 \le 1$, the inequalities

$$\|w\|_{L^2(\varepsilon,\infty)} \le \frac{1}{Z_0(\varepsilon)}\|w\|_{L^2_{Z_0^2}} \quad \text{and} \quad \|w\|_{L^2_{Z_0^2}} \le \|w\|_{L^2(0,\infty)} \tag{4.23}$$

and identical estimates for the respective Sobolev norms follow immediately for $\varepsilon > 0$. The weak formulation of equation (4.22) now reads

$$\langle w, \varphi\rangle_{Z_0^2} = -C_0 \left\langle Z_0', Z_0\varphi\right\rangle_{L^2(0,\infty)} =: F(\varphi) \quad \left(\varphi \in H^1_{Z_0^2}\right). \tag{4.24}$$

Since Z_0' decays exponentially, there holds

$$|F(\varphi)| \le |C_0|\|Z_0\varphi\|_{L^2(0,\infty)}\|Z_0'\|_{L^2(0,\infty)} = C\|\varphi\|_{Z_0^2} \le C\|\varphi\|_{H^1_{Z_0^2}},$$

which shows that F is continuous from $H^1_{Z_0^2}$ to $\mathbb{R}$. By the theorem of Lax-Milgram, or rather by the Riesz representation theorem, there exists a unique $w \in H^1_{Z_0^2}$ such that (4.24) holds for all $\varphi \in H^1_{Z_0^2}$. In particular, (4.22) holds in the sense of $L^1_{loc}(0,\infty)$. We now show that $w \in W^{2,2}_{loc}(0,\infty)$ and that the product rule is valid for the term $(Z_0^2 w')'$. This implies that $Z_1 = Z_0(1+w)$ is a solution to the original problem.
Differentiating the differential equation for Z_0, it follows that Z_0 is a C^∞-function on any fixed interval (a,∞) for $0 < a < \infty$. Since $Z_0 > 0$ on $[a,\infty)$, we conclude that any test function $\psi \in C_c^\infty(a,\infty)$ can be written as $\psi = Z_0^2\varphi$ for some test function $\varphi \in C_c^\infty(a,\infty)$. Therefore,

$$\begin{aligned}\int_a^\infty w'(x)\psi'(x)\,dx &= \int_a^\infty w'(x)\left(Z_0^2(x)\varphi'(x) + (Z_0^2)'(x)\varphi(x)\right)\,dx\\ &= -\int_a^\infty \left(w'(x)Z_0^2(x)\right)'\varphi(x)\,dx + \int_a^\infty w'(x)(Z_0^2)'(x)\varphi(x)\,dx\\ &= -\int_a^\infty \frac{1}{Z_0^2(x)}\left(w'(x)Z_0^2(x)\right)'\psi(x)\,dx + \int_a^\infty \frac{1}{Z_0^2(x)}w'(x)(Z_0^2)'(x)\psi(x)\,dx,\end{aligned}$$

which shows $w'' = \frac{1}{Z_0^2}\left((w'Z_0^2)' - w'(Z_0^2)'\right)$. The norm estimate (4.23) implies $w \in W^{1,2}(a,\infty)$ and we deduce $w'' \in L^2(a,\infty)$ by equality (4.22) so that $w \in W^{2,2}(a,\infty)$.
We prove that Z_1 is continuous on $[0,\infty)$ with $Z_1(0) = 0$. Since $w \in W^{2,2}_{loc}(0,\infty)$, the Sobolev embedding theorem A.6 yields $w \in C^1(0,\infty)$. As

$$\int_0^1 |w'(x)Z_0(x)|\,dx \le \|w'Z_0\|_{L^2(0,1)} \le \|w'\|_{Z_0^2} < \infty,$$

we may employ Lemma 4.3 and deduce $Z_1(0) = Z_0(0) + \lim_{t\searrow 0} w(t)Z_0(t) = 0$. We show that w is bounded in a vicinity of zero: Since

$$Z_1'(y) = Z_1'(1) - \int_y^1 C_0Z_0'(x) - Z_0(x) + Z_0(x)(1+w(x))(\ln(Z_0(x)) + 1)\,dx$$

for $0 < y < 1$, the existence of $\int_0^1 Z_0(x)\ln(Z_0(x))\,dx$ and

$$\int_0^1 Z_0(x)w(x)\ln(Z_0(x))\,dx \le \|Z_0w\|_{L^2(0,1)}\|\ln(Z_0)\|_{L^2(0,1)} = \|w\|_{Z_0^2}\|\ln(Z_0)\|_{L^2(0,1)} < \infty$$

show that Z_1' is bounded and continuous on $[0,1]$. L'Hôpital's rule now yields

$$\lim_{y\to 0} w(y) = \lim_{y\to 0} \frac{Z_1(y)}{Z_0(y)} - 1 = \frac{Z_1'(0)}{Z_0'(0)} - 1.$$

Therefore, w is bounded on $[0,1]$. As $w \in H^1_{Z_0^2} \subset L^\infty(1,\infty)$, we conclude $w \in L^\infty(0,\infty)$. We now confirm that w actually tends exponentially fast to zero. To this end, we remark that $w \in C^\infty(0,\infty)$ follows by rearranging and differentiating equation (4.21). Reshaping this identity once more, we obtain

$$w'' - w = \frac{Z_0'}{Z_0}\left(C_0 - 2w'\right) =: g,$$

which is an ordinary differential equation in $(1,\infty)$ whose right hand side fulfills

$$|g(y)| \le C\exp(-\alpha y) \quad (y > 1),$$

because $|Z_0'(y)| \le C\exp(-\alpha y)$ for some $\alpha \in (0,1)$ and $w \in W^{2,2}(1,\infty) \subset W^{1,\infty}(1,\infty)$. Any real-valued classical solution to this equation is given by

$$w(x) = c_1 e^x + c_2 e^{-x} + \frac{1}{2} e^x \int_1^x e^{-s} g(s)\, ds - \frac{1}{2} e^{-x} \int_1^x e^s g(s)\, ds$$

for certain constants $c_1, c_2 \in \mathbb{R}$. Employing the exponential decay of g, it is easily seen that $\left|c_2 e^{-x} - \frac{1}{2}e^{-x}\int_1^x e^s g(s)\, ds\right| \le Ce^{-\alpha x}$ for $x \ge 1$. Since $w \in W^{1,2}(1,\infty)$, we already know that $w(y)$ tends to zero for $y \to \infty$ (c.f. Lemma A.7). Therefore, the remaining part $e^x\left(c_1 + \frac{1}{2}\int_1^x e^{-s} g(s)\, ds\right)$ also tends to zero for $x \to \infty$. This implies that the factor $c_1 + \frac{1}{2}\int_1^x e^{-s} g(s)\, ds$ necessarily tends to zero as well. We make use of l'Hôpital's rule in order to find

$$\left|\lim_{x\to\infty} \frac{c_1 + \frac{1}{2}\int_1^x e^{-s} g(s)\, ds}{e^{-(1+\alpha/2)x}}\right| = \left|\lim_{x\to\infty} \frac{1}{-2(1+\alpha/2)} g(x) e^{\frac{\alpha}{2}x}\right| \le \lim_{x\to\infty} Ce^{-\frac{\alpha}{2}x} = 0.$$

From this, we deduce that there exists $R > 0$ such that $\left|\frac{c_1 + \frac{1}{2}\int_1^x e^{-s} g(s)\, ds}{e^{-(1+\alpha/2)x}}\right| \le 1$ for $x \ge R$ and therefore, $\left|c_1 + \frac{1}{2}\int_1^x e^{-s} g(s)\, ds\right| \le Ce^{-(1+\alpha/2)x}$ for $x > 1$. To summarize, we have shown that

$$|w(x)| \le Ce^{-\frac{\alpha}{2}x} \quad (x > 1).$$

The convergence result for Z_1 follows. By now, we know that $w'' = \frac{Z_0'}{Z_0}(C_0 - 2w') + w$ decays exponentially and the fundamental theorem of calculus shows that $w'(y)$ also tends exponentially fast to zero as $y \to \infty$, which yields estimate (4.20). □

Remark 4.5 (Properties of the function w).
As the function w, which was introduced in previous lemma, will appear in subsequent calculations, we gather some properties. We have seen $w \in C([0,\infty)) \cap C^\infty(0,\infty)$ in the proof of Lemma 4.4. Moreover, w is bounded. By construction it holds $wZ_0, w'Z_0 \in L^2(0,\infty)$. Since $w \in W^{2,2}(1,\infty)$, we also know $w' \in L^\infty(1,\infty)$. It seems to be unknown whether w' is bounded on $(0,\infty)$. However, $\|w'Z_0\|_{L^\infty(0,\infty)} < \infty$ is still given by boundedness of Z_1', Z_0' and w and the identity $Z_1' = w'Z_0 + (1+w)Z_0'$.

Corollary 4.6.
Let $Z_0 : [0,\infty) \longrightarrow [0,1)$ *be the solution of the boundary value problem* $\frac{1}{2T_n} Z_0'' = Z_0 \ln(Z_0)$, $Z(0) = 0$, $\lim_{y\to\infty} Z(y) = 1$. *For any* $f \in L^2(0,1)$, *the problem*

$$U'' - 2T_n\left(1 + \ln\left(Z_0\right)\right)U = f, \quad U \in W_0^{1,2}(0,1) \cap W^{2,2}(0,1),$$

is uniquely solvable. The corresponding solution operator, $f \mapsto U$, *is continuous with*

$$\|U\|_{W^{2,2}(0,1)} \le C\|f\|_{L^2(0,1)}.$$

Proof. By a scaling argument, we may assume $2T_n = 1$. We mention that any function $U \in W_0^{1,2}$ that solves the equation is automatically an element of $W^{2,2}(0,1)$ because $U \in L^\infty(0,1)$ by the Sobolev embedding theorem and $\ln(Z_0) \in L^2(0,1)$. The latter is easily seen with the substitution rule. Analogously to Lemma 4.4, we define

$$L^2_{Z_0^2} := \left\{ u \in L^1_{loc}(0,1) \ : \ \|u\|_{L^2_{Z_0^2}} := \left(\int_0^1 u(x)^2 Z_0^2(x)\, dx \right)^{1/2} < \infty \right\}$$

and the Hilbert space

$$H^1_{Z_0^2,0} := \left\{ u \in L^2_{Z_0^2} \ : \ u' \in L^2_{Z_0^2},\ u(1) = 0 \right\}$$

endowed with the scalar product $\langle u,v\rangle_{Z_0^2,0} := \langle uZ_0, vZ_0\rangle_{L^2(0,1)} + \langle u'Z_0, v'Z_0\rangle_{L^2(0,1)}$.
Similar to the beginning of the proof of Lemma 4.4, the ansatz $U = VZ_0$ leads to the discussion of the weak formulation

$$\langle V,\varphi\rangle_{Z_0^2,0} = -\langle fZ_0,\varphi\rangle_{L^2(0,1)} \quad (\varphi \in H^1_{Z_0^2,0}).$$

This problem is uniquely solvable by the Riesz representation theorem and following the argumentations of the proof of Lemma 4.4, we can show that this weak formulation is actually equivalent to the original problem via the bijection $U \mapsto \frac{U}{Z_0}$, $W_0^{1,2} \longrightarrow H^1_{Z_0^2,0}$. At this point, the essential property is that

$$\left(\frac{U}{Z_0}\right)' = \frac{U'}{Z_0} - \frac{U}{Z_0}\frac{Z_0'}{Z_0}$$

is indeed an element of $L^2_{Z_0^2}$, because according to l'Hôpital's rule $\frac{U}{Z_0} \in C([0,1])$. Conversely, for any $V \in H^1_{Z_0^2,0}$, it holds that the function $U = VZ_0$ possesses zero boundary values by Lemma 4.3 and by definition of $H^1_{Z_0^2,0}$. The Sobolev embedding theorem A.6 yields

$$\begin{aligned}\|U'' - 2T_n(1+\ln(Z_0))U\|_{L^2(0,1)} &\le \|U\|_{W^{2,2}(0,1)} + 2T_n\|1+\ln(Z_0)\|_{L^2(0,1)}\|U\|_{L^\infty(0,1)} \\ &\le C\|U\|_{W^{2,2}(0,1)}.\end{aligned}$$

Therefore, the linear mapping $U \mapsto U'' - 2T_n(1+\ln(Z_0))U$ is continuous and bijective from $W_0^{1,2}(0,1) \cap W^{2,2}(0,1)$ to $L^2(0,1)$. The claimed continuity of the solution operator follows by the bounded inverse theorem. □

4.3 Estimates to the first order asymptotic expansion

Following the preceding discussions, let V_1 be the solution to the system (4.18) and let ϱ_1 be defined by equality (4.17). Moreover, let Z_1 be the solution to

$$\frac{1}{2T_n} Z_1''(y) = \frac{2\varrho_0'(0)}{V_1(0)\varrho_0(0)} Z_0'(y) - Z_0(y) + Z_1(y)\left(\ln(Z_0(y)) + 1\right) \quad (y > 0) \tag{4.25}$$

with boundary values $Z_1(0) = 0$ and $\lim_{y\to\infty} Z_1(y) = 1$ according to Lemma 4.4.
Let Z_0 and ϱ_0 be defined as in Remark 4.2 and let

$$\begin{aligned} R_{0,V} &:= V_\varepsilon - V_0, \\ R_{1,V} &:= V_\varepsilon - V_0 - \varepsilon V_1, \\ R_{0,\varrho} &:= \varrho_\varepsilon - \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right), \\ R_{1,\varrho} &:= \varrho_\varepsilon - \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) - \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right). \end{aligned}$$

The exponential convergence of Z_0 and Z_1 implies

$$\left\|Z_i\left(\tfrac{\cdot}{\varepsilon}\right) - 1\right\|_{L^p(0,1)} \le C\varepsilon^{1/p} \quad (i = 1,2) \quad \text{and} \quad \left\|Z_0\left(\tfrac{\cdot}{\varepsilon}\right) Z_1\left(\tfrac{\cdot}{\varepsilon}\right) - 1\right\|_{L^p(0,1)} \le C\varepsilon^{1/p}$$

for $1 < p < \infty$. By Theorem 4.1 it holds

$$\|\varrho_\varepsilon - \varrho_0\|_{L^1(0,1)} \le \left\|\varrho_\varepsilon - \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right\|_{L^1(0,1)} + \left\|\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right) - 1\right)\varrho_0\right\|_{L^1(0,1)} \le C\varepsilon.$$

The potentials V_ε and their zeroth order approximation V_0 are solutions to the boundary value problems

$$-\lambda^2 V_\varepsilon'' = \varrho_\varepsilon^2 - \exp\left(\frac{V_\varepsilon}{T_p}\right) - \mathcal{C}, \quad V_\varepsilon'(0) = \beta(V_\varepsilon(0) - V_{GS}), \quad V_\varepsilon(1) = V_B,$$

and

$$-\lambda^2 V_0'' = \varrho_0^2 - \exp\left(\frac{V_0}{T_p}\right) - \mathcal{C}, \quad V_0'(0) = \beta(V_0(0) - V_{GS}), \quad V_0(1) = V_B,$$

respectively. The boundary value problem for V_1 reads as

$$-\lambda^2 V_1'' = -\frac{V_1}{T_p}\exp\left(\frac{V_0}{T_p}\right) + 2\varrho_0\varrho_1, \quad V_1'(0) = \beta V_1(0) - \frac{\varrho_0^2(0)\int_0^\infty Z_0^2(t) - 1\, dt}{\lambda^2}, \quad V_1(1) = 0,$$

c.f. (4.18) and (4.17).

Lemma 4.7 (**L^2-estimates to the first order remainders**).
The first order remainders $R_{1,V}$ and $R_{1,\varrho}$ enjoy the estimates

$$|\lambda|\sqrt{\beta}|R_{1,V}(0)| + |\lambda|\|R_{1,V}'\|_{L^2(0,1)} + \|R_{1,V}\|_{L^2(0,1)} \le C\varepsilon^{3/2} \tag{4.26}$$

and

$$\varepsilon\left\|Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\left(\frac{R_{1,\varrho}}{Z_0\left(\tfrac{\cdot}{\varepsilon}\right)}\right)'\right\|_{L^2(0,1)} + \|R_{1,\varrho}\|_{L^2(0,1)} \le C\varepsilon^{3/2} \tag{4.27}$$

for sufficiently small $\varepsilon > 0$.

Proof. $R_{1,V}$ fulfills the differential equation

$$\begin{aligned}-\lambda^2 R''_{1,V} &= \varrho_\varepsilon^2 - \varrho_0^2 - \left(\exp\left(\frac{V_\varepsilon}{T_p}\right) - \exp\left(\frac{V_0}{T_p}\right)\left(1+\varepsilon\frac{V_1}{T_p}\right)\right) - 2\varepsilon\varrho_0\varrho_1 \\ &= \varrho_\varepsilon^2 - \varrho_0^2 - \left(\exp\left(\frac{V_\varepsilon}{T_p}\right) - \exp\left(\frac{V_0+\varepsilon V_1}{T_p}\right)\right) - 2\varepsilon\varrho_0\varrho_1 + \widetilde{R_V}\end{aligned}$$

where $\left\|\widetilde{R_V}\right\|_{L^\infty(0,1)} \le C\varepsilon^2$ is verified by considering the power series of the exponential functions. Multiplying the equation by $R_{1,V}$ and integrating by parts, the mean value theorem and Young's inequality yield

$$\begin{aligned}&\lambda^2 R'_{1,V}(0)R_{1,V}(0) + \lambda^2\int_0^1 R'^2_{1,V}(x)\,dx + K_1\int_0^1 R^2_{1,V}(x)\,dx \\ \le\; &\int_0^1 \left(\varrho_\varepsilon^2(x) - \varrho_0^2(x) - 2\varepsilon\varrho_0\varrho_1\right) R_{1,V}(x)\,dx + C\varepsilon^4\end{aligned}$$

for some $K_1 > 0$. Using the identity (4.14), the boundary values simplify to

$$\begin{aligned}\lambda^2 R'_{1,V}(0)R_{1,V}(0) &= \lambda^2 R_{1,V}(0)\left(R'_{0,V}(0) - \varepsilon V'_1(0)\right) \\ &= \lambda^2 R_{1,V}(0)\left(\beta R_{0,V}(0) + \frac{\varepsilon\varrho_0^2(0)}{\lambda^2}\left(\int_0^\infty Z_0^2(t)-1\,dt\right) - \varepsilon\beta V_1(0)\right) \\ &= \lambda^2\beta R_{1,V}(0)^2 + \varepsilon\varrho_0^2(0)\left(\int_0^\infty Z_0^2(t)-1\,dt\right)R_{1,V}(0).\end{aligned}$$

A direct calculation shows

$$\begin{aligned}&\frac{1}{2}\left(\varrho_\varepsilon^2 - \varrho_0^2 - 2\varepsilon\varrho_0\varrho_1\right) \\ &= \varrho_\varepsilon R_{1,\varrho} - \frac{1}{2}R^2_{1,\varrho} + \frac{\varrho_0^2}{2}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)-1\right) + \varepsilon\varrho_0\varrho_1\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)Z_1\left(\tfrac{\cdot}{\varepsilon}\right)-1\right) + \frac{\varepsilon^2}{2}\varrho_1^2 Z_1^2\left(\tfrac{\cdot}{\varepsilon}\right)\end{aligned}$$

and the inequality

$$\begin{aligned}&\frac{\lambda^2\beta}{2}R_{1,V}(0)^2 + \frac{\lambda^2}{2}\int_0^1 R'^2_{1,V}(x)\,dx + \frac{K_1}{2}\int_0^1 R^2_{1,V}(x)\,dx \\ \le\; &\int_0^1 \varrho_\varepsilon(x)R_{1,\varrho}(x)R_{1,V}(x)\,dx \\ &+\int_0^1\left(\varepsilon\varrho_0(x)\varrho_1(x)\left(Z_0\left(\tfrac{x}{\varepsilon}\right)Z_1\left(\tfrac{x}{\varepsilon}\right)-1\right) + \frac{\varepsilon^2}{2}\varrho_1^2(x)Z_1^2\left(\tfrac{x}{\varepsilon}\right) - \frac{1}{2}R^2_{1,\varrho}(x)\right)R_{1,V}(x)\,dx \\ &+\int_0^1 \frac{\varrho_0^2(x)}{2}\left(Z_0^2\left(\tfrac{x}{\varepsilon}\right)-1\right)R_{1,V}(x)\,dx - \varepsilon\frac{\varrho_0^2(0)}{2}\left(\int_0^\infty Z_0^2(t)-1\,dt\right)R_{1,V}(0) \\ &+C\varepsilon^4 \\ =:\; & I_1 + I_2 + I_3 + C\varepsilon^4\end{aligned}$$

follows. We estimate the parts of the second integral I_2. By boundedness of ϱ_0 and ϱ_1 and

Young's inequality, it holds

$$\begin{aligned}
&\left|\int_0^1 \varepsilon\varrho_0(x)\varrho_1(x)\left(Z_0\left(\tfrac{x}{\varepsilon}\right)Z_1\left(\tfrac{x}{\varepsilon}\right)-1\right)R_{1,V}(x)\,dx\right| \\
&\le \frac{C}{C_0}\varepsilon^2\int_0^1\left(Z_0\left(\tfrac{x}{\varepsilon}\right)Z_1\left(\tfrac{x}{\varepsilon}\right)-1\right)^2\,dx + C_0\int_0^1 R_{1,V}^2(x)\,dx \\
&= \frac{C}{C_0}\varepsilon^3\int_0^{1/\varepsilon}\left(Z_0(y)Z_1(y)-1\right)^2\,dy + C_0\int_0^1 R_{1,V}^2(x)\,dx \\
&\le \frac{C}{C_0}\varepsilon^3 + C_0\int_0^1 R_{1,V}^2(x)\,dx
\end{aligned}$$

with a constant $C_0 > 0$ to be chosen later on. Again applying Young's inequality, we find

$$\left|\int_0^1 \frac{\varepsilon^2}{2}\varrho_1^2(x)Z_1^2\left(\tfrac{x}{\varepsilon}\right)R_{1,V}(x)\,dx\right| \le \frac{C}{C_0}\varepsilon^4 + C_0\int_0^1 R_{1,V}^2(x)\,dx.$$

Moreover,

$$\left|\int_0^1 \frac{1}{2}R_{1,\varrho}^2(x)R_{1,V}(x)\,dx\right| \le \frac{1}{2}\|R_{1,V}\|_{L^\infty(0,1)}\int_0^1 R_{1,\varrho}^2(x)\,dx.$$

In order to estimate the third integral I_3, we mention that exponential convergence of Z_0 implies

$$\varepsilon\int_0^\infty Z_0^2(t)-1\,dt = \varepsilon\int_0^{1/\varepsilon} Z_0^2(t)-1\,dt + \mathcal{O}(e^{-c/\varepsilon}) = \int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)-1\,dx + \mathcal{O}(e^{-c/\varepsilon})$$

so that

$$\begin{aligned}
|I_3| &= \left|\int_0^1\left(Z_0^2\left(\tfrac{x}{\varepsilon}\right)-1\right)\left(R_{1,V}(x)\frac{\varrho_0^2(x)}{2} - R_{1,V}(0)\frac{\varrho_0^2(0)}{2}\right)\right| + \mathcal{O}(e^{-c/\varepsilon}) \\
&= \left|\int_0^1\left(Z_0^2\left(\tfrac{x}{\varepsilon}\right)-1\right)\int_0^x\left(R_{1,V}\frac{\varrho_0^2}{2}\right)'(s)\,ds\,dx\right| + \mathcal{O}(e^{-c/\varepsilon}) \\
&\le C\left(\left\|R_{1,V}'\varrho_0^2\right\|_{L^\infty(0,1)} + \left\|R_{1,V}\varrho_0^{2'}\right\|_{L^\infty(0,1)}\right)\int_0^1 x\left|Z_0^2\left(\tfrac{x}{\varepsilon}\right)-1\right|\,dx + \mathcal{O}(e^{-c/\varepsilon}) \\
&\le C\varepsilon^2\left(\left\|R_{1,V}'\right\|_{L^\infty(0,1)} + \|R_{1,V}\|_{L^\infty(0,1)}\right) + \mathcal{O}(e^{-c/\varepsilon}).
\end{aligned}$$

Since we already know $\|\varrho_\varepsilon - \varrho_0\|_{L^1(0,1)} \le C\varepsilon$ and $\|R_{1,V}\|_{L^1(0,1)} \le C\varepsilon$, it follows by the differential equation for $R_{1,V}$ that $\|R_{1,V}''\|_{L^1(0,1)} \le C\varepsilon$. Since $\|R_{1,V}'\|_{L^1(0,1)} \le \|R_{1,V}'\|_{L^2(0,1)} \le C\varepsilon$, we have $\|R_{1,V}'\|_{W^{1,1}(0,1)} \le C\varepsilon$. Moreover, $\|R_{1,V}\|_{W^{1,2}(0,1)} \le \|R_{0,V}\|_{W^{1,2}(0,1)} + \|\varepsilon V_1\|_{W^{1,2}(0,1)} \le C\varepsilon$. The Sobolev embedding theorem A.6, applied with the exponents $p = 1$ and $p = 2$, then yields $\|R_{1,V}'\|_{L^\infty(0,1)} + \|R_{1,V}\|_{L^\infty(0,1)} \le C\varepsilon$ and therefore

$$|I_3| \le C\varepsilon^3 + \mathcal{O}(e^{-c/\varepsilon}) \le C\varepsilon^3.$$

Choosing $C_0 > 0$ with $2C_0 < \frac{K_1}{4}$, the estimate

$$\begin{aligned}
&\frac{\lambda^2\beta}{2}R_{1,V}(0)^2 + \frac{\lambda^2}{2}\int_0^1 R_{1,V}'^2(x)\,dx + \frac{K_1}{4}\int_0^1 R_{1,V}^2(x)\,dx \\
&\le \int_0^1 \varrho_\varepsilon(x)R_{1,\varrho}(x)R_{1,V}(x)\,dx + \frac{1}{2}\|R_{1,V}\|_{L^\infty(0,1)}\int_0^1 R_{1,\varrho}^2(x)\,dx + C\varepsilon^3 \qquad (4.28)
\end{aligned}$$

follows. In the following analysis we derive an estimate to $R_{1,\varrho}$ which will complement inequality (4.28). As seen in equality [BCD, 4.19], $R_{0,\varrho}$ fulfills the differential equation

$$\varepsilon^2 R''_{0,\varrho} = 2T_n\varrho_\varepsilon \left(\ln(\varrho_\varepsilon) - \ln\left(\varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right) + 2T_n R_{0,\varrho}\ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right) + \varrho_\varepsilon R_{0,V} - \frac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_0'\right)'$$

so that the logarithmic identities yield

$$\begin{aligned}\varepsilon^2 R''_{1,\varrho} &= 2T_n\varrho_\varepsilon\left[\ln(\varrho_\varepsilon) - \ln\left(\varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right] + 2T_n\varrho_\varepsilon \ln\left(1+\varepsilon\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)\\ &\quad +2T_n R_{0,\varrho}\ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right) + \varrho_\varepsilon R_{0,V} - \frac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_0'\right)'\\ &\quad -\varepsilon\varrho_1 Z_1''\left(\tfrac{\cdot}{\varepsilon}\right) - \frac{\varepsilon^3}{Z_1\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_1^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_1'\right)'.\end{aligned}$$

It should be mentioned that all occuring logarithms are defined for $x > 0$ and sufficiently small ε. This follows from $\varrho_\varepsilon(x) > 0$ for $x > 0$ and, with the bounded function w from Lemma 4.4 that satisfies $Z_1 = Z_0(1+w)$, from

$$\varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right) = Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\left(\varrho_0 + \varepsilon\left(1+w\left(\tfrac{\cdot}{\varepsilon}\right)\right)\varrho_1\right)$$

and

$$1+\varepsilon\frac{\varrho_1}{\varrho_0}\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)} = 1+\varepsilon\frac{\varrho_1}{\varrho_0}\left(1+w\left(\tfrac{\cdot}{\varepsilon}\right)\right),$$

since ϱ_0 is a positive function on $[0,1]$.
Employing the differential equation (4.25) for Z_1 and the identity $\varrho_1 = -\frac{V_1\varrho_0}{2T_n}$, we compute

$$\begin{aligned}-\varepsilon\varrho_1 Z_1''\left(\tfrac{\cdot}{\varepsilon}\right) &= \varepsilon V_1\left(\frac{2\varrho_0'(0)}{V_1(0)\varrho_0(0)}\varrho_0 Z_0'\left(\tfrac{\cdot}{\varepsilon}\right) + R_{0,\varrho} - \varrho_\varepsilon + \varrho_0 Z_1\left(\tfrac{\cdot}{\varepsilon}\right) + \varrho_0 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right)\\ &= \varepsilon V_1\left(\frac{2\varrho_0'(0)}{V_1(0)\varrho_0(0)}\varrho_0 Z_0'\left(\tfrac{\cdot}{\varepsilon}\right) + R_{0,\varrho}\right)\\ &\quad -\varepsilon V_1\varrho_\varepsilon - \varepsilon 2T_n\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right) - \varepsilon 2T_n\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right).\end{aligned}$$

Using this representation and the expansion

$$\ln\left(1+\varepsilon\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right) = \sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left(\varepsilon\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)^n,$$

valid for sufficiently small ε, we arrive at

$$\begin{aligned}\varepsilon^2 R''_{1,\varrho} &= 2T_n\varrho_\varepsilon\left[\ln(\varrho_\varepsilon) - \ln\left(\varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right] + 2T_n R_{1,\varrho}\ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right) + \varrho_\varepsilon R_{1,V}\\ &\quad -\frac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_0'\right)' - \frac{\varepsilon^3}{Z_1\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_1^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_1'\right)' + \varepsilon V_1\left(\frac{2\varrho_0'(0)}{V_1(0)\varrho_0(0)}\varrho_0 Z_0'\left(\tfrac{\cdot}{\varepsilon}\right) + R_{0,\varrho}\right)\\ &\quad +2T_n\left(\varrho_\varepsilon\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{n}\left(\varepsilon\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)^n - \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\right)\\ &= 2T_n\varrho_\varepsilon\left[\ln(\varrho_\varepsilon) - \ln\left(\varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right] + 2T_n R_{1,\varrho}\ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right) + \varrho_\varepsilon R_{1,V}\\ &\quad -\frac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_0'\right)' - \frac{\varepsilon^3}{Z_1\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_1^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_1'\right)' + \varepsilon V_1\left(\frac{2\varrho_0'(0)}{V_1(0)\varrho_0(0)}\varrho_0 Z_0'\left(\tfrac{\cdot}{\varepsilon}\right) + R_{0,\varrho}\right)\\ &\quad +2T_n\left(\varepsilon\varrho_1\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(\frac{\varrho_\varepsilon}{\varrho_0} - Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right) + \varrho_\varepsilon\sum_{n=2}^{\infty}\frac{(-1)^{n+1}}{n}\left(\varepsilon\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)^n\right).\end{aligned}$$

We make use of the identity

$$\varepsilon^2 R''_{1,\varrho} - 2T_n R_{1,\varrho} \ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right) = \frac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\left(\frac{R_{1,\varrho}}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)'\right)'$$

to reshape the equation as follows:

$$\begin{aligned}\frac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\left(\frac{R_{1,\varrho}}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)'\right)' &= 2T_n\varrho_\varepsilon\left[\ln(\varrho_\varepsilon) - \ln\left(\varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right] + \varrho_\varepsilon R_{1,V}\\ &\quad -\tfrac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_0'\right)' + \varepsilon 2\varrho_0'(0)\frac{V_1\varrho_0}{V_1(0)\varrho_0(0)}Z_0'\left(\tfrac{\cdot}{\varepsilon}\right)\\ &\quad +\varepsilon V_1 R_{0,\varrho} + 2T_n\varepsilon\frac{\varrho_1}{\varrho_0}\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}R_{0,\varrho}\\ &\quad -\tfrac{\varepsilon^3}{Z_1\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_1^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_1'\right)' + 2T_n\varrho_\varepsilon\sum_{n=2}^{\infty}\frac{(-1)^{n+1}}{n}\left(\varepsilon\tfrac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)^n.\end{aligned}$$

The definition of ϱ_1 yields

$$\begin{aligned}\frac{\varepsilon^2}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\left(\frac{R_{1,\varrho}}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)'\right)' &= 2T_n\varrho_\varepsilon\left[\ln(\varrho_\varepsilon) - \ln\left(\varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right] + \varrho_\varepsilon R_{1,V}\\ &\quad -2\varepsilon Z_0'\left(\tfrac{\cdot}{\varepsilon}\right)\left(\varrho_0' - \frac{V_1\varrho_0}{V_1(0)\varrho_0(0)}\varrho_0'(0)\right)\\ &\quad +\varepsilon V_1\left(1 - \frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)R_{1,\varrho}\\ &\quad +\widetilde{R_\varrho},\end{aligned} \tag{4.29}$$

where

$$\begin{aligned}\widetilde{R_\varrho} &= -\varepsilon^2 Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_0'' + \varepsilon^2\varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right)V_1\left(1 - \frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right) - \frac{\varepsilon^3}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_1^2\left(\tfrac{\cdot}{\varepsilon}\right)\varrho_1'\right)'\\ &\quad +2T_n\varrho_\varepsilon\sum_{n=2}^{\infty}\frac{(-1)^{n+1}}{n}\left(\varepsilon\tfrac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)^n,\end{aligned} \tag{4.30}$$

with $\|\widetilde{R_\varrho}\|_{L^\infty(0,1)} \leq C\varepsilon^2$. Multiplying equation (4.29) by $R_{1,\varrho}$ and integrating over $(0,1)$ by parts leads to

$$\begin{aligned}
& \varepsilon^2 \int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right) \left(\frac{R_{1,\varrho}(x)}{Z_0\left(\frac{x}{\varepsilon}\right)}\right)^{\prime 2} dx \\
& +2T_n \int_0^1 \varrho_\varepsilon(x) \left[\ln(\varrho_\varepsilon(x)) - \ln\left(\varrho_0(x) Z_0\left(\tfrac{x}{\varepsilon}\right) + \varepsilon \varrho_1(x) Z_1\left(\tfrac{x}{\varepsilon}\right)\right)\right] R_{1,\varrho}(x)\, dx \\
= & -\int_0^1 \varrho_\varepsilon(x) R_{1,\varrho}(x) R_{1,V}(x)\, dx \\
& +\varepsilon \int_0^1 2Z_0'\left(\tfrac{x}{\varepsilon}\right) \left(\varrho_0'(x) - \frac{V_1(x)\varrho_1(x)}{V_1(0)\varrho_1(0)} \varrho_0'(0)\right) R_{1,\varrho}(x)\, dx \\
& -\varepsilon \int_0^1 V_1(x) \left(1 - \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)}\right) R_{1,\varrho}^2(x)\, dx \\
& -\int_0^1 \widetilde{R_\varrho}(x) R_{1,\varrho}(x)\, dx + \mathcal{O}(e^{-c/\varepsilon}),
\end{aligned}$$

where $\mathcal{O}(e^{-c/\varepsilon})$ arises due to the boundary values. We estimate the integrals on both sides. Rewriting the following inequality in the variable $z = \frac{x}{y}$, it is easily seen that for any $\delta > 0$ there exists $K_2 > 0$ such that

$$x\left(\ln(x) - \ln(y)\right)(x-y) \geq \frac{K_2}{2T_n}(x-y)^2$$

for all $x, y > 0$ satisfying $\frac{x}{y} \geq \delta$. For sufficiently small $\varepsilon > 0$

$$\frac{\varrho_\varepsilon}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right) + \varepsilon \varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)} = \frac{\varrho_\varepsilon}{Z_0\left(\frac{\cdot}{\varepsilon}\right)} \cdot \frac{1}{\varrho_0 + \varepsilon\varrho_1(1 + w\left(\frac{\cdot}{\varepsilon}\right))} > \delta$$

actually holds for some $\delta > 0$, because $\frac{1}{\varrho_0 + \varepsilon\varrho_1(1+w(\frac{\cdot}{\varepsilon}))}$ is bounded from below and the same holds for $\frac{\varrho_\varepsilon}{Z_0(\frac{\cdot}{\varepsilon})}$, since $\frac{\varrho_\varepsilon(0)}{Z_0(0)} = \frac{\varrho_\varepsilon'(0)}{\varepsilon^{-1}Z_0'(0)} \geq C > 0$ by l'Hôpital's rule and inequality [BCD, 4.15]. We conclude

$$K_2 \int_0^1 R_{1,\varrho}^2(x)\, dx \leq 2T_n \int_0^1 \varrho_\varepsilon(x) \left[\ln(\varrho_\varepsilon(x)) - \ln\left(\varrho_0(x) Z_0\left(\tfrac{x}{\varepsilon}\right) + \varepsilon\varrho_1(x) Z_1\left(\tfrac{x}{\varepsilon}\right)\right)\right] R_{1,\varrho}(x)\, dx$$

for a certain constant $K_2 > 0$.

We consider the remaining integrals. By Young's inequality and the mean value theorem, we estimate

$$\begin{aligned}
& \left| \varepsilon \int_0^1 2Z_0'\left(\tfrac{x}{\varepsilon}\right) \left(\varrho_0'(x) - \frac{V_1(x)\varrho_1(x)}{V_1(0)\varrho_1(0)}\varrho_0'(0)\right) R_{1,\varrho}(x)\, dx \right| \\
= & \left| \varepsilon \int_0^1 2Z_0'\left(\tfrac{x}{\varepsilon}\right) f(\xi(x)) \cdot x \cdot R_{1,\varrho}(x)\, dx \right| \\
\leq & \ \varepsilon^2 \frac{C}{K_2} \int_0^1 Z_0'\left(\tfrac{x}{\varepsilon}\right)^2 x^2\, dx + \frac{K_2}{8} \int_0^1 R_{1,\varrho}^2(x)\, dx \\
\leq & \ \varepsilon^5 \frac{C}{K_2} \int_0^{1/\varepsilon} Z_0'(y)^2 y^2\, dy + \frac{K_2}{8} \int_0^1 R_{1,\varrho}^2(x)\, dx \\
\leq & \ \frac{C}{K_2}\varepsilon^5 + \frac{K_2}{8} \int_0^1 R_{1,\varrho}^2(x)\, dx.
\end{aligned}$$

with f being a bounded function. For sufficiently small $\varepsilon > 0$, there also holds

$$\left| \varepsilon \int_0^1 V_1(x) \left(1 - \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} \right) R_{1,\varrho}^2(x)\, dx \right| \leq \frac{K_2}{8} \int_0^1 R_{1,\varrho}^2(x)\, dx.$$

Using Young's inequality again, it follows that

$$\left| \int_0^1 \widetilde{R_\varrho}(x) R_{1,\varrho}(x)\, dx \right| \leq \frac{C}{K_2}\varepsilon^4 + \frac{K_2}{8} \int_0^1 R_{1,\varrho}^2(x)\, dx.$$

Altogether, we deduce

$$\begin{aligned} &\varepsilon^2 \int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right) \left(\frac{R_{1,\varrho}(x)}{Z_0\left(\frac{x}{\varepsilon}\right)} \right)'^2 dx + \frac{5}{8} K_2 \int_0^1 R_{1,\varrho}^2(x)\, dx \\ &\leq - \int_0^1 \varrho_\varepsilon(x) R_{1,\varrho}(x) R_{1,V}(x)\, dx + C\varepsilon^4. \end{aligned} \tag{4.31}$$

We already know that $\frac{1}{2}\|R_{1,V}\|_{L^\infty(0,1)} \leq C\varepsilon \leq \frac{K_2}{8}$ is given for sufficiently small $\varepsilon > 0$. Adding inequalities (4.28) and (4.31), we finally infer

$$\begin{aligned} &\frac{\lambda^2\beta}{2} R_{1,V}(0)^2 + \frac{\lambda^2}{2} \int_0^1 R_{1,V}'^2(x)\, dx + \frac{K_1}{4} \int_0^1 R_{1,V}^2(x)\, dx \\ &+\varepsilon^2 \int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right) \left(\frac{R_{1,\varrho}(x)}{Z_0\left(\frac{x}{\varepsilon}\right)} \right)'^2 dx + \frac{K_2}{2} \int_0^1 R_{1,\varrho}^2(x)\, dx \\ &\leq C\varepsilon^3. \end{aligned}$$

□

Lemma 4.8 (Preliminary L^∞-estimates to $R_{1,\varrho}$).
For sufficiently small $\varepsilon > 0$, there holds

$$\|R_{1,\varrho}\|_{L^\infty(0,1)} \leq C\varepsilon. \tag{4.32}$$

Proof. We reconsider identity (4.29). Multiplying this equality by $R_{1,\varrho}$ and integrating by parts, the same estimates as given in Lemma 4.7 yield

$$\begin{aligned} &\frac{\lambda^2\beta}{2} R_{1,V}(0)^2 + \frac{\lambda^2}{2} \int_0^1 R_{1,V}'^2(x)\, dx + \frac{K_1}{4} \int_0^1 R_{1,V}^2(x)\, dx \\ &+\varepsilon^2 \int_0^1 R_{1,\varrho}'(x)^2\, dx + \frac{K_2}{4} \int_0^1 R_{1,\varrho}^2(x)\, dx \\ &\leq C\varepsilon^3 - 2T_n \int_0^1 \ln\left(Z_0\left(\tfrac{x}{\varepsilon}\right)\right) R_{1,\varrho}^2(x)\, dx. \end{aligned}$$

In particular,

$$\begin{aligned} \varepsilon^2 \|R_{1,\varrho}\|_{W^{1,2}(0,1)}^2 &\leq C\varepsilon^3 + C\|R_{1,\varrho}\|_{L^\infty(0,1)}^2 \int_0^1 \left|\ln\left(Z_0\left(\tfrac{x}{\varepsilon}\right)\right)\right|\, dx \\ &\leq C\varepsilon^3 + C\|R_{1,\varrho}\|_{L^\infty(0,1)}^2 \varepsilon \int_0^\infty \left|\ln\left(Z_0(y)\right)\right|\, dy \\ &=: C_0\varepsilon^3 + C_1\varepsilon \|R_{1,\varrho}\|_{L^\infty(0,1)}^2. \end{aligned}$$

The existence of the last integral is easily seen with the aid of the substitution $s = Z_0(y)$ in a vicinity of $y = 0$ and the exponential convergence of Z_0 for large y. Using the interpolation inequalities A.8, we then deduce

$$\begin{aligned}\|R_{1,\varrho}\|_{L^\infty(0,1)} &\leq C\|R_{1,\varrho}\|^{1/2}_{W^{1,2}(0,1)}\|R_{1,\varrho}\|^{1/2}_{L^2(0,1)} \\ &\leq C\left(C_0\varepsilon + \frac{C_1}{\varepsilon}\|R_{1,\varrho}\|^2_{L^\infty(0,1)}\right)^{1/4}\varepsilon^{3/4}.\end{aligned}$$

For any fixed $\varepsilon > 0$, it holds $C_0\varepsilon \leq \frac{C_1}{\varepsilon}\|R_{1,\varrho}\|^2_{L^\infty(0,1)}$ or $\frac{C_1}{\varepsilon}\|R_{1,\varrho}\|^2_{L^\infty(0,1)} \leq C_0\varepsilon$. Both possibilities yield

$$\|R_{1,\varrho}\|_{L^\infty(0,1)} \leq C\varepsilon.$$

□

Lemma 4.9.
The modified remainder $\overline{R}_{1,\varrho} := \frac{R_{1,\varrho}}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}$ *fulfills*

$$\frac{\varepsilon^2}{4}\left\|\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'\right\|^2_{L^2(0,1)} + \frac{T_n}{2}\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^2_{L^2(0,1)} \leq C\varepsilon^3. \tag{4.33}$$

Proof. Abbreviate $\overline{R}_{i,\varrho} := \frac{R_{i,\varrho}}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}$ for $i = 0, 1$ and $\overline{\varrho} := \varrho_0 + \varepsilon\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\varrho_1$ so that $\frac{\varrho_\varepsilon}{Z_0\left(\frac{\cdot}{\varepsilon}\right)} = \overline{\varrho} + \overline{R}_{1,\varrho}$. Since $Z_1 = (1 + w)Z_0$ for the function w in Lemma 4.4, we have $\overline{R}_{1,\varrho} = \overline{R}_{0,\varrho} - \varepsilon\left(1 + w\left(\frac{\cdot}{\varepsilon}\right)\right)\varrho_1$ and then, using results from the proof of [BCD, Theorem 2.2],

$$\overline{R}_{1,\varrho}(1) = \overline{R}_{0,\varrho}(1) = \mathcal{O}(e^{-c/\varepsilon}) \quad \text{and} \quad \overline{R}'_{1,\varrho}(1) = \overline{R}'_{0,\varrho}(1) + \mathcal{O}(\varepsilon) = \mathcal{O}(\varepsilon^{-3/4}),$$

where we have made use of $\varrho_1(1) = 0$ for both equalities. It is easily seen with $R'_{0,\varrho}(0) = \mathcal{O}(\varepsilon^{1/2})$ (compare the proof of [BCD, Theorem 2.2]) and by boundedness of Z'_1 that

$$(Z_0^2\overline{R}'_{1,\varrho})(0) = 0 \quad \text{and} \quad Z_0^2(\tfrac{1}{\varepsilon})\overline{R}'_{1,\varrho}(1) = R'_{1,\varrho}(1) + \mathcal{O}(e^{-c/\varepsilon}).$$

Then, we also have

$$\overline{R}_{1,\varrho}(1)Z_0^2(\tfrac{1}{\varepsilon})\overline{R}'_{1,\varrho}(1) = \mathcal{O}(e^{-c/\varepsilon}) \quad \text{and} \quad \left(\overline{R}_{1,\varrho}Z_0^2\overline{R}'_{1,\varrho}\right)(0) = 0.$$

The right boundary values of $R_{1,V}$ and ϱ_1 vanish by construction, i.e.

$$R_{1,V}(1) = 0 \quad \text{and} \quad \varrho_1(1) = 0.$$

Moreover, $\|\overline{R}_{0,\varrho}\|_{L^\infty(0,1)} \leq C\varepsilon^{3/4}$ (c.f. Remark 4.2) implies the preliminary estimate

$$\|\overline{R}_{1,\varrho}\|_{L^\infty(0,1)} \leq C\varepsilon^{3/4}. \tag{4.34}$$

We multiply equation (4.29) by $M := \frac{1}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'$ and integrate over $(0, 1)$ in order to obtain

$$\varepsilon^2\int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'^2(x)\,dx$$

$$
\begin{aligned}
= \quad & 2T_n \int_0^1 \overline{R}_{1,\varrho}(x) \left(Z_0^2 \left(\tfrac{\cdot}{\varepsilon}\right) \overline{R}'_{1,\varrho} \right)'(x)\, dx \\
& + 2T_n \int_0^1 \Big((\overline{\varrho}(x) + \overline{R}_{1,\varrho}(x)) \ln(\overline{\varrho}(x) + \overline{R}_{1,\varrho}(x)) - \overline{R}_{1,\varrho}(x) - (\overline{\varrho}(x) + \overline{R}_{1,\varrho}(x)) \ln(\overline{\varrho}(x)) \Big) \\
& \qquad \times \left(Z_0^2 \left(\tfrac{\cdot}{\varepsilon}\right) \overline{R}'_{1,\varrho} \right)'(x)\, dx \\
& + \int_0^1 (\overline{\varrho}(x) + \overline{R}_{1,\varrho}(x)) R_{1,V}(x) \left(Z_0^2 \left(\tfrac{\cdot}{\varepsilon}\right) \overline{R}'_{1,\varrho} \right)'(x)\, dx \\
& - \int_0^1 2\varepsilon Z_0' \left(\tfrac{x}{\varepsilon}\right) \left(\varrho_0'(x) - \frac{V_1(x)\varrho_0(x)}{V_1(0)\varrho_0(0)} \varrho_0'(0) \right) M(x)\, dx \\
& + \int_0^1 \varepsilon V_1(x) \left(1 - \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} \right) R_{0,\varrho}(x) M(x)\, dx \\
& - \int_0^1 \varepsilon^2 \varrho_0''(x) \left(Z_0^2 \left(\tfrac{\cdot}{\varepsilon}\right) \overline{R}'_{1,\varrho} \right)'(x)\, dx \\
& - \int_0^1 \frac{\varepsilon^3}{Z_0\left(\frac{x}{\varepsilon}\right)} \left(Z_1^2 \left(\tfrac{\cdot}{\varepsilon}\right) \varrho_1' \right)'(x) M(x)\, dx \\
& + 2T_n \int_0^1 \varrho_\varepsilon(x) \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n} \left(\varepsilon \frac{\varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right)} \right)^n M(x)\, dx.
\end{aligned}
$$

Employing multiple integrations by parts, we compute

$$
\begin{aligned}
& \varepsilon^2 \int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)} \left(Z_0^2 \left(\tfrac{\cdot}{\varepsilon}\right) \overline{R}'_{1,\varrho} \right)'^2 (x)\, dx + 2T_n \int_0^1 Z_0^2 \left(\tfrac{x}{\varepsilon}\right) \overline{R}'_{1,\varrho}(x)^2\, dx \\
= \quad & -2T_n \int_0^1 \left[\overline{\varrho}'(x) \left(\ln\left(1 + \frac{\overline{R}_{1,\varrho}(x)}{\overline{\varrho}(x)} \right) - \frac{\overline{R}_{1,\varrho}(x)}{\overline{\varrho}(x)} \right) + \overline{R}'_{1,\varrho}(x) \ln\left(1 + \frac{\overline{R}_{1,\varrho}(x)}{\overline{\varrho}(x)} \right) \right] \\
& \qquad \times Z_0^2(\tfrac{x}{\varepsilon}) \overline{R}'_{1,\varrho}(x)\, dx \\
& - \int_0^1 Z_0\left(\tfrac{x}{\varepsilon}\right) \left((\overline{\varrho} + \overline{R}_{1,\varrho}) R_{1,V} \right)'(x) Z_0\left(\tfrac{x}{\varepsilon}\right) \overline{R}'_{1,\varrho}(x)\, dx \\
& - \int_0^1 2\varepsilon Z_0' \left(\tfrac{x}{\varepsilon}\right) \left(\varrho_0'(x) - \frac{V_1(x)\varrho_0(x)}{V_1(0)\varrho_0(0)} \varrho_0'(0) \right) M(x)\, dx \\
& + \int_0^1 \varepsilon V_1(x) \left(1 - \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} \right) R_{0,\varrho}(x) M(x)\, dx \\
& - \int_0^1 \varepsilon^2 \varrho_0''(x) \left(Z_0^2 \left(\tfrac{\cdot}{\varepsilon}\right) \overline{R}'_{1,\varrho} \right)'(x)\, dx \\
& - \int_0^1 2\varepsilon^2 \frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} Z_1'\left(\tfrac{x}{\varepsilon}\right) \varrho_1'(x) M(x)\, dx \\
& - \int_0^1 \varepsilon^3 \frac{Z_1^2\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)} \varrho_1''(x) M(x)\, dx \\
& + 2T_n \int_0^1 \varrho_\varepsilon(x) \sum_{n=2}^{\infty} \frac{(-1)^{n+1}}{n} \left(\varepsilon \frac{\varrho_1(x) Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x) Z_0\left(\frac{x}{\varepsilon}\right)} \right)^n M(x)\, dx + \mathcal{O}(e^{-c/\varepsilon}) \\
=: \quad & I_1 + \ldots + I_8 + \mathcal{O}(e^{-c/\varepsilon}),
\end{aligned}
$$

where $\mathcal{O}(e^{-c/\varepsilon})$ arises from to the boundary values.
We estimate the integrals I_1 to I_8. Note that $\overline{\varrho} = \varrho_0 + \varepsilon(1 + w\left(\frac{\cdot}{\varepsilon}\right))\varrho_1$ is bounded away from zero for sufficiently small $\varepsilon > 0$ and that

$$\|Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\overline{\varrho}'\|_{L^\infty(0,1)} \leq C,$$

which follows by boundedness of $Z_0 w'$ as stated in Remark 4.5.
Since $\ln\left(1 + \frac{\overline{R}_{1,\varrho}(x)}{\overline{\varrho}(x)}\right) - \frac{\overline{R}_{1,\varrho}(x)}{\overline{\varrho}(x)} = \sum_{n=2}^\infty \frac{(-1)^{n+1}}{n}\frac{\overline{R}_{1,\varrho}(x)}{\overline{\varrho}(x)}^n = \mathcal{O}(\varepsilon^{3/2})$ and $\ln\left(1 + \frac{\overline{R}_{1,\varrho}(x)}{\overline{\varrho}(x)}\right) = \mathcal{O}(\varepsilon^{3/4})$ by estimate (4.34), we can estimate I_1 by

$$\begin{aligned}
|I_1| &\leq \frac{C_0}{2}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx + \frac{C}{C_0}\varepsilon^3 + C\varepsilon^{3/4}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx \\
&\leq C_0\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx + \frac{C}{C_0}\varepsilon^3,
\end{aligned}$$

where the constant $C_0 > 0$, which will be chosen later on, arises due to Young's inequality. Using $\|R_{1,V}\|_{W^{1,2}(0,1)} \leq C\varepsilon^3$, $\|R_{1,V}\|_{L^\infty(0,1)} \leq C\varepsilon^3$ and the boundedness of $Z_0\left(\frac{\cdot}{\varepsilon}\right)\overline{\varrho}'$, we find

$$\begin{aligned}
|I_2| &\leq \left|\int_0^1 Z_0\overline{\varrho}'(x)R_{1,V}(x)Z_0\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)\,dx\right| + \left|\int_0^1 R_{1,V}(x)Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx\right| \\
&\quad + \left|\int_0^1 R_{1,V}'(x)Z_0\left(\tfrac{x}{\varepsilon}\right)(\overline{\varrho}(x) + \overline{R}_{1,\varrho}(x))Z_0\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)\,dx\right| \\
&\leq \frac{C_0}{3}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx + \frac{C}{C_0}\int_0^1 R_{1,V}^2(x)Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{\varrho}'(x)^2\,dx \\
&\quad + \|R_{1,V}\|_{L^\infty(0,1)}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx \\
&\quad + \frac{C_0}{3}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx + \frac{C}{C_0}\int_0^1 R_{1,V}'^2(x)Z_0^2\left(\tfrac{x}{\varepsilon}\right)\left(\overline{\varrho}(x) + \overline{R}_{1,\varrho}(x)\right)^2\,dx \\
&\leq C_0\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx + \frac{C}{C_0}\varepsilon^3.
\end{aligned}$$

The mean value theorem, Young's inequality and the exponential decay of Z_0' yield

$$\begin{aligned}
|I_3| &\leq \frac{C}{C_1}\int_0^1 Z_0'^2\left(\tfrac{x}{\varepsilon}\right)(f(\xi(x))x)^2\,dx + C_1\varepsilon^2\int_0^1 M^2(x)\,dx \\
&= \frac{C}{C_1}\varepsilon\int_0^{1/\varepsilon} Z_0'(y)^2(f(\xi(\varepsilon y)x)\varepsilon y)^2\,dy + C_1\varepsilon^2\int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx \\
&\leq \frac{C}{C_1}\varepsilon^3 + C_1\varepsilon^2\int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx,
\end{aligned}$$

where f is a bounded function on $[0,1]$ and $C_1 > 0$ is a constant to be chosen later on. We exploit the preliminary estimate $\|R_{0,\varrho}\|_{L^\infty(0,1)} \leq C\varepsilon$ (c.f. inequality (4.32)) and the exponential convergence of Z_0 and Z_1 to find

$$
\begin{aligned}
|I_4| &\leq \frac{C}{C_1}\varepsilon^2 \int_0^1 V_1^2(x)\left(1-\frac{Z_1\left(\frac{x}{\varepsilon}\right)}{Z_0\left(\frac{x}{\varepsilon}\right)}\right)^2 dx + C_1\varepsilon^2 \int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx \\
&= \frac{C}{C_1}\varepsilon^3 \int_0^{1/\varepsilon} V_1^2(\varepsilon y)\left(1-\frac{Z_1(y)}{Z_0(y)}\right)^2 dy + C_1\varepsilon^2 \int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx \\
&\leq \frac{C}{C_1}\varepsilon^3 + C_1\varepsilon^2 \int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx.
\end{aligned}
$$

We integrate I_5 by parts and obtain

$$
\begin{aligned}
|I_5| &\leq \left|\varepsilon^2 \int_0^1 \varrho_0'''(x) Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)\,dx\right| + \varepsilon^2\left|\varrho_0''(1) Z_0^2\left(\frac{1}{\varepsilon}\right)\overline{R}_{1,\varrho}'(1)\right| \\
&\leq \frac{C}{C_0}\varepsilon^4 + C_0\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx + C\varepsilon^2\left|Z_0^2\left(\frac{1}{\varepsilon}\right)\overline{R}_{1,\varrho}'(1)\right|.
\end{aligned}
$$

Young's inequality and the exponential decay of Z_1' yield

$$
\begin{aligned}
|I_6| &\leq \frac{C}{C_1}\int_0^1 \varepsilon^2 \frac{Z_1^2\left(\frac{x}{\varepsilon}\right)}{Z_0^2\left(\frac{x}{\varepsilon}\right)} Z_1'\left(\tfrac{x}{\varepsilon}\right)^2 \varrho_1'(x)^2\,dx + C_1\varepsilon^2\int_0^1 M^2(x)\,dx \\
&= \frac{C}{C_1}\varepsilon^3 \int_0^{1/\varepsilon} \frac{Z_1^2(y)}{Z_0^2(y)} Z_1'(y)^2 \varrho_1'(\varepsilon y)^2\,dy + C_1\varepsilon^2 \int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx \\
&\leq \frac{C}{C_1}\varepsilon^3 + C_1\varepsilon^2 \int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx.
\end{aligned}
$$

Moreover,

$$
|I_7| \leq \frac{C}{C_1}\varepsilon^4 + C_1\varepsilon^2 \int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'^2(x)\,dx.
$$

We rewrite the last integral as

$$
\begin{aligned}
I_8 &= 2T_n\int_0^1 \left(\overline{\varrho}(x)+\overline{R}_{1,\varrho}(x)\right)\left(\ln\left(1+\varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right) - \varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right)\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}_{1,\varrho}'\right)'(x)\,dx \\
&= -2T_n\int_0^1 \left[\left(\overline{\varrho}+\overline{R}_{1,\varrho}\right)\left(\ln\left(1+\varepsilon\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right) - \varepsilon\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)\right]'(x) Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)\,dx \\
&= -2T_n\int_0^1 \overline{\varrho}'(x)\left(\ln\left(1+\varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right) - \varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right) Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)\,dx \\
&\quad -2T_n\int_0^1 \left(\ln\left(1+\varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right) - \varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right) Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\,dx \\
&\quad +2T_n\int_0^1 \left(\overline{\varrho}(x)+\overline{R}_{1,\varrho}(x)\right) L(x) Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)\,dx \\
&=: I_{8,1}+I_{8,2}+I_{8,3},
\end{aligned}
$$

where

$$
L(x) := \varepsilon\left(\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)'(x)\left(\varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right)\left(1+\varepsilon\frac{\varrho_1(x)Z_1\left(\frac{x}{\varepsilon}\right)}{\varrho_0(x)Z_0\left(\frac{x}{\varepsilon}\right)}\right)^{-1} \qquad (x\in[0,1]).
$$

Note that the boundary values in the integration by parts actually vanish thanks to $\varrho_1(1) = 0$. Using $Z_1 = (1+w)Z_0$, we write L as

$$\begin{aligned} L(x) &= \varepsilon^2 \left(\tfrac{\varrho_1}{\varrho_0}\left(1 + w\left(\tfrac{\cdot}{\varepsilon}\right)\right)\right)'(x)K(x) \\ &= \varepsilon^2 \left(\tfrac{\varrho_1}{\varrho_0}\right)'(x)\left(1 + w\left(\tfrac{x}{\varepsilon}\right)\right)K(x) + \varepsilon \tfrac{\varrho_1(x)}{\varrho_0(x)} w'\left(\tfrac{x}{\varepsilon}\right)K(x) \quad (x \in [0,1]) \end{aligned}$$

with the bounded function $K := \left(\frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)\left(1 + \varepsilon \frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)^{-1}$. Using

$$\left\| \ln\left(1 + \varepsilon \frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right) - \varepsilon \frac{\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)} \right\|_{L^\infty(0,1)} \le C\varepsilon^2$$

and the boundedness of $\overline{\varrho}' Z_0\left(\frac{\cdot}{\varepsilon}\right)$, we obtain

$$\begin{aligned} |I_{8,1}| &\le \frac{C}{C_0}\varepsilon^4 \int_0^1 \overline{\varrho}'(x)^2 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\, dx + \frac{C_0}{4}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx \\ &\le \frac{C}{C_0}\varepsilon^4 + \frac{C_0}{4}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx \end{aligned}$$

by Young's inequality. Obviously there holds

$$|I_{8,2}| \le C\varepsilon^2 \int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx \le \frac{C_0}{4}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx$$

for sufficiently small $\varepsilon > 0$. Furthermore,

$$\begin{aligned} |I_{8,3}| &\le \frac{C}{C_0}\varepsilon^4 + \frac{C_0}{4}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx \\ &\quad + \frac{C}{C_0}\varepsilon^2 \int_0^1 \left(\overline{\varrho}(x) + \overline{R}_{1,\varrho}(x)\right)^2 \tfrac{\varrho_1^2(x)}{\varrho_0^2(x)} w'\left(\tfrac{x}{\varepsilon}\right)^2 K^2(x) Z_0^2\left(\tfrac{x}{\varepsilon}\right)\, dx \\ &\quad + \frac{C_0}{4}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx \\ &= \frac{C}{C_0}\varepsilon^4 + \frac{C_0}{2}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx \\ &\quad + \frac{C}{C_0}\varepsilon^3 \int_0^{1/\varepsilon} \left(\overline{\varrho}(\varepsilon y) + \overline{R}_{1,\varrho}(\varepsilon y)\right)^2 \tfrac{\varrho_1^2(\varepsilon y)}{\varrho_0^2(\varepsilon y)} w'(y)^2 K^2(\varepsilon y) Z_0^2(y)\, dy \\ &\le \frac{C}{C_0}\varepsilon^4 + \frac{C_0}{2}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx + \frac{C}{C_0}\varepsilon^3 \int_0^\infty w'(y)^2 Z_0^2(y)\, dy \\ &\le \frac{C}{C_0}\varepsilon^3 + \frac{C_0}{2}\int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx, \end{aligned}$$

because by construction $w'^2 Z_0^2$ is integrable on $(0,\infty)$, c.f. Remark 4.5. We conclude

$$|I_8| \le \frac{C}{C_0}\varepsilon^3 + C_0 \int_0^1 Z_0^2\left(\tfrac{x}{\varepsilon}\right)\overline{R}_{1,\varrho}'(x)^2\, dx.$$

Choosing $C_0 = \frac{T_n}{4}$ and $C_1 = \frac{1}{8}$, we obtain the intermediate result

$$\frac{\varepsilon^2}{2}\int_0^1 \frac{1}{Z_0^2\left(\frac{x}{\varepsilon}\right)}\left(Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'^2(x)\,dx + T_n\int_0^1 Z_0^2\left(\frac{x}{\varepsilon}\right)\overline{R}'_{1,\varrho}(x)^2\,dx \le C\varepsilon^3 + C\varepsilon^2\left|Z_0^2\left(\frac{1}{\varepsilon}\right)\overline{R}'_{1,\varrho}(1)\right|.$$

We need to handle the last summand on the right hand side. Since $0 \le Z_0 < 1$, we can drop the coefficient $\frac{1}{Z_0^2}$ in the first integral and replace Z_0^2 by Z_0^4 in the second integral to find

$$\begin{aligned}
&\frac{\varepsilon^2}{2}\left\|\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'\right\|^2_{L^2(0,1)} + T_n\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^2_{L^2(0,1)}\\
&\le C\varepsilon^3 + C\varepsilon^2\left|Z_0^2\left(\tfrac{1}{\varepsilon}\right)\overline{R}'_{1,\varrho}(1)\right|\\
&\le C\varepsilon^3 + C\varepsilon^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|_{L^\infty(0,1)}.
\end{aligned}$$

The interpolation inequalities A.8 and Young's inequality show

$$\begin{aligned}
C\varepsilon^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|_{L^\infty(0,1)} &\le C\varepsilon^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^{1/2}_{L^2(0,1)}\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^{1/2}_{W^{1,2}(0,1)}\\
&\le C\varepsilon^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|_{L^2(0,1)}\\
&\quad + C\varepsilon^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^{1/2}_{L^2(0,1)}\left\|\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'\right\|^{1/2}_{L^2(0,1)}\\
&\le C\varepsilon^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|_{L^2(0,1)} + \frac{C}{C_2}\varepsilon^3\\
&\quad + C_2^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^2_{L^2(0,1)} + \frac{\varepsilon^2}{4}\left\|\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'\right\|^2_{L^2(0,1)}\\
&\le \frac{C}{C_2}\varepsilon^4 + C_2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^2_{L^2(0,1)} + \frac{C}{C_2}\varepsilon^3\\
&\quad + C_2^2\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^2_{L^2(0,1)} + \frac{\varepsilon^2}{4}\left\|\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'\right\|^2_{L^2(0,1)},
\end{aligned}$$

where we choose $C_2 > 0$ by the condition $C_2 + C_2^2 = \frac{T_n}{2}$ to finally achieve

$$\frac{\varepsilon^2}{4}\left\|\left(Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right)'\right\|^2_{L^2(0,1)} + \frac{T_n}{2}\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|^2_{L^2(0,1)} \le C\varepsilon^3.$$

□

Corollary 4.10 (**Refined estimates to the remainders outside the boundary layer**). *The estimates*

(4.35) $$\left\|Z_0^2\left(\tfrac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho}\right\|_{L^\infty(0,1)} \le C\varepsilon,$$

(4.36) $$\left\|\overline{R}'_{1,\varrho}\right\|_{L^2(\varepsilon,1)} \le C\varepsilon^{3/2},$$

(4.37) $$\|R_{1,\varrho}\|_{L^\infty(\varepsilon,1)} \le C\varepsilon^{3/2},$$

(4.38) $$\|R'_{1,\varrho}\|_{L^2(\varepsilon,1)} \le C\varepsilon,$$

(4.39) $$\|R'_{1,\varrho}\|_{L^\infty(\varepsilon,1)} \le C\varepsilon^{1/2},$$

hold true.

Proof. With the aid of the interpolation inequalities (c.f. Lemma A.8), the first estimate follows from inequality (4.33). For $x \in [\varepsilon, 1]$, it holds $0 < Z_0(1) \leq Z_0\left(\frac{x}{\varepsilon}\right) < 1$. Then the second estimate is also obtained from (4.33). By inequality (4.27), we also deduce $\|\overline{R}_{1,\varrho}\|_{L^2(\varepsilon,1)} \leq C\varepsilon^{3/2}$ and interpolating this estimate with inequality (4.36) leads to estimate (4.37). The identity $Z_0\left(\frac{\cdot}{\varepsilon}\right) R'_{1,\varrho} = Z_0^2\left(\frac{\cdot}{\varepsilon}\right)\overline{R}'_{1,\varrho} + \frac{1}{\varepsilon}R_{1,\varrho}Z'_0\left(\frac{\cdot}{\varepsilon}\right)$ can be used to derive inequalities (4.38) and (4.39), because $\|\frac{1}{\varepsilon}R_{1,\varrho}Z'_0\left(\frac{\cdot}{\varepsilon}\right)\|_{L^\infty(\varepsilon,1)} \leq C\varepsilon^{1/2}$ by inequality (4.37) and

$$\begin{aligned}\left\|\frac{1}{\varepsilon}R_{1,\varrho}Z'_0\left(\tfrac{\cdot}{\varepsilon}\right)\right\|_{L^2(\varepsilon,1)} &= \frac{1}{\varepsilon}\left(\varepsilon\int_1^{1/\varepsilon} R_{1,\varrho}^2(\varepsilon y)Z'_0(y)^2\,dy\right)^{1/2} \\ &\leq \frac{1}{\varepsilon}\left(C\varepsilon^4\int_1^\infty Z'_0(y)^2\,dy\right)^{1/2} = C\varepsilon,\end{aligned}$$

where we have also made use of estimate (4.37). □

Lemma 4.11 (**Refined estimates to the remainders inside the boundary layer**). *Inside the boundary layer of characteristic length ε, the estimates*

$$\begin{aligned}\|R_{1,\varrho}\|_{L^2(0,\varepsilon)} &\leq C\varepsilon^2, \\ \|R'_{1,\varrho}\|_{L^2(0,\varepsilon)} &\leq C\varepsilon, \\ \|R''_{1,\varrho}\|_{L^2(0,\varepsilon)} &\leq C,\end{aligned}$$

and

$$\begin{aligned}\|R_{1,\varrho}\|_{L^\infty(0,\varepsilon)} &\leq C\varepsilon^{3/2}, \\ \|R'_{1,\varrho}\|_{L^\infty(0,\varepsilon)} &\leq C\varepsilon^{1/2},\end{aligned}$$

hold.

Proof. Since $\varrho_\varepsilon = R_{1,\varrho} + \varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)$, the differential equation $\varepsilon^2\varrho''_\varepsilon = \left(V_\varepsilon + T_n\ln(\varrho_\varepsilon^2) - F\right)\varrho_\varepsilon$ turns into

$$\begin{aligned}&\varepsilon^2 R''_{1,\varrho} + 2\varepsilon\varrho'_0 Z'_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varrho_0 Z''_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z''_1\left(\tfrac{\cdot}{\varepsilon}\right) \\ =\ &\left(R_{1,V} + \varepsilon V_1 + 2T_n\ln\left(Z_0\left(\frac{\cdot}{\varepsilon}\right)\right) + 2T_n\ln\left(1 + \varepsilon\frac{\varrho_1}{\varrho_0}\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)} + \frac{R_{1,\varrho}}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)\right) \\ &\times\left(\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right) + \varepsilon\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right) + R_{1,\varrho}\right) + \mathcal{O}(\varepsilon^2),\end{aligned}$$

compare the computations in the formal derivation of the first order asymptotic expansion, where $\varepsilon V_{1,\varepsilon} = R_{1,V} + \varepsilon V_1$. By definition of $\varrho_1 = -\frac{V_1\varrho_0}{2T_n}$ and using the differential equation (4.25) for Z_1, it holds

$$\varepsilon\varrho_1 Z''_1\left(\tfrac{\cdot}{\varepsilon}\right) = -\varepsilon V_1\varrho_0\left(\frac{2\varrho'_0(0)}{V_1(0)\varrho_0(0)}Z'_0\left(\tfrac{\cdot}{\varepsilon}\right) - Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + Z_1\left(\tfrac{\cdot}{\varepsilon}\right)\left(\ln\left(Z_0\left(\tfrac{\cdot}{\varepsilon}\right)\right) + 1\right)\right).$$

Using this identity as well as $Z_0'' = 2T_n Z_0 \ln(Z_0)$ and

$$\begin{aligned} & \ln\left(1+\varepsilon\frac{\varrho_1}{\varrho_0}\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}+\frac{R_{1,\varrho}}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right) \\ = \; & \varepsilon\frac{\varrho_1}{\varrho_0}\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}+\frac{R_{1,\varrho}}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)} \\ & +\sum_{n=2}^{\infty}\frac{(-1)^{n+1}}{n}\left(\varepsilon\frac{\varrho_1}{\varrho_0}\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}+\frac{R_{1,\varrho}}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right)^n \\ = \; & \varepsilon\frac{\varrho_1}{\varrho_0}\frac{Z_1\left(\frac{\cdot}{\varepsilon}\right)}{Z_0\left(\frac{\cdot}{\varepsilon}\right)}+\frac{R_{1,\varrho}}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}+\mathcal{O}(\varepsilon^{3/2}) \end{aligned}$$

(c.f. estimate (4.34))), we obtain the differential equation

$$\varepsilon^2 R_{1,\varrho}'' + 2\varepsilon Z_0'\left(\frac{\cdot}{\varepsilon}\right)\left(\varrho_0' - \frac{V_1\varrho_0}{V_1(0)\varrho_0(0)}\varrho_0'(0)\right) = 2T_n\ln\left(Z_0\left(\frac{\cdot}{\varepsilon}\right)\right)R_{1,\varrho} + 2T_n R_{1,\varrho} + \mathcal{O}(\varepsilon^{3/2}).$$

Here, we also used $\|R_{1,\varrho}\|_{L^\infty(0,1)} \le C\varepsilon$ (c.f. (4.32)), $\|R_{1,V}\|_{L^\infty(0,1)} \le C\varepsilon^{3/2}$ (c.f. (4.26)) and $\left\|\frac{R_{1,\varrho}}{\varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)}\right\|_{L^\infty(0,1)} \le C\varepsilon^{3/4}$ (c.f. (4.34)). The mean value theorem yields

$$2\varepsilon Z_0'\left(\frac{x}{\varepsilon}\right)\left(\varrho_0'(x) - \frac{V_1(x)\varrho_0(x)}{V_1(0)\varrho_0(0)}\varrho_0'(0)\right) = \mathcal{O}(\varepsilon^2) \quad (x\in[0,\varepsilon]).$$

We conclude that the scaled remainder $\mathcal{R}_{1,\varrho}(y) := R_{1,\varrho}(\varepsilon y)$ fulfills the differential equation

$$\mathcal{R}_{1,\varrho}''(y) - 2T_n(1+\ln(Z_0(y))\mathcal{R}_{1,\varrho}(y) = \mathcal{O}(\varepsilon^{3/2}) \quad (y\in(0,1))$$

with boundary values $\mathcal{R}_{1,\varrho}(0) = 0$ and $\mathcal{R}_{1,\varrho}(1) = \mathcal{O}(\varepsilon^{3/2})$, as seen in inequality (4.37). Now the function $U(y) = \mathcal{R}_{1,\varrho}(y) - y\mathcal{R}_{1,\varrho}(1)$ still solves an equation

$$\left\{\begin{array}{rcl} U'' - 2T_n(1+\ln(Z_0)U &=& f, \\ U(0) &=& 0, \\ U(1) &=& 0, \end{array}\right.$$

where the right hand side f admits $\|f\|_{L^2(0,1)} \le C\varepsilon^{3/2}$. Corollary 4.6 yields $\|U\|_{W^{2,2}(0,1)} \le C\varepsilon^{3/2}$, which implies $\|\mathcal{R}_{1,\varrho}\|_{W^{2,2}(0,1)} \le C\varepsilon^{3/2}$. It remains to reverse the scaling and to exploit the Sobolev embedding $W^{2,2}(0,1) \hookrightarrow C^1([0,1])$. □

Corollary 4.12 (Refined estimates to the first order remainders).
The remainders $R_{1,\varrho} = \varrho_\varepsilon - \rho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right) - \varepsilon\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)$ and $R_{1,V} = V_\varepsilon - V_0 - \varepsilon V_1$ enjoy the estimates

$$\begin{aligned} \|R_{1,\varrho}\|_{L^2(0,1)} &\le C\varepsilon^{3/2}, \\ \|R_{1,\varrho}'\|_{L^2(0,1)} &\le C\varepsilon, \\ \|R_{1,\varrho}\|_{L^\infty(0,1)} &\le C\varepsilon^{3/2}, \\ \|R_{1,\varrho}'\|_{L^\infty(0,1)} &\le C\varepsilon^{1/2} \end{aligned}$$

and

$$\|R_{1,V}\|_{W^{1,2}(0,1)} \le C\varepsilon^{3/2}$$

for $0<\varepsilon<\varepsilon_0$.

Proof. This corollary summarizes Lemma 4.7, Corollary 4.10 and Lemma 4.11. □

Remark 4.13.
The most important consequence of the estimates given in Corollary 4.12 is the optimality of the decay rates

$$\|R_{0,\varrho}\|_{L^2(0,1)} + \|R_{0,\varrho}\|_{L^\infty(0,1)} + \|R_{0,V}\|_{W^{1,2}(0,1)} \leq C\varepsilon$$

for the zeroth order remainders $R_{0,\varrho} = \varrho_\varepsilon - \rho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)$ *and* $R_{0,V} = V_\varepsilon - V_0$.
It is reasonable to assume that the first order remainders $R_{1,\varrho}$ *and* $R_{1,V}$ *decay with order* ε^2*. A rigorous proof of this assertion seems possible by proving decay rates of order* $o(\varepsilon^2)$ *for the second order remainders* $R_{2,\varrho} := \varrho_\varepsilon - \rho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right) - \varepsilon\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right) - \varepsilon^2\varrho_{2,\varepsilon}$ *and* $R_{1,V} := V_\varepsilon - V_0 - \varepsilon V_1 - \varepsilon^2 V_{2,\varepsilon}$ *with uniformly bounded functions* $\varrho_{2,\varepsilon}, V_{2,\varepsilon}$ *to be determined.*
The following section will provide numerical evidence for the conjecture of quadratic decay of the remainders $R_{1,\varrho}$ *and* $R_{1,V}$.

4.4 Numerical Results

All numerics have been done in MATLAB. We use the built-in boundary value problem solver `bvp5c` which uses a finite difference method and implements the four-stage Lobatto IIIa formula. To improve accuracy, smaller error tolerances and a grid of 80000 mesh points are used by modifying the parameter set with `bvpset('AbsTol', 12e-12, 'RelTol', 12e-12, 'Nmax', 80000)`. As the solver seems to respond rather sensitively to the choice of the initial value, it is necessary to start the computations for a large value of $\varepsilon = 0.2048$. This parameter is decreased successively until it reaches $\varepsilon = 0.0001$. The respective results for ϱ_ε and V_ε are used as initial values for the subsequent computations. As mentioned in [BCD], the solution Z to $Z'' = Z\ln(Z)$, $Z(0) = 0$, $Z(y) \to \infty$ $(y \to \infty)$ has the derivative $Z'(0) = \frac{1}{\sqrt{2}}$. We use the standard built-in solver `ode45` for ordinary differential equation with the same error tolerances as for the boundary value problems. Since the derivative $Z_1'(0)$ seems to be unknown, we replace the ordinary differential equation to Z_1 by a conform boundary value problem on $[0, 100]$ with boundary values $Z_1(0) = 0$ and $Z_1(100) = 1$ and it's solution is continuated by the constant 1. We use the same scaled parameters as in [BCD]:

V_{GS}	T_n	T_p	λ	β	$\mathcal{C}$	ϱ_B	V_B	F
-1.5	0.04	0.06	1.0	0.75	-2.0	$\sqrt{0.03}$	$T_p\ln(\varrho_B^2 - \mathcal{C})$	$V_B + T_n\ln(\varrho_B^2)$

The values of V_B and F were chosen based on the assumption $\varrho''(1) = V''(1) = 0$. The numerical results show that the remainders $\varrho_\varepsilon - \varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)$ possess a rather large negative minimum inside the boundary layer and a rather large maximum in a transitional section (c.f. Figure 4.2). This is a characteristical behavior and manifests in the non-monotonicity of Z_1 (c.f. Figure 4.3). As in the situation of the zeroth order numerics (c.f. Section 5 in [BCD]), it can be observed that the first order remainders $\varrho_\varepsilon - \varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right) - \varepsilon\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)$ have their largest magnitude in the transitional section, where the exterior and interior fittings merge. A comparison of the norms

$$R_{i,\varrho,L2} := \|R_{i,\varrho}\|_{L^2(0,1)}, \quad R_{i,\varrho,Linfinity} := \|R_{i,\varrho}\|_{L^\infty(0,1)},$$

$$R_{i,V,L2} := \|R_{i,V}\|_{L^2(0,1)}, \quad R_{i,V,Linfinity} := \|R_{i,V}\|_{L^\infty(0,1)},$$

for $i = 0, 1$ shows that the quality of the approximations actually increases for small ε when the first order summand is introduced. Extrapolating the results for ε to zero, a quadratic decay in

ε of the first order remainders can be observed for both the L^2- and the L^∞-norm (c.f. Figures 4.4 and 4.5). We refer to Appendix A.2 for a detailed overview of the computational results.

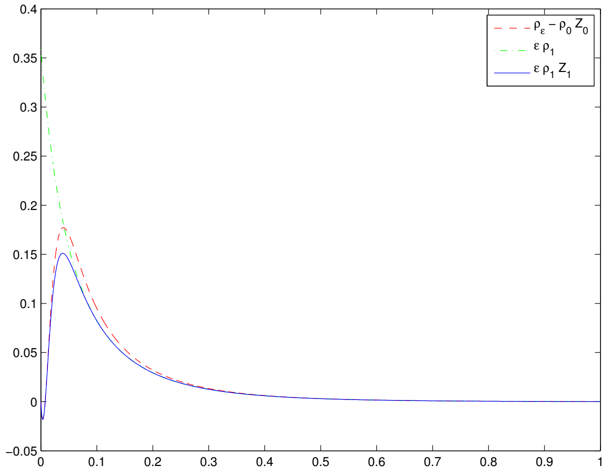

Figure 4.1: Zeroth order remainder $\varrho_\varepsilon - \varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)$, $\varepsilon\varrho_1$ and first order summand $\varepsilon\varrho_1 Z_1\left(\frac{\cdot}{\varepsilon}\right)$ for $\varepsilon = 0.0032$.

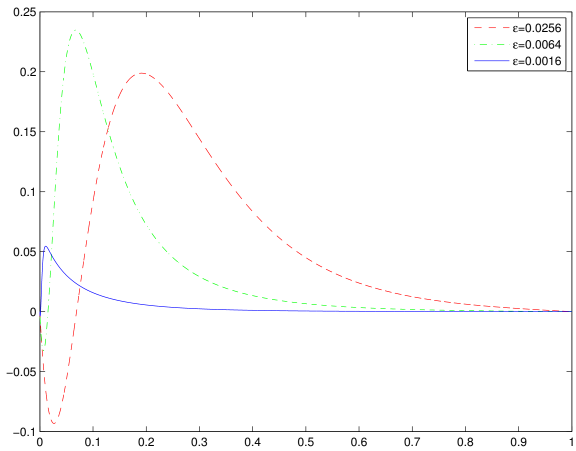

Figure 4.2: Differences $\varrho_\varepsilon - \varrho_0 Z_0\left(\frac{\cdot}{\varepsilon}\right)$.

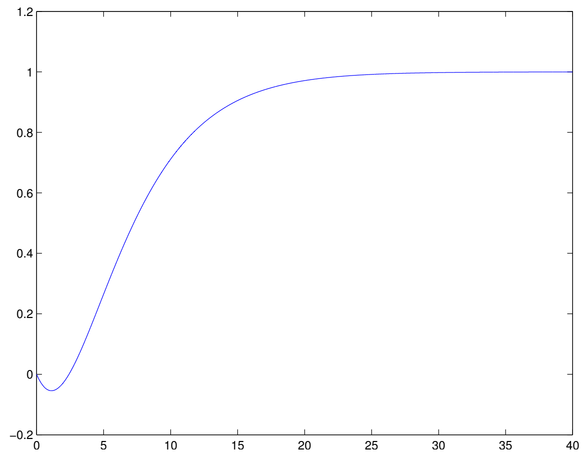

Figure 4.3: Z_1.

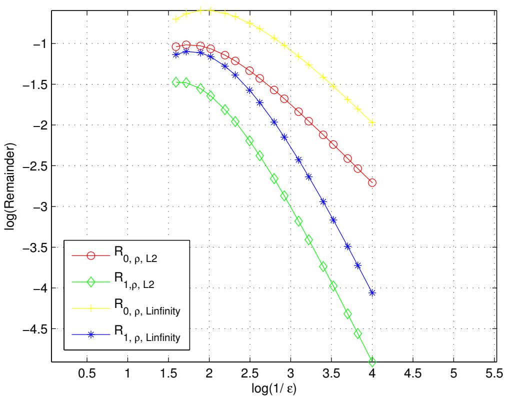

Figure 4.4: Logarithmic plots of ε^{-1} versus the norms of the zeroth- and first order remainders of ϱ.

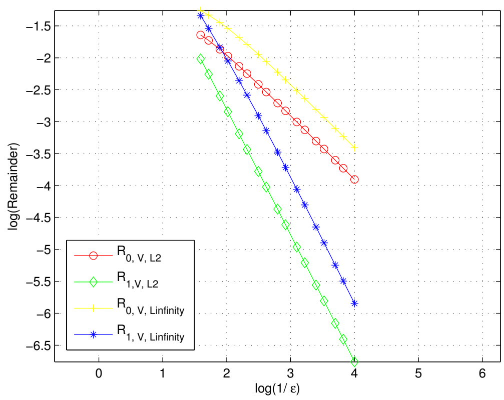

Figure 4.5: Logarithmic plots of ε^{-1} versus the norms of the zeroth- and first order remainders of V.

Appendix A

Auxiliary results

A.1 Functional analytical theorems and technical results

Definition A.1 (**Spaces of functions**).
Let $\Omega \subset \mathbb{R}^n$ be a domain. For $1 \le p \le \infty$ we denote the Lebesgue spaces by $L^p(\Omega)$ and the corresponding Sobolev spaces of order $m \in \mathbb{N}_0$ by $W^{m,p}(\Omega)$. We further define

$$W^{m,p}_{pos}(\Omega) := \{ f \in W^{m,p}(\Omega) \,:\, f > 0 \text{ almost everywhere} \}.$$

The Besov spaces $B^s_{p,q}(\Omega)$ are defined for $1 \le p, q < \infty$ and $s > 0$, $s \notin \mathbb{N}$, by real interpolation

$$B^s_{p,q}(\Omega) := \Big(L^p(\Omega), W^{\lceil s \rceil}(\Omega) \Big)_{\frac{s}{\lceil s \rceil}, q},$$

where $\lceil s \rceil$ denotes the smallest natural number larger than s. The Sobolev-Slobodeckii spaces are then given by

$$W^{s,p}(\Omega) := \begin{cases} W^{m,p}(\Omega), & s \in \mathbb{N}, \\ B^s_{p,p}(\Omega), & s \notin \mathbb{N}. \end{cases}$$

For $1 < p < \infty$ and $s, m \in \mathbb{N}$ with $1 \le s \le 2m$, assume that Ω is a $C^{2m-1,1}$-domain. Any function $u \in W^{s,p}(\Omega)$ has a boundary trace $u|_{\partial\Omega}$ and the space of all traces of all functions in $W^{s,p}(\Omega)$ is denoted by $B^{s-\frac{1}{p}}_{p,p}(\partial\Omega)$. The norm on $B^{s-\frac{1}{p}}_{p,p}(\partial\Omega)$ can be defined by

$$\|v\|_{B^{s-\frac{1}{p}}_{p,p}(\partial\Omega)} := \inf_{u \in W^{s,p}(\Omega), u|_{\partial\Omega} = v} \|u\|_{W^{s,p}(\Omega)} \quad (v \in B^{s-\frac{1}{p}}_{p,p}(\partial\Omega)),$$

or equivalently, by a localization to the spaces $B^{s-\frac{1}{p}}_{p,p}(\mathbb{R}^{n-1})$. We refer to [Gr, Chapt. 1.3] for details.

Lemma A.2.
Let $\Omega \subset \mathbb{R}^N$ be a domain and $1 \le q < p < \infty$. For any sequence $(u_n)_{n\in\mathbb{N}} \subset L^p(\Omega)$ converging to some $u \in L^p(\Omega)$, it holds $(u_n^{p/q})_{n\in\mathbb{N}} \subset L^q(\Omega)$ and $u_n^{p/q} \longrightarrow u^{p/q}$ in $L^q(\Omega)$.
Moreover, for any $f \in L^\infty(\Omega)$, the mapping $u \mapsto \int_\Omega f(x) u^p(x)\, dx$, $L^p(\Omega) \longrightarrow \mathbb{R}$, is continuous.

Proof. Evidently, $u_n^{p/q} \in L^q(\Omega)$. The function $f(s) := s^{p/q}$ fulfills

$$|f(s) - f(t)| \le \frac{p}{q} r^{p/q-1} |s - t| \quad (|s|, |t| \le r).$$

By Theorem [ApZa, 3.10], the associated Nemytskij operator $F : L^p(\Omega) \longrightarrow L^q(\Omega)$, $u \mapsto u^{p/q}$, is locally Lipschitz continuous and admits the estimate

$$\|u^{p/q} - v^{p/q}\|_{L^q(\Omega)} \leq \frac{p}{q} r^{p/q-1} \|u - v\|_{L^p(\Omega)} \quad (\|u\|_{L^p(\Omega)}, \|v\|_{L^p(\Omega)} \leq r),$$

which shows the first assertion. By the first part of the proof, we have

$$\left| \int_\Omega f(x) u_n^p(x)\, dx - \int_\Omega f(x) u^p(x)\, dx \right| \leq C \|f\|_{L^\infty(\Omega)} \|u_n^p - u^p\|_{L^1(\Omega)} \longrightarrow 0$$

as $n \to \infty$ for any $(u_n)_{n\in\mathbb{N}} \subset L^p(\Omega)$ converging to some $u \in L^p(\Omega)$. □

Lemma A.3.
Let $\Omega \subset \mathbb{R}^N$ be a domain satisfying the segment condition, $1 \leq p < \infty$ and $u \in W^{1,p}(\Omega)$. Then

$$u_+ := \max\{u, 0\}, \quad u_- := \min\{u, 0\} \quad \text{and} \quad |u|$$

are elements of $W^{1,p}(\Omega)$ with

$$\nabla u_+ = \begin{cases} \nabla u, & u > 0, \\ 0, & u \leq 0, \end{cases} \qquad \nabla u_- = \begin{cases} \nabla u, & u < 0, \\ 0, & u \geq 0 \end{cases}$$

and

$$\nabla |u| = \begin{cases} \nabla u, & u > 0, \\ -\nabla u, & u < 0, \\ 0, & u = 0. \end{cases}$$

Moreover,

$$\operatorname{Tr} |u| = |\operatorname{Tr} u|, \quad \operatorname{Tr} u^+ = (\operatorname{Tr} u)^+, \quad \operatorname{Tr} u^- = (\operatorname{Tr} u)^- \quad (u \in W^{1,p}(\Omega)).$$

Proof. A proof of the differentiability properties can be found in [Do, 5.20]. The last assertions are true for functions in $C^1(\overline{\Omega})$ and follow for arbitrary elements in $W^{1,p}(\Omega)$ by approximation, since the mappings $u \mapsto |u|$, $u \mapsto u^+$, $u \mapsto u^-$ are continuous from $W^{1,p}(\Omega)$ to $W^{1,p}(\Omega)$. □

Lemma A.4 (**A chain rule for Sobolev functions**).
Let $\Omega \subset \mathbb{R}^N$ be a domain, $f \in C^1(\mathbb{R})$, $f' \in L^\infty(\mathbb{R})$ and $u \in W^{1,1}_{loc}(\Omega)$. Then $f \circ u \in W^{1,1}_{loc}(\Omega)$ and the representation

$$\partial_i (f \circ u) = (f' \circ u) \partial_i u \quad (i = 1, \dots, n)$$

holds almost everywhere in Ω.

Proof. A proof can be found in [GiTr, Lem. 7.5]. □

Lemma A.5.
Let $\Omega \subset \mathbb{R}^N$ be a domain and $u \in W^{1,2}(\Omega)$. Then $u^2 \in W^{1,1}_{loc}(\Omega)$ and $\partial_i u^2 = 2(\partial_i u)u$. In particular, if $u\nabla u = 0$, then u is a constant function.

Proof. Since $u \in W^{1,2}(\Omega)$, one has $u, \partial_i u \in L^2(\Omega)$ and therefore $u\partial_i u \in L^1_{loc}(\Omega)$ for $i = 1, \dots, n$. Then

$$\int_\Omega (\partial_i u) u\varphi = -\int_\Omega u \partial_i (u\varphi) = -\int_\Omega u^2 \partial_i \varphi - \int_\Omega u (\partial_i u) \varphi,$$

so that $\partial_i u^2 = 2(\partial_i u)u$. If $u\nabla u = 0$, then $\nabla u^2 = 0$ and therefore u is a constant function. □

Theorem A.6 (**Embeddings of Sobolev and Besov spaces**).
Let $\Omega \subset \mathbb{R}^N$ be a domain satisfying the cone condition. Then the following embeddings hold for $1 < p < \infty$, $j \in \mathbb{N}_0$ and $m \in \mathbb{N}$.
If $mp > N$, then

$$\begin{aligned} W^{j+m,p}(\Omega) &\hookrightarrow C^j(\overline{\Omega}), \\ W^{j+m,p}(\Omega) &\hookrightarrow W^{j,q}(\Omega) \quad (p \leq q \leq \infty), \end{aligned}$$

if $mp = N$, then

$$W^{j+m,p}(\Omega) \hookrightarrow W^{j,q}(\Omega) \quad (p \leq q < \infty)$$

and if $mp < N$, then

$$W^{j+m,p}(\Omega) \hookrightarrow W^{j,q}(\Omega) \quad (p \leq q \leq \tfrac{Np}{N-mp}).$$

The embedding constants only depend on N, m, p, q, j and the the dimensions of the cone providing the cone condition for Ω.
Assuming that Ω is a bounded domain, all embeddings are also compact, provided $q \neq \infty$. In the case of bounded domains, all embeddings are still given, if $m > 0$ is not integer.

Proof. A more detailed overview for integer orders can be found in [Adams, Thm. 4.12]. The compactness results are known as the Rellich-Kondrachov theorems, c.f. [Adams, Thm. 6.3]. For embedding results on Besov spaces, we refer to [Tri, 4.6.1]. □

Lemma A.7 (**Asymptotics of functions in $W^{1,2}(\mathbb{R})$**).
Let $u \in W^{1,2}(\mathbb{R})$. Then

$$\lim_{t \to \pm\infty} u(t) = 0.$$

Proof. It holds

$$\left|u^2(y) - u^2(x)\right| = \left|\int_x^y (u^2)'(s)\, ds\right| = \left|\int_x^y 2u(s)u'(s)\, ds\right| \leq 2\|u\|_{L^2(x,y)}\|u'\|_{L^2(x,y)} \longrightarrow 0$$

for $x < y$, $x, y \longrightarrow \pm\infty$. Therefore, $u^2(t)$ has a limit for $t \longrightarrow \pm\infty$. Since $u \in L^2(\mathbb{R})$, this limit must be zero and then also $\lim_{t \to \pm\infty} u(t) = 0$. □

Lemma A.8 (**Interpolation inequalities**).
Let $\Omega \subset \mathbb{R}^N$ be a domain and let $1 \leq p < q < r \leq \infty$ satisfy $\frac{1}{q} = \frac{\theta}{p} + \frac{1-\theta}{r}$ for some $0 < \theta < 1$. Then $u \in L^p(\Omega) \cap L^r(\Omega)$ implies $u \in L^q(\Omega)$ with

$$\|u\|_{L^q(\Omega)} \leq \|u\|_{L^p(\Omega)}^{\theta}\|u\|_{L^r(\Omega)}^{1-\theta}.$$

Let $\Omega \subset \mathbb{R}^N$ be a domain satisfying the cone condition. If either

(i) $mp > N$ and $p \leq q \leq \infty$,

(ii) $mp = N$ and $p \leq q < \infty$, or

(iii) $mp < N$ and $p \leq q \leq \frac{Np}{N-mp}$,

then

$$\|u\|_{L^q(\Omega)} \leq C\|u\|_{W^{m,p}(\Omega)}^{\theta}\|u\|_{L^p(\Omega)}^{1-\theta} \quad (u \in W^{m,p}(\Omega)),$$

where $\theta = \frac{N}{mp} - \frac{N}{mq}$. The constant C probably depends on m, N, p, q and the dimensions of the cone providing the cone condition for Ω.

Proof. We refer to [Adams, Thm. 5.8]. □

Definition A.9 (**Second order elliptic operator**).
Let $a^{ij}, b^i, c : \mathbb{R}^N \longrightarrow \mathbb{R}$ $(i, j = 1, \dots n)$ be bounded and measurable functions satisfying

$$a^{ij} = a^{ji} \quad \text{and} \quad |a^{ij}(x) - a^{ij}(y)| \leq \omega(|x-y|)$$

for $i, j = 1, \dots, n$ and some increasing function $\omega : [0, \infty) \longrightarrow [0, \infty)$ fulfilling $\lim_{\varepsilon \searrow 0} \omega(\varepsilon) = 0$. Then the (formal) expression

$$L = \sum_{i,j=1}^{n} a^{ij} \partial_i \partial_j + \sum_{i=1}^{n} b^i \partial_i + c$$

is called a second-order elliptic differential operator if there exists a constant of ellipticity $C > 0$ such that

$$C^{-1}|\xi|^2 \geq \sum_{i,j=1}^{n} a^{ij}(x) \xi_i \xi_j \geq C|\xi|^2 \quad (x, \xi \in \mathbb{R}^N).$$

Lemma A.10 (**A maximum principle for elliptic operators with constant coefficients**).

Assume $a^{ij}, b^i \in \mathbb{R}$ and $c \leq 0$ $(i, j = 1, \dots, n)$ in Definition A.9. Let $\Omega \subset \mathbb{R}^N$ be a domain, $u \in W^{1,2}(\Omega)$ and $Lu \geq 0$ (resp. $Lu \leq 0$). If for some ball $B \subset \Omega$ with $\operatorname{dist}(B, \partial\Omega) > 0$

$$\text{ess-sup}_{x \in B}\, u(x) = \text{ess-sup}_{x \in \Omega}\, u(x) \geq 0, \quad \textit{resp.} \quad \text{ess-inf}_{x \in B}\, u(x) = \text{ess-inf}_{x \in \Omega}\, u(x) \leq 0,$$

then u is a constant function in Ω.

Proof. A proof can be found in [GiTr, Thm. 8.19]. The authors even consider more general operators in divergence form. □

Lemma A.11 (**A Harnack inequality for elliptic operators**).
Let $\Omega \subset \mathbb{R}^N$ be a domain and L be an elliptic operator in the sense of Definition A.9. For $u \in W^{1,2}(\Omega)$ satisfying $Lu = 0$ and $u \geq 0$ in Ω, it holds

$$\text{ess-sup}_{x \in B(y,r)}\, u(x) \leq C\, \text{ess-inf}_{x \in B(y,r)}\, u(x)$$

for any ball $B(y, r)$ with $B(y, 4r) \subset \Omega$. The constant C only depends on r, N and the coefficients of L.

Proof. We refer to [GiTr, Thm. 8.20]. □

Theorem A.12 (**A variant of the Schauder fixed point theorem**).
Let V be a Banach space and $\emptyset \neq X \subset V$ be a bounded, closed, convex subset. Assume that $F : X \longrightarrow X$ is compact. Then F has a fixed point in X.

Proof. A proof can be found in [We, Thm. IV.7.18]. □

Proposition A.13.
Suppose that $(V, \|\cdot\|)$ is a reflexive Banach space and let $M \subset V$ be a weakly closed subset. Assume that $E : M \longrightarrow \mathbb{R} \cup \{\infty\}$ fulfills

(i) *E is coercive, i.e. $E(u) \longrightarrow \infty$ as $\|u\| \longrightarrow \infty$,*

(ii) *E is sequentially weakly lower semi-continuous on M with respect to V, i.e. for any sequence $(u_n)_{n\in\mathbb{N}} \subset M$ such that $u_n \rightharpoonup u \in M$ weakly in V, there holds*

$$E(u) \leq \liminf_{n\to\infty} E(u_n).$$

Then E is bounded from below on M and attains its minimum in M.

Proof. A proof is given in [Str, Thm. 1.2]. □

Proposition A.14.
Let $\Omega \subset \mathbb{R}^N$ be a domain and assume that $J : \Omega \times \mathbb{R}^m \times \mathbb{R}^{Nm} \longrightarrow \mathbb{R}$ is a Caratheodory function, i.e. J is measurable with respect to $x \in \Omega$ and continuous with respect to $z \in \mathbb{R}^m \times \mathbb{R}^{Nm}$. Moreover, assume that

(i) *there exists $\Phi \in L^1(\Omega)$: $J(x, u, p) \geq \Phi(x)$ for almost all $(x, u, p) \in \Omega \times \mathbb{R}^m \times \mathbb{R}^{Nm}$,*

(ii) *$J(x, u, \cdot)$ is convex for almost all $(x, u) \in \Omega \times \mathbb{R}^m$.*

Then, if $u_n, u \in W^{1,1}_{loc}(\Omega)$ and $u_n \longrightarrow u$ in $L^1(\Omega')$, $\nabla u_n \rightharpoonup \nabla u$ weakly in $L^1(\Omega')$ for all bounded $\Omega' \subset\subset \Omega$, it follows that

$$E(u) \leq \liminf_{n\to\infty} E(u_n),$$

where

$$E(u) := \int_\Omega J(x, u(x), \nabla u(x))\, dx.$$

Proof. This can be found in [Str, Thm. 1.6]. □

Definition A.15 (Gâteaux-derivative).
Let X, Y be Banach spaces and $U \subset X$ be an open subset. A mapping $f : U \longrightarrow Y$ is said to be Gâteaux-differentiable in $u \in U$ if

$$h \mapsto \lim_{t\to 0} \frac{1}{t} \left(f(u + th) - f(u) \right) \quad (h \in X)$$

defines a continuous and linear operator $f'_G(u) \in L(X, Y)$.

Definition and Remark A.16 (Fréchet-derivative).
Let X, Y be Banach spaces and $U \subset X$ be an open subset. A mapping $f : U \longrightarrow Y$ is said to be Fréchet-differentiable in $u \in U$ if there exists a linear and continuous operator $f'(u) \in L(X, Y)$ such that

$$\frac{\|f(u + h) - f(u) - f'(u)h\|_Y}{\|h\|_X} \longrightarrow 0$$

whenever $\|h\|_X \longrightarrow 0$.
f is called Fréchet-differentiable in U, if f is Fréchet-differentiable in any $u \in U$. In this case f is said to be continuously differentiable, if the mapping $u \mapsto f'(u)$, $U \to L(X, Y)$ is continous.
If f is Fréchet-differentiable in $u \in U$, then f is Gâteaux-differentiable in u and $f'_G(u) = f'(u)$.

Theorem A.17 ([Str], **C.1 Thm.**).
Let $\Omega \subset \mathbb{R}^N$ be a bounded domain and assume that $F : \Omega \times \mathbb{R} \times \mathbb{R}^N \longrightarrow \mathbb{R}$ is measurable with respect to $x \in \Omega$ and continuously differentiable with respect to $u \in \mathbb{R}$ and $p \in \mathbb{R}^N$. If there exist $C, s_1, s_2, s_3, t > 0$ such that

(i) $|F(x,u,p)| \le C(1 + |u|^{s_1} + |p|^2)$, *where* $s_1 \le \frac{2N}{N-2}$, *if* $N \ge 3$,

(ii) $|\partial_u F(x,u,p)| \le C(1 + |u|^{s_2} + |p|^t)$, *where* $t < 2$, *if* $N \le 2$ *and* $s_2 \le \frac{N+2}{N-2}$, $t \le \frac{N+2}{N}$, *if* $N \ge 3$,

(iii) $|\partial_p F(x,u,p)| \le C(1 + |u|^{s_3} + |p|)$, *where* $s_3 \le \frac{N}{N-2}$, *if* $N \ge 3$,

then the functional $E : H^1(\Omega) \longrightarrow \mathbb{R}$,

$$E(u) := \int_\Omega F(x, u(x), \nabla u(x))\, dx \quad (u \in H^1(\Omega)),$$

is continuously Fréchet-differentiable in $H^1(\Omega)$ *and*

$$E'(u)h = \int_\Omega \partial_u F(x, u(x), \nabla u(x)) h(x) + \langle \partial_p F(x, u(x), \nabla u(x)), \nabla h(x) \rangle \, dx.$$

Lemma A.18.
The solution operator Φ, $f \mapsto u$, *to the equation*

$$u''(x) = f(x) \quad (x \in (0,1)), \quad u(0) = u(1) = 0$$

is continuous from $L^2(0,1)$ *to* $W^{2,2}(0,1)$ *and continuous from* $L^1(0,1)$ *to* $C^1([0,1])$.
The solution u *to the equation*

$$u''(x) = f(x) \quad (x \in (0,1)), \quad u(0) = u_0,\ u(1) = u_1$$

fulfills

$$\|u\|_{C^1(0,1)} \le 2\left(\|f\|_{L^1(0,1)} + |u_0| + |u_1|\right).$$

If $f \ge 0$ ($f \le 0$), *then* $\Phi(f) \le 0$ ($\Phi(f) \ge 0$).

Proof. The first asserted continuity is well-known. Note that the solution operator is explicitly given by

$$(\Phi f)(x) = \int_0^x \int_0^y f(s)\, dsdy - x \int_0^1 \int_0^y f(s)\, dsdy \quad (x \in [0,1]).$$

Then

$$\left| \int_0^x \int_0^y f(s)\, dsdy - x \int_0^1 \int_0^y f(s)\, dsdy \right| \le 2 \int_0^1 \int_0^y |f(s)|\, dsdy \le 2\|f\|_{L^1(0,1)} \quad (x \in [0,1])$$

implies

$$\|(\Phi f)\|_\infty \le 2\|f\|_{L^1(0,1)}.$$

Analogously

$$\left| \int_0^x f(s)\, ds - \int_0^1 \int_0^y f(s)\, dsdy \right| \le 2\|f\|_{L^1(0,1)} \quad (x \in [0,1]),$$

so that

$$\|(\Phi f)'\|_\infty \le 2\|f\|_{L^1(0,1)}.$$

The estimate for inhomogeneous boundary values follows from

$$u(x) = (\Phi f)(x) + u_0 + x(u_1 - u_0) \quad (x \in [0,1]).$$

The assertions concerning the signs of the solutions are an immediate consequence of the maximum principle A.10. □

Lemma A.19.
Let $h : (0,\infty) \longrightarrow \mathbb{R}$ be continuously differentiable. Let $I = [a,b] \subset (0,\infty)$ be an interval such that

$$h'(x) \ge C_0 > 0 \quad (x \in I).$$

Then, for fixed $\tau > 0$ and $k_\nu := h + \frac{\nu}{\tau}\ln$, it holds that

$$\|h^{-1} - k_\nu^{-1}\|_{L^\infty(J)} \le C\nu \quad (0 < \nu < \nu_0),$$

where $J := k_{\nu_0}(I)$.

Proof. Note that J is is still contained in the range of h for sufficiently small ν_0, because

$$J \subset [h(a) - \nu_0\|\ln\|_{L^\infty(I)}, h(b) + \nu_0\|\ln\|_{L^\infty(I)}] \subset h((0,\infty))$$

by monotonicity. Let $y \in J$ and define α_y by

$$\tan\alpha_y := \frac{|y - k_\nu(h^{-1}(y))|}{|h^{-1}(y) - k_\nu^{-1}(y)|}.$$

Then

$$|h^{-1}(y) - k_\nu^{-1}(y)| = \frac{|h(h^{-1}(y)) - k_\nu(h^{-1}(y))|}{\tan\alpha_y} \le \frac{\nu\|\ln\|_{L^\infty(h^{-1}(J))}}{\tan\alpha_y} \le C\nu,$$

since $\tan\alpha_y \ge C > 0$ for $y \in J$ follows by $k' \ge C_0 + \frac{\nu}{\tau b}$ on I. □

A.2 Numerical tables

ε	$\lVert R_{0,\varrho}\rVert_{L^2(0,1)}$	$\lVert R_{1,\varrho}\rVert_{L^2(0,1)}$	$\lVert R_{0,\varrho}\rVert_{L^\infty(0,1)}$	$\lVert R_{1,\varrho}\rVert_{L^\infty(0,1)}$
0.2048	0.036014	0.063789	0.058474	0.17107
0.1536	0.036609	0.045875	0.07746	0.14362
0.1024	0.042444	0.029774	0.10377	0.10242
0.0768	0.047948	0.02545	0.11698	0.074982
0.0512	0.06183	0.026858	0.12133	0.047332
0.0384	0.075094	0.03001	0.1378	0.053627
0.0256	0.091092	0.033483	0.19883	0.072893
0.0192	0.096204	0.032987	0.23122	0.079604
0.0128	0.093461	0.027952	0.25355	0.076993
0.0096	0.086173	0.022754	0.25316	0.068629
0.0064	0.07196	0.015402	0.23473	0.052612
0.0048	0.061013	0.011008	0.21319	0.040939
0.0032	0.046423	0.0064041	0.1772	0.026678
0.0024	0.03737	0.0041867	0.1509	0.018796
0.0016	0.026845	0.0021942	0.11625	0.010845
0.0012	0.020937	0.0013497	0.094643	0.0070908
0.0008	0.014535	0.00065979	0.069165	0.0037379
0.0006	0.011131	0.00039024	0.054601	0.0023149
0.0004	0.00758	0.00018272	0.038515	0.0011449
0.0003	0.0057467	0.00010557	0.029796	0.00068318
0.0002	0.0038732	0.00004822	0.020545	0.00032386
0.00015	0.0029209	0.000027499	0.015693	0.00018867
0.0001	0.0019581	0.00001239	0.010669	0.000087047

ε	$\lVert R_{0,V}\rVert_{L^2(0,1)}$	$\lVert R_{1,V}\rVert_{L^2(0,1)}$	$\lVert R_{0,V}\rVert_{L^\infty(0,1)}$	$\lVert R_{1,V}\rVert_{L^\infty(0,1)}$
0.2048	0.035588	0.22069	0.076797	0.72748
0.1536	0.035455	0.15697	0.076617	0.52668
0.1024	0.034929	0.093648	0.07588	0.32643
0.0768	0.034009	0.062628	0.074524	0.22728
0.0512	0.031328	0.033297	0.070278	0.131
0.0384	0.028244	0.020299	0.065011	0.085973
0.0256	0.022744	0.0096226	0.054826	0.045839
0.0192	0.018694	0.0055489	0.046711	0.028783
0.0128	0.013598	0.0025189	0.035695	0.014623
0.0096	0.010631	0.0014326	0.028807	0.0089231
0.0064	0.0073774	0.00064622	0.020776	0.0043708
0.0048	0.0056427	0.00036766	0.016253	0.0026035
0.0032	0.0038358	0.00016623	0.011333	0.0012356
0.0024	0.0029051	0.000094655	0.0087039	0.00072121
0.0016	0.0019559	0.000042749	0.0059488	0.00033381
0.0012	0.0014743	0.000024284	0.0045197	0.00019193
0.0008	0.00098782	0.000010917	0.0030535	0.000087302
0.0006	0.00074276	$6.179 \cdot 10^{-6}$	0.0023058	0.000049703
0.0004	0.00049646	$2.7643 \cdot 10^{-6}$	0.0015479	0.000022364
0.0003	0.00037283	$1.5597 \cdot 10^{-6}$	0.001165	0.000012658
0.0002	0.00024888	$6.951 \cdot 10^{-7}$	0.00077946	$5.6595 \cdot 10^{-6}$
0.00015	0.00018678	$3.912 \cdot 10^{-7}$	0.00058564	$3.1922 \cdot 10^{-6}$
0.0001	0.0001246	$1.7382 \cdot 10^{-7}$	0.00039113	$1.4219 \cdot 10^{-6}$

Zusammenfassung in deutscher Sprache

Aufgrund der stetig voranschreitenden Miniaturisierung von mikroelektronischen Halbleiter-Elementen wie beispielsweise Tunneldioden oder Feldeffekttransistoren wurde es in den letzten Jahrzehnten notwendig, klassische Modelle des Stromflusses in derartigen Bauteilen zu erweitern. In dieser Arbeit werden zwei makroskopische Modelle des Stromflusses in Halbleitern betrachtet, welche quantenmechanische Effekte berücksichtigen und auf fluiddynamischen Prinzipien beruhen. In Kapitel 2 wird eine eindimensionale, stationäre Variante des viskosen Quanten-Hydrodynamikmodells

$$\begin{cases} \partial_t n - \operatorname{div} J &= \nu \Delta n, \\ \partial_t J - \operatorname{div}\left(\frac{J \otimes J}{n}\right) - \nabla(Tn) + n\nabla V + \frac{\varepsilon^2}{6} n \nabla \frac{\Delta\sqrt{n}}{\sqrt{n}} &= \nu \Delta J - \frac{J}{\tau} + \mu \nabla n, \\ \partial_t(ne) - \operatorname{div}\left(\frac{J}{n}(ne + P)\right) + J \cdot \nabla V &= -\frac{2}{\tau}\left(ne - \frac{d}{2}n\right) + \nu\Delta(ne) + \mu \operatorname{div} J, \\ P &= Tn \operatorname{id}_{\mathbb{R}^d} - \frac{\varepsilon^2}{12} n \left(\nabla \otimes \nabla\right) \ln(n), \\ ne &= \frac{|J|^2}{2n} + \frac{d}{2}Tn - \frac{\varepsilon^2}{24} n \Delta \ln(n), \\ \lambda^2 \Delta V &= n - \mathcal{C} \end{cases}$$

betrachtet, welche durch die Gleichungen

$$\begin{cases} J' &= -\nu n'', \\ 2\varepsilon^2 n \left(\frac{\sqrt{n}''}{\sqrt{n}}\right)' - \nu J'' - (p(n))' + \frac{1}{\tau} J &= \left(\frac{J^2}{n}\right)' - n(V + V_B)', \\ \lambda^2 V'' &= n - \mathcal{C} \end{cases}$$

im Intervall $(0,1)$ beschrieben wird. Hierbei stellt p einen generischen Druckterm dar, der gewissen Regularitätsbedingungen genügen muss (Definition 2.2). V_B ist ein zusätzliches Barrierepotential. Die Konstanten ε, λ, ν und τ stehen für die skalierte Planck-Konstante $\hbar$, die Debye-Länge, die Viskosität und die Relaxationskonstante. Eine weitere gegebene Größe ist das Dotierungsprofil $\mathcal{C}$, welches die Materialeigenschaften des Halbleiters beschreibt. Die unbekannten Funktionen sind die Elektronendichte n, das elektrische Potential V sowie die elektrische Flussdichte J. Da das Barrierepotential üblicherweise eine stückweise konstante Funktion und damit nicht klassisch differenzierbar ist, ist es notwendig einen geeigneten schwachen Lösungsbegriff zu definieren (Definition 2.1). Den Ausgangspunkt für die Lösungstheorie des eindimensionalen stationären viskosen Quanten-Hydrodynamikmodells bildet das äquivalente System von

Gleichungen

$$\text{(A.1)}\qquad \begin{cases} F &= -(V+V_B)+h(n)+\frac{\nu}{\tau}\ln(n)-2(\varepsilon^2+\nu^2)\frac{\sqrt{n}''}{\sqrt{n}}, \\ nF' &= -\left(\frac{J_0^2}{n}\right)'+2J_0\nu\left(2\frac{\sqrt{n}''}{\sqrt{n}}-\frac{(n')^2}{2n^2}\right)+\frac{J_0}{\tau}, \\ \lambda^2 V'' &= n-\mathcal{C}, \end{cases}$$

im Intervall $(0,1)$. In diesem Gleichungssystem kann F als eine viskose Variante eines Fermi-Potentials aufgefasst werden. Die Enthalpie h stellt eine Lösung der Differentialgleichung $sh'(s)=p'(s)$, $s>0$, dar.
Es wird zunächst der Fall eines konstanten Fermi-Potentials F betrachtet. Mit Hilfe von Variationsmethoden werden Existenzresultate für Dirichlet-Randbedingungen (Lemma 2.9), homogene Neumann-Randbedingungen (Lemma 2.13) und periodische Randbedingungen (Lemma 2.14) für die Elektronendichte n hergeleitet. Für den Fall von periodischen Randbedingungen beziehungsweise homogenen Neumann-Randbedingungen betrachten wir weiterhin die zusätzliche Bedingung, dass die Gesamtmasse $\int_0^1 n(x)\,dx$ der Elektronen eine vorgegebene Größe ist (Lemma 2.17 und Lemma 2.18). In allen Fällen werden Dirichlet-Randbedingungen an das elektrische Potential V gestellt. In den jeweiligen Lemmas wird mit Hilfe des Maximumsprinzip zudem bewiesen, dass die Elektronendichten strikt positiv sind.
In Lemma 2.21 wird mit Hilfe von Fixpunktargumenten das Existenzresultat für periodische Randbedingungen mit vorgegebener Gesamtmasse der Elektronen auf beliebig große, nichtkonstante Fermi-Potentiale erweitert. Unter einer Kleinheitsbedingung konnte ein entsprechendes Resultat auch für den Fall von homogenen Neumann-Randbedingungen unter Vorgabe der Gesamtmasse der Elektronen gezeigt werden (Lemma 2.29).
Durch die Umformulierung (A.1) wird die Relevanz eines charakteristischen Parameters des viskosen Quanten-Hydrodynamikmodells ersichtlich. Es ist zu erwarten, dass der Koeffizient $\kappa := \varepsilon^2+\nu^2$ der höchsten auftretenden Ableitung einen signifikanten Einfluss auf die Lösungen hat. In Kapitel 3 wird das qualitative Verhalten der Lösungen $n=n_\kappa$ und $V=V_\kappa$ untersucht, wenn κ gegen Null konvergiert. Wir betrachten konstante Fermi-Potentiale und die Fälle von homogenen Neumann-Randbedingungen und periodischen Randbedingungen für die Elektronendichten. Es werden zudem die jeweiligen Fälle betrachtet, wenn zusätzlich die Gesamtmasse der Elektronen vorgeschrieben wird. In Lemma 3.1 werden zunächst gleichmäßige punktweise Abschätzungen $0<C_0\le n_\kappa\le C_1$ für hinreichend kleine κ für die Elektronendichten nachgewiesen. Wir betrachten im Anschluss den Fall stückweise konstanter Barrierepotentiale V_B. Es werden Normabschätzungen für die Ableitungen von $u_\kappa := \sqrt{n_\kappa}$ im Inneren von Teilintervallen, in denen V_B konstant ist, hergeleitet (Lemma 3.5). Dies ermöglicht es, die $W^{1,2}$-Konvergenz der elektrischen Potentiale V_κ gegen eine Grenzfunktion V_0 nachzuweisen, wenn κ gegen Null konvergiert. Für ein maximales Intervall $[x_0,x_1]$ der Länge L, in dem das Barrierepotential V_B konstant ist, wird in Lemma 3.8 bewiesen, dass die Wurzeln u_κ der Elektronendichten der Abschätzung

$$\|u_0^2-u_\kappa^2\|_{L^\infty(s_0+\kappa^{1/4}L,s_1-\kappa^{1/4}L)} \le C\kappa^{1/4} \quad (0<\kappa<\kappa_0)$$

für eine gewisse Grenzfunktion u_0 genügen. Es stellt sich heraus, dass diese Grenzfunktion an allen Sprungstellen von V_B ebenfalls unstetig ist. Wir befassen uns mit dem Existenznachweis und der expliziten Darstellung von fluiddynamischen Grenzschichten, welche sich an den jeweiligen Sprungstellen s_0 der Grenzfunktion u_0 ausbilden. In Korollar 3.12 wird zunächst gezeigt, dass die Ableitungen $u'_\kappa(s_0)$ von der Größenordnung $\kappa^{-1/2}$ sind. In Lemmas 3.13 und 3.15 wird eine lokale Darstellung

$$u_\kappa(s_0+\cdot) = \frac{u_0(s_0+\cdot)}{u_0(s_0+)} w\left(\tfrac{\cdot}{\kappa^{1/2}} + c_\kappa\right) + \mathcal{O}(\kappa^{1/8})$$

der asymptotischen Entwicklung nullter Ordnung der Funktionen u_κ mit einer gewissen Funktion $w : (0,\infty) \longrightarrow \mathbb{R}$ und eindeutigen positiven Konstanten c_κ hergeleitet. In Korollar 3.19 wird die globale Darstellung

$$u_\kappa = \frac{u_0}{c_0} W_\kappa + R_\kappa$$

im Intervall $(0,1)$ mit gewissen Funktionen c_0 und W_κ eingeführt. Es wird abschließend gezeigt, dass die verbesserten Resttermabschätzungen

$$\|R_\kappa\|_{L^2(0,1)} \le C\kappa^{1/2} \quad \text{und} \quad \|R_\kappa\|_{L^\infty(0,1)} \le C\kappa^{1/4}$$

erfüllt sind (Lemma 3.20).
Im letzten Kapitel befasst sich diese Arbeit mit einer Variante des stationären bipolaren Quanten-Drift-Diffusionsmodells

$$\begin{cases} F &= V + h_n(n) - \varepsilon^2 \frac{\Delta\sqrt{n}}{\sqrt{n}}, \\ G &= -V + h_p(p) - \xi\varepsilon^2 \frac{\Delta\sqrt{p}}{\sqrt{p}}, \\ \operatorname{div}(\mu_n n \nabla F) &= R_0(n,p) R_1(F,G), \\ \operatorname{div}(-\mu_p p \nabla G) &= -R_0(n,p) R_1(F,G), \\ -\lambda^2 \Delta V &= n - p - \mathcal{C}, \end{cases}$$

welche die Enthalpien

$$h_n(n) = T_n \ln(n) \quad \text{und} \quad h_p(p) = T_p \ln(p)$$

verwendet und durch die quasi 1D Approximation

$$\text{(A.2)} \qquad \begin{cases} F &= V + T_n \ln(n) - \varepsilon^2 \frac{\sqrt{n}''}{\sqrt{n}}, \\ -\lambda^2 V'' &= n - \exp(V/T_p) - \mathcal{C} \end{cases}$$

im Intervall $(0,1)$ gegeben ist. Hier bezeichnet $\mathcal{C}$ wieder das Dotierungsprofil des Halbleiters, ε die skalierte Planck-Konstante und λ die Debye-Länge. T_n und T_p sind die Temperaturkonstanten der Elektronen n beziehungsweise der positiven Teilchen p. Es werden die Randwerte

$$n(0) = 0, \quad n(1) = n_B, \quad V'(0) = \beta(V(0) - V_{GS}), \quad V'(1) = 0$$

und das konstante Fermi-Potential $F = V_B + T_n \ln(n_B)$ betrachtet. Die Wahl des Randwertes $n(0) = 0$ bewirkt die Bildung einer fluiddynamischen Grenzschicht an der Stelle $x = 0$, deren Nachweis in [BCD] von S. Bian, L. Chen und M. Dreher erbracht wurde. Dort wurde gezeigt, dass die Elektronendichten $n = n_\varepsilon$ und die elektrischen Potentiale $V = V_\varepsilon$ für $\varepsilon \to 0$ gegen Grenzfunktionen n_* und V_* konvergieren und dass die asymptotischen Entwicklungen nullter Ordnung

$$\varrho_\varepsilon = \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + R_{0,\varrho} \quad \text{und} \quad V_\varepsilon = V_0 + R_{0,V}$$

gegeben sind. Hierbei ist $\varrho_\varepsilon = \sqrt{n_\varepsilon}$, $\varrho_0 = \sqrt{n_*}$, $V_0 = V_*$ und Z_0 die Lösung der Differentialgleichung $Z_0'' = 2T_n Z_0 \ln(Z_0)$, $Z_0(0) = 0$, $\lim_{y\to\infty} Z_0(y) = 1$. Darüber hinaus wurde in [BCD] gezeigt, dass die Restterme den Abschätzungen

$$\|R_{0,\varrho}\|_{L^2(0,1)} \leq C\varepsilon, \quad \|R_{0,\varrho}\|_{L^\infty(0,1)} \leq C\varepsilon^{3/4} \quad \text{und} \quad \|R_{0,V}\|_{W^{1,2}(0,1)} \leq C\varepsilon$$

genügen. In Kapitel 4 werden durch formale Rechnungen Differentialgleichungen für Funktionen ϱ_1, V_1 und Z_1 hergeleitet, welche die asymptotischen Entwicklungen zu

$$\varrho_\varepsilon = \varrho_0 Z_0\left(\tfrac{\cdot}{\varepsilon}\right) + \varepsilon \varrho_1 Z_1\left(\tfrac{\cdot}{\varepsilon}\right) + R_{1,\varrho} \quad \text{und} \quad V_\varepsilon = V_0 + \varepsilon V_1 + R_{1,V}$$

erweitern. Die Differentialgleichung für die Funktion Z_1 (vgl. (4.25)) ist singulär und ein entsprechendes Existenz- und Eindeutigkeitsresultat ist der Inhalt von Lemma 4.4. Umfangreiche Rechnungen zeigen die Resttermabschätzung

$$\|R_{1,\varrho}\|_{L^2(0,1)} + \|R_{1,\varrho}\|_{L^\infty(0,1)} + \|R_{1,V}\|_{W^{1,2}(0,1)} \leq C\varepsilon^{3/2}$$

(Korollar 4.12). Anschließende numerische Ergebnisse weisen darauf hin, dass in dieser Abschätzung sogar die Konvergenzrate ε^2 zu erwarten ist.

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