universität wien

MASTERARBEIT | MASTER'S THESIS

Titel | Title

On the blow-up for the L2-critical power-nonlinear Schrödinger equation

verfasst von | submitted by

Lara Lichtnecker BSc

angestrebter akademischer Grad | in partial fulfilment of the requirements for the degree of

Master of Science (MSc)

Wien | Vienna, 2025

Studienkennzahl lt. Studienblatt | Degree programme code as it appears on the student record sheet:	UA 066 821
Studienrichtung lt. Studienblatt | Degree programme as it appears on the student record sheet:	Masterstudium Mathematik
Betreut von | Supervisor:	Univ.-Prof. Mag. Dr. Roland Donninger

Abstract

This thesis presents an introduction to the L^2-critical power nonlinear Schrödinger equation. We focus on proving a result from *The blow-up dynamics and upper bound on the blow-up rate for critical non-linear Schrödinger equation* by Frank Merle and Pierre Raphaël [10], which has so far been conjectured to hold based on numerical estimates. This result specifically addresses the existence and properties of particular solutions to inhomogeneous linear Schrödinger problems, playing a crucial role in establishing a key positivity property of a quadratic form used in their analysis.

The proof provided in this thesis is computer-assisted and employs a pseudo-spectral method and a contraction argument, which allows us to rigorously prove the finite time blow-up and upper bound on the blow-up rate given in [10] in dimension one for even initial data with negative energy and L^2-mass close to the Ground State.

Abstrakt

Inhalt dieser Masterarbeit ist eine Einführung in die L^2-kritische nichtlineare Schrödingergleichung. Der Fokus liegt darauf, ein Resultat aus *The blow-up dynamics and upper bound on the blow-up rate for critical non-linear Schrödinger equation* von Frank Merle und Pierre Raphaël [10] zu beweisen, dessen Gültigkeit bislang nur auf numerischen Abschätzungen basiert. Insbesondere geht es hier um die Existenz und Eigenschaften spezieller Lösungen inhomogener linearer Schrödinger Gleichungen, die die Positivität einer bestimmten quadratischen Form gewährleisten.
Basierend auf einer Pseudospektral-Methode sowie einem Kontraktionsargument erbringt diese Arbeit einen rigorosen computergestützten Beweis für die in [10] behauptete obere Schranke an die Blow-Up-Rate im eindimensionalen Fall für symmetrische Anfangsdaten mit negativer Energie und L^2-Norm nahe dem Grundzustand.

Contents

1 Introduction **3**

2 The Ground State for the L^2-critical p-NLS **11**

3 A blow-up result in dimension 1 **19**
3.1 ε-decomposition 20
3.2 Time-reparametrization 24
3.3 Conservation laws and a priori bounds 27
3.4 Dynamics of the scaling parameter 31

4 Linear Schrödinger operators and Sturm Liouville theory **45**
4.1 Spectra of linear Schrödinger operators with exponentially decaying potential 59
4.2 Proof of Proposition 3.11 65

5 Proof of Theorem 4.33 i) **74**
5.1 Methods 77
5.2 Approximation of Q and V_1 81
5.3 Smallness of $\mathcal{R}(g_1)$ 102
5.4 Approximation of $\mathcal{L}_{c,1}$ 105
5.5 The contraction argument 112
5.6 The positivity estimate 114

6 Proof of Theorem 4.33 ii) **121**
6.1 Approximation of Q_3 and V_2 122
6.2 Smallness of $\mathcal{R}(g_2)$ 137
6.3 Approximation of $\mathcal{L}_{c,2}$ 141
6.4 The contraction argument 145
6.5 The positivity estimate 146

A Sobolev Spaces **154**

B Littlewood-Paley decomposition **155**

C Euler-Lagrange equations **157**

D Self-adjoint operators on Hilbert spaces **158**

E Chebychev polynomials **160**

F Coefficient tables **161**

1 Introduction

This Section is based on [6] and [15].

Physical Motivation

The Schrödinger equation is the partial differential equation governing the dynamics of the wave function of a quantum mechanical particle, which can be understood to describe such a particle in a probabilistic sense.

A classical particle can be described by its position x and momentum

$$p = m\dot{x}$$

where $\dot{x}$ denotes the particle velocity, m denotes the particle mass and the (kinetic) energy is given by

$$E = \frac{p^2}{2m}.$$

By *de Broglie's hypothesis*, the dynamics of a quantum mechanical particle can by described using a a plane wave ansatz

$$u(t,x) = Ae^{i(kx-\omega t)},$$

and the relations

$$p = \hbar k, \qquad\qquad E = k\omega,$$

where ω denotes the (time-)frequency and k denotes the wave vector or spatial frequency of the wave function u, which gives the *dispersion relation*

$$\omega = \frac{E}{k} = \frac{p^2}{2mk} = \frac{\hbar^2 k}{2m}$$

for the Schrödinger equation, in particular

$$i\hbar\partial_t u(t,x) = \frac{\hbar^2 k^2}{2m}u(t,x) = -\frac{\hbar^2}{2m}\triangle u(t,x).$$

The free Schrödinger equation

Non-dimensionalizing the differential equation above gives the (normalized) free Schrödinger equation

$$\begin{cases} i\partial_t u(t,x) = -\triangle u(t,x), & t \in \mathbb{R},\ x \in \mathbb{R}^d \\ u(0,x) = u_0(x), \end{cases} \tag{1.1}$$

with initial data u_0 which we assume to be in $H^s(\mathbb{R}^d)$ ($s \geq 0$) and describes a quantum particle in the absence of potential energy. In this case the corresponding solution can be obtained via Fourier transform.

Recall the identity

$$\mathcal{F}(\partial_j f)(\xi) = i\xi_j \mathcal{F}(f)(\xi).$$

Applying the Fourier transform in the spatial variable to (1.1) gives the ODE

$$\begin{cases} \partial_t \mathcal{F}(u)(t,\xi) = i|\xi|^2 \mathcal{F}(u)(t,\xi), \\ \mathcal{F}(u)(0,\xi) = \mathcal{F}(u_0)(\xi) \end{cases}$$

with solution

$$\mathcal{F}(u)(t,\xi) = e^{-it|\xi|^2} \mathcal{F}(u_0)(\xi),$$

and hence we can take the inverse Fourier transform to obtain a solution to (1.1) in terms of a *Fourier multiplier*

$$u(t,x) = \mathcal{F}^{-1}\left(e^{-it|.|^2}\mathcal{F}(u_0)\right)(x) = e^{-it\,\triangle}(u_0)(x).$$

We denote the *evolution operator* $U(t) \coloneqq e^{-it\,\triangle}$, such that

$$u(t,x) = U(t)u_0(x).$$

Moreover the evolution operator is a unitary operator on $L^2(\mathbb{R}^d)$ and preserves Sobolev norms

$$\|U(t)u_0\|_{H^s(\mathbb{R}^d)} = \|u_0\|_{H^s(\mathbb{R}^d)}.$$

The subject of this thesis is to study the prototype of the Schrödinger equation with some non-linear potential function V

$$\begin{cases} i\partial_t u(t,x) = -\triangle u(t,x) + V(u(t,x)), & t \in \mathbb{R},\ x \in \mathbb{R}^d \\ u(0,x) = u_0(x). \end{cases} \tag{1.2}$$

The power-nonlinear Schrödinger equation

Let

$$V(u) = \pm|u|^{p-1}u,\ p > 1,$$

such that (1.2) takes the form

$$\begin{cases} i\partial_t u = -\triangle u \pm |u|^{p-1}u, \\ u(0,x) = u_0(x), \end{cases} \tag{1.3}$$

known as the *power-nonlinear Schrödinger equation* (p-NLS).
At the end of this Section it will be clear that the sign in front of the potential term has a strong impact on the evolution of solutions. We refer to these different cases as *defocusing* (+) and *focusing* (-) case.

Conservation Laws

Let u be a solution of (1.3) with $u_0 \in H^1(\mathbb{R}^d)$, $1 < p < \frac{d+2}{d-2}$ and consider the following transformations:

- **space-time translation**
  $u \mapsto u_{t_0,x_0}$ for $t_0 \in \mathbb{R}$ and $x_0 \in \mathbb{R}^d$ and $u_{t_0,x_0}(t,x) \coloneqq u(t+t_0, x+x_0)$,
- **phase shift**
  $u \mapsto u_\gamma$ for $\gamma \in \mathbb{R}$ and $u_\gamma(t,x) \coloneqq e^{i\gamma}u(t,x)$,
- **scaling**
  $u \mapsto u_\lambda$ for $\lambda > 0$ and $u_\lambda(t,x) \coloneqq \lambda^{\frac{2}{p-1}}u(\lambda^2 t, \lambda x)$,
- **Galilean transformation**
  $u \mapsto u_\beta$ for $\beta \in \mathbb{R}$ and $u_\beta(t,x) \coloneqq u(t, x-\beta t)e^{i\frac{\beta}{2}t}$.

It is easy to check that any of the transformations above solves (1.3). We say that such a transformation is a *symmetry* or *invariance* of the power-nonlinear Schrödinger equation.

Remark. Note that the scaling $u \mapsto u_\lambda$ is adapted to the structure of (1.3), in the sense that the factors λ^2 and λ balance out the time derivative and the spatial Laplacian. The amplitude scaling $\lambda^{\frac{2}{p-1}}$ is the unique choice to balance out the nonlinear term such that the dynamics of the equation are preserved. This suggests that this space-time scaling is of significant importance when investigating the behaviour of solutions to (1.3).

By *Noether's theorem* (see [14]), every symmetry yields a corresponding *conservation law* - a quantity which is conserved under the time-evolution of (1.3):

- **L^2-conservation** (induced by phase-shift)

$$\|u(t,.)\|_{L^2(\mathbb{R}^d)} = \|u_0\|_{L^2(\mathbb{R}^d)} \tag{1.4}$$

- **Energy-conservation** (induced by time-translation)

$$E[u](t) \coloneqq \frac{1}{2}\|\nabla u(t,.)\|^2_{L^2(\mathbb{R}^d)} \pm \frac{1}{p+1}\|u(t,.)\|^{p+1}_{L^{p+1}(\mathbb{R}^d)} = E[u](0) \tag{1.5}$$

  (where the sign on the right hand side depends on (de-)focusing)

- **Conservation of momentum** (induced by space-translation)

$$\mathrm{Im}\left(\int_{\mathbb{R}^d} \nabla u(t,x)\bar{u}(t,x)dx\right) = \mathrm{Im}\left(\int_{\mathbb{R}^d} \nabla u_0(x)\bar{u}_0(x)dx\right) \tag{1.6}$$

Remark. The significance of L^2-conservation is easily seen by normalizing $\|u_0\|_{L^2(\mathbb{R}^d)} = 1$ and regarding $\rho(x) = |u(x)|^2$ as probability distribution of the position of a quantum particle (*Copenhagen Interpretation*).

Duhamel's principle

A fundamental tool to examine solutions of (1.3) is the corresponding intergral form

$$u(t,x) = U(t)u_0(x) - i\int_0^t U(t-s)(|u(s,x)|^{p-1}u(s,x))ds. \tag{1.7}$$

A solution u to (1.9) of this form is called *distributional solution.* If in addition $u \in C([-T,T], H^s(\mathbb{R}^d))$ for some $T > 0$, then u is called a *strong H^s-solution.*

Well-posedness

For some cases of initial data it is possible to construct explicit solutions to (1.3), but these cases are the exception. In general, the first question that arises is whether solutions exist at all.

Problem (1.3) is called *locally well-posed* (in $H^s(R^d)$) if

- for all $R > 0$ there exists some $T > 0$ such that for all u_0 with $\|u_0\|_{H^s(\mathbb{R}^d)} < R$ there exists a unique strong H^s-solution to (1.3), in particular $u_0 = \tilde{u}_0$ implies $u(t,.) = \tilde{u}(t,.)$ for all $t \in [-T,T]$
- solutions depend continuously on initial data, i.e. the solution map $u_0 \mapsto u$ is continuous from $H^s(\mathbb{R}^d)$ to some suitable solution space $X \subseteq C([-T,T], H^s(\mathbb{R}^d))$.

The time of existence guaranteed by local well-posedness is in general not maximal, and the question arises if it can be extended such that a solution exists for all times. In this case we refer to a problem as *globally well-posed.*

Criticality of the exponent

The exponent p in (1.3) plays a crucial role when it comes to well-posedness of the problem.
Recall the scaling symmetry $u \mapsto u_\lambda$ with $u_\lambda(t,x) \coloneqq \lambda^{\frac{2}{p-1}} u(\lambda^2 t, \lambda x)$. In order for the highest derivative norm in the space H^s to be conserved under this scaling, i.e. $\|u_\lambda\|_{\dot{H}^s(\mathbb{R}^d)} = \|u\|_{\dot{H}^s(\mathbb{R}^d)}$ (see Appendix A), we need to require

$$(p-1)\left(\frac{d}{2} - s\right) = 2. \tag{1.8}$$

We call p *(H^s)-critical* if (1.8) is satisfied, *subcritical* if $(p-1)\left(\frac{d}{2}-s\right) < 2$ and *supercritical* if $(p-1)\left(\frac{d}{2}-s\right) > 2$.

Heuristically speaking, the dispersive effects and the nonlinearity balance each other for critical p, whereas the dispersive effects dominate for subcritical p and the nonlinearity dominates for supercritical p.

Note that p is L^2-critical for $p = 1 + \frac{4}{d}$ and H^1-critical for $p = 1 + \frac{4}{d-2}$.

We give a brief sketch of how Duhamel's principle can be used to show local well-posedness (see [15] for details):

For $\|u_0\|_{H^s(\mathbb{R}^d)} < R$ let

$$K_{u_0}(u)(t) \coloneqq U(t)u_0 - i\int_0^t U(t-s)(|u(s,.)|^{p-1}u(s,.))ds$$

and let $X_T \subseteq C([-T,T], H^s(\mathbb{R}^d)$ be a Banach space with corresponding norm $\|.\|_{X_T}$ and $T > 0$ yet to be determined. In particular we want K_{u_0} to be a contraction on X_T by choosing a suitable solution space.
The norm $\|.\|_{X_T}$ is usually chosen to be some L^p-based space-time norm on $[-T,T] \times \mathbb{R}^d$ (e.g. Strichartz norms or a temporal sup over weighted Sobolev spaces), such that

$$\|K_{u_0}(u) - K_{u_0}(v)\|_{X_T} = \left\| \int_0^t U(t-s)\Big(|u(s,.)|^{p-1}u(s,.) - |v(s,.)|^{p-1}v(s,.) \Big) ds \right\|_{X_T}.$$

The goal is now, to control both the evolution operator $U(t)$ and the nonlinearity in a suitable sense, in particular the latter one is attained by using arguments based on subcriticality of p and leads to the following well-known results:

Theorem 1.1. (Local well-posedness in L^2) *Let $1 < p < 1 + \frac{4}{d}$ (L^2-subcritical).*
Then (1.3) is locally well-posed in $L^2(\mathbb{R}^d)$. (See [15] Prop.3.15.)

Theorem 1.2. (Local well-posedness in H^1) *Let $1 < p < 1 + \frac{4}{d-2}$ (H^1-subcritical).*
Then (1.3) is locally well-posed in $H^1(\mathbb{R}^d)$. (See [5].)

Global well-posedness

The idea is to use conservation laws to obtain a bound on the H^s-norm of a solution which is uniform in time. Since the time of existence guaranteed by local well-posedness depends only on the size of the initial data in H^s, this means that it can always be prolonged by a time interval of same length, leading to global existence.

In the L^2-case, global well-posedness follows directly from L^2-conservation:

Corollary 1.3. *(Global well-posedness in L^2)*
Let $1 < p < 1 + \frac{4}{d}$ (L^2-subcritical). Then (1.3) is globally well-posed in $L^2(\mathbb{R}^d)$.

For global well-posedness in H^1 we need to distinguish between the focusing and defocusing case. While the L^2-norm is conserved, we need to find a uniform bound on the $\dot{H}^1$ norm and would like to use energy conservation, which is straight forward in the defocusing case, while in the focusing case we will need to impose additional conditions on p.

Corollary 1.4. *(Global well-posedness in H^1, defocusing case)*
Let $1 < p < 1 + \frac{4}{d-2}$ (H^1-subcritical). Then the defocusing case of (1.3) is globally well-posed in $H^1(\mathbb{R}^d)$.

Proof. By energy conservation (1.5) for the defocusing case we have

$$\|\nabla u(t,.)\|^2_{L^2(\mathbb{R}^d)} \leq 2E[u](0) \text{ for all } t \in \mathbb{R}.$$

□

Corollary 1.5. *(Global well-posedness in H^1, focusing case)*
Let $1 < p < 1 + \frac{4}{d}$ (L^2-subcritical). Then the focusing case of (1.3) is globally well-posed in $H^1(\mathbb{R}^d)$.

Proof. By energy conservation (1.5) for the focusing case we have

$$E[u](0) = \frac{1}{2}\|\nabla u(t,.)\|^2_{L^2(\mathbb{R}^d)} - \frac{1}{p+1}\|u(t,.)\|^{p+1}_{L^{p+1}(\mathbb{R}^d)}$$

and by Gagliardo-Nirenberg (2.1) with $\tilde{p} = p+1, \tilde{q} = 2, s = 1$:

$$\|u(t,.)\|_{L^{p+1}(\mathbb{R}^d)} \leq C\|u(t,.)\|^{1-\theta}_{L^2(\mathbb{R}^d)}\|\nabla u(t,.)\|^{\theta}_{L^2(\mathbb{R}^d)}$$

for some constant $C > 0$ with $\theta = \frac{d}{2}\frac{p-1}{p+1}$. Hence,

$$\frac{1}{2}\|\nabla u(t,.)\|^2_{L^2(\mathbb{R}^d)} \leq E[u](0) + \frac{C}{p+1}\|u(t,.)\|^{(1-\theta)(p+1)}_{L^2(\mathbb{R}^d)}\|\nabla u(t,.)\|^{\frac{d}{2}(p-1)}_{L^2(\mathbb{R}^d)}$$

such that for $2 - \frac{d}{2}(p-1) > 0$, which is equivalent to $p < 1 + \frac{4}{d}$, we get a uniform bound on $\|\nabla u\|_{L^2(\mathbb{R}^d)}$ despite the negative sign in the energy conservation. □

At L^2-critical $p = 1 + \frac{4}{d}$, global well-posedness for the focusing case of (1.3) is just no longer given. This is the setting we will fix from now on.

$$\begin{cases} i\partial_t u = -\triangle u - |u|^{p-1}u, \ p = 1 + 4/d \\ u(0,.) = u_0 \in H^1(\mathbb{R}^d). \end{cases} \tag{1.9}$$

Blow-up

A solution u to (1.9) is said to *blow up* at time T if

$$\|\nabla u(t,.)\|_{L^2(\mathbb{R}^d)} \xrightarrow{t\to T} \infty.$$

In that case, for $T \in \mathbb{R}$ one speaks of *finite time blow-up*, which is equivalent to T being the maximal time of existence of u by Theorem (1.2).
In the case of a global solution u, it is still possible that the spatial gradient of u diverges as $t \to \infty$, in which case we speak of *infinite time blow-up*.

The main content of this thesis is the investigation of blow-up for solutions of (1.9), in particular we will prove finite time blow-up under certain conditions on the initial data and exploit an upper bound on the blow-up rate. To end this Section, we give a simple argument for a well-known lower bound on the blow-up rate.

Lemma 1.6. *Let u be a solution of (1.9) with finite blow-up time $T \in (0, \infty)$. Then*

$$\|\nabla u(t,.)\|_{L^2(\mathbb{R}^d)} \gtrsim^1 \frac{1}{\sqrt{T-t}}.$$

[1]Throughout this thesis we denote $A \lesssim B \iff (A \leq CB$ for some constant $C > 0)$ and $A \simeq B \iff (A \lesssim B$ and $A \gtrsim B)$.

Proof. For $t \in [0,T)$ arbitrary and fixed define

$$\lambda_t \coloneqq \|\nabla u(t,.)\|^{-1}_{L^2(\mathbb{R}^d)}, \qquad v^t(\tau,z) \coloneqq \lambda_t^{d/2} u(t+\lambda_t^2\tau, \lambda_t z).$$

By scaling and translational invariance, v^t is a solution of (1.9) and

$$\|v^t(0,.)\|_{L^2(\mathbb{R}^d)} = \|u(0,.)\|_{L^2(\mathbb{R}^d)}, \qquad \|\nabla v^t(0,.)\|_{L^2(\mathbb{R}^d)} = 1 \qquad \text{for all } t \in [0,T).$$

Hence by Theorem 1.2, there exists some time $\tau_0 > 0$ independent of t, such that v^t exists on $[0,\tau_0)$. It follows that

$$t + \lambda_t^2 \tau_0 \leq T \text{ for all } t \in [0,T),$$

i.e.

$$\|\nabla u(t,.)\|^{-2}_{L^2(\mathbb{R}^d)} \lesssim T - t \text{ for all } t \in [0,T).$$

□

2 The Ground State for the L^2-critical p-NLS

Stationary solutions

One special type of solutions which are of great importance for the $L^2 - critical$ p-NLS are stationary solutions (or *solitons*) to (1.9) of the form

$$u(t,x) = e^{i\omega t} W_\omega(x)$$

with some frequency $\omega > 0$.
Inserting this ansatz into (1.9) gives the corresponding elliptic differential equation for W:

$$\omega W_\omega = \triangle W_\omega + |W_\omega|^{p-1} W_\omega \tag{2.1}$$

and it follows that for any $\omega > 0$, if Q is a solution of (2.1) with $\omega = 1$, then

$$Q_\omega(x) \coloneqq \omega^{4/d} Q(\omega x)$$

is a solution to (2.1).

As we will see at the end of this Section, there exists a unique positive solution Q to (2.1) with $\omega = 1$, which is called the *Ground State*.

Perturbation theory

The following is based on [17]. We consider perturbations of the Ground State of the form

$$u(t,x) = e^{it}(Q(x) + \varepsilon(t,x))$$

where Q denotes the Ground State and $\varepsilon \in H^1$ is a small (in the sense of H^1-norm) perturbation such that u is a solution of (1.9). This yields the differential equation for ε:

$$i\partial_t \varepsilon = Q + \varepsilon - \triangle(Q+\varepsilon) - |Q+\varepsilon|^{p-1}(Q+\varepsilon),$$

and denoting $\varepsilon_1 = \mathrm{Re}(\varepsilon),\ \varepsilon_2 = \mathrm{Im}(\varepsilon)$ we have

$$\begin{cases} \partial_t \varepsilon_1 = -\varepsilon_2 - \triangle \varepsilon_2 - |Q+\varepsilon|^{p-1}\varepsilon_2, \\ \partial_t \varepsilon_2 = -Q - \varepsilon_1 + \triangle Q + \triangle \varepsilon_1 + |Q+\varepsilon|^{p-1}(Q+\varepsilon_1). \end{cases} \tag{2.2}$$

Now since

$$|Q+\varepsilon|^{p-1} = Q^{p-1} + (p-1)Q^{p-2}\varepsilon_1 + \mathcal{O}(\varepsilon^2),$$

using (2.1), we obtain

$$\begin{cases} \partial_t \varepsilon_1 = L_- \varepsilon_2 + \mathcal{O}(\varepsilon^2), \\ \partial_t \varepsilon_2 = -i L_+ \varepsilon_1 + \mathcal{O}(\varepsilon^2), \end{cases} \tag{2.3}$$

or in matrix-form:

$$\partial_t \varepsilon = L\varepsilon + \mathcal{O}(\varepsilon^2),$$

where

$$L_+ \coloneqq -\triangle + 1 - pQ^{p-1}, \qquad L_- \coloneqq -\triangle + 1 - Q^{p-1} \tag{2.4}$$

and

$$L = \begin{bmatrix} 0 & L_- \\ -L_+ & 0 \end{bmatrix}$$

is called the *linearized operator close to the Ground State*.

Moreover, L_+, L_- are self-adjoint operators on $L^2(\mathbb{R}^d)$ and L_- is non-negative, the null spaces are given by

$$N(L_+) = \operatorname{span}\{\nabla Q\}, \qquad N(L_-) = \operatorname{span}\{Q\},$$

and

$$L_+\left(\frac{d}{2}Q + (.)\nabla Q\right) = -2Q, \qquad L_-((.)Q) = -2\nabla Q,$$

which leads to the generalized null space of L:

$$N_g(L) = \operatorname{span}\left\{ \begin{pmatrix} 0 \\ Q \end{pmatrix}, \begin{pmatrix} \nabla Q \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ (.)Q \end{pmatrix}, \begin{pmatrix} \frac{d}{2}Q + (.)\nabla Q \\ 0 \end{pmatrix} \right\}.$$

This non-trivial null space is induced from the symmetries of (1.9), which can be seen by considering the derivatives of the following transformations of Q with respect to the corresponding transformation parameter:

- scaling: $\partial_\lambda(\lambda^{d/2}Q(\lambda\ .))\big|_{\lambda=1} = \frac{d}{2}Q + (.)\nabla Q$
- translation: $\partial_{x_0}(Q(.+x_0))\big|_{x_0=0} = \nabla Q$
- phase shift: $\partial_\gamma(e^{i\gamma}Q)\big|_{\gamma=0} = iQ$
- Galilean transformation: $\partial_\beta(e^{i\frac{\beta}{2}x}Q)\big|_{\beta=0} = i\frac{\beta}{2}(.)Q$.

Variational characterization of the Ground State

The aim of this Section is to exploit the best constant of the Gagliardo-Nirenberg inequality in the H^1 setting with L^2-critical p. This will lead to a variational characterization of the Ground State which was shown by Michael I. Weinstein in 1983 (see [18] and [15]).

Theorem 2.1. (Gagliardo-Nirenberg)
Let $1 < \tilde{q} < \tilde{p} \leq \infty$, $s > 0$, $\theta \in (0,1)$ *such that* $\frac{1}{\tilde{p}} = \frac{1}{\tilde{q}} - \frac{\theta s}{d}$.
Then

$$\|u\|_{L^{\tilde{p}}(\mathbb{R}^d)} \lesssim_{\tilde{p},\tilde{q},s,d} \|u\|^{1-\theta}_{L^{\tilde{q}}(\mathbb{R}^d)} \|u\|^{\theta}_{\dot{W}^{s,\tilde{q}}(\mathbb{R}^d)} \quad \text{for all } u \in \dot{W}^{s,\tilde{q}}(\mathbb{R}^d).$$

We fix $\tilde{p} = 1 + \frac{4}{d}$ with $\tilde{q} = 2$ and $s = 1$, which gives $\theta = \frac{d}{2}\frac{p-1}{p+1}$ and the corresponding Gagliardo-Nirenberg inequality

$$\|u\|^{p+1}_{L^{p+1}(\mathbb{R}^d)} \leq C_d \|u\|^{4/d}_{L^2(\mathbb{R}^d)} \|\nabla u\|^2_{L^2(\mathbb{R}^d)} \tag{2.5}$$

For $u \in H^1(\mathbb{R}^d) \setminus \{0\}$ we introduce the Weinstein functional

$$W[u] \coloneqq \frac{\|u\|^{p+1}_{L^{p+1}(\mathbb{R}^d)}}{\|u\|^{4/d}_{L^2(\mathbb{R}^d)} \|\nabla u\|^2_{L^2(\mathbb{R}^d)}}.$$

The first step is to show that maximizers of the Weinstein functional do indeed exist, more precisely we claim that

$$W[v] = W_{\max} \coloneqq \sup\{W[u] : u \in H^1(\mathbb{R}^d) \setminus \{0\}\}$$

is attained for some function $v \in H^1(\mathbb{R}^d)$.

First note that this functional in invariant both under homogeneous transformation $u \mapsto \mu u$ with $\mu \in \mathbb{R}$ and scaling $u \mapsto u_\lambda$ with $\lambda > 0$. Moreover, we can without loss of generality assume $v \geq 0$ for a maximizer of W:

Lemma 2.2. (Diamagnetic inequality) *Let* $u \in H^1(\mathbb{R}^d)$. *Then*

$$-|\nabla u| \leq \nabla |u| \leq |\nabla u| \text{ for all } u \in H^1(\mathbb{R}^d)$$

in a distributional sense. In partibular $W[|u|] \geq W[u]$ *for all* $u \in H^1(\mathbb{R}^d)$.

Proof. Let $u \in \mathcal{S}(\mathbb{R}^d)$. Then $\nabla(\varepsilon^2 + |u|^2)^{1/2} = \nabla u \frac{u}{(\varepsilon^2+|u|^2)^{1/2}}$ and hence $|\nabla(\varepsilon^2 + |u|^2)^{1/2}| \leq |\nabla u|$, which gives

$$-|\nabla u| \leq \nabla(\varepsilon^2 + |u|^2)^{1/2} \leq |\nabla u|$$

for all $\varepsilon > 0$. This now holds for any H^1 function u as limit of Schwartz-functions and the claim follows by taking the distributional limit $\varepsilon \to 0$. □

The existence of an extremizer is based on a compactness argumentation involving the following results:

Lemma 2.3. (Rellich compactness) *Let $(u_n)_{n\in\mathbb{N}}$ be a uniformly bounded sequence in $H^1(\mathbb{R}^d)$ that converges weakly to u in $H^1(\mathbb{R}^d)$ and $p \geq 1$.*
Then u_n converges to u locally in L^{p+1}, i.e. $\|u_n - u\|_{L^{p+1}(B_R^d)} \to 0$ for any ball $B_R^d \subset \mathbb{R}^d$.
(See [15], Lemma B.3)

Lemma 2.4. (Spatial localization of near-maximizers of W)
For all $R \geq 1, \eta > 0$ there exist $R_1 > R$ and $\varepsilon > 0$, such that for all $u \in H^1(\mathbb{R}^d) \setminus \{0\}$ with $\|u\|_{L^2(\mathbb{R}^d)} = \|\nabla u\|_{L^2(\mathbb{R}^d)} = 1$, $W[u] \geq W_{\max} - \varepsilon$ and $\|u\|^{p+1}_{L^{p+1}(B_R^d)} \geq \eta$:

$$\|u\|^{p+1}_{L^{p+1}(\mathbb{R}^d \setminus B_{R_1}^d)} \leq \eta.$$

(See [15], Lemma B.4)

Theorem 2.5. (Existence of extremizers of W)
There exists $v \in H^1(\mathbb{R}^d) \setminus \{0\}$, $v \geq 0$ such that $W[v] = W_{\max}$

Proof. There exists a maximizing sequence $(v_n)_{n\in\mathbb{N}} \subset H^1(\mathbb{R}^d) \setminus \{0\}$, such that

$$\lim_{n\to\infty} W[v_n] = W_{\max}.$$

By Lemma(2.2) and invariance of W with respect to homogeneous transformation and scaling we can without loss of generality assume $v_n \geq 0$ and $\|v_n\|_{L^2(\mathbb{R}^d)} = \|\nabla v\|_{L^2(\mathbb{R}^d)} = 1$, hence

$$\lim_{n\to\infty} \|v_n\|^{p+1}_{L^{p+1}(\mathbb{R}^d)} = W_{\max}.$$

We use the Littlewood-Paley decomposition (see Section B) to investigate the structure of $(v_n)_{n\in\mathbb{N}}$.
By triangle inequality and Lemma B.3:

$$0 < \limsup_{n\to\infty} \|v_n\|_{L^{p+1}(\mathbb{R}^d)} \leq \limsup_{n\to\infty} \sum_{N\in\mathbb{N}} \|P_N v_n\|_{L^{p+1}(\mathbb{R}^d)} \leq \sum_{N\in\mathbb{N}} \limsup_{n\to\infty} \|P_N v_n\|_{L^{p+1}(\mathbb{R}^d)}$$

and hence

$$\limsup_{n\to\infty} \|P_{N_0} v_n\|_{L^{p+1}(\mathbb{R}^d)} > 0$$

for some frequency $N_0 \in \mathbb{N}$.

By the Bernstein inequalities (Proposition B.2) and Hölder:

$$\|P_{N_0} f\|_{L^{p+1}(\mathbb{R}^d)} \lesssim 2^{N_0(\frac{d}{3} - \frac{d}{p+1})} \|P_{N_0} f\|_{L^3(\mathbb{R}^d)} \lesssim \|P_{N_0} f\|^{1/3}_{L^\infty(\mathbb{R}^d)} \|P_{N_0} f\|^{2/3}_{L^2(\mathbb{R}^d)}$$

and hence

$$\limsup_{n\to\infty} \|P_{N_0} v_n\|_{L^\infty(\mathbb{R}^d)} > 0.$$

By translational invariance of W we can shift every v_n individually such that passing to a subsequence we have

$$|P_{N_0} v_n(0)| > c > 0 \text{ for all } n \in \mathbb{N}.$$

Now we can expand $P_{N_0} v_n(0)$ using the convolution property of the Fourier transform:

$$\begin{aligned}
|P_{N_0} v_n(0)| &= |\int_{\mathbb{R}^d} \mathcal{F}^{-1}(\psi_{N_0})(y) v_n(y) dy| \\
&\leq \int_{B_R^d} |\mathcal{F}^{-1}(\psi_{N_0})(y) v_n(y)| dy + \int_{\mathbb{R}^d \setminus B_R^d} |\mathcal{F}^{-1}(\psi_{N_0})(y) v_n(y)| dy \\
&\lesssim \|v_n\|_{L^2(B_R^d)} + \|v_n\|_{L^2(R^d)} \left(\int_{\mathbb{R}^d \setminus B_R^d} |\mathcal{F}^{-1}(\psi_{N_0})(y)|^2 \right)^{1/2}
\end{aligned}$$

for any radius $R > 0$ and observe that for all $|y| > R$

$$|\mathcal{F}^{-1}(\psi_{N_0})(y)| = \left| \int_{\mathbb{R}^d} e^{i\xi \cdot y} \psi_{N_0}(\xi) d\xi \right| = \frac{1}{|y|^d} \left| \int_{\mathbb{R}^d} e^{ix \cdot \frac{y}{|y|}} \psi_{N_0}\left(\frac{x}{|y|}\right) dx \right| \lesssim \frac{1}{R^d}.$$

In particular choosing R sufficiently large

$$\|v_n\|_{L^2(B_R^d)} > \tilde{c} \text{ for all } n \in \mathbb{N}$$

for some $\tilde{c} > 0$, and hence by Hölder

$$\|v_n\|_{L^{p+1}(B_R^d)} > \eta \text{ for all } n \in \mathbb{N} \tag{2.6}$$

for some $\eta > 0$.

This suffices to find a subsequence that converges in $L^{p+1}(\mathbb{R}^d)$:

Since $(v_n)_{n\in\mathbb{N}}$ is uniformly bounded in $H^1(\mathbb{R}^d)$, by Banach-Alaoglu there is a subsequence that converges weakly to some v in $H^1(\mathbb{R}^d)$ and by Lemma 2.3 $v_n \to v$ locally in $L^{p+1}(\mathbb{R}^d)$.
Moreover, by (2.6) and Lemma 2.4: for all $\eta' \in (0, \eta]$ there exists a radius $R(\eta') > 0$ such that

$$\|v_n\|_{L^{p+1}(\mathbb{R}^d \setminus B^d_{R(\eta')})} \leq \eta' \text{ for all } n \in \mathbb{N}$$

and by weak lower semi-continuity

$$\|v\|_{L^{p+1}(\mathbb{R}^d \setminus B^d_{R(\eta')})} \leq \eta'.$$

Hence, we obtain

$$\|v_n - v\|_{L^{p+1}(\mathbb{R}^d)} \leq \|v_n - v\|_{L^{p+1}(B^d_{R(\eta')})} + \|v_n\|_{L^{p+1}(\mathbb{R}^d \setminus B^d_{R(\eta')})} + \|v\|_{L^{p+1}(\mathbb{R}^d \setminus B^d_{R(\eta')})}$$

for all $\eta' \in (0, \eta]$, i.e. $v_n \to v$ in $L^{p+1}(\mathbb{R}^d)$, in particular

$$\|v\|^{p+1}_{L^{p+1}(\mathbb{R}^d)} = W_{\max}.$$

Now by weak lower semi-continuity $\|v\|_{L^2(\mathbb{R}^d)} = \|\nabla v\|_{L^2(\mathbb{R}^d)} \leq 1$,
and on the other hand

$$\|v\|^{p+1}_{L^{p+1}(\mathbb{R}^d)} \leq W_{\max} \|v\|^{4/d}_{L^2(\mathbb{R}^d)} \|\nabla v\|^2_{L^2(\mathbb{R}^d)},$$

which gives

$$\|v\|_{L^2(\mathbb{R}^d)} = \|\nabla v\|_{L^2(\mathbb{R}^d)} = 1,\ W[v] = W_{\max}$$

and $v \geq 0$ since $v_n \geq 0$ for all $n \in \mathbb{N}$. □

Now that we know that maximizers of W do exist, we can exploit the corresponding Euler-Lagrange equations:

Let $v \in H^1(\mathbb{R}^d) \setminus \{0\}$ such that $W[v] = W_{\max}$ and (again by 2.2 and invariance) without loss of generality $v \geq 0$ and

$$\|v\|_{L^2(\mathbb{R}^d)} = \|\nabla v\|_{L^2(\mathbb{R}^d)} = 1,\ \|v\|^{p+1}_{L^{p+1}(\mathbb{R}^d)} = W_{\max}.$$

Determining the functional derivatives of the individual norms and applying the product rule yields

$$\frac{\delta W[v]}{\delta v} = (p+1)v^p - 2W_{\max}\left(\frac{2v}{d} - \triangle v\right),$$

and since v is an extremizer of W, the functional derivative $\frac{\delta W[v]}{\delta v}$ must vanish by the Euler-Lagrange equations (see Appendix C) and we obtain

$$\triangle v + \frac{p+1}{2W_{\max}} v^p = \frac{2}{d} v.$$

Solutions to this nonlinear elliptic equation, which in its general form is given by

$$\triangle u + Au^p = Bu \tag{2.7}$$

with $A, B > 0$, are equivalent up to homogeneous transformation and scaling.
In particular we can define $Q \coloneqq \mu v_\lambda$ with $\mu = (\frac{p+1}{2W_{\max}})^{\frac{1}{p-1}}$ and $\lambda = \sqrt{\frac{d}{2}}$, such that

$$\triangle Q + Q^p = Q, \tag{2.8}$$

$$W[Q] = W[v] = W_{\max}$$

and

$$\|Q\|_{L^2(\mathbb{R}^d)}^{4/d} = \frac{p+1}{2W_{\max}}\|v\|_{L^2(\mathbb{R}^d)} = \frac{p+1}{2W_{\max}}.$$

This gives the best constant in (2.5)

$$W_{\max} = \frac{p+1}{2}\|Q\|_{L^2(\mathbb{R}^d)}^{-4/d}$$

where $Q \geq 0$ is the solution to (2.8) of maximal L^2-norm.
Note that equation (2.8) is precisely equation (2.1) with $\omega = 1$ and hence Q is the Ground State.

The Ground State has been shown to be unique in general dimension d by Kwong [7] in 1989. A particularly simple proof of this result by McLoad [9] can be found in [15].

Theorem 2.6. *The positive solution $Q \in H^1(\mathbb{R}^d) \setminus \{0\}$ of 2.8 is unique up to translation. Moreover Q is strictly positive, smooth, exponentially decaying and radial (up to translation).*

In dimension 1 the Ground State is explicitly known:

$$Q(x) = \left(\frac{3}{\cosh(2x)^2}\right)^{1/4}.$$

Corollary 2.7. (Sharp Gagliardo-Nirenberg inequality) *Let $p = 1 + \frac{4}{d}$, $u \in H^1(\mathbb{R}^d)$. Then*

$$\frac{1}{p+1}\|u\|_{L^{p+1}(\mathbb{R}^d)}^{p+1} \leq \frac{1}{2}\|Q\|_{L^2(\mathbb{R}^d)}^{-\frac{4}{d}}\|\nabla u\|_{L^2(\mathbb{R}^d)}^2\|u\|_{L^2(\mathbb{R}^d)}^{\frac{4}{d}}.$$

Corollary 2.8. (Variational characterization of the Ground State) *Let $p = 1 + \frac{4}{d}$, $u \in H^1(\mathbb{R}^d)$ with $E[u] = 0$ and $\|u\|_{L^2(\mathbb{R}^d)} = \|Q\|_{L^2(\mathbb{R}^d)}$. Then there exist $x_0, \gamma \in \mathbb{R}$, $\lambda > 0$ such that*

$$u(x) = e^{i\gamma}\lambda^{\frac{d}{2}}Q(\lambda(x - x_0))$$

Proof. First suppose $u \geq 0$. Then u is a maximizer of W and hence solves 2.7 for some $A, B > 0$, i.e.

$$u(x) = \mu\lambda^{\frac{d}{2}}Q(\lambda(x - x_0))$$

for some $\mu, x_0 \in \mathbb{R}, \lambda > 0$ by Theorem 2.6. But from $\|u\|_{L^2(\mathbb{R}^d)} = \|Q\|_{L^2(\mathbb{R}^d)}$ we have $\mu = 1$, i.e.

$$u(x) = \lambda^{\frac{d}{2}} Q(\lambda(x - x_0))$$

for some $x_0 \in \mathbb{R}, \lambda > 0$.

Now for a general complex-valued function u, by Lemma 2.2 $E[|u|] \leq E[u] = 0$ and by Corollary 2.7 $E[|u|] \geq 0$, hence $E[|u|] = 0 = E[u]$ and

$$|u(x)| = \lambda^{\frac{d}{2}} Q(\lambda(x - x_0))$$

for some $x_0 \in \mathbb{R}, \lambda > 0$.

Writing $u(x) = |u(x)|e^{i\gamma(x)}$ we have

$$\begin{aligned} |\nabla u(x)|^2 &= |\nabla(|u(x)|e^{i\gamma(x)})|^2 = |\nabla|u(x)|e^{i\gamma(x)} + i|u(x)|e^{i\gamma(x)}\gamma'(x)|^2 \\ &= |\nabla|u(x)||^2 + |u(x)|^2|\gamma'(x)|^2 \end{aligned}$$

and since $E[|u|] = E[u]$ we conclude $\gamma = const.$ □

Remark. Note that this characterization holds for any function $H^1(\mathbb{R}^d)$, not only to solutions of p-NLS. Merely the energy- and L^2 -condition already determine the shape of such a function.

Along the way we obtain a sufficient condition for global existence of solutions from Corollary (2.7):

Corollary 2.9. *Let $p = 1 + \frac{4}{d}$, $u \in H^1(\mathbb{R}^d)$ with $\|u_0\|_{L^2(\mathbb{R}^d)} < \|Q\|_{L^2(\mathbb{R}^d)}$. Then the corresponding solution u to (1.9) is a global solution.*

Proof. By Corollary (2.7) and L^2-conservation we have

$$E[u](0) = E[u](t) \geq \frac{1}{2}\|\nabla u(t,.)\|^2_{L^2(\mathbb{R}^d)}(1 - \|u_0\|^{\frac{4}{d}}_{L^2(\mathbb{R}^d)}\|Q\|^{-\frac{4}{d}}_{L^2(\mathbb{R}^d)}) = C\|\nabla u(t,.)\|^2_{L^2(\mathbb{R}^d)} \text{ for all } t$$

for some constant $C > 0$ and hence we have a uniform bound in time on $\|u(t,.)\|_{H^1(\mathbb{R}^d)}$. □

This motivates the investigation of solutions to (1.9) with $0 < \|u_0\|_{L^2(\mathbb{R}^d)} - \|Q\|_{L^2(\mathbb{R}^d)} < \alpha_0$ for some small $\alpha_0 > 0$.

3 A blow-up result in dimension 1

From now on we fix $d = 1$ and denote $L^p = L^p(\mathbb{R})$, $H^1 = H^1(\mathbb{R})$.
We consider the one-dimensional power-nonlinear Schrödinger equation

$$\begin{cases} i\partial_t u(t,x) = -\triangle u(t,x) - |u(t,x)|^4 u(t,x), \\ \quad u(0,.) = u_0 \in H^1. \end{cases} \tag{3.1}$$

In this Section we will prove the following result from "*The blow-up dynamic and upper bound on the blow-up rate for critical nonlinear Schrödinger equation*" [10], published by Frank Merle and Pierre Raphael in 2005, for the case of initial data $u_0 \in H^1_{\text{even}}$, the space of even H^1-functions:

Theorem 3.1. *There exists some $\alpha^* > 0$ and a constant $C^* > 0$ such that for all $u_0 \in H^1_{\text{even}}$ satisfying*

$$0 < \|u_0\|_{L^2}^2 - \|Q\|_{L^2}^2 < \alpha^* \tag{3.2}$$

and

$$E_0 = E[u_0] < 0, \tag{3.3}$$

the corresponding solution u to (3.1) blows up in finite time, i.e. there exists some $T \in (0, \infty)$ such that

$$\lim_{t \to T} \|u(t,.)'\|_{L^2} = \infty.$$

Moreover for t close to T

$$\|u(t,.)'\|_{L^2} \leq \frac{C^*}{\sqrt{|E_0|}(T-t)}.$$

The proof of this result heavily relies on a positivity property of a quadratic form (see Proposition 3.11), which is conjectured to hold based on numerical estimates in [10]. In Sections 5 and 6 we will give a rigorous proof of Proposition 3.11 using a pseudo-spectral method.

Outline of the proof

- In Section 3.1 we decompose the solution u into a modulation of the Ground State plus a perturbation ε which is small in H^1. More precisely, the variational characterization of the Ground State allows us to find time-dependent scaling and phase-shift parameters λ and γ, such that the corresponding modulation of u can be regarded as a perturbation of the Ground State. In particular, while u might eventually even blow up, its modulation remains close to the Ground State and ε is small in H^1 throughout the whole time-evolution of u.

The key feature of the ε-decomposition is that the scaling parameter is inverse proportional to the L^2-norm of the gradient of u and thus the investigation of blow-up dynamics of u can be traced back to the behaviour of the scaling parameter.
By a time-reparametrization $t \mapsto = \int_0^t \frac{1}{\lambda^2}$ we simplify the differential equation for ε such that the linear terms can be described by the linear operator close to the Ground State L plus terms arising from the modulation dynamics.

- The main task in this proof is to relate the behavior of the scaling parameter to the L^2-inner product $\big(\varepsilon_2 \big| Q_1\big)$, where ε_2 denotes the imaginary part of ε. This is achieved by imposing orthogonality conditions on ε which lead to cancellations of the linear terms in the time derivative of $\big(\varepsilon_2 \big| Q_1\big)$ and expressing the quadratic terms by a quadratic form H which can essentially be bounded from below in terms of the norms $\|\varepsilon\|_{L^2_w}^2 + \|\partial_1 \varepsilon\|_{L^2}^2$[2], where $\|\varepsilon\|_{L^2_w}$ is a localized version of the L^2-norm, and in particular turns out to be controlled by the time-derivative of $\big(\varepsilon_2 \big| Q_1\big)$ in a time-averaging sense.
This will allow to determine the asymptotic sign of $\big(\varepsilon_2 \big| Q_1\big)$ and yield an almost-monotonicity property for λ, proving (finite or infinite) blow-up.[3]

- The blow-up bound is proven by choosing suitable time-intervals on which the variation of λ is controlled, leading to a uniform upper bound on λ in terms of $\big(\varepsilon_2 \big| Q_1\big)$.
Using this upper bound and choosing a sequence of times t_n such that $\lambda(t_n) = 2^{-n}$ we determine a bound on the length of time intervals $|t_{n+1} - t_n| \lesssim 2^{-n}$, proving finite time blow-up, and obtain a lower bound on $\lambda(t)$ for t close to the blow-up time T, or equivalently an upper bound on $\|u(t,.)'\|_{L^2}$.

3.1 ε-decomposition

We denote the modulation of a function $u \in H^1$ as

$$M_{\lambda,\gamma,x_0}(u) \coloneqq e^{-i\gamma} \lambda^{1/2} u(\lambda(. - x_0))$$

and

$$\alpha(u) \coloneqq \|u\|_{L^2}^2 - \|Q\|_{L^2}^2.$$

Lemma 3.2. (Existence of a modulation close to the Ground State)
For any $\delta_0 > 0$ there exists some $\alpha_0 > 0$, such that for all $u \in H^1$ with

$$\alpha(u) < \alpha_0 \text{ and } E[u] < 0$$

there exist some $\gamma,\ x_0 \in \mathbb{R}$ such that

$$\|M_{\lambda,\gamma,x_0}(u) - Q\|_{H^1} < \delta_0$$

[2]Throughout this thesis we denote ∂_j as the derivative with respect to the j^{th} slot of a function, starting to count at 0.
[3]Note that ε is a time and space dependent function. Inner products or norms of time-dependent functions are to be understood as spatial inner products or norms which depend on time.

with

$$\lambda = \|Q'\|_{L^2}/\|u'\|_{L^2}.$$

Proof. Let $(u_n)_{n\in\mathbb{N}} \subset H^1$ with

$$\lim_{n\to\infty} \alpha(u_n) = 0 \text{ and } \lim_{n\to\infty} E[u_n]/\|u_n\|_{L^2}^2 \leq 0.$$

It suffices to show that there exist some $\gamma, x_0 \in \mathbb{R}$ such that the corresponding modulation of u_n with γ, x_0 and $\lambda_n \coloneqq \|Q'\|_{L^2}/\|u_n'\|_{L^2}$ converges to Q in H^1 as $n \to \infty$.

We suitably scale the individual u_n by $v_n = \lambda_n^{1/2} u_n(\lambda_n(.))$ such that

$$\|v_n\|_{L^2}^2 = \|u_n\|_{L^2}^2, \qquad \|v_n'\|_{L^2}^2 = \lambda_n^2\|u_n'\|_{L^2}^2, \qquad \|v_n\|_{L^6}^6 = \lambda_n^2\|u_n\|_{L^6}^6,$$

and hence

$$\lim_{n\to\infty} \alpha(v_n) = 0, \qquad \lim_{n\to\infty} E[v_n] \leq 0, \qquad \|v_n'\|_{L^2} = \|Q'\|_{L^2} \text{ for all } n.$$

On the other hand by (2.7) we have

$$\lim_{n\to\infty} E[v_n] \geq \lim_{n\to\infty} \frac{1}{2}\|v_n'\|_{L^2}(1 - \|v_n\|_{L^2}^4/\|Q\|_{L^2}^4) = 0$$

and hence $\lim_{n\to\infty} E[v_n] = 0$.

By the same compactness argument as in the proof of Theorem 2.5 we conclude $v_n \to v$ in H^1 for some v with $E[v] = 0$ and $\|v_n'\|_{L^2} = \|Q'\|_{L^2}$, i.e. $v = e^{i\gamma}Q(. + x_0)$ for some $\gamma, x_0 \in \mathbb{R}$ and

$$e^{-i\gamma}\lambda_n u_n(\lambda_n(. - x_0)) \xrightarrow{n\to\infty} Q \text{ in } H^1.$$

□

Remark. Note that in the proof above the condition $E[u] < 0$ is crucial for H^1-convergence.

From now on we will restrict to the case $u \in H^1_{\text{even}}$ such that we can disregard space translation and the statement above holds with $M_{\lambda,\gamma} \coloneqq M_{\lambda,\gamma,0}$ and we define

$$\begin{aligned}
\varepsilon(\lambda,\gamma,u) &\coloneqq M_{\lambda,\gamma}(u) - Q \\
\varepsilon_1(\lambda,\gamma,u) &\coloneqq \mathrm{Re}(\varepsilon(\lambda,\gamma,u)), \\
\varepsilon_2(\lambda,\gamma,u) &\coloneqq \mathrm{Im}(\varepsilon(\lambda,\gamma,u)).
\end{aligned}$$

As the next result shows, we can even put some constraints on such a modulation of u, such that the corresponding difference to the Ground State $\varepsilon(\lambda,\gamma,u)$ satisfies certain orthogonality conditions, while still maintaining smallness in H^1 and $\lambda \sim \|Q'\|_{L^2}/\|u'\|_{L^2}$ (in the sense of Lemma 3.2).

Lemma 3.3. (Imposing orthogonality conditions) *Let $f_1, f_2 \in H^1$ with*

$$\big(Q/2 + (.)Q'\big|f_1\big) \neq 0 \text{ and } \big(Q\big|f_2\big) \neq 0, \tag{3.4}$$

where $\big(.\big|.\big)$ denotes the L^2-inner product.
Then for any $\delta_0 > 0$, there exists some $\alpha_0 > 0$ such that for all $u \in H^1_{\text{even}}$ with

$$\alpha(u) < \alpha_0 \text{ and } E[u] < 0$$

there exist some $\lambda > 0$, $\gamma \in \mathbb{R}$ such that

$$\big(\varepsilon_1(\lambda,\gamma,u)\big|f_1\big) = \big(\varepsilon_2(\lambda,\gamma,u)\big|f_2\big) = 0$$

and

$$\left|1 - \lambda\frac{\|u'\|_{L^2}}{\|Q'\|_{L^2}}\right| + \|\varepsilon(\lambda,\gamma,u)\|_{H^1} < \delta_0.$$

Proof. We define

$$\Phi:\ (0,\infty)\times\mathbb{R}\times H^1_{\text{even}} \to \mathbb{R}^2,$$

$$(\lambda,\gamma,u) \mapsto \big(\big(\varepsilon_1(\lambda,\gamma,u)\big|f_1\big),\ \big(\varepsilon_2(\lambda,\gamma,u)\big|f_2\big)\big),$$

such that for $u_1 = \mathrm{Re}(u)$, $u_2 = \mathrm{Im}(u)$

$$\begin{aligned}
\partial_\lambda\varepsilon_1(\lambda,\gamma,u)\big|_{\lambda=1,\gamma=0} &= \frac{u_1}{2} + (.)u_1', \qquad & \partial_\gamma\varepsilon_1(\lambda,\gamma,u)\big|_{\lambda=1,\gamma=0} &= u_2,\\
\partial_\lambda\varepsilon_2(\lambda,\gamma,u)\big|_{\lambda=1,\gamma=0} &= \frac{u_2}{2} + (.)u_2', \qquad & \partial_\gamma\varepsilon_1(\lambda,\gamma,u)\big|_{\lambda=1,\gamma=0} &= -u_1,
\end{aligned}$$

and hence the Frechet derivative of Φ with respect to (λ,γ) at the point $(\lambda,\gamma,u) = (1,0,Q)$ given by

$$D(\Phi)_{\lambda,\gamma}\big|_{\lambda=1,\gamma=0,u=Q} = \begin{bmatrix} \frac{\partial\Phi_1}{\partial\lambda} & \frac{\partial\Phi_1}{\partial\gamma} \\ \frac{\Phi_2}{\partial\lambda} & \frac{\Phi_2}{\partial\gamma} \end{bmatrix}\Bigg|_{\lambda=1,\gamma=0,u=Q} = \begin{bmatrix} \left(\frac{Q}{2} + (.)Q'\big|f_1\right) & 0 \\ 0 & -(Q\big|f_2) \end{bmatrix}$$

is non-vanishing by assumption.
By the implicit function theorem for Banach spaces, there exist some neighbourhood $U_R = \{u \in H^1 : \|u-Q\|_{H^1} < R\}$ of Q in H^1, some neighbourhood V of $(1,0)$ in $\mathbb{R}^2$ and a Frechet-differentiable map $F : U_R \to V$ such that for all $u \in U_R$ there exist unique $(\lambda,\gamma) \in V$ with $\big(\varepsilon_1(\lambda,\gamma,u)\big|f_1\big) = \big(\varepsilon_2(\lambda,\gamma,u)\big|f_2\big) = 0$.

By Lemma (3.2), there is some α_0 such that for any u with $E[u] < 0$ and $\alpha(u) < \alpha_0$, we obtain $\|M_{\tilde{\lambda},\tilde{\gamma}}(u) - Q\|_{H^1} < R$ for some $\tilde{\gamma} \in \mathbb{R}$ and $\tilde{\lambda} = \|Q'\|_{L^2}/\|u'\|_{L^2}$, and hence there are unique $\lambda > 0$, $\gamma \in \mathbb{R}$ such that

$$\varepsilon(\lambda, \gamma, M_{\tilde{\lambda},\tilde{\gamma}}(u)) = \varepsilon(\lambda\tilde{\lambda}, \gamma + \tilde{\gamma}, u)$$

satisfies

$$\big(\varepsilon_1(\lambda\tilde{\lambda}, \gamma + \tilde{\gamma}, u)\big|f_1\big) = \big(\varepsilon_2(\lambda\tilde{\lambda}, \gamma + \tilde{\gamma}, u)\big|f_2\big) = 0.$$

Moreover, by continuity of F we have $\lambda \to 0$ and $\gamma \to 1$ as $\alpha_0 \to 0$, and hence by choosing α_0 sufficiently small:

$$\left|1 - \lambda\tilde{\lambda}\frac{\|u'\|_{L^2}}{\|Q'\|_{L^2}}\right| + \|\varepsilon(\lambda\tilde{\lambda}, \gamma + \tilde{\gamma}, u)\|_{H^1} = |1 - \lambda| + \|\varepsilon(\lambda\tilde{\lambda}, \gamma + \tilde{\gamma}, u)\|_{H^1} < \delta,$$

i.e. the parameters $\lambda\tilde{\lambda}$ and $\gamma + \tilde{\gamma}$ do the job. □

So far, this decomposition applies to functions $u \in H^1_{\text{even}}$. However, since for a strong H^1-solution u of (1.9) with $u_0 \in H^1_{\text{even}}$

- $t \mapsto u(t, .) \in H^1$ is continuous,
- $\alpha(u(t, .)) = \alpha(u_0)$, $E[u(t, .)] = E[u_0]$
- the modulation we just derived depends continuously on u,
- $u(t, .)$ remains even throughout the time evolution

we obtain a decomposition for solutions u of (3.1) which is continuous in t:

Theorem 3.4. *Let $\delta_0 > 0$, α_0 as in Lemma 3.3, u a strong H^1-solution to (3.1) with initial data $u_0 \in H^1_{\text{even}}$ such that*

$$\alpha(u_0) < \alpha_0 \text{ and } E[u_0] < 0$$

and $f_1, f_2 \in H^1$ such that (3.4) is satisfied. Then there exist continuous functions $\lambda : (-T_-, T_+) \to (0, \infty)$, $\gamma : (-T_-, T_+) \to \mathbb{R}$ such that

$$\varepsilon(t, x) \coloneqq e^{i\gamma(t)}\lambda(t)^{1/2}u(t, \lambda(t)x) - Q(x)$$

satisfies

$$\big(\varepsilon_1(t, .)\big|f_1\big) = \big(\varepsilon_2(t, .)\big|f_2\big) = 0$$

and

$$\left|1 - \lambda(t)\frac{\|u(t, .)'\|_{L^2}}{\|Q'\|_{L^2}}\right| + \|\varepsilon(t, .)\|_{H^1} < \delta_0$$

for all $t \in (-T_-, T_+)$, where T_-, $T_+ \in (0, \infty)$ denote the maximal negative and positive times of existence of u.

Remark. In this construction, neither the modulation of u, nor ε is a solution to (1.9). In particular we cannot directly apply conservation laws of (1.9) to any of them. Still, by construction, $\varepsilon(t,.)$ will remain small in H^1 uniformly in time.

Moreover note that δ_0 depends continuously on $\alpha(u_0)$ and we will refine the smallness condition on $\alpha(u_0)$ multiple times throughout the analysis according to how small we need δ_0.

We apply Theorem 3.4 to an even initial condition u_0 satisfying (3.2) and (3.3), imposing orthogonality conditions adapted to the analysis of the time-derivative of $\big(\varepsilon_2\big|Q_1\big)$ (which turns out to be strongly related to the dynamics of the scaling parameter λ, see Section 3.4): On the one hand they lead to cancellation of linear terms (see (3.16)) and on the other hand they allow us to control the quadratic terms by means of a quadratic form H (see Proposition 3.11 and Corollary 3.12).

Let

$$Q_1(x) \coloneqq \frac{Q(x)}{2} + xQ'(x), \qquad Q_2(x) \coloneqq \frac{Q_1(x)}{2} + xQ_1'(x),$$

then

$$\big(\tfrac{Q}{2} + (.)Q'\big|Q_1\big) = \|Q_1\|_{L^2}^2 \text{ and } \big(Q\big|Q_2\big) = -\|Q_1\|_{L^2}^2$$

and hence we obtain a decomposition

$$\varepsilon(t,x) = e^{i\gamma(t)}\lambda(t)^{1/2}u(t,\lambda(t)x) - Q(x) \tag{3.5}$$

with

$$\big(\varepsilon_1(t,.)\big|Q_1\big) = \big(\varepsilon_2(t,.)\big|Q_2\big) = 0 \tag{3.6}$$

and

$$\left|1 - \lambda(t)\frac{\|u(t,.)'\|_{L^2}}{\|Q'\|_{L^2}}\right| + \|\varepsilon(t,.)\|_{H^1} < \delta_0 \tag{3.7}$$

for $t \in (-T_-, T_+)$.

3.2 Time-reparametrization

In order to get rid of as many linear terms as possible in the differential equation for ε, we want the scaling in the modulation of u to be as close to an admissable scaling (see Section 1) as possible. For that aim we reparametrise ε by introducing a new time scale

$$s(t) \coloneqq \int_0^t \frac{1}{\lambda(\tau)^2}d\tau. \tag{3.8}$$

Remark. It follows that $\{s(t) :\ t \in (-T_-, T_+)\} = \mathbb{R}$:
From the condition $E_0 < 0$ and Gagliardo-Nirenberg (Corollary 2.7) we obtain

$$0 > E_0 = \frac{1}{2}\|u(t,.)'\|_{L^2}^2 - \frac{1}{6}\|u(t,.)\|_{L^6}^6 > -C\|u(t,.)'\|_{L^2}^2,$$

for some $C > 0$, in particular λ is uniformly bounded from above for all $t \in (-T_-, T_+)$.
For $T_+ = \infty$, it follows that $\{s(t) :\ t \in [0, T_+)\} = [0, \infty)$. If u blows up at finite time $T_+ < \infty$, then the lower bound on the blow-up rate (1.6)

$$\|u(t,.)'\|_{L^2} \gtrsim \frac{1}{\sqrt{T_+ - t}}$$

gives $\lambda(t) \lesssim \sqrt{T_+ - t}$ for t close to T_+ and again $\{s(t) :\ t \in [0, T_+)\} = [0, \infty)$. The claim follows by the same argument for T_-.

To determine the differential equation for the reparametrized function ε, we define a transformation of variables by

$$\psi(t) \coloneqq \int_0^t \frac{1}{\lambda(\tau)^2} d\tau, \qquad \bar{\lambda}(s) \coloneqq \lambda(\psi^{-1}(s)), \qquad \bar{\gamma}(s) \coloneqq \gamma(\psi^{-1}(s)),$$

such that $\psi'(t) = \lambda(t)^{-2} = \bar{\lambda}(\psi(t))^{-2}$.
Recall that by (3.5)

$$u(t,x) = e^{-i\gamma(t)}\lambda(t)^{-1/2}\left(\varepsilon\left(t, \frac{x}{\lambda(t)}\right) + Q\left(\frac{x}{\lambda(t)}\right)\right).$$

Using the Ansatz

$$\begin{aligned} u(t,x) &= e^{-i\gamma(t)}\lambda(t)^{-1/2}\left(\varepsilon\left(\psi(t), \frac{x}{\lambda(t)}\right) + Q\left(\frac{x}{\lambda(t)}\right)\right) \\ &= e^{-i\bar{\gamma}(\psi(t))}\bar{\lambda}(\psi(t))^{-1/2}\left(\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) + Q\left(\frac{x}{\bar{\lambda}(\psi(t))}\right)\right) \end{aligned}$$

and the differential equation (1.9) for u we obtain

$$\begin{aligned} \partial_0\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) &= i\bar{\gamma}'(\psi(t))\left(\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) + Q\left(\frac{x}{\bar{\lambda}(\psi(t))}\right)\right) + \frac{\bar{\lambda}'(\psi(t))}{2\bar{\lambda}(\psi(t))}\left(\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) + Q\left(\frac{x}{\bar{\lambda}(\psi(t))}\right)\right) \\ &\quad + \frac{\bar{\lambda}'(\psi(t))x}{\bar{\lambda}(\psi(t))^2}\left(\partial_1\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) + Q'\left(\frac{x}{\bar{\lambda}(\psi(t))}\right)\right) + i\left(\partial_1^2\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) + Q''\left(\frac{x}{\bar{\lambda}(\psi(t))}\right)\right) \\ &\quad + i\left|\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) + Q\left(\frac{x}{\bar{\lambda}(\psi(t))}\right)\right|^4\left(\varepsilon\left(\psi(t), \frac{x}{\bar{\lambda}(\psi(t))}\right) + Q\left(\frac{x}{\bar{\lambda}(\psi(t))}\right)\right). \end{aligned}$$

In terms of new variables s and y this gives

$$\partial_0\varepsilon(s,y) = i\bar{\gamma}'(s)\left(\varepsilon(s,y)+Q(y)\right) + \frac{\bar{\lambda}'(s)}{2\bar{\lambda}(s)}\left(\varepsilon\left(s,y\right)+Q\left(y\right)\right) + \frac{\bar{\lambda}'(s)y}{\bar{\lambda}(s)}\left(\partial_1\varepsilon\left(s,y\right)+Q'\left(y\right)\right)$$
$$+ i\left(\partial_1^2\varepsilon\left(s,y\right)+Q''\left(y\right)\right) + i\left|\varepsilon\left(s,y\right)+Q\left(y\right)\right|^4\left(\varepsilon\left(s,y\right)+Q\left(y\right)\right)$$

and we obtain the following differential equations for $\varepsilon_1 = \mathrm{Re}(\varepsilon)$ and $\varepsilon_2 = \mathrm{Im}(\varepsilon)$:

$$\begin{cases} \partial_s\varepsilon_1(s,y) = -\partial_y^2\varepsilon_2(s,y) - \varepsilon_2(s,y)|\varepsilon(s,y)+Q(y)|^4 - \bar{\gamma}'(s)\varepsilon_2(s,y) \\ \qquad\qquad + \dfrac{\bar{\lambda}'(s)}{2\bar{\lambda}(s)}(\varepsilon_1(s,y)+Q(y)) + \dfrac{\bar{\lambda}'(s)y}{\bar{\lambda}(s)}(\partial_y\varepsilon_1(s,y)+Q'(y)), \\ \partial_s\varepsilon_2(s,y) = \partial_y^2\varepsilon_1(s,y) + Q''(y) + (\varepsilon_1(s,y)+Q(y))|\varepsilon(s,y)+Q(y)|^4 \\ \qquad\qquad + \bar{\gamma}'(s)(\varepsilon_1(s,y)+Q(y)) + \dfrac{\bar{\lambda}'(s)}{2\bar{\lambda}(s)}\varepsilon_2(s,y) + \dfrac{\bar{\lambda}'(s)y}{\bar{\lambda}(s)}\partial_y\varepsilon_2(s,y)). \end{cases}$$

So far, writing our decomposition in s and y, we have

$$Q(y)+\varepsilon(s,y) = e^{i\bar{\gamma}(s)}\bar{\lambda}(s)^{1/2}u(\psi^{-1}(s),\bar{\lambda}(s)y)$$

and with $\tilde{\gamma}(s) \coloneqq -s - \bar{\gamma}(s)$,

$$e^{is}(Q(y)+\varepsilon(s,y)) = e^{-i\tilde{\gamma}(s)}\bar{\lambda}(s)^{1/2}u(\psi^{-1}(s),\bar{\lambda}(s)y). \tag{3.9}$$

Remark. Note that if the modulation parameters λ and γ were constant, then in particular $\psi(t) = \bar{\lambda}^{-2}t$ and $\psi^{-1}(s) = \bar{\lambda}^2 s$, and hence the left hand side of (3.9) would be an invariant transformation of u, hence satisfy (3.1). In this case, the linear terms of $\partial_s\varepsilon(s,y)$ would be precisely $L\varepsilon(s)$, where L is the linearized operator close to the Ground State (2.4). While we clearly cannot expect λ and γ to be constant, the time-reparametrization and phase shift $\bar{\gamma} \mapsto \tilde{\gamma}$ allows us to write the linear terms of $\partial_s\varepsilon(s,y)$ as $L\varepsilon(s,y)$ plus terms which appear due to the dynamics of the modulation parameters.

From now on, we will for simplicity denote $\bar{\lambda}$ as λ and $\bar{\gamma}$ as γ if not mentioned otherwise.

We define

$$R_1(\varepsilon)(s,y) \coloneqq (Q(y)+\varepsilon_1(s,y))|Q(y)+\varepsilon(s,y)|^4 - Q(y)^5 - 5Q(y)^4\varepsilon_1(s,y), \tag{3.10}$$
$$R_2(\varepsilon)(s,y) \coloneqq \varepsilon_2(s,y)|Q(y)+\varepsilon(s,y)|^4 - \varepsilon_2(s,y)Q(y)^4, \tag{3.11}$$

and obtain

$$\begin{aligned}
\partial_s\varepsilon_1(s,y) =& -\partial_y^2\varepsilon_2(s,y) - \varepsilon_2(s,y)|Q(y)+\varepsilon(s,y)|^4 - \gamma'\varepsilon_2(s,y) + \frac{\lambda'(s)}{\lambda(s)}\left(\frac{Q(y)}{2}+yQ'(y)\right) + \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_1(s,y)}{2}+y\partial_y\varepsilon_1(s,y)\right)\\
=& -\partial_y^2\varepsilon_2(s,y) - R_2(\varepsilon)(s,y) + Q(y)^4\varepsilon_2(s,y) + \tilde{\gamma}'(s)\varepsilon_2(s,y) + \varepsilon_2(s,y)\\
&+ \frac{\lambda'(s)}{\lambda(s)}Q_1(y) + \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_1(s,y)}{2}+y\partial_y\varepsilon_1(s,y)\right),\\
\partial_s\varepsilon_2(s,y) =& Q''(y) + \partial_y^2\varepsilon_1(s,y) + (Q(y)+\varepsilon_1(s,y))|Q(y)+\varepsilon(s,y)|^4\\
&- \tilde{\gamma}'(s)Q(y) - Q(y) - \tilde{\gamma}'(s)\varepsilon_1(s,y) - \varepsilon_1(s,y) + \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_2(s,y)}{2}+y\partial_y\varepsilon_2(s,y)\right)\\
=& \partial_y^2\varepsilon_1(s,y) + R_1(\varepsilon)(s,y) + 5Q(y)^4\varepsilon_1(s,y) - \tilde{\gamma}'(s)Q(y) - \tilde{\gamma}'(s)\varepsilon_1(s,y) - \varepsilon_1(s,y) + \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_2(s,y)}{2}+y\partial_y\varepsilon_2(s,y)\right),
\end{aligned}$$

where we used $\gamma' = -\tilde{\gamma}' - 1$ and $Q'' + Q^5 = Q$, and hence

$$\begin{cases}
\partial_s\varepsilon_1(s,y) = L_-\varepsilon_2(s,y) + \dfrac{\lambda'(s)}{\lambda(s)}Q_1(y) + \tilde{\gamma}'(s)\varepsilon_2(s,y) + \dfrac{\lambda'(s)}{\lambda(s)}\left(\dfrac{\varepsilon_1(s,y)}{2}+y\partial_y\varepsilon_1(s,y)\right) - R_2(\varepsilon)(s,y),\\
\partial_s\varepsilon_2(s,y) = -L_+\varepsilon_1(s,y) - \tilde{\gamma}'(s)Q(y) - \tilde{\gamma}'(s)\varepsilon_1(s,y) + \dfrac{\lambda'(s)}{\lambda(s)}\left(\dfrac{\varepsilon_2(s,y)}{2}+y\partial_y\varepsilon_2(s,y)\right) + R_1(\varepsilon)(s,y).
\end{cases} \tag{3.12}$$

Remark. In contrast to classical approaches to equations like (3.12), where one would aim for solving the equation or showing that the perturbation ε vanishes asymptotically, this is not the case here. We already have full control in the time evolution of ε. The only thing we are interested in is the scaling parameter λ.

3.3 Conservation laws and a priori bounds

Lemma 3.5. (ε-version of L^2-conservation) *We have*

$$\|\varepsilon(s,.)\|_{L^2}^2 = \alpha(u_0) - 2\big(\varepsilon_1(s,.)\big|Q\big)$$

for all $s \in \mathbb{R}$.

Proof. From the L^2-conservation (1.4) for u we have

$$\|u_0\|_{L^2}^2 = \|u(\psi^{-1}(s),.)\|_{L^2}^2 = \|Q+\varepsilon(s,.)\|_{L^2}^2 = \|\varepsilon(s,.)\|_{L^2}^2 + \|Q\|_{L^2}^2 + 2\big(\varepsilon_1(s,.)\big|Q\big),$$

and hence,

$$\|\varepsilon(s,.)\|_{L^2}^2 = \|u_0\|_{L^2}^2 - \|Q\|_{L^2}^2 - 2\big(\varepsilon_1(s,.)\big|Q\big) = \alpha(u_0) - 2\big(\varepsilon_1(s,.)\big|Q\big).$$

□

Lemma 3.6. (ε-version of energy-conservation) *We have*

$$-2|E_0|\lambda(s)^2 = -\frac{1}{3}\int_{\mathbb{R}} F(\varepsilon)(s,y)dy + \|\varepsilon(s,.)'\|_{L^2}^2 - 2\big(\varepsilon_1(s,.)\big|Q\big) - 5\big(\varepsilon_1(s,.)^2\big|Q^4\big) - \big(\varepsilon_2(s,.)^2\big|Q^4\big)$$

for all $s \in \mathbb{R}$, where

$$F(\varepsilon)(s,y) \coloneqq |\varepsilon(s,y)+Q(y)|^6 - Q(y)^6 - 6Q(y)^5\varepsilon_1(s,y) - 15Q(y)^4\varepsilon_1(s,y) - 3Q(y)^4\varepsilon_2(s,y)^2$$

denotes the cubic terms in ε of $|Q(y)+\varepsilon(s,y)|^6$.

Proof. From the energy conservation (1.5) for u we have

$$E_0 = E[u](\psi^{-1}(s)) = \lambda(s)^{-2}E[Q+\varepsilon](s)$$

and since $E_0 < 0$

$$\begin{aligned}
-2|E_0|\lambda(s)^2 = 2E[Q+\varepsilon](s) &= \|Q'+\varepsilon(s,.)'\|_{L^2}^2 - \frac{1}{3}\|Q+\varepsilon(s,.)\|_{L^6}^6 \\
&= \|Q'\|_{L^2}^2 + 2\big(\varepsilon_1(s,.)'\big|Q'\big) + \|\varepsilon(s,.)'\|_{L^2}^2 - \frac{1}{3}\|Q+\varepsilon(s,.)\|_{L^6}^6 \\
&= \|Q'\|_{L^2}^2 - 2\big(\varepsilon_1(s,.)\big|Q''\big) + \|\varepsilon(s,.)'\|_{L^2}^2 - \frac{1}{3}\|Q+\varepsilon(s,.)\|_{L^6}^6.
\end{aligned}$$

Now inserting

$$\|Q+\varepsilon(s,.)\|_{L^6}^6 = \int F(\varepsilon)(s,y)dy + \|Q\|_{L^6}^6 + 6\big(Q^5\big|\varepsilon_1(s,.)\big) + 15\big(Q^4\big|\varepsilon_1(s,.)^2\big) + 3\big(Q^4\big|\varepsilon_2(s,.)^2\big)$$

and using $E[Q]=0$ and $Q''+Q^5-Q=0$ gives the claimed identity. □

Definition 3.7. *We define a weighted L^2 norm by*

$$\begin{aligned}
w(y) &\coloneqq e^{-\frac{9}{5}|y|}, \\
\|\varepsilon(s,.)\|_{L^2_w} &\coloneqq \left(\int_{\mathbb{R}} |\varepsilon(s,y)|^2 w(y)dy\right)^{1/2}.
\end{aligned}$$

Remark. This localized version of the L^2-norm is introduced in order to be controlled in terms of the inner product $\big(\varepsilon_2\big|Q_1\big)$ (see Section 3.4), which is clearly not possible using the L^2-norm.

Lemma 3.8. *For any polynomial P, $k \in \mathbb{N}_0$ and δ_0 as in Theorem 3.4, the estimates*

i) $\left|\left(\varepsilon(s,.)\middle|PQ^{(k)}\right)\right| \lesssim \|\varepsilon(s,.)\|_{L^2_w}$

ii) $\left|\left(R(\varepsilon)(s,.)\middle|PQ^{(k)}\right)\right| \lesssim \|\varepsilon(s,.)'\|^2_{L^2} + \|\varepsilon(s,.)\|^2_{L^2_w}$

iii) $\int |F(\varepsilon)(s)| + \left|\left(\tilde{R}_1(\varepsilon)(s,.)\middle|PQ^{(k)}\right)\right| \lesssim \delta_0 \left(\|\varepsilon(s,.)'\|^2_{L^2} + \|\varepsilon(s,.)\|^2_{L^2_w}\right)$

hold for all $s \in \mathbb{R}$, where $R(\varepsilon) \coloneqq R_1(\varepsilon) + iR_2(\varepsilon)$ and $\tilde{R}_1(\varepsilon) \coloneqq R_1(\varepsilon) - 10Q^3\varepsilon_1^2 - 2Q^3\varepsilon_2^2$ denotes the cubic part in ε of $R_1(\varepsilon)$.

Proof. i) Recall that Q and all derivatives $Q^{(k)}$ are exponentially decaying, i.e. $|Q^{(k)}(y)| \lesssim e^{-|y|}$, and for any polynomial P and $\alpha > 0$ we have $|P(y)| \lesssim e^{-\alpha|y|}$. In particular

$$|P(y)Q^{(k)}(y)| \lesssim e^{-\frac{19}{20}|y|},$$

which gives

$$\left|\left(\varepsilon(s,.)\middle|PQ^{(k)}\right)\right| \lesssim \int |\varepsilon(s,y)|e^{-\frac{19}{20}|y|}dy \leq \left(\int |\varepsilon(s,y)|^2 e^{-\frac{9}{5}|y|}dy\right)^{1/2} \left(\int e^{-\frac{1}{10}|y|}dy\right)^{1/2} \lesssim \|\varepsilon(s,.)\|_{L^2_w}$$

ii) Note that all terms in $R(\varepsilon)$ are of the form ε^5 or $\varepsilon^n Q^m$ with $n \geq 2$, $m \leq 3$ and hence we can estimate

$$|R(\varepsilon)| \lesssim (|\varepsilon|^2 Q^3 + |\varepsilon|^5)$$

and

$$\begin{aligned}\left|\left(R(\varepsilon)(s,.)\middle|PQ^{(k)}\right)\right| &\lesssim \int (|\varepsilon(s,y)|^2 Q(y)^3 + |\varepsilon(s,y)|^5) e^{-\frac{19}{20}|y|}dy \\ &\lesssim \int |\varepsilon(s,y)|^2 e^{-\frac{9}{5}|y|}dy + \int |\varepsilon(s,y)|^5 e^{-\frac{19}{20}|y|}dy.\end{aligned}$$

By Gagliardo-Nirenberg (Theorem 2.1) we have

$$\|\varepsilon(s,.)\|_{L^\infty} \lesssim \|\varepsilon(s,.)'\|^{1/2}_{L^2} \|\varepsilon(s,.)\|^{1/2}_{L^2},$$

and hence

$$\begin{aligned}\int |\varepsilon(s,y)|^5 e^{-\frac{19}{20}|y|}dy \lesssim \|\varepsilon(s,.)^5\|_{L^2} &\leq \|\varepsilon(s,.)\|^4_{L^\infty} \|\varepsilon(s,.)\|_{L^2} \lesssim \|\varepsilon(s,.)'\|^2_{L^2} \|\varepsilon(s,.)\|^3_{L^2} \\ &\lesssim \|\varepsilon(s,.)'\|^2_{L^2} \|\varepsilon(s,.)\|^3_{H^1} \leq \|\varepsilon(s,.)'\|^2_{L^2} \delta_0^3 \lesssim \|\varepsilon(s,.)'\|^2_{L^2}.\end{aligned}$$

iii) By the same argument as above we can estimate

$$|F(\varepsilon)| \lesssim (|\varepsilon|^3 Q^3 + |\varepsilon|^6), \qquad |\tilde{R}_1(\varepsilon)| \lesssim (|\varepsilon|^3 Q^2 + |\varepsilon|^5),$$

such that by Corollary 2.7

$$\begin{aligned}\int |F(\varepsilon)(s,y)|dy &\lesssim \int |\varepsilon(s,y)|^3 Q(y)^3 dy + \|\varepsilon\|_{L^6}^6 \lesssim \int |\varepsilon(s,y)|^3 e^{-\frac{9}{5}|y|} dy + \|\varepsilon(s,.)'\|_{L^2}^2 \|\varepsilon(s,.)\|_{L^2}^4 \\ &\lesssim \|\varepsilon(s,.)\|_{L^\infty} \|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2 \|\varepsilon(s,.)\|_{H^1} \\ &\lesssim \delta_0 \left(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2 \right)\end{aligned}$$

and analogously

$$\left| \left(\tilde{R}_1(\varepsilon)(s,.) \middle| P Q^{(k)} \right) \right| \lesssim \int |\varepsilon(s,y)|^3 e^{\frac{9}{5}|y|} dy + \int |\varepsilon(s,y)|^5 e^{\frac{19}{20}|y|} dy \lesssim \delta_0 \|\varepsilon(s,.)\|_{L^2_w}^2 .$$

□

Recall the ε-energy conservation (Lemma 3.6) and note that the only linear term in ε appearing, is the inner product $\left(\varepsilon_1 \middle| Q\right)$. In particular estimating the higher order terms with the previous Lemma provides the following bound.

Corollary 3.9. *For all $s \in \mathbb{R}$ we have*

$$\left| E_0 \lambda(s)^2 + \left(\varepsilon_1(s,.) \middle| Q \right) \right| \lesssim \left(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2 \right).$$

In particular, $\varepsilon(s,.) = 0$ implies $\lambda(s) = 0$.

Proof. From Lemmas 3.6 and 3.8 we obtain

$$\begin{aligned}\left| E_0 \lambda(s)^2 + \left(\varepsilon_1(s,.) \middle| Q \right) \right| &\lesssim \left| \int F(\varepsilon)(s,y) dy \right| + \|\varepsilon(s,.)'\|_{L^2}^2 + \left| \left(\varepsilon_1(s,.)^2 \middle| Q^4 \right) \right| + \left| \left(\varepsilon_2(s,.)^2 \middle| Q^4 \right) \right| \\ &\lesssim \left(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2 \right).\end{aligned}$$

□

Lemma 3.10. (A bound on the modulation parameters)
For all $s \in \mathbb{R}$ we have

$$\left| \frac{\lambda'(s)}{\lambda(s)} \right| + |\tilde{\gamma}(s)| \lesssim \|\varepsilon(s,.)\|_{L^2_w} + \|\varepsilon(s,.)'\|_{L^2}.$$

Proof. By (3.12)

$$\begin{aligned}0 =&\partial_s\big(\varepsilon_1(s,.)\big|Q_1\big) = \big(L_-\varepsilon_2(s,.)\big|Q_1\big) + \frac{\lambda'(s)}{\lambda(s)}\big(Q_1\big|Q_1\big) + \tilde\gamma'(s)\big(\varepsilon_2(s,.)\big|Q_1\big)\\ &+ \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_1(s,.)}{2} + (.)\varepsilon_1(s,.)'\middle|Q_1\right) - \big(R_2(\varepsilon)(s,.)\big|Q_1\big)\\ =&\big(\varepsilon_2(s,.)\big|L_-Q_1\big) + \frac{\lambda'(s)}{\lambda(s)}\|Q_1\|_{L^2}^2 + \tilde\gamma'(s)\big(\varepsilon_2(s,.)\big|Q_1\big) - \frac{\lambda'(s)}{\lambda(s)}\big(\varepsilon_1(s,.)\big|Q_2\big) - \big(R_2(\varepsilon)(s,.)\big|Q_1\big)\end{aligned}$$

and

$$\begin{aligned}0 =&\partial_s\big(\varepsilon_2(s,.)\big|Q_2\big) = -\big(L_+\varepsilon_1(s,.)\big|Q_2\big) - \tilde\gamma'(s)\big(Q\big|Q_2\big) - \tilde\gamma'(s)\big(\varepsilon_1(s,.)\big|Q_2\big)\\ &+ \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_2(s,.)}{2} + (.)\varepsilon_2'(s,.)\middle|Q_2\right) + \big(R_1(\varepsilon)(s,.)\big|Q_2\big)\\ =&-\big(\varepsilon_1(s,.)\big|L_+Q_2\big) + \tilde\gamma'(s)\|Q_1\|_{L^2}^2 - \tilde\gamma'(s)\big(\varepsilon_1(s,.)\big|Q_2\big) - \frac{\lambda'(s)}{\lambda(s)}\left(\varepsilon_2(s,.)\middle|\frac{Q_2}{2} + (.)Q_2'\right) + \big(R_1(\varepsilon)(s,.)\big|Q_2\big)\end{aligned}$$

which gives

$$\begin{aligned}\frac{\lambda'(s)}{\lambda(s)}\Big(\|Q_1\|_{L^2}^2 - \big(\varepsilon_1(s,.)\big|Q_2\big)\Big) &= -\big(\varepsilon_2\big|L_-Q_1\big) - \tilde\gamma'(s)\big(\varepsilon_2(s,.)\big|Q_1\big) + \big(R_2(\varepsilon)(s,.)\big|Q_1\big),\\ \tilde\gamma'(s)\Big(\|Q_1\|_{L^2}^2 - \big(\varepsilon_1(s,.)\big|Q_2\big)\Big) &= \big(\varepsilon_1(s,.)\big|L_+Q_2\big) + \frac{\lambda'(s)}{\lambda(s)}\left(\varepsilon_2(s,.)\middle|\frac{Q_2}{2} + (.)Q_2'\right) - \big(R_1(\varepsilon)(s,.)\big|Q_2\big).\end{aligned}$$

Choosing δ_0 sufficiently small such that

$$\|Q_1\|_{L^2}^2 - \big(\varepsilon_1(s,.)\big|Q_2\big) \geq C \quad \text{and} \quad \big|\big(\varepsilon_2(s,.)\big|Q_1\big)\big|,\ \left|\left(\varepsilon_2(s,.)\middle|\frac{Q_2}{2} + (.)Q_2'\right)\right| < \frac{C}{2}$$

for all $s \in \mathbb{R}$ and some constant $C < 0$ we obtain

$$\begin{aligned}C\left(\left|\frac{\lambda'(s)}{\lambda(s)}\right| + |\tilde\gamma'(s)|\right) \leq &\big|\big(\varepsilon_2\big|L_-Q_1\big)\big| + \frac{C}{2}\cdot|\tilde\gamma'(s)| + \big|\big(R_2(\varepsilon)(s,.)\big|Q_1\big)\big|\\ &+ \big|\big(\varepsilon_1(s,.)\big|L_+Q_2\big)\big| + \frac{C}{2}\cdot\left|\frac{\lambda'(s)}{\lambda(s)}\right| + \big|\big(R_1(\varepsilon)(s,.)\big|Q_2\big)\big|\end{aligned}$$

and the claim follows from Lemma 3.8. □

3.4 Dynamics of the scaling parameter

The key point in the proof of Theorem 3.1 is to relate the quantity $\frac{\lambda'(s)}{\lambda(s)}$ to the inner product $\big(\varepsilon_2(s,.)\big|Q_1\big)$ and to control the quadratic terms of the time derivative $\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big)$ using the ε-version of energy conservation (Lemma 3.6) and a quadratic form H, which is shown to be positive under the orthogonality conditions (3.6) (see Proposition 3.11).

The first important step is to project the differential equation for ε_1 onto the preimage of Q_1 under L_-. This way, using the self-adjointness of L_-, we do not need to care about the action of L_- on ε_2:

From $L_-((.)^2Q) = -4Q_1$ and (3.12) we obtain

$$\begin{aligned}\partial_s\big(\varepsilon_1(s,.)\big|(.)^2Q\big) =& \big(L_-\varepsilon_2(s,.)\big|(.)^2Q\big) + \frac{\lambda'(s)}{\lambda(s)}\big(Q_1\big|(.)^2Q\big) + \tilde{\gamma}'(s)\big(\varepsilon_2(s,.)\big|(.)^2Q\big)\\ &+ \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_1(s,.)}{2} + (.)\varepsilon_1(s,.)'\Big|(.)^2Q\right) - \big(R_2(\varepsilon)(s,.)\big|(.)^2Q\big)\\ =& -4\big(\varepsilon_2(s,.)\big|Q_1\big) - \frac{\lambda'(s)}{\lambda(s)}\|(.)Q\|_{L^2}^2 + \tilde{\gamma}'(s)\big(\varepsilon_2(s,.)\big|(.)^2Q\big)\\ &+ \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_1(s,.)}{2} + (.)\varepsilon_1(s,.)'\Big|(.)^2Q\right) - \big(R_2(\varepsilon)(s,.)\big|(.)^2Q\big).\end{aligned}$$

We integrate this identity to get rid of the time-derivative $\partial_s\big(\varepsilon_1(s,.)\big|(.)^2Q\big)$:

$$\begin{aligned}&4\int_{s_1}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds + \|(.)Q\|_{L^2}^2\ln\left(\frac{\lambda(s_2)}{\lambda(s_2)}\right)\\ &= -\big(\varepsilon_1(s,.)\big|(.)^2Q)\big)\big|_{s=s_1}^{s=s_2} + \int_{s_1}^{s_2}\left(\tilde{\gamma}'(s)\big(\varepsilon_2(s,.)\big|(.)^2Q\big) + \frac{\lambda'(s)}{\lambda(s)}\left(\frac{\varepsilon_1(s,.)}{2} + (.)\varepsilon_1(s,.)'\Big|(.)^2Q\right) - \big(R_2(\varepsilon)(s,.)\big|(.)^2Q\big)\right)ds\end{aligned}$$

and estimating the right hand side with Lemma 3.8 and Lemma 3.10 we obtain a relation between $\big(\varepsilon_2\big|Q_1\big)$ and λ in a time-averaging sense:
For all $s_1 \le s_2$

$$\left|4\int_{s_1}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds + \|(.)Q\|_{L^2}^2\ln\left(\frac{\lambda(s_2)}{\lambda(s_1)}\right)\right| \lesssim \delta_0 + \int_{s_1}^{s_2}\Big(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2\Big)\,ds. \tag{3.13}$$

This suggests to find a suitable control on the right hand side of (3.13). We will derive such a bound in terms of the inner product $\big(\varepsilon_2\big|Q_1\big)$ (see Corollary 3.15), which in light of having this same expression on both sides of inequality (3.13) is more than convenient and together with understanding the dynamics of $\big(\varepsilon_2\big|Q_1\big)$ will yield an almost monotonicity property for λ. We start by analyzing the evolution of $\big(\varepsilon_2\big|Q_1\big)$.

Recall that from the ε-version of energy conservation (Lemma 3.6)

$$2\big(\varepsilon_1(s,.)\big|Q\big) = \|\varepsilon(s,.)'\|_{L^2}^2 + 2|E_0|\lambda(s)^2 - \frac{1}{3}\int F(\varepsilon)(s,y)dy - 5\big(Q^4\big|\varepsilon_1(s,.)^2\big) - \big(Q^4\big|\varepsilon_2(s,.)^2\big).$$

Using $L_+Q_1 = -2Q$, $\big(Q\big|Q_1\big) = 0$ and the orthogonality conditions (3.6) we obtain from (3.12)

$$\begin{aligned}\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big) =& 2\big(\varepsilon_1(s,.)\big|Q\big) + \big(R_1(\varepsilon)(s,.)\big|Q_1\big)\\ =& \|\varepsilon(s,.)'\|_{L^2}^2 - 5\big(Q^4\big|\varepsilon_1(s,.)^2\big) - \big(Q^4\big|\varepsilon_2(s,.)^2\big) + 10\big(Q^3\varepsilon_1(s,.)^2\big|Q_1\big) + 2\big(Q^3\varepsilon_2(s,.)^2\big|Q_1\big)\\ &+ 2|E_0|\lambda(s)^2 - \frac{1}{3}\int F(\varepsilon)(s,y)dy + \big(\tilde{R}_1(\varepsilon)(s,.)\big|Q_1\big)\\ =& \|\varepsilon(s,.)'\|_{L^2}^2 + 10\big((.)Q^3Q'\big|\varepsilon_1(s,.)^2\big) + 2\big((.)Q^3Q'\big|\varepsilon_2(s,.)^2\big) + 2|E_0|\lambda(s)^2\\ &- \frac{1}{3}\int F(\varepsilon)(s,y)dy + \big(\tilde{R}_1(\varepsilon)(s,.)\big|Q_1\big),\end{aligned}$$

where the last equality follows from

$$2\big(Q^3Q_1\big|\varepsilon_j(s,.)^2\big) - \big(Q^4\big|\varepsilon_j(s,.)^2\big) = 2\big((.)Q^3\partial_yQ\big|\varepsilon_j(s,.)^2\big).$$

Defining

$$H(\varepsilon,\varepsilon)(s) = H_1(\varepsilon_1,\varepsilon_1)(s) + H_2(\varepsilon_2,\varepsilon_2)(s) \coloneqq \big(\mathcal{L}_1\varepsilon_1(s,.)\big|\varepsilon_1(s,.)\big) + \big(\mathcal{L}_2\varepsilon_2(s,.)\big|\varepsilon_2(s,.)\big) \tag{3.14}$$

with

$$\mathcal{L}_1 \coloneqq -\triangle + 10(.)Q^3Q', \qquad\qquad \mathcal{L}_2 \coloneqq -\triangle + 2(.)Q^3Q' \tag{3.15}$$

and

$$G(\varepsilon)(s) \coloneqq -\frac{1}{3}\int F(\varepsilon)(s,y)dy + \big(\tilde{R}_1(\varepsilon)(s,.)\big|Q_1\big),$$

we can summarize

$$\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big) = H(\varepsilon,\varepsilon)(s) + 2|E_0|\lambda(s)^2 + G(\varepsilon)(s) \tag{3.16}$$

where $H(\varepsilon,\varepsilon)$ contains all quadratic terms in ε, the terms in $G(\varepsilon)$ are of order ≥ 3 in ε and the linear terms vanish thanks to the orthogonality conditions.

Proposition 3.11. (Positivity of the quadratic form H)
There exists a constant $\tilde{\eta}_1 > 0$ such that for all $f = f_1 + if_2 \in H^1_{even}$ with $\big(f_1\big|Q\big) = 0$, $\big(f_2\big|Q_1\big) = 0$ and $\big(f_2\big|Q_2\big) = 0$ the lower bound

$$H(f,f) \geq \tilde{\eta}_1\left(\|f\|_{L^2_w}^2 + \|f'\|_{L^2}^2\right)$$

holds.

Remark. This result is proven in Section 4.2. The point is that although the negative directions of H_1 and H_2 are not explicitly known, it suffices to avoid the directions Q, Q_1 and Q_2 to ensure positivity of H, in particular H dominates the norms $\|f\|_{L^2_w}^2$, $\|f'\|_{L^2}^2$. Moreover the following result allows us to measure the negativity of $H(\varepsilon,\varepsilon)$ by means of the projections $\big(\varepsilon_1\big|Q\big)$ and $\big(\varepsilon_2\big|Q_2\big)$.

Corollary 3.12. *There exists a constant $\eta_1 > 0$ such that for $\alpha(u_0)$ sufficiently small, we have*

$$H(\varepsilon,\varepsilon)(s) \geq \eta_1 \left(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2 \right) - \frac{1}{\eta_1} \left(\big(\varepsilon_1(s,.)\big|Q\big)^2 + \big(\varepsilon_2(s,.)\big|Q_1\big)^2 \right)$$

for all $s \in \mathbb{R}$.

Proof. Set $\tilde{\varepsilon} = \varepsilon - aQ - ibQ_1$ with $a = \big(\varepsilon_1\big|Q\big)/\|Q\|_{L^2}^2$ and $b = \big(\varepsilon_2\big|Q_1\big)/\|Q_1\|_{L^2}^2$, then $\big(\tilde{\varepsilon_1}\big|Q\big) = 0$, $\big(\tilde{\varepsilon_2}\big|Q_1\big) = 0$, $\big(\tilde{\varepsilon_2}\big|Q_2\big) = 0$ (since $\big(Q\big|Q_2\big) = 0$) and hence $\tilde{\varepsilon}$ satisfies the conditions of Proposition 3.11 which for δ_0 sufficiently small gives

$$\begin{aligned}
H(\varepsilon,\varepsilon) =& H(\tilde{\varepsilon},\tilde{\varepsilon}) + a^2 H_1(Q,Q) + b^2 H_2(Q_1,Q_1) + 2a\big(\mathcal{L}_1 Q\big|\tilde{\varepsilon}_1\big) + 2b\big(\mathcal{L}_2 Q_1\big|\tilde{\varepsilon}_2\big) \\
\geq& \tilde{\eta}_1 \left(\|\tilde{\varepsilon}\|_{L^2_w}^2 + \|\partial_1 \tilde{\varepsilon}\|_{L^2}^2 \right) - C_1(a^2+b^2) - C_2\delta_0 \|\tilde{\varepsilon}\|_{L^2_w} \\
\geq& \frac{\tilde{\eta}_1}{2} \left(\|\tilde{\varepsilon}\|_{L^2_w}^2 + \|\partial_1 \tilde{\varepsilon}\|_{L^2}^2 \right) - C_1(a^2+b^2) \\
\geq& \frac{\tilde{\eta}_1}{2} \left(\|\varepsilon\|_{L^2_w}^2 + \|\partial_1 \varepsilon\|_{L^2}^2 \right) - \frac{\tilde{\eta}_1}{2} C(\delta_0)(|a|+|b|) - C_1(a^2+b^2)
\end{aligned}$$

where the last inequality follows from

$$\left(\|\tilde{\varepsilon}\|_{L^2_w}^2 + \|\partial_1 \tilde{\varepsilon}\|_{L^2}^2 \right) \geq \left(\|\varepsilon\|_{L^2_w}^2 + \|\partial_1 \varepsilon\|_{L^2}^2 \right) - C(\delta_0)(|a|+|b|),$$

and hence for $|a|,\ |b| < \frac{\tilde{\eta}_1}{2}$ we obtain

$$\begin{aligned}
H(\varepsilon,\varepsilon) \geq& \frac{\tilde{\eta}_1}{2} \left(\|\varepsilon\|_{L^2_w}^2 + \|\partial_1 \varepsilon\|_{L^2}^2 \right) - C(a^2+b^2) \\
\geq& \eta_1 \left(\|\varepsilon\|_{L^2_w}^2 + \|\partial_1 \varepsilon\|_{L^2}^2 \right) - \frac{1}{\eta_1} \left(\big(\varepsilon_1\big|Q\big)^2 + \big(\varepsilon_2\big|Q_1\big)^2 \right)
\end{aligned}$$

for some η_1 sufficiently small.

□

Corollary 3.13. *There exists a constant $\eta_1 > 0$ such that for δ_0 sufficiently small, we have*

$$\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big) \geq \frac{\eta_1}{2} \left(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2 \right) - \frac{2}{\eta_1} \left(\big(\varepsilon_1(s,.)\big|Q\big)^2 + \big(\varepsilon_2(s,.)\big|Q_1\big)^2 \right) + 2|E_0|\lambda(s)^2 \tag{3.17}$$

for all $s \in \mathbb{R}$.

Proof. Inserting the lower bound on $H(\varepsilon,\varepsilon)$ from Corollary 3.12 into (3.16) and estimating $|G(\varepsilon)|$ with Lemma 3.8

gives

$$\begin{aligned}\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big) &\geq \eta_1\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)-\frac{1}{\eta_1}\left(\big(\varepsilon_1(s,.)\big|Q\big)^2+\big(\varepsilon_2(s,.)\big|Q_1\big)^2\right)+2|E_0|\lambda(s)^2+G(\varepsilon)(s)\\ &\geq \frac{\eta_1}{2}\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)-\frac{2}{\eta_1}\left(\big(\varepsilon_1(s,.)\big|Q\big)^2+\big(\varepsilon_2(s,.)\big|Q_1\big)^2\right)+2|E_0|\lambda(s)^2\end{aligned}$$

for δ_0 sufficiently small. □

The following result will allow us to bound the right hand side of (3.13) and at the same time analyze the dynamics of $\big(\varepsilon_2\big|Q_1\big)$:

Proposition 3.14. *There exists a constant $\eta_0>0$ such that for δ_0 sufficiently small, we have*

$$\partial_s\left(\left(1+\frac{1}{4\eta_0}\big(\varepsilon_1(s,.)\big|Q\big)\right)\big(\varepsilon_2(s,.)\big|Q_1\big)\right)\geq \eta_0\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)-\frac{1}{\eta_0}\big(\varepsilon_2(s,.)\big|Q_1\big)^2+2|E_0|\lambda(s)^2$$

for all $s\in\mathbb{R}$.

Proof. Notice that the term $\big(\varepsilon_1(s,.)\big|Q\big)^2$ can be replaced by the time-derivative $\partial_s\left(\big(\varepsilon_2(s,.)\big|Q_1\big)\big(\varepsilon_1(s,.)\big|Q\big)\right)$:

From (3.12), $L_-Q=0$, $L_+Q_1=-2Q$, $\big(Q\big|Q_1\big)=0$ and Lemma 3.8 we have

$$\big|\partial_s\big(\varepsilon_1(s,.)\big|Q\big)\big|\lesssim\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right),\qquad \big|\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big)-2\big(\varepsilon_1(s,.)\big|Q\big)\big|\lesssim\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)$$

which gives

$$\begin{aligned}\Big|\partial_s\left(\big(\varepsilon_2(s,.)\big|Q_1\big)\big(\varepsilon_1(s,.)\big|Q\big)\right)-2\big(\varepsilon_1(s,.)\big|Q\big)^2\Big| &= \big|\big(\varepsilon_2(s,.)\big|Q_1\big)\partial_s\big(\varepsilon_1(s,.)\big|Q\big)+\big(\varepsilon_1(s,.)\big|Q\big)\left[\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big)-2\big(\varepsilon_1(s,.)\big|Q\big)\right]\big|\\ &\lesssim \delta_0\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)\end{aligned}$$

and hence by Corollary 3.13

$$\begin{aligned}\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big) &\geq \frac{\eta_1}{2}\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)-\frac{1}{\eta_1}\partial_s\left(\big(\varepsilon_1(s,.)\big|Q\big)\big(\varepsilon_2(s,.)\big|Q\big)\right)-C\delta_0\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)\\ &\quad-\frac{2}{\eta_1}\big(\varepsilon_2(s,.)\big|Q_1\big)^2+2|E_0|\lambda(s)^2\\ &\geq \frac{\eta_1}{4}\left(\|\varepsilon(s,)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)-\frac{1}{\eta_1}\partial_s\left(\big(\varepsilon_1(s,.)\big|Q\big)\big(\varepsilon_2(s,.)\big|Q\big)\right)-\frac{4}{\eta_1}\big(\varepsilon_2(s,.)\big|Q_1\big)^2+2|E_0|\lambda(s)^2\\ &= \eta_0\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)-\frac{1}{4\eta_0}\partial_s\left(\big(\varepsilon_1(s,.)\big|Q\big)\big(\varepsilon_2(s,.)\big|Q\big)\right)-\frac{1}{\eta_0}\big(\varepsilon_2(s,.)\big|Q_1\big)^2+2|E_0|\lambda(s)^2\end{aligned}$$

for δ_0 sufficiently small and $\eta_0 \coloneqq \frac{\eta_1}{4}$, and we obtain

$$\begin{aligned}\partial_s\left(\left(1+\frac{1}{4\eta_0}\big(\varepsilon_1(s,.)\big|Q\big)\right)\big(\varepsilon_2(s,.)\big|Q_1\big)\right) &= \partial_s\big(\varepsilon_2(s,.)\big|Q_1\big)+\frac{1}{4\eta_0}\partial_s\left(\big(\varepsilon_1(s,.)\big|Q\big)\big(\varepsilon_2(s,.)\big|Q_1\big)\right)\\ &\geq \eta_0\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)-\frac{1}{\eta_0}\big(\varepsilon_2(s,.)\big|Q_1\big)^2+2|E_0|\lambda(s)^2.\end{aligned}$$

□

Integrating the inequality in Proposition 3.14 yields

$$\left[\left(1+\tfrac{1}{4\eta_0}\big(\varepsilon_1\big|Q\big)\right)\big(\varepsilon_2\big|Q_1\big)\right]_{s_1}^{s_2}\geq\eta_0\int_{s_1}^{s_2}\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)ds-\tfrac{1}{\eta_0}\int_{s_1}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)^2ds+2|E_0|\int_{s_1}^{s_2}\lambda(s)^2ds \tag{3.18}$$

for all $s_1\leq s_2$.

Corollary 3.15. *The following estimate holds for δ_0 sufficiently small and η_0 as in Proposition 3.14:*

$$\left|4\int_{s_1}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds+\|(.)Q\|_{L^2}^2\ln\left(\frac{\lambda(s_2)}{\lambda(s_1)}\right)\right|\leq C(\eta_0)\delta_0+\int_{s_1}^{s_2}\left|\big(\varepsilon_2(s,.)\big|Q_1\big)\right|ds \tag{3.19}$$

for all $s_1\leq s_2$.

Proof. By choosing making δ_0 sufficiently small we can assume

$$\left|1+\frac{1}{4\eta_0}\big(\varepsilon_1\big|Q\big)\right|\in\left[\tfrac{1}{2},\tfrac{3}{2}\right] \tag{3.20}$$

and inserting (3.18) into (3.13) gives

$$\begin{aligned}&\left|4\int_{s_1}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds+\|(.)Q\|_{L^2}^2\ln\left(\frac{\lambda(s_2)}{\lambda(s_1)}\right)\right|\leq C\delta_0+C\int_{s_1}^{s_2}\left(\|\varepsilon(s,.)\|_{L^2_w}^2+\|\varepsilon(s,.)'\|_{L^2}^2\right)ds\\ \leq& C\delta_0+\frac{C}{\eta_0}\left[\left(1+\frac{1}{4\eta_0}\big(\varepsilon_1\big|Q\big)\right)\big(\varepsilon_2\big|Q_1\big)\right]_{s_1}^{s_2}+\frac{C}{\eta_0^2}\int_{s_1}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)^2ds-\frac{2C|E_0|}{\eta_0}\int_{s_1}^{s_2}\lambda(s)^2ds\\ \leq& C(\eta_0)\delta_0+\int_{s_1}^{s_2}\left|\big(\varepsilon_2(s,.)\big|Q_1\big)\right|ds\end{aligned}$$

for δ_0 sufficiently small and $s_1\leq s_2$. □

With Proposition 3.14 and Corollary 3.15 in hand, we are now able to determine the sign of $\big(\varepsilon_2\big|Q_1\big)$ and prove an *almost monotonicity property* for λ.

Proposition 3.16. *There exists a unique $s_0 \in \mathbb{R}$ such that*

i)

$$\big(\varepsilon_2(s_0,.)\big|Q_1\big) = 0, \qquad \big(\varepsilon_2(s,.)\big|Q_1\big) < 0 \text{ for } s < s_0, \qquad \big(\varepsilon_2(s,.)\big|Q_1\big) > 0 \text{ for } s > s_0$$

ii) for all $s_2 \geq s_1 \geq s_0$:

$$3\int_{s_1}^{s_2} \big(\varepsilon_2(s,.)\big|Q_1\big)\, ds - C(\eta_0)\delta_0 \leq -\|(.)Q\|_{L^2}^2 \ln\left(\frac{\lambda(s_2)}{\lambda(s_1)}\right) \leq 5\int_{s_1}^{s_2} \big(\varepsilon_2(s,.)\big|Q_1\big)\, ds + C(\eta_0)\delta_0 \tag{3.21}$$

$$\text{and} \quad \lambda(s_2) < 2\lambda(s_1). \tag{3.22}$$

Proof. i) First note that $\big(\varepsilon_2(s,.)\big|Q_1\big) = 0$ implies $\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big) > 0$, since otherwise by Proposition 3.14 we have $\Big(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2\Big) = 0$, i.e. $\varepsilon(s) = 0$, and by Corollary 3.9 $\lambda(s) = 0$, which is impossible. Consequently is suffices to show that $\big(\varepsilon_2(s_0,.)\big|Q_1\big) = 0$ for some $s_0 \in \mathbb{R}$.

Suppose $\big(\varepsilon_2(s,.)\big|Q_1\big) < 0$ for all $s \in \mathbb{R}$. Then by (3.19)

$$-\|(.)Q\|_{L^2}^2 \ln\left(\frac{\lambda(s_2)}{\lambda(s_1)}\right) \leq C(\eta_0)\delta_0 + 3\int_{s_1}^{s_2} \big(\varepsilon_2(s,.)\big|Q_1\big) ds.$$

In particular $\int_0^\infty \big(\varepsilon_2(s,.)\big|Q_1\big) ds = -\infty$ would imply $\lambda(s) \xrightarrow{s\to\infty} \infty$ and hence by (3.7)
$\|u(t,.)'\|_{L^2} \xrightarrow{t\to T_+} 0$ and by Corollary 2.7 (Gagliardo-Nirenberg) $E[u] = 0$, a contradiction.
We conclude $\int_0^\infty \big(\varepsilon_2(s,.)\big|Q_1\big) ds > -\infty$ and deduce:

- Since $\int_0^s \big(\varepsilon_2(\tilde{s},.)\big|Q_1\big) d\tilde{s}$ is bounded from below (uniformly in s), (3.19) gives

$$0 < \lambda^- < \lambda(s) < \lambda^+ < \infty \qquad (*)$$

  for all $s \geq 0$ and some constants $\lambda^-,\ \lambda^+ > 0$.
- From (3.12) and Lemma 3.8 we see that $\partial_s\big(\varepsilon_2(s,.)\big|Q_1\big)$ is bounded uniformly in s, which together with $\int_0^\infty \big(\varepsilon_2(s,.)\big|Q_1\big) ds > -\infty$ and $\big(\varepsilon_2\big|Q_1\big) < 0$ implies

$$\big(\varepsilon_2(s,.)\big|Q_1\big) \xrightarrow{s\to\infty} 0. \qquad (**)$$

Now recall that by Proposition 3.14

$$\partial_s\left(\left(1 + \frac{1}{4\eta_0}\big(\varepsilon_1(s,.)\big|Q\big)\right)\big(\varepsilon_2(s,.)\big|Q_1\big)\right) \geq \eta_0\left(\|\varepsilon(s,.)\|_{L^2_w}^2 + \|\varepsilon(s,.)'\|_{L^2}^2\right) - \frac{1}{\eta_0}\big(\varepsilon_2(s,.)\big|Q_1\big)^2.$$

Since $\left(\left(1 + \frac{1}{4\eta_0}\big(\varepsilon_1(s,.)\big|Q\big)\right)\big(\varepsilon_2(s,.)\big|Q_1\big)\right)$ is (again by Lemma 3.8) uniformly bounded in s, there exists some sequence $s_n \xrightarrow{n\to\infty} \infty$ such that $\partial_s\left(\left(1 + \frac{1}{4\eta_0}\big(\varepsilon_1(s,.)\big|Q\big)\right)\big(\varepsilon_2(s,.)\big|Q_1\big)\right)\big|_{s=s_n} \xrightarrow{n\to\infty} 0$, and hence

$\left(\|\varepsilon(s_n,.)\|^2_{L^2_w} + \|\varepsilon'(s_n,.)\|^2_{L^2}\right) \xrightarrow{n\to\infty} 0$ by $(**)$, which in turn implies $\lambda(s_n) \xrightarrow{n\to\infty} 0$ by Corollary 3.9 and contradicts $(*)$.

Analogously, by investigation of the asymptotics for $s \to -\infty$, $\left(\varepsilon_2(s,.)\middle|Q_1\right) > 0$ for all $s \in \mathbb{R}$ is impossible and (i) is proven.

ii) The inequality follows directly from Corollary 3.19 for $s_2 \geq s_1 \geq s_0$.
Now suppose $\lambda(s_2) \geq 2\lambda(s_1)$ for some $s_2 \geq s_1 \geq s_0$, then by (3.19)

$$\|(.)Q\|^2_{L^2} \ln(2) - C(\eta_0)\delta_0 \leq \|(.)Q\|^2_{L^2} \ln\left(\frac{\lambda(s_2)}{\lambda(s_1)}\right) - C(\eta_0)\delta_0 \leq -3\int_{s_1}^{s_2} \left(\varepsilon_2(s,.)\middle|Q_1\right) ds < 0$$

for δ_0 sufficiently small, which is a contradiction.

□

Remark. By time-translation invariance we assume without loss of generality $s_0 = 0$.

Corollary 3.17. (Blow-up in finite or infinite time) *There exists some $\alpha_1 > 0$ such that any solution u of (3.1) with initial condition u_0 satifying the assumptions of Theorem 3.1 with $\alpha* < \alpha_1$ blows up in finite or infinite time, i.e.*

$$\lim_{s\to\infty} \lambda(s) = 0.$$

Proof. Suppose there exists some sequence $(s_n)_{n\in\mathbb{N}} \subset \mathbb{R}$ s.t. $s_n \xrightarrow{n\to\infty} \infty$ and $\lambda(s_n) > C$ for all $n \in \mathbb{N}$ for some constant $C > 0$. Then by the almost-monotonicity property (3.22) $\lambda(s) > \frac{\lambda(s_n)}{2} > \frac{C}{2}$ for all $0 < s < s_n$ and hence

$$\lambda(s) > \frac{C}{2} > 0$$

for all $s > 0$.
From (3.21) we obtain

$$3\int_0^s \left(\varepsilon_2(s,.)\middle|Q_1\right) ds \leq C(\eta_0)\delta_0 - \|(.)Q\|_{L^2} \ln\left(\frac{\lambda(s)}{\lambda(0)}\right) < \tilde{C}$$

for all $s > 0$ and some constant $\tilde{C} > 0$, in particular

$$0 < \int_0^\infty \left(\varepsilon_2(s,.)\middle|Q_1\right) ds < \infty.$$

Together with $\left(\varepsilon_2(s,.)\middle|Q_1\right) > 0$ for $s > 0$ and $\left|\partial_s\left(\varepsilon_2(s,.)\middle|Q_1\right)\right|$ being uniformly bounded in s (by (3.12) and Lemma 3.8) this gives

$$\left(\varepsilon_2(s,.)\middle|Q_1\right) \xrightarrow{s\to\infty} 0$$

and as in the proof of Proposition 3.16 we deduce from Proposition 3.14 the existence of some sequence $\tilde{s}_n \xrightarrow{n\to\infty} \infty$ such that $\lambda(\tilde{s}_n) \xrightarrow{n\to\infty} 0$, a contradiction. □

The final result of finite time blow-up and the corresponding upper bound is shown by finding appropriate time intervals on which the variation of λ is small, such that Proposition 3.16 will lead to a uniform control of λ by the inner product $\big(\varepsilon_2\big|Q_1\big)$.

Let $k_0 > 1$ and δ_0 sufficiently small such that

$$0 < \frac{2}{\|(.)Q\|_{L^2}^2} C(\eta_0)\delta_0 \leq \ln(k_0) < \frac{\eta_0}{10\|(.)Q\|_{L^2}^2}. \tag{3.23}$$

Now since by Proposition (3.17) $\lambda(s) \xrightarrow{s\to\infty} 0$, there exists some $\tilde{s}_0$ such that $\lambda(s) < \lambda(0)/k_0$ for all $s \geq \tilde{s}_0$, in particular for all $s_2 \geq \tilde{s}_0$ we have $k_0\lambda(s_2) \in (\lambda(s_2), \lambda(0))$ and by continuity of λ there is some $s \in (0, s_2)$ such that $\lambda(s) = k_0\lambda(s_2)$.

We define for $s_2 \geq \tilde{s}_0$

$$s_1(s_2) \coloneqq \sup\big\{s \in (0, s_2) : \lambda(s) = k_0\lambda(s_2)\big\}$$

and

$$I(s_2) \coloneqq [s_1(s_2), s_2].$$

Lemma 3.18. (Controll of $I(s_2)$) *Let $s_2 \geq \tilde{s}_0$ and $s \in I(s_2)$. Then*

$$\frac{\lambda(s_2)}{2} \leq \lambda(s) \leq k_0\lambda(s_2) \tag{3.24}$$

and

$$\big(\varepsilon_2(s,.)\big|Q_1\big) \leq 4\big(\varepsilon_2(s_2,.)\big|Q_1\big). \tag{3.25}$$

Proof. (3.24) follows directly from the almost monotonicity property (3.22) and the definition of $I(s_2)$.
Let $K(s_2) \coloneqq \sup\left\{\frac{\big(\varepsilon_2(s,.)\big|Q_1\big)}{\big(\varepsilon_2(s_2,.)\big|Q_1\big)} : \ s \in I(s_2)\right\} > 0$, then $\big(\varepsilon_2(s,.)\big|Q_1\big) \leq K(s_2)\big(\varepsilon_2(s_2,.)\big|Q_1\big)$ for all $s \in I(s_2)$.
Now fix any $s \in I(s_2)$. From (3.18) we have

$$\left(1 + \frac{1}{4\eta_0}\big(\varepsilon_1(s,.)\big|Q\big)\right)\big(\varepsilon_2(s,.)\big|Q_1\big) \leq \left(1 + \frac{1}{4\eta_0}\big(\varepsilon_1(s_2,.)\big|Q\big)\right)\big(\varepsilon_2(s_2,.)\big|Q_1\big) + \frac{1}{\eta_0}\int_s^{s_2}\big(\varepsilon_2(\tilde{s},.)\big|Q_1\big)^2 d\tilde{s}$$

and (3.20) gives

$$\frac{1}{2}\big(\varepsilon_2(s,.)\big|Q_1\big) \leq \frac{3}{2}\big(\varepsilon_2(s_2,.)\big|Q_1\big) + \frac{1}{\eta_0}\int_s^{s_2}\big(\varepsilon_2(\tilde{s},.)\big|Q_1\big)^2 d\tilde{s}.$$

Since $\big(\varepsilon_2(\tilde{s},.)\big|Q_1\big)^2 \leq K(s_2)\big(\varepsilon_2(s_2,.)\big|Q_1\big)\cdot\big(\varepsilon_2(\tilde{s},.)\big|Q_1\big)$ for all $\tilde{s}\in(s,s_2)$, we obtain

$$\begin{aligned}\big(\varepsilon_2(s,.)\big|Q_1\big) &\leq 3\big(\varepsilon_2(s_2,.)\big|Q_1\big)+\frac{2}{\eta_0}K(s_2)\big(\varepsilon_2(s_2,.)\big|Q_1\big)\int_s^{s_2}\big(\varepsilon_2(\tilde{s},.)\big|Q_1\big)d\tilde{s}\\ &= \big(\varepsilon_2(s_2,.)\big|Q_1\big)\cdot\left(3+\frac{2}{\eta_0}K(s_2)\int_s^{s_2}\big(\varepsilon_2(\tilde{s},.)\big|Q_1\big)d\tilde{s}\right).\end{aligned}$$

From the definition of $K(s_2)$ we obtain the upper bound

$$K(s_2)=\sup\left\{\frac{\big(\varepsilon_2(s,.)\big|Q_1\big)}{\big(\varepsilon_2(s_2,.)\big|Q_1\big)}:\ s\in I(s_2)\right\}\leq 3+\frac{2}{\eta_0}K(s_2)\int_{s_1(s_2)}^{s_2}\big(\varepsilon_2(\tilde{s},.)\big|Q_1\big)d\tilde{s} \tag{3.26}$$

and by (3.24)

$$-\ln\left(\frac{\lambda(s_2)}{\lambda(s_1(s_2))}\right)\leq \ln(k_0)$$

such that by (3.21) and (3.23) we can bound the integral on the right hand side of (3.26):

$$\begin{aligned}3\int_{s_1(s_2)}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds &\leq C(\eta_0)\delta_0-\|(.)Q\|_{L^2}^2\ln\left(\frac{\lambda(s_2)}{\lambda(s_1(s_2))}\right)\leq \frac{\|(.)Q\|_{L^2}^2}{2}\ln(k_0)+\|(.)Q\|_{L^2}^2\ln(k_0)\\ &= \frac{3}{2}\|(.)Q\|_{L^2}^2\ln(k_0),\end{aligned}$$

Together with (3.23) this gives

$$K(s_2)\leq 3+\frac{1}{\eta_0}K(s_2)\|(.)Q\|_{L^2}^2\ln(k_0)\leq 3+\frac{K(s_2)}{10}$$

and hence

$$K(s_2)<4.$$

□

Proposition 3.19. (Uniform control of λ by $\big(\varepsilon_2\big|Q_1\big)$)
There exists a constant $B>0$ such that for δ_0 sufficiently small

$$|E_0|\lambda(s)^2\leq B\big(\varepsilon_2(s,.)\big|Q_1\big)^2$$

for all $s\geq\tilde{s}_0$.

Proof. Let $s_2\geq\tilde{s}_0$ and $\tilde{B}>0$ such that

$$|E_0|\lambda(s_2)^2\geq\tilde{B}\big(\varepsilon_2(s_2,.)\big|Q_1\big)^2. \tag{3.27}$$

By applying Proposition 3.14 and (3.21) to the interval $I(s_2) = [s_1(s_2), s_2]$, we show that $\tilde{B}$ has to be bounded from above by some constant independent of s_2, and hence any B greater than $\tilde{B}$ does the job.

By (3.24), (3.25) and (3.27)

$$2|E_0|\lambda(s)^2 - \frac{1}{\eta_0}\big(\varepsilon_2(s,.)\big|Q_1\big)^2 \geq 2|E_0|\frac{\lambda(s_2)^2}{4} - \frac{16}{\eta_0}\big(\varepsilon_2(s_2,.)\big|Q_1\big)^2 \geq \left(\frac{\tilde{B}}{2} - \frac{16}{\eta_0}\right)\big(\varepsilon_2(s_2,.)\big|Q_1\big)^2 \tag{3.28}$$

for all $s \in I(s_2)$.

If $\left(\frac{\tilde{B}}{2} - \frac{16}{\eta_0}\right) \leq 0$, we are done with $\tilde{B} \leq \frac{8}{\eta_0}$.
If $\left(\frac{\tilde{B}}{2} - \frac{16}{\eta_0}\right) > 0$, then by (3.20), (3.18) and (3.28)

$$\begin{aligned}\frac{3}{2}\big(\varepsilon_2(s_2,.)\big|Q_1\big) - \frac{1}{2}\big(\varepsilon_2(s_1(s_2),.)\big|Q_1\big) &\geq 2|E_0|\int_{s_1(s_2)}^{s_2}\lambda(s)^2 ds - \frac{1}{\eta_0}\int_{s_1(s_2)}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)^2 ds \\ &\geq \left(\frac{\tilde{B}}{2} - \frac{16}{\eta_0}\right)(s_2 - s_1(s_2))\big(\varepsilon_2(s_2,.)\big|Q_1\big)^2,\end{aligned}$$

i.e.

$$\frac{3}{2} \geq \left(\frac{\tilde{B}}{2} - \frac{16}{\eta_0}\right)(s_2 - s_1(s_2))\big(\varepsilon_2(s_2,.)\big|Q_1\big)$$

and it remains to find a uniform lower bound on $(s_2 - s_1(s_2))\big(\varepsilon_2(s_2,.)\big|Q_1\big)$.
By (3.24), (3.21) and (3.23) we have

$$\begin{aligned}\|(.)Q\|_{L^2}^2 \ln(k_0) \leq -\|(.)Q\|_{L^2}^2 \ln\left(\frac{\lambda(s_2)}{\lambda(s_1(s_2))}\right) &\leq 5\int_{s_1(s_2)}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds + C(\eta_0)\delta_0 \\ &\leq 5\int_{s_1(s_2)}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds + \frac{\|(.)Q\|_{L^2}^2}{2}\ln(k_0),\end{aligned}$$

i.e.

$$\|(.)Q\|_{L^2}^2 \ln(k_0) \leq 10\int_{s_1(s_2)}^{s_2}\big(\varepsilon_2(s,.)\big|Q_1\big)ds \leq 40\big(\varepsilon_2(s_2,.)\big|Q_1\big)(s_2 - s_1(s_2)),$$

where the last inequality follows from (3.25), and hence

$$(s_2 - s_1(s_2)) \geq \frac{\|(.)Q\|_{L^2}^2 \ln(k_0)}{40\big(\varepsilon_2(s_2,.)\big|Q_1\big)},$$

which gives

$$\frac{3}{2} \geq \left(\frac{\tilde{B}}{2} - \frac{16}{\eta_0}\right)\frac{\|(.)Q\|_{L^2}^2 \ln(k_0)}{40},$$

in particular

$$\tilde{B} \leq 2\left(\frac{60}{\|(.)Q\|_{L^2}^2 \ln(k_0)} + \frac{16}{\eta_0}\right).$$

□

Proposition 3.20. (Finite time blow-up with and upper bound)
There exists some $\alpha^* > 0$ such that any solution u of (3.1) with initial condition u_0 satisfying the assumptions of Theorem 3.1 blows up at finite time $T \in (0, \infty)$ and

$$\|u(t,.)'\|_{L^2} \lesssim \left(\frac{1}{\sqrt{|E_0|}(T-t)}\right)^{1/2}$$

for t close to T.

Proof. Let S be the (finite or infinite) blow-up time from Corollary 3.17, $T \coloneqq \psi^{-1}(S)$, $(t_n)_{n\in\mathbb{N}}$ such that $\lambda(\psi(t_n)) = 2^{-n}$, $\tilde{t_0}$ such that $\psi(\tilde{t_0}) = \tilde{s}_0$ and n_0 such that $t_n > \tilde{t}_0$ for all $n \geq n_0$.
By (3.22) $0 < s_n < s_{n+1}$ and hence $0 < t_n < t_{n+1}$ for all $n \geq n_0$, $t_n \xrightarrow{n\to\infty} T$, and

$$2^{-(n+2)} \leq \lambda(s) \leq 2^{-(n-1)} \tag{3.29}$$

for all $s \in [s_n, s_{n+1}]$.

Moreover by Proposition 3.19

$$\int_{s_n}^{s_{n+1}} \lambda(s)ds \leq \frac{\sqrt{B}}{\sqrt{|E_0|}} \int_{s_n}^{s_{n+1}} \big(\varepsilon_2(s,.)\big|Q_1\big)ds$$

and by (3.21) and (3.29)

$$3\int_{s_n}^{s_{n+1}} \big(\varepsilon_2(s,.)\big|Q_1\big)ds \leq C(\eta_0)\delta_0 + \|(.)Q\|_{L^2}^2 \ln(8) \leq 3\|(.)Q\|_{L^2}^2 \ln(8)$$

for δ_0 sufficiently small. Combing the two inequalities above gives

$$\begin{aligned}\frac{\sqrt{B}}{\sqrt{|E_0|}}\|(.)Q\|_{L^2}^2 \ln(8) \geq \int_{s_n}^{s_{n+1}} \lambda(s)ds &= \int_{s_n}^{s_{n+1}} \frac{\lambda(s)^2}{\lambda(s)}ds \geq 2^{n-1}\int_{s_n}^{s_{n+1}} \lambda(s)^2 ds = 2^{n-1}\int_{t_n}^{t_{n+1}} \lambda(\psi(t))^2\psi'(t)dt \\ &= 2^{n-1}\int_{t_n}^{t_{n+1}} dt = 2^{n-1}(t_{n+1}-t_n)\end{aligned}$$

and hence

$$(t_{n+1}-t_n) \leq \frac{C}{\sqrt{|E_0|}}2^{-(n+2)}$$

for some constant $C > 0$ for all $n \geq n_0$, in particular

$$T = \lim_{n\to\infty} t_n < \infty$$

and

$$T - t_n = \sum_{k=n}^{\infty} (t_{k+1} - t_k) \leq \frac{C}{\sqrt{|E_0|}} 2^{-(n+1)} = \frac{C}{\sqrt{|E_0|}} \lambda(\psi(t_{n+1})).$$

Now note that for t sufficiently large, there exists some $n \geq n_0$ such that $t_n < t < t_{n+1}$ which gives

$$T - t \leq T - t_n \leq \frac{C}{\sqrt{|E_0|}} \lambda(\psi(t_{n+1})) < \frac{2C}{\sqrt{|E_0|}} \lambda(\psi(t)),$$

i.e.

$$\lambda(\psi(t)) \gtrsim (T-t)\sqrt{|E_0|}.$$

Finally, with λ in terms of the original time-parameter t (since λ here is actually $\bar{\lambda}$ from Section 3.2) and recalling (3.7)

$$\left| 1 - \lambda(t) \frac{\|u(t,.)'\|_{L^2}}{\|Q'\|_{L^2}} \right| + \|\varepsilon(t,.)\|_{H^1} < \delta_0 \ \forall t \in [0,T)$$

gives

$$1 + \delta_0 > \lambda(t) \frac{\|u(t,.)'\|_{L^2}}{\|Q'\|_{L^2}} \gtrsim (T-t)\sqrt{|E_0|} \|u(t,.)'\|_{L^2}.$$

□

This concludes the proof of Theorem 3.1.

Remark. The case of general (not even) initial data gives an additional modulation parameter for space-translation. However, this modulation is the least problematic to deal with and can be estimated with an additional factor of δ_0 compared to γ and λ. (see [10], Lemma 5.iii).
Moreover the additional parameter allows to impose a third orthogonality condition which ensures an analogue of Corollary 3.12, provided that the general version of Proposition 3.11 (see [10], Proposition 2) holds true.

Remark. The bound in Proposition 3.19 can be improved to

$$\big(\varepsilon_2(s,.)\big|Q_1\big) \geq \frac{B}{|\ln(\lambda(s))|^{1/2}}$$

by refining the inequality in Proposition 3.14, and leads to the sharper blow-up bound

$$\|u(t,.)'\|_{L^2} \lesssim \left(\frac{|\ln(T-t)|^{1/2}}{T-t} \right)^{1/2}$$

(see [10], Section 4.3).

Remark. In 2001 Galina Perelman proved the existence of solutions with blow-up rate $\|u(t,.)'\|_{L^2} = C\sqrt{\frac{\ln|\ln(T-t)|}{T-t}}$ as $t \to T$ in dimension 1, by considering a specific perturbation of the Ground State as even initial data u_0 with

negative energy. Most importantly, u_0 is in the space $\Gamma := \{f \in H^1 : \ (.)f \in L^2\}$ where the additional symmetry of pseudo-conformal transformation applied to solitons yields a four-parameter family of solutions to (1.9). Her argument uses the same ε-decomposition as in Section 3.1 and a change of coordinates which allows to split the evolution of solution into one part which stays in the above mentioned family of solutions, and one part which remains small in a suitable sense. This leads to the specific representation $u(t,x) = e^{i\gamma(t)}\lambda(t)^{-1/2}\left(Q(\frac{x}{\lambda(t)}) + f(t,\frac{x}{\lambda(t)})\right)$ with $\lambda,\ \gamma \in C^1([0,T))$, $\lambda(t) = C\sqrt{\frac{T-t}{\ln|\ln(T-t)|}}$ and some function f with $f(t,.)$ small in $L^2 \cap L^\infty$ uniformly in $t \in [0,T)$ and $\|f(t,.)\|_{L^\infty} \xrightarrow{t\to T} 0$. (See [11].)

The blow-up bound in [10] in contrast applies to a broader class of initial data, which does not rely on pseudo-conformal invariance. Moreover the argument is based on the non-linear dynamics, while Perelman exploits estimates from the linearized problem.

4 Linear Schrödinger operators and Sturm Liouville theory

In order to get a better understanding of linear Schrödinger operators, before proving Proposition 3.11, we will give an introduction to basic *Sturm-Liouville theory*, which deals with a more general class of linear second order differential operators. The key insight here is that by a suitable spectral transformation, we can relate the absolutely continuous spectrum to the asymptotic behaviour of solutions.
Moreover, the exponential decay of the potential V allows for an uncomplicated analysis of the spectrum. In fact, by Weyl's Theorem 4.20, the essential spectrum of a linear operator $L = -\triangle + V$ coincides with the essential spectrum of the free Schrödinger operator $\sigma_{\text{ess}}(-\triangle) = [0, \infty)$ and from Sturm's Theorem we will see that L has finitely many eigenvalues on the negative real line.
This Section is mainly based on [16]. We use some basic results about self-adjoint operators, which can be found in Appendix D.

Let $I \coloneqq (a, b) \subseteq \mathbb{R}$ be open, $r \in L^1_{loc}(I, (0, \infty))$ and consider the Hilbert space

$$\mathcal{H} \coloneqq L^2(I, r(x)dx) \qquad \text{with} \qquad \langle f, g\rangle \coloneqq \int_I f(x)^* g(x) r(x) dx.$$

Definition 4.1. (Sturm-Liouville operator)
Let $p^{-1} \in L^1_{loc}(I, (0, \infty))$, $q \in L^1_{loc}(I, \mathbb{R})$. An operator τ of the form

$$\tau f \coloneqq \frac{1}{r}\left(-p'f' - pf'' + qf\right), \qquad \mathcal{D}(\tau) = \{f \in \mathcal{H} : f, pf' \in AC(I), \tau f \in \mathcal{H}\},$$

where $AC(a, b) \coloneqq \left\{f \in C(a, b) : \ f(x) = f(c) + \int_a^c g(t)dt, \ g \in L^1_{loc}(a, b)\right\}$, is called Sturm-Liouville operator.

We call τ regular at a, if $a \in \mathbb{R}$ and p^{-1}, q, r are integrable near a and regular, if τ is regular at both endpoints.

Definition 4.2. (Modified Wronskian)

$$W(f, g)(x) \coloneqq \left(p(fg' - f'g)\right)(x)$$

Note that if f, g are solutions of $(\tau - z)u = 0$ for some $z \in \mathbb{C}$, then

$$W(f, g)' = p'fg' - p'f'g + pfg'' - pf''g = (-p'f' - pf'')g + (p'g' + pg'')f = (rz - q)fg - (rz - q)fg = 0,$$

i.e. $W(f, g)(x) = W(f, g) = const.$ Moreover, in that case $W(f, g) = 0$ iff f and g are linearly dependent.

Lemma 4.3. (Lagrange Identity) *Let $f, pf', g, pg' \in AC(I)$, $c \leq d \in (a,b)$, then*

$$\langle g, \tau f\rangle_{(c,d)} - \langle \tau g, f\rangle_{(c,d)} = \int_c^d g^*(y)\tau f(y)r(y)dy - \int_c^d (\tau g)^*(y)f(y)r(y)dy = W(g^*, f)(d) - W(g^*, f)(c). \quad (4.1)$$

Moreover for $f, g \in \mathcal{D}(\tau)$, taking the limits $c \to a$, $d \to b$:

$$\langle g, \tau f\rangle - \langle \tau g, f\rangle = W(g^*, f)(b) - W(g^*, f)(a) \quad (4.2)$$

where $W(g^*, f)(b) \coloneqq \lim_{d\to b} W(g^*, f)(d)$, $W(g^*, f)(a) \coloneqq \lim_{c\to a} W(g^*, f)(c)$.

Proof. By partial integration. □

Theorem 4.4. *Let $rg \in L^1_{loc}(I)$, $z, \alpha, \beta \in \mathbb{C}$ and $c \in I$.*
Then there exists a unique solution $f, pf' \in AC(I)$ of the problem

$$\begin{cases} (\tau - z)f = g, \\ f(c) = \alpha,\ (pf')(c) = \beta. \end{cases} \quad (4.3)$$

Moreover the map $z \mapsto f$ is entire and f, pf' can be extended continuously to a regular endpoint.

Proof. Let

$$u = \begin{pmatrix} f \\ pf' \end{pmatrix}, \qquad v = \begin{pmatrix} 0 \\ rg \end{pmatrix}, \qquad A = \begin{pmatrix} 0 & \frac{1}{p} \\ zr - q & 0 \end{pmatrix},$$

then (4.3) is equivalent to the linear first order system

$$u' - Au = v, \qquad u(c) = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

Integrating

$$u(x) - \int_c^x A(y)u(y)dy = u(c) + \int_c^x v(y)dy$$

and denoting

$$Ku(x) \coloneqq \int_c^x A(y)u(y)dy, \qquad w(x) \coloneqq u(c) + \int_c^x v(y)dy$$

gives the *Volterra integral equation*

$$u - Ku = w.$$

For any $d \in (c, b)$ consider the integral operator K on the Banach space $C([c,d])$ with $\|.\| = \|.\|_{L^\infty[c,d]}$ and let $a(x) \coloneqq \|A(x)\|$, $a_1(x) \coloneqq \int_c^x a(y)dy$.

We claim that $|K^n h(x)| \leq \|h\| \frac{a_1(x)^n}{n!}$ for all $h \in C([c,d])$, $x \in [c,d]$ and $n \in \mathbb{N}$. Indeed, $n = 1$ gives

$$|Kh(x)| = \left| \int_c^x A(y)h(y)dy \right| \leq \left| \int_c^x a(y)\|h\|dy \right| = \|h\|a_1(x)$$

and by induction $n \mapsto n+1$

$$|K^{n+1}h(x)| = \left| \int_c^x A(y)K^n h(y)dy \right| \leq \frac{\|h\|}{n!} \int_c^x a(y)a_1(y)^n dy = \frac{\|h\|}{n!} \int_c^x a_1'(y)a_1(y)^n dy = \|h\| \frac{a_1(x)^{(n+1)}}{(n+1)!}.$$

Arguing analogously for $d \in (a,c)$ it follows that the Neumann series $(1-K)^{-1} = \sum_{k=0}^{\infty} K^k$ converges uniformly on any compact subset of (a,b) and hence $u = (1-K)^{-1} w$ is the unique solution of (4.3). Moreover $\sum_{k=0}^{N} K^k w$ is entire in z for all $n \in \mathbb{N}$ and by uniform convergence on compact subsets the same holds for u. □

Remark. Note that we do not know anything about f at the endpoints a and b, in particular f might fail to be in $L^2(I, r(x)dx)$ and hence is in general not in $\mathcal{D}(\tau)$.

Remark. Choosing the boundary conditions

$$\begin{pmatrix} u_1 \\ pu_1' \end{pmatrix}(c) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad \begin{pmatrix} u_2 \\ pu_2' \end{pmatrix}(c) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

yields solutions u_1, u_2 of $(\tau - z)u = 0$ which are linearly independent with $W(u_1, u_2) = 1$ and entire in z.

A simple computation shows that if u_1, u_2 are solutions of $(\tau - z)u = 0$ with $W(u_1, u_2) = 1$, then any solution of (4.3) can be written as

$$\begin{aligned} f(x) &= u_1(x) \left(\alpha + \int_c^x u_2(y)g(y)r(y)dy \right) + u_2(x) \left(\beta - \int_c^x u_1(y)g(y)r(y)dy \right), \\ f'(x) &= u_1'(x) \left(\alpha + \int_c^x u_2(y)g(y)r(y)dy \right) + u_2'(x) \left(\beta - \int_c^x u_1(y)g(y)r(y)dy \right) \end{aligned} \tag{4.4}$$

for some α, $\beta \in \mathbb{C}$.

Boundary conditions

Restricting τ to compactly supported functions, by Lemma 4.3, we obtain a symmetric operator

$$A_0 f \coloneqq \tau f, \qquad \mathcal{D}(A_0) = \mathcal{D}(\tau) \cap AC_c(I).$$

Furthermore A_0 is densely defined with

$$\begin{aligned} \bar{A_0} f &= \tau f, \qquad & \mathcal{D}(\bar{A_0}) &= \{f \in \mathcal{D}(\tau) : W(f,g)(a) = W(f,g)(b) = 0 \text{ for all } g \in \mathcal{D}(\tau)\}, \\ A_0^* f &= \tau f, \qquad & \mathcal{D}(A_0^*) &= \mathcal{D}(\tau) \end{aligned}$$

(see [16], Lemma 9.4 for a proof), where A_0^* denotes the adjoint and $\bar{A_0}$ the closure A_0^{**} of A_0.
Hence, any self-adjoint extension of A_0 must lie between $\bar{A_0}$ and A_0^* and we proceed by investigating necessary conditions at the endpoints.

Definition 4.5. (Limit Point and Limit Circle)
We call τ limit point at an endpoint a if

$$W(f,g)(a) = 0 \qquad \text{for all } f, g \in \mathcal{D}(\tau).$$

Otherwise τ is called limit circle at a.

Lemma 4.6. (Characterization of limit circle endpoints)
A Sturm-Liouville operator τ is limit circle at an endpoint a iff there exists some $v \in \mathcal{D}(\tau)$ with $W(v, v^*)(a) = 0$ and $W(v, f)(a) \neq 0$ for atleast one $f \in \mathcal{D}(\tau)$. Moreover we can assume v to be real-valued.

Proof. If τ is limit circle at a, then by definition there exist some $f, v \in \mathcal{D}(\tau)$ with $0 \neq W(f,v)(a) = W(f, \mathrm{Re}(v))(a) + iW(f, \mathrm{Im}(v))$, i.e. either $W(f, \mathrm{Re}(v))(a) \neq 0$ or $(f, \mathrm{Im}(v))(a) \neq 0$ and we can assume v to be real-valued and $W(v, v*)$ holds trivially. The opposite implication is trivial. □

The following result from [16], Lemma 9.5 gives rise to sufficient boundary conditions at limit circle endpoints to define a self-adjoint extension of A_0:

Let τ be limit circle at a and v as in Lemma 4.6, then

$$\begin{aligned} W(v,f)(a) = 0 \quad &\Leftrightarrow \quad W(v,f^*)(a) = 0 \quad \text{for all } f \in \mathcal{D}(\tau), \\ W(v,f)(a) = W(v,g)(a) = 0 \quad &\Rightarrow \quad W(g^*,f)(a) = 0 \quad \text{for all } f, g \in \mathcal{D}(\tau) \end{aligned} \tag{4.5}$$

Theorem 4.7. *The operator*

$$Af \coloneqq \tau f, \qquad \mathcal{D}(A) \coloneqq \left\{ f \in \mathcal{D}(\tau) : \; W(v,f)(a) = 0, \text{ if } \tau \text{ is limit circle at } a, \; W(w,f)(b) = 0, \text{ if } \tau \text{ is limit circle at } b \right\}$$

with v as in Lemma 4.6 and w analogous for b, is self-adjoint. (See [16], Theorem 9.6 for a proof.)

Now let τ be limit circle at a, $\tau u_j = 0$, $j = 1, 2$, $W(u_1, u_2) = 1$, v as in Lemma 4.6 real-valued and $f \in \mathcal{D}(\tau)$. Then the *Pflücker identity* for functions in $\mathcal{D}(\tau)$ gives

$$W(u_1, v)(a)W(u_2, f)(a) + W(u_1, u_2)(a)W(f, v)(a) + W(u_1, f)(a)W(v, u_2)(a) = 0$$

and hence by denoting $BC_a^j(v) \coloneqq W(u_j, v)(a)$,

$$W(f, v)(a) = 0 \qquad \Leftrightarrow \qquad \frac{W(u_1, f)(a)}{W(u_2, f)(a)} = \frac{BC_a^1(v)}{BC_a^2(v)}$$

where the right hand side is real-valued and already determined by τ from the uniqueness of u_1 and u_2 by Theorem 4.4, such that all possible boundary conditions can be parametrized by $\alpha \in [0, \pi)$ and

$$W(f, v)(a) = 0 \qquad \Leftrightarrow \qquad \cos(\alpha)W(u_2, f)(a) + \sin(\alpha)W(u_1, f)(a) = 0, \qquad \tan(\alpha) = -\frac{BC_a^2(v)}{BC_a^1(v)}.$$

In particular if a is regular, choosing u_1, u_2 such that $u_1(a) = 1$, $(pu_1')(a) = 0$, $u_2(a) = 0$, $(pu_2')(a) = 1$ the boundary conditions read

$$\cos(\alpha)f(a) + \sin(\alpha)(pf')(a) = 0. \tag{4.6}$$

At points z where $(A - z)$ is invertible, for each endpoint we can always find a solution of $(\tau - z)u = 0$ which behaves nicely at this endpoint and we can use these *fundamental solutions* to construct the inverse $(A - z)^{-1}$:

Theorem 4.8. (Green function and fundamental solutions)
Let $z \in \mathrm{Res}(A)$. Then there exist fundamental solutions $u_a(z, .)$, $u_b(z, .)$ of $(\tau - z)u = 0$, which are square-integrable near a and b respectively, i.e.

$$u_a(z, .) \in L^2((a, c), r(x)dx), \qquad u_b(z, .) \in L^2((d, b), r(x)dx), \qquad \text{for all } c, d \in (a, b),$$

and satisfy the boundary conditions at a and b respectively (in case that a, b are limit circle).
Moreover u_a and u_b can be chosen to be holomorphic in z and such that $u_a(z, .)^* = u_a(z^*, .)$, $u_b(z, .)^* = u_b(z^*, .)$.

The resolvent map of A, $z \mapsto (A - z)^{-1}$, is given by

$$(A - z)^{-1}g(x) = \int_a^b G(z, x, y)g(y)r(y)dy$$

where

$$G(z, x, y) \coloneqq \frac{1}{W(u_b(z), u_a(z))} \begin{cases} u_b(z, x)u_a(z, y), & x \geq y \\ u_a(z, x)u_b(z, y), & x \leq y \end{cases} \tag{4.7}$$

is called the Green function.

Proof. Let $z \in \mathrm{Res}(A)$, $g \in L^2_c(I, r(x)dx) = \{f \in L^2(I, r(x)dx) : \mathrm{supp}(f) \subset I \text{ compact}\}$ and $f = (A-z)^{-1}g \in \mathcal{D}(A)$. Near a we set $u_a = f$ such that $(\tau - z)u_a = g = 0$ and using Theorem 4.3 we can extend u_a to (a, b), analogously for u_b. The only thing we need to ensure in order to obtain non-trivial solutions is that f does not vanish identically near the endpoints.
Let u_1, u_2 be solutions of the homogeneous problem $(\tau - z)u = 0$ with $W(u_1, u_2) = 1$ such that by (4.4) we can write

$$f(x) = u_1(x)\left(\alpha + \int_a^x u_2(y)g(y)r(y)dy\right) + u_2(x)\left(\beta + \int_x^b u_1(y)g(y)r(y)dy\right) \qquad (*).$$

In particular since g vanishes near the endpoints, $f \equiv 0$ near both a and b is only possible if $\int_a^b u_j g r = 0$, $j = 1, 2$, which we avoid by choosing a suitable g such that without loss of generality $f \not\equiv 0$ near b and u_b is defined and non-trivial.
Now consider $(*)$ with $\mathrm{supp}(g) \subseteq (c, d) \subset (a, b)$, $u_1 = u_b$ and any u_2 with $(\tau - z)u_2 = 0$ and $W(u_b, u_2) = 1$:

- If $u_2 \notin L^2((d, b), r(x)dx)$, then $\beta u_2 = f - \left(\alpha + \int_a^d u_2 g r\right) \in L^2((d, b), r(x)dx)$ gives $\beta = 0$.
- If $u_2 \in L^2((d, b), r(x)dx)$, then taking any $\tilde{u}_b, \tilde{u}_1 \in \mathcal{D}(\tau)$ that coincide with u_b, u_2 near b (any absolutely continuous extentions that are square-integrable near a) gives $W(\tilde{u}_b, \tilde{u}_2) = W(u_b, u_2) = 1$ and hence τ must be limit circle at b. In particular (since $f \in \mathcal{D}(\tau)$ and u_b satisfies the boundary conditions at b) $W(w, f)(b) = W(w, u_b)(b) = 0$ and by (4.6) $0 = W(f, u_b)(b) = \beta W(u_2, u_b) = \beta$.

We conclude that a representation of f as in $(*)$ with $u_1 = u_b$ necessarily implies $\beta = 0$.
Analogously choosing g such that u_a is defined, we see that a representation of f as in $(*)$ with $u_2 = u_a$ implies $\alpha = 0$, such that

$$f(x) = u_b(x)\int_a^x u_a(y)g(y)r(y)dy + u_a(x)\int_x^b u_b(y)g(y)r(y)dy = \int_a^b G(z, x, y)g(y)dy$$

for $f = (\tau - z)^{-1}g$, $g \in L^2_c(I, r(x)dx)$ and the claim follows from the density of $L^2_c(I, r(x)dx)$ in $L^2(I, r(x)dx)$.
For the holomorphicity and complex-conjugation property of u_a, u_b see [16], Lemma 9.8. □

Remark. Note that if there is more than one square-integrable solution near a, then for the Green function to be well-defined we need a boundary condition at a, i.e. a must be limit circle This is known as the *Weyl alternative*.

Theorem 4.9. (Weyl alternative)
A Sturm-Liouville operator τ is limit circle at an endpoint a iff there exists some $z_0 \in \mathbb{C}$ such that all solutions of $(\tau - z_0)u = 0$ are square-integrable near a. In that case, this holds for all $z \in \mathbb{C}$.

Proof. Let τ be limit circle at a and $v, \tilde{v} \in \mathcal{D}(\tau)$ real-valued such that $W(v, \tilde{v})(a) \neq 0$ (as in Lemma 4.6). Let $A, \tilde{A}$

be the corresponding self-adjoint operators with

$$\mathcal{D}(A) = \left\{ f \in \mathcal{D}(\tau) : \ W(v,f)(a) = 0, \ W(w,f)(b) = 0 \text{ if } \tau \text{ is limit circle at } b \right\},$$
$$\mathcal{D}(\tilde{A}) = \left\{ f \in \mathcal{D}(\tau) : \ W(\tilde{v},f)(a) = 0, \ W(w,f)(b) = 0 \text{ if } \tau \text{ is limit circle at } b \right\}$$

with any suitable w for the endpoint b. Then $A \neq \tilde{A}$ since $v \in \mathcal{D}(A) \setminus \mathcal{D}(\tilde{A})$.
Let $z_0 \in \mathrm{Res}(A) \cap \mathrm{Res}(\tilde{A})$ and $u_a(z_0,.), \tilde{u}_a(z_0,.)$ solutions of $(\tau - z_0)u = 0$ as in Theorem 4.8, i.e. $W(v, u_a(z_0))(a) = 0$, $W(\tilde{v}, \tilde{u}_a(z_0))(a) = 0$ and both $u_a(z_0,.)$ and $\tilde{u}_a(z_0,.)$ are square-integrable near a. Then $u_a(z_0,.)$ and $\tilde{u}_a(z_0,.)$ are linearly independent, since $A \neq \tilde{A}$. In particular any solution of $(\tau - z_0)u = 0$ is a linear combination of $u_a(z_0,.)$ and $\tilde{u}_a(z_0,.)$ and hence square-integrable near a.
For general $z \in \mathbb{C}$ let u_1, u_2 be linearly independent solutions of $(\tau - z_0)u = 0$ with $W(u_1,u_2) = 0$ and such that u_1, u_2 are both square-integrable near a. If $(\tau - z)u = 0$, then $(\tau - z_0)u = (z - z_0)u$ and hence by (4.4) with $g = (z - z_0)u$ we have

$$u(x) = \alpha u_1(x) + \beta u_2(x) + (z - z_0) \int_c^x (u_1(x)u_2(y) - u_1(y)u_2(x))u(y)r(y)dy.$$

Choosing c close to a such that $|z - z_0|^2 M^2 < \frac{1}{36}$ for $M := \int_a^c |u_j(y)|^2 r(y)dy$ we can estimate

$$\begin{aligned} B(x)^2 := \left| \int_c^x (u_1(x)u_2(y) - u_1(y)u_2(x))u(y)r(y)dy \right|^2 &\leq \int_a^c \left| u_1(x)u_2(y) - u_1(y)u_2(x) \right|^2 r(y)dy \int_a^x u(y)^2 r(y)dy \\ &\leq 3M \left(u_1(x)^2 + u_2(x)^2 \right) \int_a^x u(y)^2 r(y)dy \end{aligned}$$

for all $x \in (a,c)$, and hence

$$\int_a^c B(x)^2 r(x)dx \leq 3M \int_a^c \left(u_1(x)^2 + u_2(x)^2 \right) \left(\int_a^x u(y)^2 r(y)dy \right) r(x)dx \leq 6M^2 \int_a^c u(x)^2 r(x)dx$$

which gives

$$\begin{aligned} \int_a^c u(x)^2 r(x)dx &\leq 3 \left(\int_a^c \left| \alpha u_1(x) + \beta u_2(x) \right|^2 r(x)dx + |z - z_0|^2 \int_a^x B(x)^2 r(x)dx \right) \\ &\leq 3 \left(3(\alpha^2 + \beta^2)M + 6|z - z_0|^2 M^2 \int_a^c u(x)^2 r(x)dx \right) \\ &\leq 9(\alpha^2 + \beta^2)M + \frac{1}{2} \int_a^c u(x)^2 r(x)dx < \infty. \end{aligned}$$

Conversely if all solutions of $(\tau - z_0)u = 0$ are square-integrable near a, then in particular there exist two linearly independent functions $f, g \in \mathcal{D}(\tau)$, hence $W(f,g)(a) \neq 0$ and τ is limit circle at a. □

Let us summarize some implications of the previous results:

- If τ is regular at a, then taking any real-valued $v \in \mathcal{D}(\tau)$ with $(v(a), (pv')(a) \neq (0,0)$ gives

$$W(v,f)(a) = v(a)(pf')(a) - (pv')(a)f(a),$$

  such that we can always find some $f \in \mathcal{D}(\tau)$ with $W(v,f)(a) \neq 0$ and hence τ is limit circle at a.

- If τ is regular at both endpoints, then $u_a(z,.)$ and $u_(z,.)$ can be constructed for all $z \in \mathbb{C}$ and the only case where $(A-z)^{-1}$ does not exist is for $W(u_b(z), u_a(z)) = 0$, meaning that u_b and u_a are linearly dependent, in particular z is an eigenvalue of A and hence $\sigma(A) = \sigma_p(A)$.

- If τ is limit circle at both endpoints, then the spectrum of any self-adjoint extension of A_0 is purely discrete. This follows from the well-known fact that for a self-adjoint operator A with compact resolvent for every $z \in \mathrm{Res}(A)$, the spectrum of A is discrete. The representation of the resolvent in Theorem 4.8, shows that the resolvent $(A-z)^{-1}$ is a Hilbert Schmidt-operator and hence compact for every $z \in \mathrm{Res}(A)$. (See [16] for details.)

- If A is a self-adjoint extension of A_0, then all eigenvalues of A are simple:
  Indeed, if τ is limit point at one endpoint a, then by Theorem 4.9 there can be atmost one solution of $(\tau - \lambda)u = 0$ which is square-integrable near a, and if both endpoints are limit circle, then $(A-\lambda)u_{1,2} = 0$, $u_{1,2} \in \mathcal{D}(A) \subseteq \mathcal{D}(\tau)$ implies $W(u_1, u_2) = 0$ and u_1, u_2 are linearly dependent.

The Weyl-m functions

Recall that by Theorem 4.4, fixing some $c \in (a,b)$ we can always find two linearly independent solutions of $(\tau - z)u_{1,2}(z,.) = 0$ which are entire in z. On the other hand for $z \in \mathrm{Res}(A)$, there are fundamental solutions $u_a(z,.)$ and $u_b(z,.)$, holomorphic in $z \in \mathrm{Res}(A)$.
The idea is, to describe the fundamental solutions as linear combinations of $u_{1,2}(z,.)$, for $z \in \mathrm{Res}(A)$, and to investigate the corresponding coefficients (the *Weyl-m functions*) in the limit as z moves towards $\sigma(A) \subseteq \mathbb{R}$.

Let $c \in (a,b)$ be arbitrary, $c(z,.)$, $s(z,.)$ be solutions of $(\tau - z)u = 0$ for all $z \in \mathbb{C}$ as in Theorem 4.4 with $c(z,c) = 1$, $c'(z,c) = 0$, $s(z,c) = 0$, $s'(z,c) = 1$ such that $W(c(z,.), s(z,.)) = 1$, and $u_a(z,.)$, $u_b(z,.)$ be solutions of $(\tau - z)u = 0$ for all $z \in \mathrm{Res}(A)$ which are in L^2 near a and b respectively as in Theorem 4.8.

Definition 4.10. (Weyl-m functions) *For $z \in \mathrm{Res}(A)$ we define*

$$m_a(z) := \frac{W(u_a(z,.), c(z,.))}{W(u_a(z,.), s(z,.))} = -\frac{p(c)u_a'(z,c)}{u_a(z,c)},$$
$$m_b(z) := -\frac{W(u_b(z,.), c(z,.))}{W(u_b(z,.), s(z,.))} = \frac{p(c)u_b'(z,c)}{u_b(z,c)}.$$

From the representation (4.4) we see that (up to a factor which we can normalize)

$$u_a(z,.) = c(z,.) - m_a(z)s(z,.), \qquad u_b(z,.) = c(z,.) - m_b(z)s(z,.) \qquad \text{for all } z \in \mathrm{Res}(A). \tag{4.8}$$

Moreover we have

$$\mathrm{Im}(m_a(z)) = \mathrm{Im}(z)\int_a^c |u_a(z,x)|^2 r(x)dx, \qquad \mathrm{Im}(m_b(z)) = \mathrm{Im}(z)\int_c^b |u_b(z,x)|^2 r(x)dx \tag{4.9}$$

and since u_a and u_b are holomorphic in z on $\mathrm{Res}(A) \supseteq \mathbb{C}\setminus\mathbb{R}$ and satisfy $u_a(z,.)^* = u_a(z^*,.)$, the same holds for the Weyl-m functions. In fact they are even *Herglotz functions* (see [16], Lemma 9.14):

Let $\mathbb{C}_\pm = \{z \in \mathbb{C} : \pm\mathrm{Im}(z) > 0\}$ be the upper and lower complex halfplanes.
A holomorphic function $F : \mathbb{C}_+ \to \overline{\mathbb{C}}_+$ is called *Herglotz function* and can be defined on $\mathbb{C}_-$ by $F(z^*) = F(z)^*$.
Moreover, F is a Herglotz function iff it can be written as

$$F(z) = a + bz + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right) d\mu(\lambda) \tag{4.10}$$

for some $a \in \mathbb{R}$, $b \geq 0$ and a finite Borel measure μ on $\mathbb{R}$ such that $\int_{\mathbb{R}} \frac{1}{1+\lambda^2} d\mu(\lambda) < \infty$.
This gives a one-to-one correspondence between F and μ in (4.10):

Every Herglotz function corresponds to a unique finite Borel measure μ on $\mathbb{R}$ given by the Stieltjes inversion formula

$$\mu(\lambda) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{\pi}\int_{-\infty}^{\lambda+\delta} \mathrm{Im}(F(t+i\varepsilon))dt.$$

Conversely, given a finite Borel measure μ, the Borel-transform $F(z) = \int_{\mathbb{R}} \frac{1}{\lambda - z} d\mu(\lambda)$ is a Herglotz function.
As one might suspect in light of the Stietjes inversion formula, the values of μ can be read off from the boundary behaviour of F in the limit towards the real line by

$$\mu(\{\lambda\}) = \lim_{\varepsilon\downarrow 0} \mathrm{Im}(F(\lambda + i\varepsilon)).$$

The key to understanding the spectrum of A will be to find a spectral measure associated to the Weyl-m functions. For that aim we define

Definition 4.11. (The Weyl-m matrix)

$$M(z) := \frac{1}{m_a(z) + m_b(z)} \begin{pmatrix} -1 & \frac{1}{2}(m_a(z) - m_b(z)) \\ \frac{1}{2}(m_a(z) - m_b(z)) & m_a(z)m_b(z) \end{pmatrix}$$

and note that $W(u_a(z), u_b(z)) = m_a(z) + m_b(z)$ and by (4.8) and the Definition 4.7 of the Green function, we can write the Weyl-m-matrix as

$$M(z) = \begin{pmatrix} G(z,x,x) & \frac{1}{2}(p(x)\partial_x + p(y)\partial_y)G(z,x,y) \\ \frac{1}{2}(p(x)\partial_x + p(y)\partial_y)G(z,x,y) & p(x)\partial_x p(y)\partial_y G(z,x,y) \end{pmatrix}\Bigg|_{x=y=c}. \tag{4.11}$$

Now consider the following spectral mapping:

Lemma 4.12. *There exists a measure μ and a non-negative 2×2-matrix-valued function R with $\operatorname{tr}(R) = 1$, such that*

$$U : L^2(I, r(x)dx) \to L^2(\mathbb{R}, Rd\mu), \qquad Uf(\lambda) = \int_I \underline{s}(\lambda, x) f(x) r(x) dx =: \underline{f}(\lambda)$$

is a spectral mapping for A as in Theorem D.5 with inverse

$$U^{-1}\underline{f}(x) = \int_{\mathbb{R}} \underline{s}(\lambda, x) R(\lambda) \underline{f}(\lambda) d\mu(\lambda),$$

where

$$\underline{s}(z,x) \coloneqq \begin{pmatrix} c(z,x) \\ s(z,x) \end{pmatrix}$$

and

$$L^2(\mathbb{R}, Rd\mu) = \{f : \mathbb{R} \to \mathbb{C}^2 \text{ measurable and } \int_{\mathbb{R}} \underline{f}^* R \underline{f} d\mu < \infty\} \quad \text{with} \quad \langle \underline{f}, \underline{g} \rangle_{L^2(\mathbb{R}, Rd\mu)} = \int_{\mathbb{R}} \underline{f}^* R \underline{g} d\mu.$$

Remark. Note that since A is a second order linear differential operator, it come as no surprise that we can write any spectral mapping as in Theorem D.5 as $U_0 : L^2(I, r(x)dx) \to \oplus_{j=1}^2 L^2(\mathbb{R}, d\mu_j)$. Moreover U_0 is of the form

$$U_0 f(\lambda) = \int_I \underline{u}(\lambda, x) f(x) r(x) dx = \int_I u_1(\lambda, x) f(x) r(x) dx + \int_I u_2(\lambda, x) f(x) r(x) dx$$

where $\underline{u}(\lambda, x) = (u_1(\lambda, x), u_2(\lambda, x))$, and u_1, u_2 are linearly independent solutions of $(\tau - \lambda)u = 0$.
Taking the 2×2-matrix $C(\lambda)$ that maps $\underline{s}(\lambda, .)$ to $\underline{u}(\lambda, .)$ and $\tilde{\mu} = \mu_1 + \mu_2$, such that $\tilde{\mu} << \mu_j$ and hence $d\mu_j = r_j d\mu$ for some densities r_1, r_2, we can define $\tilde{R} = C^* \left(\begin{smallmatrix} r_1 & 0 \\ 0 & r_2 \end{smallmatrix}\right) C$ and $R = \tilde{R}\operatorname{tr}(\tilde{R})^{-1}$. In particular be obtain a measure $\mu = \operatorname{tr}(\tilde{R})^{-1}\tilde{\mu}$ such that $\mu_j << \mu$ and $Rd\mu = \tilde{R}d\tilde{\mu}$. (See [16], Lemma 9.28 for details.)

We will show that the trace of the Weyl-m matrix is a Herglotz-function and corresponds to the spectral measure μ in Lemma 4.12.

Lemma 4.13. *Let U be as in Lemma 4.12. Then*

$$UG(z,x,.)(\lambda) = \frac{1}{\lambda - z}\underline{s}(\lambda, x),$$
$$Up(x)\partial_x G(z,x,.)(\lambda) = \frac{1}{\lambda - z}p(x)\underline{s}'(\lambda, x)$$

for all $x \in (a,b)$, $z \in \mathrm{Res}(A)$.

Proof. By (4.8) and Definition 4.7 $G(z,x,.) \in L^2(I, r(x)dx)$ for all $x \in I$, $z \in \mathrm{Res}(A)$.
Moreover since $R_A(z) = g(A)$ with $g(z) = \frac{1}{1-z}$:

$$UR_A(z) = M_{\frac{1}{.-z}}U, \qquad \text{i.e.} \qquad R_A(z)f = U^{-1}\left(\frac{1}{.-z}Uf\right)$$

in L^2 sense, and we obtain

$$\left\langle UG(z,x,.), Uf\right\rangle_{L^2(\mathbb{R}, Rd\mu)} = \left\langle G(z,x,.), f\right\rangle_{L^2(I.r(x)dx)} = \int_a^b G(z,x,y)f(y)r(y)dy = R_A(z)f(x)$$
$$\overset{\text{for a.e. x}}{=} U^{-1}\left(\frac{1}{1-z}Uf\right)(x) = \int_{\mathbb{R}} \frac{1}{\lambda - z}\underline{s}(\lambda, x)R(\lambda)Uf(\lambda)d\mu(\lambda) = \left\langle \frac{\underline{s}(.,x)}{.-z}, Uf\right\rangle_{L^2(\mathbb{R}, Rd\mu)}.$$

for all $f \in L^2(I, r(x)dx)$, in particular

$$UG(z,x,.) = \frac{\underline{s}(.,x)}{.-z}$$

for almost every x. Now since the left hand side of this equation is continuous with respect to x, so is the right hand side if Uf has compact support (since U is a convolution operator with s which is absolutely continuous). The equality hence holds pointwise, since such Uf are dense in $L^2(\mathbb{R}, Rd\mu)$. The second identity follows similary. □

Theorem 4.14. *The Weyl-m matrix is given by*

$$M(z) = D + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right) R(\lambda)d\mu(\lambda) \tag{4.12}$$

with $D = \mathrm{Re}(M(i))$. Moreover

$$\int_{\mathbb{R}} \frac{1}{1+\lambda^2}R(\lambda)d\mu(\lambda) = \mathrm{Im}(M(i)).$$

Proof. From Lemma 4.13 and $\underline{s}(.,c) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ we have

$$\|G(z,c,.)\|^2_{L^2(I,r(x)dx)} = \|UG(z,c,.)\|^2_{L^2(\mathbb{R},Rd\mu)} = \int_{\mathbb{R}} \frac{1}{|\lambda - z|^2} \underline{s}(.,c)^* R(\lambda) \underline{s}(.,c) d\mu(\lambda) = \int_{\mathbb{R}} \frac{1}{|\lambda - z|^2} R_{1,1}(\lambda) d\mu(\lambda).$$

On the other hand by (4.9)

$$\begin{aligned}
\|G(z,x,.)\|^2_{L^2(I,r(x)dx)} &= \int_a^b |G(z,c,y)|^2 r(y) dy \\
&= \frac{1}{|W(u_a(z), u_b(z))|^2} \left(|u_b(z,c)|^2 \int_a^c |u_a(z,y)|^2 r(y) dy + |u_a(z,c)|^2 \int_c^b |u_b(z,y)|^2 r(y) dy \right) \\
&= \frac{1}{|m_a(z) + m_b(z)|^2} \frac{\mathrm{Im}(m_a(z) + m_b(z))}{\mathrm{Im}(z)} = \frac{\mathrm{Im}(M_{1,1}(z))}{\mathrm{Im}(z)},
\end{aligned}$$

and hence

$$\mathrm{Im}(z) \int_{\mathbb{R}} \frac{1}{|\lambda - z|^2} R_{1,1}(\lambda) d\mu(\lambda) = \mathrm{Im}(M_{1,1}(z)).$$

Similarly

$$\mathrm{Im}(z) \int_{\mathbb{R}} \frac{1}{|\lambda - z|^2} R_{i,j}(\lambda) d\mu(\lambda) = \mathrm{Im}(M_{i,j}(z)) \qquad \text{for all } i,j \in 1,2$$

and using $Im\left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right) = \mathrm{Im}(z) \frac{1}{|\lambda - z|^2}$ we obtain

$$Im\left(\int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) R(\lambda) d\mu(\lambda) \right) = \mathrm{Im}(z) \int_{\mathbb{R}} \frac{1}{|\lambda - z|^2} R(\lambda) d\mu(\lambda) = \mathrm{Im}(M(z)).$$

Since a holomophic function is up to a real constant determined by its imaginary part, we see

$$M(z) = D + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) R(\lambda) d\mu(\lambda)$$

and setting $z = i$ shows the remaining properties. □

As consequence of this theorem, since $\mathrm{tr}(R) = 1$, we infer from (4.10) that

$$\mathrm{tr}(M(z)) = M_{1,1}(z) + M_{2,2}(z) = \mathrm{tr}(D) + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) d\mu(\lambda)$$

is the Herglotz function corresponding to the spectral measure μ.

Recall that the spectrum of a finite Borel measure on $\mathbb{R}$ is defined the set of growth points

$$\sigma(\mu) = \{\lambda \in \mathbb{R} : \ \mu((\lambda - \varepsilon, \lambda + \varepsilon)) > 0 \text{ for all } \varepsilon > 0\}$$

and the set

$$M \coloneqq \{\lambda \in \mathbb{R} :\ 0 < \limsup_{\varepsilon \downarrow 0} \operatorname{Im}(F(\lambda + i\varepsilon))\}$$

defines a minimal support for μ in terms of the corresponding Herglotz function.
Moreover, the sets

$$M_{\mathrm{ac}} \coloneqq \{\lambda \in \mathbb{R} :\ 0 < \limsup_{\varepsilon \downarrow 0} \operatorname{Im}(F(\lambda + i\varepsilon)) < \infty\}, \qquad M_{\mathrm{s}} \coloneqq \{\lambda \in \mathbb{R} :\ \limsup_{\varepsilon \downarrow 0} \operatorname{Im}(F(\lambda + i\varepsilon)) = \infty\}$$

are minimal supports for μ_{ac} and μ_s, and since μ is a maximal spectral measure for A, we have

$$\sigma(A) = \sigma(\mu) \qquad \text{and} \qquad \sigma_{\mathrm{ac}}(A) = \sigma(\mu_{\mathrm{ac}}) = \overline{M_{\mathrm{ac}}}^{\mathrm{ess}},$$

where $\overline{M_{\mathrm{ac}}}^{\mathrm{ess}} = \{\lambda \in \mathbb{R} :\ |(\lambda - \varepsilon, \lambda + \varepsilon) \cap M_{\mathrm{ac}}| > 0 \text{ for all } \varepsilon > 0\}$ denotes the essential closure of M_{ac}.

We proceed by investigating the absolutely continuous spectrum of A and assume that b is limit point, since otherwise the spectrum of A is purely discrete.

Definition 4.15. *Let v_1 and v_2 be solutions of $(\tau - z)u = 0$, then v_1 is called subordinate with respect to v_2 at b if*

$$\liminf_{x \to b} \frac{\|v_1\|_{(c,x)}}{\|v_2\|_{(c,x)}} = 0$$

where $\|f\|_{(c,x)} \coloneqq \sqrt{\int_c^x |f(y)|^2 r(y) dy}$.

Remark. Note that if v_1 is subordinate with respect to v_2 at b, then v_1 is subordinate with respect to any linearly independent solution of $(\tau - z)u = 0$.

Lemma 4.16. *Let $\lambda \in \mathbb{R}$. Then there exists a subordinate solution $u(\lambda, .)$ at b iff there exists a sequence $\varepsilon_n \downarrow 0$ such that $m_b(\lambda + i\varepsilon_n)$ converges in $\mathbb{R} \cup \{\infty\}$ as $n \to \infty$.*

Sketch of the proof. We will use the following result from [16], Lemma 9.23:

$$5 - \sqrt{24} \leq |m_b(\lambda + i\varepsilon)| \frac{\|s(\lambda)\|_{(c,x)}}{\|c(\lambda)\|_{(c,x)}} \leq 5 + \sqrt{24} \tag{4.13}$$

where $\varepsilon = \left(2\|s(\lambda)\|_{(c,x)}\|c(\lambda)\|_{(c,x)}\right)^{-1}$ and since b is limit point, by Theorem 4.9, there is a one-to-one correspondence between $\varepsilon \in (0, \infty)$ and $x \in (c, b)$.
Generalizing the functions $s(\lambda)$, $c(\lambda)$ to $s_\alpha(\lambda)$, $c_\alpha(\lambda)$ satisfying a general condition $\cos(\alpha)f(a) + \sin(\alpha)(pf')(a) = 0$ at c for some $\alpha \in [0, \pi)$ as in (4.6), gives a corresponding Weyl-m function $m_{b,\alpha}$ which depends on α. In particular

$m_{b,\alpha}$ and $m_{b,\beta}$ for different conditions α and β at c are related by

$$m_{b,\alpha}(z) = \frac{\cos(\alpha-\beta)m_{b,\beta}(z) + \sin(\alpha-\beta)}{\cos(\alpha-\beta) - \sin(\alpha-\beta)m_{b,\beta}(z)}. \tag{4.14}$$

Now let $u(\lambda)$ be a solution of $(\tau-\lambda)u = 0$, then depending on the values $u(\lambda, c)$, $p(c)u'(\lambda, c)$ we can always write $u(\lambda)$ as $s_\alpha(\lambda)$ for some suitable α and by (4.13) $u(\lambda)$ is subordinate at b iff $\lim_{n\to\infty} m_{b,\alpha}(\lambda + i\varepsilon_n) = \infty$ for some $\varepsilon_n \downarrow 0$. By (4.14) this is the case iff $\lim_{n\to\infty} m_b(\lambda + i\varepsilon_n) = \lim_{n\to\infty} m_{b,0}(\lambda + i\varepsilon_n) = \cot(-\alpha) \in \mathbb{R} \cup \{\infty\}$. □

Definition 4.17.

$$N_a(\tau) \coloneqq \left\{\lambda \in \mathbb{R} : \text{ there exists no solution of } (\tau-\lambda)u = 0 \text{ which is subordinate at } a\right\}$$
$$N_b(\tau) \coloneqq \left\{\lambda \in \mathbb{R} : \text{ there exists no solution of } (\tau-\lambda)u = 0 \text{ which is subordinate at } b\right\}$$

Theorem 4.18. *$N_a(\tau) \cup N_b(\tau) \subseteq M_{\mathrm{ac}}$ is a minimal support for μ_{ac}.*
In particular $\overline{N_a(\tau) \cup N_b(\tau)}^{\mathrm{ess}} = \sigma_{\mathrm{ac}}(A)$.

Sketch of the proof. We only show $N_a(\tau) \cup N_b(\tau) \subseteq M_{\mathrm{ac}}$ (see [16], Theorem 9.31 for a complete proof).
By Lemma 4.16 $\lambda \in N_a(\tau)$ iff $\liminf_{\varepsilon\to 0} \operatorname{Im}(m_a(\lambda + i\varepsilon)) > 0$ and $\limsup_{\varepsilon\to 0} |m_a(\lambda + i\varepsilon)| < \infty$.
Now recall $M_{\mathrm{ac}} = \{\lambda \in \mathbb{R} : \ 0 < \limsup_{\varepsilon\downarrow 0} \operatorname{Im}(\operatorname{tr}(M(\lambda + i\varepsilon))) < \infty\}$, $M_{1,1} = -\frac{1}{m_a + m_b}$ and let $\lambda \in N_a(\tau)$.
If $\limsup |M_{1,1}| = \infty$, then $0 = \liminf |m_a + m_b| \geq \liminf \operatorname{Im}(m_a) > 0$, a contradiction.
Suppose $\limsup |m_b| < \infty$, then

$$\liminf \operatorname{Im}(M_{1,1}) = \liminf \frac{\operatorname{Im}(m_a + m_b)}{|m_a + m_b|^2} \geq \frac{\liminf \operatorname{Im}(m_a)}{\limsup |m_a|^2 + \limsup |m_b|^2} > 0,$$

and otherwise, if $\limsup |m_b| = \infty$, then

$$\liminf \operatorname{Im}(M_{1,1}) = \liminf \operatorname{Im}\left(\frac{m_a}{1 + \frac{m_a}{m_b}}\right) \geq \liminf \operatorname{Im}(m_a) > 0.$$

Arguing similarly for $M_{2,2}$ we conclude

$$\limsup_{\varepsilon\downarrow 0} |\operatorname{tr}(M(\lambda + i\varepsilon))| < \infty \qquad \text{and} \qquad \liminf_{\varepsilon\downarrow 0} \operatorname{Im}(\operatorname{tr}(M(\lambda + i\varepsilon))) > 0,$$

i.e. $\lambda \in M_{\mathrm{ac}}$. □

4.1 Spectra of linear Schrödinger operators with exponentially decaying potential

Consider the (self-adjoint) free Schrödinger operator $-\triangle$ with $\mathcal{D}(-\triangle) = H^2(\mathbb{R})$.
Since $-\triangle$ is (via Fourier transform) unitarily equivalent to the multiplication operator

$$M_{(.)^2} : \psi \mapsto (.)^2\psi, \qquad \mathcal{D}(M_{(.)^2}) = \{\psi \in L^2(\mathbb{R}) : \ (.)^2\psi \in L^2(\mathbb{R})\},$$

we have

$$\langle \psi, R_{-\triangle}(z)\psi\rangle = \langle \mathcal{F}\psi, R_{M_{(.)^2}}(z)\mathcal{F}\psi\rangle = \int_{\mathbb{R}} \frac{1}{\xi^2 - z}|\mathcal{F}\psi(\xi)|^2 d\xi = \frac{1}{2}\int_0^\infty \frac{1}{\lambda - z}|\mathcal{F}\psi(\sqrt{\lambda})|^2\lambda^{-1/2}d\lambda = \int_{\mathbb{R}} \frac{1}{\lambda - z}d\mu_\psi(\lambda)$$

where $d\mu_\psi(\lambda) = \frac{1}{2}\chi_{[0,\infty)}(\lambda)|\mathcal{F}\psi(\sqrt{\lambda})|^2\lambda^{-1/2}d\lambda$, and hence every spectral measure μ_ψ is absolutely continuous with respect to Lebesgue measure and supported on $[0,\infty)$ and we conclude

$$\sigma(-\triangle) = \sigma_{\mathrm{ac}}(-\triangle) = [0,\infty).$$

Now let

$$V : \psi \mapsto V\psi, \qquad \mathcal{D}(V) = L^2(\mathbb{R})$$

be the (self-adjoint) multiplication operator by the function V (we will sloppily denote both the operator and the function by V), where V is symmetric, bounded and exponentially decaying.

Lemma 4.19. *Let A be a self-adjoint operator on $\mathcal{H}$ and B be a bounded self-adjoint operator defined on all of $\mathcal{H}$. Then the operator*

$$A + B : \psi \mapsto A\psi + B\psi, \qquad \mathcal{D}(A + B) = \mathcal{D}(A)$$

is self-adjoint. (see [6], Proposition 9.13)

We infer that

$$L \coloneqq -\triangle + V, \qquad \mathcal{D}(L) = H^2(\mathbb{R})$$

is a self-adjoint operator.

Theorem 4.20. (Weyl) *Let A, B be self-adjoint operators with compact resolvent difference $R_A(z) - R_B(z) \in \mathcal{C}(\mathcal{H})$ for some $z \in \mathrm{Res}(A) \cap \mathrm{Res}(B)$. Then the essential spectra of A and B coincide:*

$$\sigma_{\mathrm{ess}}(A) = \sigma_{\mathrm{ess}}(B).$$

Proof. We will use the characterization of the essential spectrum of a self-adjoint operator via *singular Weyl-sequences*:

$$\lambda \in \sigma_{\text{ess}}(A) \quad \Leftrightarrow \quad \text{there exists a sequence } (\psi_n)_n \subseteq \mathcal{D}(A) \text{ s.t. } \|\psi_n\| = 1,\ \psi_n \xrightarrow{\text{wk}} 0 \text{ and } \|(A-\lambda)\psi_n\| \to_n 0$$

("⇒" can be seen by taking an orthonormal basis of eigenfunctions in case that λ is an eigenvalue of infinite multiplicity and for an accumulation point, setting $P_n \coloneqq P_A([\lambda - \frac{1}{n}, \lambda - \frac{1}{n+1}) \cup (\lambda + \frac{1}{n+1}, \lambda + \frac{1}{n}])$, there must be a subsequence (n_j) with $rank(P_{n_j}) > 0$ for all j and we can take $\psi_j \in Ran(P_{n_j}))$, see [16], Lemma 6.17 for a complete proof) and show that a singular Weyl-sequence for $\lambda \in \sigma_{\text{ess}}(A)$ gives a singular Weyl-sequence for λ corresponding to B (an vice versa).
Let $\lambda \in \sigma_{\text{ess}}(A)$ and note that

$$\frac{R_A(z)}{z-\lambda}(A-\lambda) = \frac{R_A(z)}{z-\lambda}\big((A-z)-(\lambda-z)\big) = \frac{1}{z-\lambda}\big(I - R_A(z)(\lambda - z)\big) = R_A(z) - \frac{1}{\lambda - z}$$

such that

$$\left\| \left(R_A(z) - \frac{1}{z-\lambda} \right) \psi_n \right\| = \left\| \frac{R_A(z)}{z-\lambda}(A-\lambda)\psi_n \right\| \leq \left\| \frac{R_A(z)}{z-\lambda} \right\| \|(A-\lambda)\psi_n\| \to 0.$$

Since $\psi_n \xrightarrow{\text{wk}} 0$ and $R_A(z) - R_B(z)$ is compact, also $\|(R_A(z) - R_B(z))\psi_n\| \to 0$ and hence

$$\left\| \left(R_B(z) - \frac{1}{z-\lambda} \right) \psi_n \right\| = \left\| \left(R_B(z) - R_A(z)\right) \psi_n + \left(R_A(z) - \frac{1}{z-\lambda} \right) \psi_n \right\| \to 0$$

and

$$\|(B-\lambda)\, R_B(z)\psi_n\| = \left\| (\lambda - z) \left(\frac{1}{z-\lambda} - R_B(z) \right) \psi_n \right\| \to 0.$$

Moreover $|\langle R_B(z)\psi_n, \phi\rangle| \leq \|R_B(z)\| |\langle \psi_n, \phi\rangle| \to 0$ for all $\phi \in \mathcal{H}$ and normalizing $\{R_B(z)\psi_n\}$ gives a singular Weyl-sequence for λ corresponding to B, i.e. $\sigma_{\text{ess}}(A) \subseteq \sigma_{\text{ess}}(B)$. □

To see that the resolvent difference $R_L(z) - R_{-\triangle}(z)$ is compact, we refer to [16], Lemmas 9.33, 9.12 and 6.29. (The relevant point in this argument is the rapid decay of V, in particular $\sup_{n\in\mathbb{Z}} \int_n^{n+1} |V|^2 < \infty$.)

Hence, from Weyl's Theorem 4.20 we infer that the essential spectrum of $L = -\triangle + V$ is given by

$$\sigma_{\text{ess}}(L) = \sigma_{\text{ess}}(-\triangle) = [0, \infty).$$

However, the essential spectrum can contain eigenvalues. We will regard L as a Sturm-Liouville operator and use Theorem 4.18 to show that $\sigma_{\text{ess}}(L)$ is in fact absolutely continuous. In particular the point spectrum $\sigma_p(L)$ must be contained in $(-\infty, 0]$.

We set $I = \mathbb{R}$, $p = r = 1$, $q = V$, $\mathcal{H} = L^2(\mathbb{R})$ such that

$$\tau = -\triangle + V = L, \qquad \mathcal{D}(\tau) = \left\{ f \in \mathcal{H} : \ f, f' \in AC(\mathbb{R}), \ \tau f \in \mathcal{H} \right\} = H^2(\mathbb{R}) \tag{4.15}$$

is self-adjoint and hence limit point at both endpoints $-\infty$ and ∞.

Remark. The self-adjointness of L can also be seen from the *Sobolev embedding*

$$H^s(\mathbb{R}^d) \hookrightarrow C^k_\infty(\mathbb{R}^d) = \{ f \in C^k(\mathbb{R}^d) : \ f \text{ vanishes at } \infty \} \qquad \text{for all } s > k + d/2,$$

in particular

$$H^2(\mathbb{R}) \hookrightarrow C^1_\infty(\mathbb{R}),$$

which gives

$$W(f,g)(x) \xrightarrow{|x| \to \infty} 0 \qquad \text{for all } f, g \in \mathcal{D}(\tau).$$

Now recall the characterization of the absolutely continuous spectrum by means of subordinacy, as in Theorem 4.18. We show that for $\lambda > 0$, there are no solutions of $(\tau - \lambda)u = 0$ that are subordinate at ∞ by constructing two linearly independent solutions that are are not subordinate with respect to one another near ∞.

Lemma 4.21. (Volterra iteration) *Let $a \in \mathbb{R}$, $g \in L^\infty(a, \infty)$, $M \coloneqq \int_a^\infty \sup_{a<x<s} |K(x,s)| ds < \infty$. Then there exists a unique solution to the Volterra integral equation*

$$f(x) = g(x) + \int_x^\infty K(x,s) f(s) ds \tag{4.16}$$

given by

$$f(x) = g(x) + \sum_{n=1}^\infty \int_a^\infty \cdots \int_a^\infty \prod_{i=1}^n \chi_{\{x_{i-1} < x_i\}} K(x_{i-1}, x_i) g(x_n) dx_n \dots dx_1$$

where $x_0 = x$. Moreover

$$\|f\|_{L^\infty(a,\infty)} \leq e^M \|g\|_{L^\infty(a,\infty)}.$$

Proof. We proceed as in [13], Lemma 2.4. Let

$$K_0(s) \coloneqq \sup_{a<x<s} |K(x,s)|, \qquad \phi(f)(s) \coloneqq \int_a^\infty \chi_{\{x<y\}} K(x,y) f(y) dy,$$

$$f_0 \coloneqq g \qquad \text{and} \qquad f_{n+1}(x) \coloneqq \phi(f_n)(x) \qquad \text{for } n \geq 0.$$

Then

$$
\begin{aligned}
|f_n(x)| &= \left| \int_a^\infty \cdots \int_a^\infty \prod_{i=1}^n \chi_{\{x_{i-1}<x_i\}} K(x_{i-1}, x_i) g(x_n) dx_n \dots dx_1 \right| \\
&\le \int_a^\infty \cdots \int_a^\infty \prod_{i=1}^n \chi_{\{x_{i-1}<x_i\}} K_0(x_i) |g(x_n)| dx_n \dots dx_1 \\
&\le \|g\|_{L^\infty(a,\infty)} \int_a^\infty \cdots \int_a^\infty \prod_{i=1}^n \chi_{\{x_{i-1}<x_i\}} K_0(x_i) dx_n \dots dx_1 \\
&\le \|g\|_{L^\infty(a,\infty)} \frac{1}{n!} \int_a^\infty \cdots \int_a^\infty \prod_{i=1}^n K_0(x_i) dx_n \dots dx_1 = \|g\|_{L^\infty(a,\infty)} \frac{1}{n!} \left(\int_a^\infty K_0(s) ds \right)^n = \|g\|_{L^\infty(a,\infty)} \frac{M^n}{n!}
\end{aligned}
$$

where the last inequality can be seen by $\phi_0(x) \coloneqq \int_x^\infty K_0(x)dx$, $K_0(x) = -\phi_0'(x)$ such that

$$
\begin{aligned}
&\int_a^\infty \cdots \int_a^\infty \prod_{i=1}^n \chi_{\{x_{i-1}<x_i\}} K_0(x_i) dx_n \dots dx_1 \\
&= \int_{x_0}^\infty K_0(x_1) \int_{x_1}^\infty K_0(x_2) \cdots \int_{x_{n-3}}^\infty K_0(x_{n-2}) \left(\int_{x_{n-2}}^\infty K_0(x_{n-1}) \int_{x_{n-1}}^\infty K_0(x_n) dx_n dx_{n-1} \right) dx_{n-2} \dots dx_2 dx_1 \\
&= \int_{x_0}^\infty K_0(x_1) \int_{x_1}^\infty K_0(x_2) \cdots \int_{x_{n-3}}^\infty K_0(x_{n-2}) \left(\int_{x_{n-2}}^\infty (-\phi_0'(x_{n-1})) \phi_0(x_{n-1}) dx_{n-1} \right) dx_{n-2} \dots dx_2 dx_1 \\
&= \int_{x_0}^\infty K_0(x_1) \int_{x_1}^\infty K_0(x_2) \cdots \int_{x_{n-3}}^\infty K_0(x_{n-2}) \left(\frac{1}{2} \int_{x_{n-2}}^\infty \phi_0(x_{n-2})^2 \right) dx_{n-2} \dots dx_2 dx_1 = \cdots = \frac{1}{n!} \phi_0(x_0)^n \le \frac{1}{n!} \phi_0(a).
\end{aligned}
$$

Now let $f^N \coloneqq \sum_{n=0}^N f_n$, then $f^N(x)$ converges uniformly and absolutely on (a,∞) to $f \coloneqq \lim_{N\to\infty} f^N$,

$$
|f(x)| \le \|g\|_{L^\infty(a,\infty)} \sum_{n=0}^\infty \frac{M^n}{n!} = \|g\|_{L^\infty(a,\infty)} e^M \qquad \text{for all } x \in (a,\infty)
$$

and

$$
\begin{aligned}
f(x) &= \lim_{N\to\infty} f^N(x) = g(x) + \lim_{N\to\infty} \sum_{n=1}^N f_n(x) = g(x) + \lim_{N\to\infty} \sum_{n=1}^N \phi(f_{n-1})(x) \\
&= g(x) + \lim_{N\to\infty} \phi \left(\sum_{n=1}^N f_{n-1} \right)(x) = g(x) + \lim_{N\to\infty} \phi(f^{N-1})(x) = g(x) + \lim_{N\to\infty} \int_x^\infty K(x,y) f^{N-1}(y) dy \\
&= g(x) + \int_x^\infty K(x,y) f(y) dy.
\end{aligned}
$$

□

Lemma 4.22. *Let $\lambda > 0$ and τ as in (4.15). Then there exists linearly independent solutions f_+ and f_- of $(\tau - \lambda)f = 0$ such that*

$$f_\pm(x) \xrightarrow{x\to\infty} e^{\pm i\sqrt{\lambda}x}$$

Proof. We proceed similarly as in [13]. Let $\tilde{\lambda} \coloneqq \sqrt{\lambda} > 0$ and observe that (by simple differentiation) the problem is equivalent to

$$f_\pm(x) = e^{\pm i\tilde{\lambda}x} + \int_x^\infty \frac{\sin(\tilde{\lambda}(y-x))}{\tilde{\lambda}} V(y) f_\pm(y) dy.$$

Applying a Volterra iteration as in Lemma 4.21 for $g(x) = e^{\pm i\tilde{\lambda}x} \in L^\infty(\mathbb{R})$, $K(x,y) = \frac{\sin(\tilde{\lambda}(y-x))}{\tilde{\lambda}} V(y)$ such that by the exponential decay of V: $M = \int_a^\infty \sup_{a<x<s} |K(x,s)| ds < \infty$ for all $a \in \mathbb{R}$, gives unique solutions $f_\pm$. Moreover $W(f_+, f_-)(x) \xrightarrow{x\to\infty} 2i\sqrt{\lambda} \neq 0$ and hence f_+, f_- are linearly independent. □

Corollary 4.23. *Let L be as in Definition 4.15. Then*

$$\sigma_{\mathrm{ac}}(L) = [0,\infty), \qquad \sigma_{\mathrm{sc}}(L) = \emptyset, \qquad \sigma_p(L) \subseteq (-\infty, 0].$$

Proof. Let $\lambda > 0$, then any solution of $(\tau - \lambda) = 0$ must be a linear combination of f_+, f_- as in Lemma 4.22 and hence there are no subordinate solutions at ∞, which by Definition 4.17 and Theorem 4.18 means $(0,\infty) \subseteq N_\infty \subseteq M_{\mathrm{ac}}$. Now since $\sigma_{\mathrm{ess}}(L) = [0,\infty)$ and $\sigma_{\mathrm{ac}} = \overline{M_{\mathrm{ac}}}^{\mathrm{ess}}$, we infer $\sigma_{\mathrm{ac}}(L) = [0,\infty)$ and $\sigma_{\mathrm{sc}}(L) \subseteq \{0\}$, but the the singular continuous spectrum cannot be supported on a single point and hence $\sigma_{\mathrm{sc}}(L) = \emptyset$ and $\sigma_p(L) \subseteq (-\infty, 0]$. □

Remark. In fact this result applies to any operator $-\triangle + q$ with $q \in L^1_{loc}$ and $\lim_{|n|\to\infty} \int_n^{n+1} |q| = 0$ (see [16], Lemma 9.38).

To end this Section, we turn to the question weather the number of negative eigenvalues is finite.

Theorem 4.24. (Sturm comparison)
Let $\tau_0 = -\triangle + q_0$, $\tau_1 = -\triangle + q_1$ on $I = (a,b)$ with $q_0 \leq q_1$, $\tau_0 u = 0$, $\tau_1 v = 0$ and $(c,d) \subseteq I$.
Suppose $W(u,v)(c) = W(u,v)(d) = 0$ or, if $c, d \in (a,b)$, $u(c) = u(d) = 0$. Then either u and v are linearly dependent or there exists some $x \in (c,d)$ with $v(x) = 0$.

Proof. By possible decreasing d and flipping the sign u we can assume $u > 0$ on (c,d). Suppose that v has no zeros in (c,d), then we can assume also $v > 0$ on (c,d).
At c we have either $W(u,v)(c) = 0$ or $u = 0, u' > 0, v \geq 0$, i.e. $W(u,v)(c) \leq 0$, and at d we have either

$W(u,v)(d) = 0$ or $u = 0, u' < 0, v \geq 0$, i.e. $W(u,v)(d) \geq 0$.
From $-u''v = q_0uv$, $-v''u = q_1vu$ and $W(u,v)' = u''v - uv''$ we have

$$0 \leq W(u,v)(d) - W(u,v)(c) = \int_c^d (q_0 - q_1)(x)u(x)v(x)dx \leq 0,$$

but this is only possible if $q_0 \equiv q_1$ on (c,d) (in particular $\tau_0 = \tau_1$ on (c,d)) and $W(u,v)(c) = W(u,v)(d) = 0$, which implies that u and v are linearly dependent. □

Corollary 4.25. *Let $\tau = -\triangle + q$, $\tau u = \lambda_0 u$, $\tau v = \lambda_1 v$ with $\lambda_0 \leq \lambda_1$ and $u(x_1) = u(x_2) = 0$ for some $x_1, x_2 \in I$. Then either u and v are linearly dependent or v has a zero in (x_1, x_2).*

Proof. Set $q_0 = q - \lambda_0$, $\tau_0 = -\triangle + q_0$ and $q_1 = q - \lambda_1$, $\tau_1 = -\triangle + q_1$, then $\tau_0 u = 0$, $\tau_1 v = 0$ and the above Theorem applies. □

Theorem 4.26. *Let L as in (4.15) and $\lambda_0 < \cdots < \lambda_n < \ldots$ be its eigenvalues in $(-\infty, 0]$ with corresponding eigenfunctions $\psi_0, \ldots, \psi_n, \ldots$, then ψ_n has n zeros.*

Proof. Suppose ψ_n has m zeros $x_1, \ldots x_m$.
Then by Corollary 4.25 ψ_{n+1} has atleast one zero in each interval $(-\infty, x_1), (x_1, x_2) \ldots, (x_{m-1}, x_m), (x_m, \infty)$,
i.e. ψ_{n+1} has atleast $m+1$ zeros and hence by induction $m \geq n$.
Now let

$$\eta_0 \coloneqq \chi_{(-\infty, x_1)}\psi_n, \qquad \eta_m \coloneqq \chi_{(x_m, \infty)}\psi_n, \qquad \eta_j \coloneqq \chi_{(x_j, x_{j+1})}\psi_n \qquad \text{for } 1 \leq j \leq m-1.$$

We will use the following results from [16], Lemma 9.33 and Theorem 4.15:

- Let $q \in L^1_{loc}(\mathbb{R})$ and $\sup_{n\in\mathbb{Z}} \int_n^{n+1} |q| < \infty$.
  Then the form domain of $-\triangle + q$ coincides with the form domain of $-\triangle$:

$$\mathbf{D}(-\triangle + q) = \mathbf{D}(-\triangle) = H^1(\mathbb{R}).$$

- Let A be self-adjoint, $(\psi_j)_1^k \subseteq \mathbf{D}(A)$ linearly independent and $\lambda \in \mathbb{R}$.
  If $\langle \psi, A\psi \rangle < \lambda \|\psi\|^2$ for any linear combination $\psi = \sum_{j=1}^k c_j\psi_j$, then *dim Ran*$(P_A((-\infty, \lambda)) \geq k$.

We infer that $\mathbf{D}(L) = H^1(\mathbb{R})$ and since $\eta_j \in \mathcal{D}(L) = H^2(\mathbb{R}) \subseteq H^1(\mathbb{R})$, $\langle \eta_j, L\eta_j \rangle = \lambda_n \|\eta_j\|^2$ and $\langle \eta, L\eta \rangle = \lambda_n \|\eta\|^2 < \lambda_{n+1}\|\eta\|^2$ for any linear combination $\eta = \sum_{j=0}^m c_j\eta_j$:

$$\dim \operatorname{Ran}(P_L((-\infty, \lambda_{n+1}))) \geq m+1,$$

i.e. L has atleast $m+1$ eigenvalues in $(-\infty, \lambda_n]$ and in particular $m > n$ is not possible. □

Definition 4.27. *The equation $(\tau - \lambda)u = 0$ is called oscillating if there exists a solution with infinitely many zeros. In that case, this holds for any solution (by Theorem 4.24).*

Theorem 4.28. *Let L as in (4.15). Then L has finitely many negative eigenvalues.*

Proof. This result is based on *Kneser's Theorem*, see [16] Theorem 9.42.
Consider the operator $\tau_0 = -\triangle + q_0$ with $q_0(x) = \frac{C}{x^2}$. Then $\tau_0 u = 0$ has two linearly independent solutions $u_{1,2}(x) = x^{1/2 \pm \sqrt{C+1/4}}$.
If $C \geq -1/4$, then $u_{1,2}$ vanish only at $x = 0$ and if $C < -1/4$, then $\mathrm{Re}(u_j)$ and $\mathrm{Im}(u_j)$, $j = 1, 2$ are solutions with infinitely many zeros near ∞.
Now since V is exponentially decaying, we have $\liminf_{|x| \to \infty} x^2 V(x) > -1/4$ and hence by Theorem 4.24 $(L-0)u = 0$ is not oscillatory, which by Theorem 4.26 is equivalent to L having finitely many eigenvalues below zero. □

4.2 Proof of Proposition 3.11

Recall the definition of H (3.14) as quadratic form corresponding to the linear Schrödinger operators

$$\mathcal{L}_1 = -\triangle + 10(.)Q^3Q', \qquad \mathcal{L}_2 = -\triangle + 2(.)Q^3Q'.$$

We define

$$\bar{H}(f,f) = \bar{H}_1(f_1,f_1) + \bar{H}_2(f_2,f_2) \coloneqq \big(\bar{\mathcal{L}}_1 f_1 \big| f_1\big) + \big(\bar{\mathcal{L}}_2 f_2 \big| f_2\big) \tag{4.17}$$

with

$$\bar{\mathcal{L}}_1 \coloneqq -\triangle + \frac{10}{9}\left(10(.)Q^3Q'\right) - \frac{1}{9}\left(\cosh(\tfrac{9}{10}(.))^{-2}\right), \tag{4.18}$$

$$\bar{\mathcal{L}}_2 \coloneqq -\triangle + \frac{10}{9}\left(2(.)Q^3Q'\right) - \frac{1}{9}\left(\cosh(\tfrac{9}{10}(.))^{-2}\right) \tag{4.19}$$

which gives

$$\bar{H}(f,f) = \|f'\|_{L^2}^2 + \frac{10}{9}\Big(10\big((.)Q^3Q'\big|f_1^2\big) + 2\big((.)Q^3Q'\big|f_2^2\big)\Big) - \frac{1}{9}\|f\cosh(\tfrac{9}{10}(.))\|_{L^2}^2.$$

From

$$H(f,f) = \|f'\|_{L^2}^2 + 10\big((.)Q^3Q'\big|f_1^2\big) + 2\big((.)Q^3Q'\big|f_2^2\big)$$

and

$$\cosh(\tfrac{9}{10}(.))^{-2} = \frac{2}{\cosh(\frac{9}{5}(.)) + 1} \geq w(.)$$

we see

$$\begin{aligned}\frac{9}{10}\bar{H}(f,f) &= H(f,f) - \frac{1}{10}\left(\|f'\|_{L^2}^2 + \|f\cosh(\tfrac{9}{10}(.))\|_{L^2}^2\right) \\ &\leq H(f,f) - \frac{1}{10}\left(\|f'\|_{L^2}^2 + \|f\|_{L^2_w}^2\right),\end{aligned}$$

and hence it suffices to show $\bar{H}(f,f) \geq 0$ for all $f = f_1 + if_2 \in H^1_{\text{even}}$ with $\left(f_1 \middle| Q\right) = 0$, $\left(f_2 \middle| Q_1\right) = 0$ and $\left(f_2 \middle| Q_2\right) = 0$.

For that aim first determine the number of negative directions of $\bar{H}$.

Definition 4.29. (Index of a bilinear form)
Let B be a bilinear form on a vector space V. Then

$$\operatorname{ind}_V(B) \coloneqq \max\{k \in \mathbb{N} : \text{ there exists a subspace } P \subseteq V \text{ of codimension } k \text{ such that } B\big|_P \text{ is positive}\}$$

is called the index of B on V.

Moreover, denoting H^1_{odd} as the space of odd H^1 functions, and assuming that H^1_{even} is B-orthogonal to H^1_{odd}, i.e. $B(f,g) = 0$ for all $f \in H^1_{\text{even}}$, $g \in H^1_{\text{odd}}$, we write

$$\operatorname{ind}_{H^1}(B) = i + j \qquad \text{iff} \qquad \operatorname{ind}_{H^1_{\text{even}}}(B) = i \text{ and } \operatorname{ind}_{H^1_{\text{odd}}}(B) = j.$$

Remark. Note that the index of a quadratic form corresponding to a linear Schrödinger operator L with exponentially decaying potential coincides with the number of negative eigenvalues of L. This is easily seen from the spectral representation

$$f = \sum_{k=1}^{n} c_k\psi_k + \int_0^\infty \left(f\middle|\phi_\lambda\right)\phi_\lambda d\lambda$$

of any L^2-function f, where $\{\psi_k\}_{k=1}^n$ are the eigenfunctions of L corresponding the discrete spectrum and $\{\phi_\lambda\}_{\lambda\geq 0}$ are the generalized eigenfunctions of L corresponding to the continuous spectrum of L.

The indices of $\bar{H}_1$ and $\bar{H}_2$ can be determined by comparison of $\bar{\mathcal{L}}_1$ and $\bar{\mathcal{L}}_2$ to operators with known spectrum:

Lemma 4.30. *Let*

$$\tilde{L}_1 \coloneqq -\triangle - \frac{243}{25}\cosh(\tfrac{9}{10}(.))^{-2}, \qquad \tilde{L}_2 \coloneqq -\triangle - \frac{81}{50}\cosh(\tfrac{9}{10}(.))^{-2}$$

and

$$C_1(f) = \|f_1 \cosh(\tfrac{9}{10}(.))^{-1}\|_{L^2}^2, \qquad C_2(f) = \|f_2 \cosh(\tfrac{9}{10}(.))^{-1}\|_{L^2}^2.$$

Then

$$\bar{H}_1(f_1, f_1) \geq \big(\tilde{L}_1 f_1 \big| f_1\big) + 2C_1(f) \qquad \textit{and} \qquad \bar{H}_2(f_2, f_2) \geq \big(\tilde{L}_2 f_2 \big| f_2\big) + \frac{1}{30} C_2(f)$$

for all $f = f_1 + if_2 \in H^1$.

Proof. We claim that

$$10(.)Q^3Q' \geq -\frac{13}{2}\cosh(\tfrac{9}{10}(.))^{-2}.$$

First note that determining the unique maximum of the function $y \mapsto \frac{60y}{13}\cosh(y)^2\cosh(2y)^{-2}\tanh(2y) - 1$ on $[0, \infty)$ (similarly to the proof of (173) in [8]), gives the inequality

$$\tanh(2y)\cosh(2y)^{-2} \leq \frac{13}{60y}\cosh(y)^{-2} \qquad \text{for all } y \geq 0 \qquad (*).$$

From the explicit form of Q we obtain

$$10(.)Q^3Q' = -\frac{10(.)}{3}\tanh(2y)\cosh(2y)^{-1} = -\frac{10(.)}{3}\tanh(2y)\cosh(2y)^{-2}\cosh(2y).$$

Now using (*)

$$\begin{aligned}\frac{10y}{3}\tanh(2y)\cosh(2y)^{-2}\cosh(2y) &\leq \frac{13}{18}\cosh(y)^{-2}\cosh(2y) \leq \frac{13}{2}\cosh(y)^{-2} \\ &\leq \frac{13}{2}\cosh(9y/10)^{-2} \qquad \text{for all } y \geq 0\end{aligned}$$

and the claim follows from $10(.)Q^3Q'$ being even.
Estimating

$$\begin{aligned}\bar{H}_1(f_1, f_1) &= \|f_1'\|_{L^2}^2 + \frac{10}{9}\cdot 10\big((.)Q^3Q'\big|f_1^2\big) - \frac{1}{9}C_1(f) \\ &\geq \|f_1'\|_{L^2}^2 - \frac{10}{9}\frac{13}{2}C_1(f) - C_1(f) \\ &\geq \|f_1'\|_{L^2}^2 - \frac{243}{25}C_1(f) + 2C_1(f) = \big(\tilde{L}_1 f_1\big|f_1\big) + 2C_1\end{aligned}$$

and

$$\begin{aligned}\bar{H}_2(f_2, f_2) &= \|f_2'\|_{L^2}^2 + \frac{2}{9}\cdot 10\big((.)Q^3Q'\big|f_2^2\big) - \frac{1}{9}C_2(f) \\ &\geq \|f_2'\|_{L^2}^2 + \frac{2}{9}\cdot\frac{13}{2}C_2(f) - \frac{1}{9}C_2(f) \\ &\geq \|f_2'\|_{L^2}^2 - \frac{81}{50}C_2(f) - \frac{1}{30}C_2(f) = \big(\tilde{L}_2 f_2\big|f_2\big) + \frac{1}{30}C_2\end{aligned}$$

concludes the proof. □

Lemma 4.31. *Let*

$$L_n := -\triangle - \frac{n(n+1)}{4\cosh(\frac{\cdot}{2})^2}.$$

Then L_n has exactly $\left[\frac{n}{2}\right]+1$ negative eigenvalues and continuous spectrum on $[0,\infty)$.
In particular L_3 has two and L_1 has one negative eigenvalues.

Proof. This follows from knowing the eigenfunctions $L_n f_n = 0$ explicitly and applying Theorem 4.26. □

Corollary 4.32. Indices of $\bar{H}_1$ and $\bar{H}_2$

$$\operatorname{ind}_{H^1}(\bar{H}_1) = 1+1 \qquad\qquad \operatorname{ind}_{H^1}(\bar{H}_2) = 1+0.$$

Proof. For $f \in H^2$ let $\tilde{f}(y) := f(\frac{5y}{9})$. Then $\triangle\tilde{f}(y) = \frac{25}{81}\triangle f(\frac{5y}{9})$ and

$$\tilde{L}_1 f_1(y) = \frac{81}{25} L_3 \tilde{f}_1(\tfrac{9y}{5}), \qquad \tilde{L}_2 f_2(y) = \frac{81}{25} L_1 \tilde{f}_2(\tfrac{9y}{5})$$

for $\tilde{L}$ as in Lemma 4.30 and L_n as in Lemma 4.31. In particular

$$\tilde{L}_1 f = \lambda f \iff L_3 \tilde{f}(\tfrac{9(.)}{5}) = \frac{25}{81}\lambda\tilde{f}(\tfrac{9(.)}{5}) \quad \text{and} \quad \tilde{L}_2 f = \lambda f \iff L_1 \tilde{f}(\tfrac{9(.)}{5}) = \frac{25}{81}\lambda\tilde{f}(\tfrac{9(.)}{5})$$

and hence by Lemma 4.31, $\tilde{L}_1$ and $\tilde{L}_2$ have two and one negative eigenvalues.
From Lemma 4.30 we infer that $\bar{\mathcal{L}}_1$ and $\bar{\mathcal{L}}_2$ have atmost two and one negative eigenvalues and hence $\operatorname{ind}_{H^1}(\bar{H}_1) \le 2$ and $\operatorname{ind}_{H^1}(\bar{H}_2) \le 1$.

Now observe that we can write H in terms of the linearized operator close to the Ground State (2.4):

$$H_1(f_1,f_1) = \big(L_+ f_1 \big| \tfrac{f_1}{2} + (.)f_1'\big), \qquad H_2(f_2,f_2) = \big(L_- f_2 \big| \tfrac{f_2}{2} + (.)f_2'\big) \tag{4.20}$$

which simplifies the computations

$$\begin{aligned} H_1(Q',Q') &= \big(L_+Q' \big| \tfrac{Q'}{2} + (.)Q''\big) = 0, \\ H_1(Q,Q) &= \big(L_+Q \big| \tfrac{Q}{2} + (.)Q'\big) = -4\big(Q^5 \big| \tfrac{Q}{2} + (.)Q'\big) = -\frac{4}{3}\|Q\|_{L^6}^6 < 0, \\ H_2(Q,Q) &= \big(L_-Q \big| \tfrac{Q}{2} + (.)Q'\big) = 0. \end{aligned}$$

Observing that Q is even, Q' odd and $\bar{H} < H$ concludes the proof. □

Theorem 4.33. *i) There exists a unique regular even function $\phi_1 \in L^\infty$ such that $\bar{\mathcal{L}}_1\phi_1 = Q$.*
Moreover

$$\phi_1' \in L^2$$

and

$$-\big(\phi_1|Q\big)\left(1 - \bar{H}_1(Q,Q)\frac{\big(\phi_1|Q\big)}{\big(Q|Q\big)^2}\right) > 0.$$

ii) Let $Q_3 = Q_1 + \frac{Q_2}{2}$. There exists a unique regular even function $\phi_2 \in L^\infty$ such that $\bar{\mathcal{L}}_2\phi_2 = Q_3$.
Moreover

$$\phi_2' \in L^2$$

and

$$-\big(\phi_2|Q_3\big)\left(1 - \bar{H}_2(Q,Q)\frac{\big(\phi_2|Q_3\big)}{\big(Q|Q_3\big)^2}\right) > 0.$$

Remark. In [10], existence and uniqueness of ϕ_1 and ϕ_2 were shown by proving coercivity of $\bar{\mathcal{L}}_1$ and $\bar{\mathcal{L}}_1$ and applying a Volterra iteration (see Lemma 4.21), while the positivity estimates were checked numerically. In Sections 5 and 6 we will give a rigorous proof using a pseudo-spectral method and a contraction argument.

We are now ready to prove Proposition 3.11 by decomposing H^1_{even} into suitable subspaces. Note that the functions ϕ_j from Theorem 4.33 are not in H^1 and we need to use an approximation argument:

Let χ be a smooth cut-off function with $\text{supp}(\chi) \subseteq [-1,1]$ and denote $\chi_A(y) \coloneqq \chi(\frac{y}{A})$, $\phi_{j,A} \coloneqq \chi_A\phi_j \in H^1_{\text{even}}$. Define

$$\|f\|_j \coloneqq \left(\|f'\|_{L^2}^2 + \int_{\mathbb{R}} |V_j||f|^2\right)^{1/2}$$

where $\bar{\mathcal{L}}_j = -\triangle + V_j$, then

$$\begin{aligned}\big|\bar{H}_j(f,g)\big| = \big|\big(\bar{\mathcal{L}}_j f|g\big)\big| &\leq \big|\big(f'|g'\big)\big| + \left|\left(|V_j|^{1/2}|f|\middle||V_j|^{1/2}|g|\right)\right| \\ &\leq \|f'\|_{L^2}\|g'\|_{L^2} + \left(\int_{\mathbb{R}} |V_j||f|^2\right)^{1/2}\left(\int_{\mathbb{R}} |V_j||g|^2\right)^{1/2} \leq \|f\|_j\|g\|_j \end{aligned} \tag{4.21}$$

and

$$\|\phi_{j,A} - \phi_j\|_j = \left(\|\phi_{j,A}' - \phi_j'\|_{L^2} + \int_{\mathbb{R}} |V_j||\phi_{j,A} - \phi_j|^2\right) \xrightarrow{A\to\infty} 0 \tag{4.22}$$

since V_j is exponentially decaying and $\phi_j' \in L^2$ by Theorem 4.33.

We prove $\bar{H}_1(f,f) \geq 0$ for all $f \in H^1_{\text{even}}$ with $\big(f\big|Q\big) = 0$:

1) Let $P_{1,A} \coloneqq \operatorname{span}\{Q, \phi_{1,A}\}$, then $\bar{H}_1\big|_{P_{1,A}}$ is non-degenerate for A sufficiently large:
Consider the matrix representation of $\bar{H}_1\big|_{P_{1,A}}$ in terms of the basis $\{Q, \phi_{1,A}\}$ with determinant

$$D_{1,A} = \begin{vmatrix} \bar{H}_1(Q,Q) & \bar{H}_1(Q,\phi_{1,A}) \\ \bar{H}_1(Q,\phi_{1,A}) & \bar{H}_1(\phi_{1,A},\phi_{1,A}) \end{vmatrix} = \bar{H}_1(Q,Q)\bar{H}_1(\phi_{1,A},\phi_{1,A}) - \bar{H}_1(Q,\phi_{1,A})^2.$$

Note that from $\bar{\mathcal{L}}_1\phi_1 = Q$ and (4.21)

$$\begin{aligned} \bar{H}_1(\phi_{1,A},\phi_{1,A}) &= \bar{H}_1(\phi_{1,A},\phi_{1,A}-\phi_1) + \bar{H}_1(\phi_{1,A},\phi_1) = \bar{H}_1(\phi_{1,A},\phi_{1,A}-\phi_1) + \big(\phi_{1,A}\big|Q\big) \\ &= \bar{H}_1(\phi_{1,A},\phi_{1,A}-\phi_1) + \big(\phi_{1,A}-\phi_1\big|Q\big) + \big(\phi_1\big|Q\big) \\ &\leq \|\phi_{1,A}\|_1\|\phi_{1,A}-\phi_1\|_1 + \|\phi_{1,A}-\phi_1\|_1\|Q\|_1 + \big(\phi_1\big|Q\big) \end{aligned}$$

and

$$\begin{aligned} \bar{H}_1(Q,\phi_{1,A}) &= \bar{H}_1(Q,\phi_{1,A}-\phi_1) + \bar{H}_1(Q,\phi_1) = \bar{H}_1(Q,\phi_{1,A}-\phi_1) + \big(Q\big|Q\big) \\ &\leq \|Q\|_1\|\phi_{1,A}-\phi_1\|_1 + \big(Q\big|Q\big) \end{aligned}$$

and hence by (4.22) and Theorem 4.33

$$\begin{aligned} D_{1,A} &= \bar{H}_1(Q,Q)\big(\phi_1\big|Q\big) - \big(Q\big|Q\big)^2 + o(1) \\ &= -\big(Q\big|Q\big)^2\left(1 - \bar{H}_1(Q,Q)\frac{(\phi|Q)}{\big(Q\big|Q\big)^2}\right) + o(1) \neq 0 \qquad \text{as } A \to \infty. \end{aligned}$$

By this non-degeneracy we can decompose $H^1_{\text{even}} = P_{1,A} \oplus P^{\perp}_{1,A}$ for all A sufficiently large, where

$$P^{\perp}_{1,A} \coloneqq \{f \in H^1_{\text{even}} : \bar{H}_1(f,g) = 0 \text{ for all } g \in P_{1,A}\}$$

denotes the orthogonal complement of $P_{1,A}$ with respect to $\bar{H}_1$ in H^1_{even}.
Since $\bar{H}_1(Q,Q) < H_1(Q,Q) = 0$ and $\operatorname{ind}_{H^1_{\text{even}}}(\bar{H}_1) = 1$ we conclude

$$\bar{H}_1 \geq 0 \text{ on } P^{\perp}_{1,A}.$$

2) Let $A_n \xrightarrow{n\to\infty} \infty$ and $(f_n)_{n\in\mathbb{N}} \subseteq H^1_{\text{even}}$ with $f_n \in P_{1,A_n}$ and $\big(f_n\big|Q\big) \xrightarrow{n\to\infty} 0$. Then $\liminf_{n\to\infty} \bar{H}_1(f_n,f_n) \geq 0$:
Writing $f_n = \alpha_n Q + \beta_n \phi_{1,A_n}$ gives

$$\big(f_n\big|Q\big) = \alpha_n\big(Q\big|Q\big) + \beta_n\left(\phi_{1,A_n}\big|Q\right) \xrightarrow{n\to\infty} 0$$

and if $\beta_n = 0$ for all $n \geq N_0$ for some $N_0 \in \mathbb{N}$, then $\big(f_n\big|Q\big) = \alpha_n\|Q\|_{L^2}$ for $n \geq N_0$, and hence $\alpha_n \xrightarrow{n\to\infty} 0$, i.e. $f_n \xrightarrow{n\to\infty} 0$ and $\lim_{n\to\infty} \bar{H}_1(f_n,f_n) = 0$.

Otherwise by choosing a subsequence with $\beta_n \neq 0$ for all n sufficiently large

$$\lim_{n\to\infty} \frac{\alpha_n}{\beta_n} = -\lim_{n\to\infty} \frac{\big(\phi_{1,A_n}\big|Q\big)}{\big(Q\big|Q\big)} = \frac{\big(\phi_1\big|Q\big)}{\big(Q\big|Q\big)}$$

and

$$\begin{aligned}\frac{\bar{H}_1(f_n,f_n)}{\beta_n^2} &= \left(\frac{\alpha_n}{\beta_n}\right)^2 \bar{H}_1(Q,Q) + 2\frac{\alpha_n}{\beta_n}\bar{H}_1(Q,\phi_{1,A_n}) + \bar{H}_1(\phi_{1,A_n},\phi_{1,A_n}) \\ &\xrightarrow{n\to\infty} \frac{\big(\phi_1\big|Q\big)^2}{\big(Q\big|Q\big)^2}\bar{H}_1(Q,Q) - \big(\phi_1\big|Q\big) = -\big(Q,\phi_1\big)\left(1 - \frac{\big(Q\big|\phi_1\big)}{\big(Q\big|Q\big)^2}\bar{H}_1(Q,Q)\right) > 0\end{aligned}$$

by Theorem 4.33.

3) Now let $f \in H^1_{\text{even}} \setminus \{0\}$ with $\big(f\big|Q\big) = 0$ and write $f = f^A + f^A_\perp$ with $f^A \in P_{1,A}$ and $f^A_\perp \in P^\perp_{1,A}$. Then

$$\bar{H}_1(f,f) = \bar{H}_1(f^A,f^A) + \bar{H}_1(f^A_\perp,f^A_\perp) \geq \bar{H}_1(f^A,f^A)$$

for A sufficiently large and we claim that

$$\big(f^A\big|Q\big) \xrightarrow{A\to\infty} 0,$$

which concludes the proof.
Indeed, since $\big(f\big|Q\big) = 0$ gives $\big(f^A_\perp\big|Q\big) = -\big(f^A\big|Q\big)$ and $0 = \bar{H}_1(f^A_\perp,\phi_{1,A}) = \big(f^A_\perp\big|\bar{\mathcal{L}}_1\phi_{1,A}\big)$,

$$\begin{aligned}\big|\big(f^A\big|Q\big)\big| = \big|\big(f^A_\perp\big|Q\big)\big| &= \big|\big(f^A_\perp\big|\bar{\mathcal{L}}_1\phi_1\big)\big| \leq \big|\big(f^A_\perp\big|\bar{\mathcal{L}}_1(\phi_1-\phi_{1,A})\big)\big| + \big|\big(f^A_\perp\big|\bar{\mathcal{L}}_1\phi_{1,A}\big)\big| \\ &\leq \|f^A\|_1\|\phi_1-\phi_{1,A}\|_1 \xrightarrow{A\to\infty} 0\end{aligned}$$

by (4.22) and $\|f^A_\perp\|_1 \lesssim \|f\|_{H^1}$.

Analogously we prove $\bar{H}_2(f,f) \geq 0$ for all $f \in H^1_{\text{even}}$ with $\big(f\big|Q_1\big)$ and $\big(f\big|Q_1\big)$, which by definition of Q_3 (Theorem 4.33, ii) implies $\big(f\big|Q_3\big) = 0$:

1) For $P_{2,A} \coloneqq \operatorname{span}\{Q,\phi_{2,A}\}$ we obtain

$$\begin{aligned}D_{2,A} &= \bar{H}_2(Q,Q)\bar{H}_2(\phi_{2,A},\phi_{2,A}) - \bar{H}_2(Q,\phi_{2,A})^2 \\ &= -\big(Q\big|Q_3\big)^2\left(1 - \bar{H}_2(Q,Q)\frac{\big(\phi_2\big|Q_3\big)}{\big(Q\big|Q_3\big)^2}\right) + o(1) \neq 0 \qquad \text{as } A\to\infty\end{aligned}$$

and hence $H^1_{\text{even}} = P_{2,A} \oplus P^\perp_{2,A}$ for all A sufficiently large and

$$\bar{H}_2 \geq 0 \text{ on } P^\perp_{2,A}.$$

2) If $A_n \xrightarrow{n\to\infty} \infty$ and $(f_n)_{n\in\mathbb{N}} \subseteq H^1_{\text{even}}$ with $f_n \in P_{2,A_n}$ and $\big(f_n\big|Q_3\big) \xrightarrow{n\to\infty} 0$. Then $\liminf_{n\to\infty} \bar{H}_2(f_n,f_n) \geq 0$

since $f_n = \alpha_n Q + \beta_n \phi_{2,A_n}$ gives $\lim_{n\to\infty} \frac{\alpha_n}{\beta_n} = -\frac{(\phi_2|Q_3)}{(Q|Q_3)}$ and

$$\frac{\bar{H}_2(f_n,f_n)}{\beta_n^2} = \left(\frac{\alpha_n}{\beta_n}\right)^2 \bar{H}_2(Q,Q) + 2\frac{\alpha_n}{\beta_n}\bar{H}_2(Q,\phi_{2,A_n}) + \bar{H}_2(\phi_{2,A_n},\phi_{2,A_n})$$
$$\xrightarrow{n\to\infty} \frac{(\phi_2|Q_3)^2}{(Q|Q_3)^2}\bar{H}_2(Q,Q) - (\phi_2|Q) = -(\phi_2,Q_3)\left(1 - \bar{H}_2(Q,Q)\frac{(\phi_2|Q_3)}{(Q|Q_3)^2}\right) > 0$$

by Theorem 4.33.

3) For $f \in H^1_{\text{even}} \setminus \{0\}$ with $(f|Q_3) = 0$ we argue as above for $\bar{H}_1$.

Remark. As mentioned at the end of Section 3, the blow-up bound in Theorem 3.1 was shown for general (not even) initial data in [10]. Moreover this bound is conjectured to hold true in general dimension $d \geq 1$, under the assumption of the following spectral property:

Let $\mathcal{L}_1 = -\triangle + V_1$, $\mathcal{L}_2 = -\triangle + V_2$ with

$$V_1(r) = \frac{2}{d}\left(\frac{4}{d}+1\right) rQ^{4/d+1}(r)Q'(r), \qquad V_2(r) = \frac{2}{d} rQ^{4/d+1}(r)Q'(r), \qquad r = |y|,\ y \in \mathbb{R}^d,$$

$$H(\varepsilon,\varepsilon) = H_1(\varepsilon_1,\varepsilon_1) + H_2(\varepsilon,\varepsilon) = (\varepsilon_1|\mathcal{L}_1\varepsilon_1) + (\varepsilon_2|\mathcal{L}_2\varepsilon_2) \qquad \text{for } \varepsilon \in H^1(\mathbb{R}^d),$$

and

$$Q_1(y) = \frac{d}{2}Q(y) + y\cdot\nabla Q(y), \qquad \frac{d}{2}Q_1(y) + y\cdot\nabla Q_1(y).$$

Then there exists a universal constant $\tilde{\eta}_1 > 0$ such that

$$H(\varepsilon,\varepsilon) \geq \tilde{\eta}_1\left(\|\nabla\varepsilon\|_{L^2(\mathbb{R}^d)} + \int_{\mathbb{R}^d} |\varepsilon(y)|^2 e^{-|y|}dy\right)$$

for $\varepsilon \in H^1(\mathbb{R}^d)$ with

$$(\varepsilon_1|Q) = (\varepsilon_1|Q_1) = (\varepsilon_2|Q_1) = (\varepsilon_2|Q_2) = 0 \qquad (*)$$

and

$$(\varepsilon_1|(.)Q) = (\varepsilon_2|\nabla Q) = 0.$$

This spectral property was numerically checked for $d = 2, ..., 6$ in [4], shortly after [10] was published. We briefly sketch how the case of radial initial data (with orthogonality conditions $(*)$) was handled:

- Again, H_1 and H_2 are being estimated from below by $\bar{H}_1$ and $\bar{H}_2$ with corresponding operators $\bar{\mathcal{L}}_1$ and $\bar{\mathcal{L}}_2$, such that the problem reduces to showing positivity of $\bar{H}_j$ under the given orthogonality conditions.

- The index of $\bar{H}_j$ on the space of radial H^1 functions $H^1_{\text{radial}}(\mathbb{R}^d)$ is determined by numerically constructing the solutions to the homogeneous radial problem $\bar{\mathcal{L}}_j u(r) = -u''(r) - \frac{d-1}{r}u'(r) + \bar{V}_j(r)u(r) = 0$, $u(0) = 1$, $u'(0) = 0$. From Sturm's Theorem 4.24 and $\sigma_p(-\triangle) = \emptyset$ it follows that if the potential V_j is very small, then the solution u has no zeros. Now since $\bar{V}_j$ is basically made from Q, which is explicitly known, one can determine some radius R such that $\bar{V}_j(r)$ is sufficiently small for $r > R$ and it suffices compute u on $[-R, R]$ and count its zeros. This shows that $\text{ind}_{H^1_{\text{radial}}(\mathbb{R}^d)}(\bar{H}_1) = 1$ for $d = 2, 3$ and $\text{ind}_{H^1_{\text{radial}}(\mathbb{R}^d)}(\bar{H}_1) = 2$ for $d \in [4, 6]$, while $\text{ind}_{H^1_{\text{radial}}(\mathbb{R}^d)}(\bar{H}_2) = 1$ for $d \in [2, 6]$.

- The non-degeneracy of $\bar{H}_1$ on $(P_0)_A = \text{span}\{u_{0,A}\}$ for A sufficiently large is shown by numerically approximating the unique solutions of $\bar{\mathcal{L}}_1 u_0 = Q$ and $\bar{\mathcal{L}}_1 u_3 = Q_1$ such that $(1 + (.)^{d-2})u_j \in L^\infty$, $j = 0, 3$, and computing $\big(u_0\big|Q\big)\big(u_3\big|Q_1\big) - \big(u_0\big|Q_1\big)^2 =: K_1$. For $K_1 > 0$, the claimed positivity of $\bar{H}_1$ then follows similary as in the one-dimensional case by decomposition $H^1_{\text{radial}}(\mathbb{R}^d) = (P_0)_A \oplus (P_0)_A^\perp$ and similarly for $\bar{H}_2$ (with corresponding computation of K_2).

- The numerical accuracy is is claimed to be high by observing $\big(u_3\big|Q\big) = \big(u_3\big|\bar{\mathcal{L}}_1 u_0\big) = \big(\bar{\mathcal{L}}_1 u_3\big|u_0\big) = \big(Q_1\big|u_0\big)$ and computationally showing that $\big(u_3\big|Q\big) - \big(Q_1\big|u_0\big)$ is small for the numerical approximations u_0 and u_3.

- The point is, that while K_2 could be shown to be positive for all $d \in [2, 6]$, it seemed that $K_1 > 0$ only holds for $d \in [2, 4]$ and the operator $\bar{H}_1$ restricted to P_0 becomes degenerate at $d \in [5, 6]$. However, the case of $d = 5$ could be recovered by replacing the condition $\big(\varepsilon_1\big|Q_1\big) = 0$ by $\big(\varepsilon_1\big||.|^2 Q\big) = 0$, showing that $\bar{H}_1$ is not degenerate at $d = 5$ and the whole proof of the upper bound on the blow-up rate goes through aswell. Unfortunately this approach of using different orthogonality conditions did not work at $d = 6$.

The higher dimensional spectral property was checked with a very similar numerical approach in [19] in 2018, successfully showing non-degeneracy of $\bar{H}_1$ and $\bar{H}_2$ on the corresponding spaces for the radial case with $d \in [2, 12]$. The key here was to use more precise boundary conditions in the approximation of solutions to the inhomogeneous problem. From $(1 + (.)^{d-2})u \in L^\infty$ it follows that $|u'(r)| \xrightarrow{r\to\infty} 0$ for $d \geq 2$, which was used in [4], whereas in [19] the stronger asymptotics $|u(r)| \xrightarrow{r\to\infty} 0$ for $d \geq 3$ were used.
Moreover the spectral property for general functions in $H^1(\mathbb{R}^d)$ was numerically verified for $d \in [2, 10]$ in [19].

5 Proof of Theorem 4.33 i)

For notational simplicity we will denote the operator $\bar{\mathcal{L}}_1$ from Theorem 4.33 i) as $\mathcal{L}_1$ and restate the claim:

Let

$$Q(x) = 3^{1/4}\cosh(2x)^{-1/2},$$
$$V_1(x) = \frac{100}{9}xQ(x)^3Q'(x) - \frac{1}{9}\cosh(\tfrac{9x}{10})^{-2}$$

and

$$\mathcal{L}_1 f = -f'' + V_1 f, \qquad \bar{H}_1(f,f) = \big(\mathcal{L}_1 f\big|f\big).$$

Then there exists a unique regular function $\phi_1 \in L^\infty$ such that

$$\mathcal{L}_1\phi_1 = Q. \tag{5.1}$$

Moreover

$$\phi_1' \in L^2 \tag{5.2}$$

and the **positivity estimate**

$$-\big(\phi_1\big|Q\big)\left(1 - \bar{H}_1(Q,Q)\frac{\big(\phi_1\big|Q\big)}{\big(Q\big|Q\big)^2}\right) > 0. \tag{5.3}$$

holds.

The proof we give is computer assisted in the sense that we will numerically approximate solutions of differential equations, using a Chebychev pseudo-spectral method, and show existence of the true solutions by a contraction argument (similarly as in [2]). In particular, the approximation errors are rigorously being proved to be sufficiently small, based on estimates which are obtained from evaluation of rational functions at rational points.

Outline of the proof

1. Compactification of the problem

Let

$$\psi:\ (-1,1) \to \mathbb{R},\ y \mapsto \frac{y}{1-y^2}$$

and

$$\Phi_1 := \phi_1 \circ \psi.$$

We define

$$\mathcal{L}_{c,1} f := -f'' + \frac{\psi''}{\psi'} f' + (\psi')^2 \big(V_1 \circ \psi\big) f$$

and

$$\mathcal{R}(\Phi_1) := \mathcal{L}_{c,1} \Phi_1 - (\psi')^2 \big(Q \circ \psi\big)$$

such that (5.1) on $\mathbb{R}$ is equivalent to

$$\mathcal{R}(\Phi_1) = 0 \tag{5.4}$$

or in explicit form

$$-\Phi_1''(y) + \tfrac{2y(y^2+3)}{(1+y^2)(1-y^2)} \Phi_1'(y) + \tfrac{(1+y^2)^2}{(1-y^2)^4} V_1(\psi(y)) \Phi_1(y) - \tfrac{(1+y^2)^2}{(1-y^2)^4} Q(\psi(y)) = 0 \tag{5.5}$$

on $[-1, 1]$.

2. Approximation of Φ_1

We approximate Φ_1 by a polynomial g_1 on $[-1, 1]$ using a Chebychev pseudo-spectral method. The exponential decay of both Q and V_1 in (5.5) gives

$$\lim_{y \to 1} \Phi_1'(y) = 0$$

and

$$\begin{aligned} \lim_{y \to 1} \Phi_1''(y) &= \lim_{y \to 1} \frac{2y(y^2+3)}{(1+y^2)(1-y^2)} \Phi_1'(y) = \lim_{y \to 1} \frac{\frac{d}{dy}\big[2y(y^2+3)\Phi_1'(y)\big]}{\frac{d}{dy}\big[(1+y^2)(1-y^2)\big]} \\ &= \lim_{y \to 1} \frac{-(y^2+3)\Phi_1''(y)}{2y} = -2\Phi_1''(1), \end{aligned}$$

hence g_1 must satisfy the boundary conditions

$$\begin{cases} g_1'(1) = 0, \\ g_1''(1) = 0. \end{cases} \tag{5.6}$$

Using the ansatz

$$g_1(y) = \sum_{n=0}^{N} a_n T_{2n}(y),$$

where T_n is the n^{th} Chebychev polynomial of first kind, implementation of (5.6) gives

$$a_{N-1} = \sum_{0}^{N-2} a_n d_n, \qquad\qquad a_N = \sum_{0}^{N-2} a_n \big[c_n + d_n c_{N-1}\big],$$

with

$$c_n = -\frac{T''_{2n}(1)}{T''_{2N}(1)}, \qquad\qquad d_n = \frac{(\frac{n}{N-1})^2 + c_n(\frac{N}{N-1})^2}{1 + c_{N-1}(\frac{N}{N-1})^2},$$

and hence

$$g(y) = \sum_{n=0}^{N-2} a_n \Psi_n(y)$$

with

$$\Psi_n = T_{2n} + d_n T_{2(N-1)} + (c_n + d_n c_{N-1}) T_{2N}. \tag{5.7}$$

We numerically solve the problem

$$\mathcal{R}\Big(\sum_{n=0}^{N-2} a_n \Psi_n\Big)(y_i) = 0$$

with $y_i = 1 - (\frac{i}{N+1})^2$, $i = 3, ..., N+1$ and $N = 55$.
Rationalizing the obtained coefficients gives $(a_n)_{n=0}^{53} \subset \mathbb{Q}$ listed in Appendix F, Table 1, and we obtain a polynomial g_1 of degree 110.

Remark. The points $y_i = 1 - \left(\frac{i}{N+1}\right)$ are empirically found to give better results in this case than the usual Gauss-Lobato points which are used in Section 5.4.

3. Contraction argument

We claim that there exists a unique $\delta_1 \in W^{1,\infty}(-1,1)$ such that

$$\mathcal{R}(g_1 + \delta_1) = 0, \tag{5.8}$$

which proves (5.1).

For that aim we approximate the fundamental solutions of the homogeneous problem

$$\mathcal{L}_{c,1} u = 0$$

by u_+ and u_-. The unique linear operator $\tilde{\mathcal{L}}_{c,1}$ corresponding to the approximations u_+ and u_- can be inverted by variation of constants (similarly as in Theorem 4.8), which gives

$$\tilde{\mathcal{L}}_{c,1}\delta_1 = \mathcal{L}_{c,1}\delta_1 + \big(\tilde{\mathcal{L}}_{c,1} - \mathcal{L}_{c,1}\big)\delta_1 = -\mathcal{R}(g_1) + \big(\tilde{\mathcal{L}}_{c,1} - \mathcal{L}_{c,1}\big)\delta_1$$

and we can rewrite (5.8) as fixed point problem

$$\delta_1 = -\tilde{\mathcal{L}}_{c,1}^{-1}\mathcal{R}(g_1) + \tilde{\mathcal{L}}_{c,1}^{-1}\big(\tilde{\mathcal{L}}_{c,1} - \mathcal{L}_{c,1}\big)\delta_1 =: \mathcal{K}(\delta_1). \tag{5.9}$$

By showing that $\mathcal{R}(g_1)$ is small and $\tilde{\mathcal{L}}_{c,1}$ close to $\mathcal{L}_{c,1}$ in a suitable sense and deriving bounds on the operator $\tilde{\mathcal{L}}_{c,1}^{-1}$,

we prove that $\mathcal{K}$ is a contraction on some closed ball in $W^{1,\infty}(-1,1)$ which again proves (5.8).

4. Properties of ϕ_1
Property (5.2) follows immediately from the exponential decay of Q and V_1. To show (5.3), we compute $\left(\phi_1 \middle| Q\right)$ and $\bar{H_1}(Q,Q)$ using a trapezoidal rule and approximations for Q and V_1 and estimating the resulting errors.

Remark. From now on we will denote $\|.\|_{L^\infty} := \|.\|_{L^\infty([-1,1])}$. Moreover since we are mainly dealing with even functions, we will mostly only consider them on $[0,1]$. The only exceptions appear in the approximation of $\mathcal{L}_{1,c}$, working with the fundamental solutions $u_\pm$.

5.1 Methods

The functions we are working with can by divided into two types. On the one hand we have approximations $\tilde{V}_{1,j}$ for the potential V_1 and $\tilde{Q}_i$ of the inhomogeneity Q on $\mathbb{R}$, which leads to the rational functions $\tilde{Q}_i \circ \psi$ and $\tilde{V}_{1,j} \circ \psi$ on $[1,1]$. The corresponding derivatives are computed explicitly and bounds for second derivatives are obtained from monotonicity arguments (see Section 5.2). The lower derivatives can then be estimated by Lemma 5.6 which is based on the mean-value theorem.
The other type are polynomials in Chebychev basis on $[-1,1]$. This representation provides an easy method to estimate the $L^\infty[-1,1]$ norm from the Chebychev coefficients (Lemma 5.5). To compute the derivatives of a polynomial in Chebychev basis, we will make use of an algorithm for a change of basis between Lagrange, Chebychev and monomial basis from [3].

Basis change

Definition 5.1. Lagrange representation of a polynomial
Let $d \in \mathbb{N}$ and $\xi = (\xi^0, ..., \xi^d) \in \mathbb{R}^{d+1}$ with $\xi^j \neq \xi^k$ for $j \neq k$ and

$$l_j^\xi(x) := \prod_{\substack{0 \leq j \leq d \\ j \neq k}} \frac{x - \xi^k}{\xi^j - \xi^k},\ x \in \mathbb{R}.$$

Then any polynomial $p : \mathbb{R} \to \mathbb{R}$ of degree d can be written in Lagrange representation

$$p(x) = \sum_{0 \leq j \leq d} p(\xi^j) l_j^\xi(x).$$

The *Lagrange basis polynomials* l_j^ξ can now be represented in monomial basis using recursively defined coefficients.

Lemma 5.2. *Let $d \in \mathbb{N}$ and $\xi = (\xi^0, ..., \xi^d) \in \mathbb{R}^{d+1}$ with $\xi^j \neq \xi^k$ for $j \neq k$ and $\xi_{(k)} := (\xi^0, ..., \xi^{k-1}, \xi^{k+1}, ..., \xi^d) \in \mathbb{R}^d$ for $0 \leq k \leq d$. Then*

$$l_j^\xi(x) = \sum_{0 \leq k \leq d} L(\xi)_j^k x^k$$

with

$$L(\xi)_k^j := \frac{a_{d,j}(-\xi_{(k)})}{\prod_{\substack{0 \leq l \leq d \\ l \neq k}} (\xi^k - \xi^l)} \text{ for } 0 \leq j, k \leq d$$

and $a_{d,j}(\xi)$ defined by the following recursion for $0 \leq j \leq k \leq d$ and $\xi = (\xi^1, ..., \xi^d) \in \mathbb{R}^d$:

$$\begin{aligned} a_{k,0}(\xi) &:= \prod_{0 \leq l \leq k} \xi^l, \\ a_{k,j}(\xi) &:= a_{k-1,j-1}(\xi) + \xi^k a_{k-1,j}(\xi), \ 1 \leq j \leq k-1, \\ a_{k,k}(\xi) &:= 1. \end{aligned}$$

Proof. We claim that

$$\prod_{1 \leq l \leq d} (x + \xi^l) = \sum_{0 \leq j \leq d} a_{d,j}(\xi) x^j,$$

from which the statement follows directly.
Indeed, $d = 1$ gives $a_{1,0}(\xi) + a_{1,1}(\xi)x = \xi^1 x$ and by induction $d \mapsto d+1$:

$$\begin{aligned} \prod_{1 \leq l \leq d+1} (x + \xi^l) &= (x + \xi^{d+1}) \sum_{0 \leq j \leq d} a_{d,j}(\xi) x^j = (x + \xi^{d+1}) \left(a_{d,0}(\xi) + \sum_{1 \leq j \leq d} a_{d,j}(\xi) x^j \right) \\ &= a_{d,0}(\xi)x + a_{d+1,0}(\xi) + \sum_{1 \leq j \leq d} a_{d,j}(\xi) x^{j+1} + \xi^{d+1} \left(\sum_{1 \leq j \leq d} a_{d,j}(\xi) x^j \right) \\ &= a_{d+1,0}(\xi) + \sum_{0 \leq j \leq d} a_{d,j}(\xi) x^{j+1} + \xi^{d+1} \left(\sum_{1 \leq j \leq d} a_{d,j}(\xi) x^j \right) \\ &= a_{d+1,0}(\xi) + x^{d+1} + \sum_{0 \leq j \leq d-1} \left[a_{d,j}(\xi) + \xi^{d+1} a_{d,j+1}(\xi) \right] x^{j+1} \\ &= a_{d+1,0}(\xi) + x^{d+1} + \sum_{0 \leq j \leq d-1} a_{d+1,j+1}(\xi) x^{j+1} \\ &= a_{d+1,0}(\xi) + x^{d+1} + \sum_{1 \leq j \leq d} a_{d+1,j}(\xi) x^j = \sum_{0 \leq j \leq d+1} a_{d+1,j}(\xi) x^j \end{aligned}$$

□

In particular the derivatives $p^{(m)}$ of a polynomial p in monomial representation

$$p(x) = \sum_{0 \leq k \leq d} \sum_{0 \leq j \leq d} p(\xi^j) L(\xi)_j^k x^k$$

are easy to compute and given by

$$p^{(m)}(x) = \sum_{0\le k\le d-m} \frac{(k+m)!}{k!} \sum_{0\le j\le d} p(\xi^j) L(\xi)_j^{k+m} x^k.$$

Moreover we can expand monomials in Chebychev basis:

Lemma 5.3. *Let $n \in \mathbb{N}$ and $x \in \mathbb{R}$. Then*

$$x^k = \sum_{0\le j\le k} C_k^j T_j(x)$$

with

$$C_k^j := \begin{cases} 0 & \text{if } j > k, \\ \frac{1}{2^{k-1}} \binom{k}{\frac{k-1}{2} - \frac{j-1}{2}} & \text{if } j \le k,\ j,k \text{ odd}, \\ \frac{1}{2^k} \binom{k}{\frac{k}{2}} & \text{if } k \text{ even},\ j = 0, \\ \frac{1}{2^{k-1}} \binom{k}{\frac{k-1}{2}} & \text{if } k \text{ even},\ j \ge 2 \text{ even}, \\ 0 & \text{otherwise.} \end{cases}$$

Proof. Using the defining property $T_n(\cos(x)) = \cos(nx)$ for the Chebychev polynomials of first kind (see Appendix E) and $\cos(x)^k = \frac{1}{2^k}(e^{ix} + e^{-ix})^k$ gives for k odd

$$\begin{aligned} \cos(x)^k &= \frac{1}{2^k} \sum_{0\le j\le k} \binom{k}{j} e^{i(k-2j)x} = \frac{1}{2^k} \left[\binom{k}{0} e^{ikx} + \cdots + \binom{k}{\frac{k-1}{2}} e^{ix} + \binom{k}{\frac{k+1}{2}} e^{-ix} + \cdots + \binom{k}{k} e^{-ikx} \right] \\ &= \frac{1}{2^k} \sum_{0\le j\le \frac{k-1}{2}} \left(\binom{k}{\frac{k-1}{2} - j} \right) \left[e^{i(2j+1)x} + e^{-i(2j+1)x} \right] = \frac{1}{2^k} \sum_{0\le j\le \frac{k-1}{2}} \left(\binom{k}{\frac{k-1}{2} - j} \right) \cos((2j+1)x) \end{aligned}$$

and hence by the change of variable $x \mapsto \cos(x)$

$$x^k = \frac{1}{2^k} \sum_{0\le j\le \frac{k-1}{2}} \left(\binom{k}{\frac{k-1}{2} - \frac{j-1}{2}} \right) T_{2j+1}(x)$$

for k odd. Similarly for k even

$$x^k = \frac{1}{2^k} \binom{k}{\frac{k}{2}} + \frac{1}{2^{k-1}} \sum_{1\le j\le \frac{k}{2}} \left(\binom{k}{\frac{k}{2} - j} \right) T_{2j}(x),$$

which gives

$$x^k = \sum_{0 \le j \le k} C_k^j T_j(x)$$

for all $k \geq 0$. □

Finally we can use a composition of basis changes to obtain the Chebychev representation of a polynomial directly from its Lagrange representation.

Lemma 5.4. *Let $d \in \mathbb{N}$ and $\xi = (\xi^0, ..., \xi^d) \in \mathbb{R}^{d+1}$ with $\xi^j \neq \xi^k$ for $j \neq k$. Then any polynomial $p : \mathbb{R} \to \mathbb{R}$ of degree d can be written in Chebychev representation*

$$p(x) = \sum_{0 \le l \le d} \sum_{0 \le j \le d} p(\xi^j) T(\xi)_j^l T_l(x)$$

with

$$T(\xi)_j^l := \sum_{0 \le k \le d} C_k^l L(\xi)_j^k.$$

Proof. From Lemmas 5.2 and 5.3 we have

$$\begin{aligned} p(x) &= \sum_{0 \le j \le d} p(\xi^j) l_j^\xi(x) = \sum_{0 \le j \le d} \sum_{0 \le k \le d} p(\xi^j) L(\xi)_j^k x^k = \sum_{0 \le j \le d} \sum_{0 \le k \le d} \sum_{0 \le l \le k} p(\xi^j) L(\xi)_j^k C_k^l T_l(x) \\ &= \sum_{0 \le j \le d} \sum_{0 \le l \le k} p(\xi^j) T(\xi)_j^l T_l(x). \end{aligned}$$

□

The representation of a polynomial on $[-1, 1]$ in Chebychev basis allows an easy estimate for its L^∞-norm:

Lemma 5.5. *Let $p = \sum_0^N a_n T_n$ with $\{a_n\}_{n=0}^N \subset \mathbb{R}$, $N \in \mathbb{N}$ be a polynomial on $[-1, 1]$, where T_n denotes the first kind Chebychev-polynomial of degree n. Then*

$$\|p\|_{L^\infty} \le \sum_{n=0}^N |a_n|, \qquad \|p'\|_{L^\infty} \le \sum_{n=0}^N n^2 |a_n|.$$

Proof. This follows directly from $\|T_n\|_{L^\infty} \leq 1$ and $\|T_n'\|_{L^\infty} \leq n^2$. □

Monotonicity arguments

Lemma 5.6. *Let $I = [a, b] \subset \mathbb{R}$, $a < b \in \mathbb{Q}$, $f \in C^1(I)$ and for $N \in \mathbb{N}$ set*

$$\Omega_N := \{a + k \cdot \frac{b-a}{N} : \ k = 0, ..., N\} \subset \mathbb{Q}.$$

Then

$$\max_{[a,b]} f \leq \max_{\Omega_N} f + \|f'\|_{L^\infty([a,b])} \cdot \frac{b-a}{N},$$
$$\max_{[a,b]} |f| \leq \max_{\Omega_N} |f| + \|f'\|_{L^\infty([a,b])} \cdot \frac{b-a}{N},$$
$$\min_{[a,b]} f \geq \min_{\Omega_N} f - \|f'\|_{L^\infty([a,b])} \cdot \frac{b-a}{N}.$$

Proof. This result follows directly from the mean-value theorem. □

Lemma 5.7. *Let $f(y) = f_1(y)f_2(y)$, $f_1 \geq 0$ increasing and $f_2 \geq 0$ decreasing in y. Then*

$$f(y) \leq f_1(y_1)f_2(y_2) \qquad \text{for all } y \in [y_1, y_2].$$

Moreover for $[a, b] \subset \mathbb{R}$, $a, b \in \mathbb{Q}$ and

$$\Omega_N^{mon} = \{(y_k, y_{k+1}) : \ y_k = a + k \cdot \frac{b-a}{N}, \ k = 0, ..., N-1\}$$

we have

$$\|f\|_{L^\infty([a,b])} \leq \max\{f_1(y_1)f_2(y_2) : (y_1, y_2) \in \Omega_N^{mon}\}.$$

5.2 Approximation of Q and V_1

Truncated series expansions and error estimates

To approximate the function $x \mapsto e^{-x}$ we use the truncated Taylor expansion

$$e_N^-(x) := \sum_0^N (-1)^n \frac{x^n}{n!},$$

and demand $N \in \mathbb{N}$ to be even, such that

$$e_N^-(x) = \sum_0^N (-1)^n \frac{x^n}{n!} = 1 - x + \frac{x^2}{2} - \frac{x^3}{6} + ... + \frac{x^N}{N!}.$$

We claim that in that case

$$e_N^-(x) \geq e^{-x} \geq 0 \tag{5.10}$$

for all $x \in [0, N+1]$.

Indeed, we have

$$\begin{aligned} e^{-x} - e_N^-(x) &= \sum_{n=0}^{\infty} (-1)^n \frac{x^n}{n!} - \sum_{n=0}^{N} (-1)^n \frac{x^n}{n!} = \sum_{n=N+1}^{\infty} (-1)^n \frac{x^n}{n!} \\ &= \sum_{n=N+1,N+3,N+5,...}^{\infty} \left(\frac{x^{n+1}}{(n+1)!} - \frac{x^n}{n!} \right) \leq 0 \text{ for all } x \in [0, N+1]. \end{aligned}$$

We obtain a non-negative remainder

$$R_N(x) = e_N^-(x) - e^{-x}$$

with

$$0 \leq R_N(x) \leq \frac{x^{N+1}}{(N+1)!}.$$

Moreover

$$(e_N^-)'(x) = -e_{N-1}^-(x)$$

and

$$e_{N-3}^-(x) \leq e_{N-1}^-(x) \leq e_N^-(x) \leq e_{N-2}^-(x) \qquad \text{for } N \geq 3 \text{ even.}$$

Finally for e_N^- on $\psi([a,b])$ for an interval $[a,b] \subseteq [0,1]$, we demand

$$\psi(b) \leq N - 3, \qquad \text{and} \qquad e_{N-3}^-(\psi(b)) \geq 0. \tag{5.11}$$

The first condition ensures $e_N^-(x),\ e_{N-2}^-(x),\ e_{N-4}^-(x) \geq e^{-x} \geq 0$ for $x \in \psi([a,b])$, in particular $e_{N-3}^-,\ e_{N-1}^-$ are decreasing and the second condition ensures $e_{N-3}^-,\ e_{N-1}^- \geq 0$ on $\psi([a,b])$ and we inherit the natural property

$$e_{N-k}^- \in [0,1] \text{ and decreasing on } \psi([a,b]) \text{ for } 0 \leq k \leq 3.$$

From now on we will only use the approximations e_N^- on domains that satisfy these conditions, which is sufficient

as we will only be working with up to three derivatives.

To approximate the function $x \mapsto (1+x)^{1/2}$ we use the truncated Taylor expansion

$$sr_N(x) := 1 + \frac{x}{2} + \sum_{n=2}^{N} (-1)^{n-1} \frac{(2n-3)!!}{2^n \cdot n!} x^n, \qquad x \in [0,1]$$

such that

$$|(1+x)^{1/2} - sr_N(x)| \leq R_N^{sr}(x)$$

with

$$R_N^{sr}(x) := \frac{(2N-1)!!}{2^{N+1}} \frac{x^{N+1}}{(N+1)!}, \qquad x \in [0,1]. \tag{5.12}$$

Moreover, note that $sr_N(x) \geq 1$ for all $x \in [0,1]$, which by the mean-value theorem implies

$$|(1+x)^{-1/2} - sr_N(x)^{-1}| \leq R_N^{sr}(x) \tag{5.13}$$

for all $x \in [0,1]$ and we define

$$(1+x)^{-1/2,N} := sr_N(x)^{-1}. \tag{5.14}$$

Approximation of Q

We rewrite

$$\begin{aligned} Q(x) &= 3^{1/4} \left(\frac{2}{e^{2x} + e^{-2x}} \right)^{1/2} = 3^{1/4} 2^{1/2} (e^{2x}(1 + e^{-4x}))^{-1/2} \\ &= 3^{1/4} 2^{1/2} e^{-x} (1 + e^{-4x})^{-1/2} \end{aligned}$$

and define the following approximations for Q

$$\begin{aligned} \tilde{Q}_0(x) &:= C e_{22}^-(x)(1 + e_{56}^-(4x))^{-1/2}, \\ \tilde{Q}_1(x) &:= C e_{90}^-(x), \\ \tilde{Q}_2(x) &:= 0 \end{aligned}$$

with

$$C := 3^{1/4} 2^{1/2} \tag{5.15}$$

and

$$I_0 := \left[0, \frac{88}{100}\right], \qquad I_1 := \left[\frac{88}{100}, \frac{98}{100}\right], \qquad I_2 := \left[\frac{98}{100}, 1\right].$$

Remark. Observing that $\psi(\frac{88}{100}) < 4$ and $\psi(\frac{98}{100}) < 25$ and evaluating

$$e_{19}^{-}\left(\psi\left(\tfrac{88}{100}\right)\right) > 0 \qquad e_{53}^{-}\left(4\psi\left(\tfrac{88}{100}\right)\right) > 0, \qquad e_{87}^{-}\left(\psi\left(\tfrac{98}{100}\right)\right) > 0$$

we see that all functions e_N^- appearing in $\tilde{Q}_i$ satisfy (5.11) on the interval I_i.

Lemma 5.8. *The approximations $\tilde{Q}_0$, $\tilde{Q}_1$ and $\tilde{Q}_2$ satisfy the following estimates:*

$$\begin{aligned}
\|(\psi')^2(Q-\tilde{Q}_0)\circ\psi\|_{L^\infty(I_0)} &< 4\cdot 10^{-6},\\
\|(\psi')^2(Q-\tilde{Q}_1)\circ\psi\|_{L^\infty(I_1)} &< 6\cdot 10^{-6},\\
\|(\psi')^2(Q-\tilde{Q}_2)\circ\psi\|_{L^\infty(I_2)} &< 6\cdot 10^{-5}.
\end{aligned}$$

Proof. By the mean-value theorem we have

$$\begin{aligned}
|Q(x)-\tilde{Q}_0(x)| &= C|e^{-x}(1+e^{-4x})^{-1/2} - e_{22}^{-}(x)(1+e_{56}^{-}(4x))^{-1/2}|\\
&\le 2\Big(e_{22}^{-}(x)\big|(1+e_{56}^{-}(4x))^{-1/2}-(1+e^{-4x})^{-1/2}\big| + (1+e^{-4x})^{-1/2}|e_{22}^{-}(x)-e^{-x}|\Big)\\
&\le 2\Big(e_{22}^{-}(x)R_{56}(4x)/2 + R_{22}(x)\Big)
\end{aligned}$$

and from the monotonicity of e_N^-, R_N, ψ and ψ', it follows that

$$\psi'(y)^2|Q(\psi(y))-\tilde{Q}_0(\psi(y))| \le 2\psi'(y_2)^2\Big(e_{22}^{-}(\psi(y_1))R_{56}(4\psi(y_2)/2 + R_{22}(\psi(y_2))\Big)$$

for all $y\in[y_1,y_2]\subseteq I_0$. From Lemma 5.7 on I_0 with $N=88$ we conclude

$$\psi'(y)^2|Q(\psi(y))-\tilde{Q}_0(\psi(y))| < 4\cdot 10^{-6}$$

for all $y\in I_0$.

Similarly we estimate

$$\begin{aligned}
|Q(x)-\tilde{Q}_1(x)| &= C|e_{90}^{-}(x) - e^{-x}(1+e^{-4x})^{-1/2}|\\
&\le 2\big(e_{90}^{-}(x)\big|1-(1+e^{-4x})^{-1/2}\big| + (1+e^{-4x})^{-1/2}\big|e_{90}^{-}(x)-e^{-x}\big|\big)\\
&\le 2\big(e_{90}^{-}(x)e^{-4x}/2 + R_{90}(x)\big) \le 2\big(e_{90}^{-}(x)e_{200}^{-}(4x)/2 + R_{90}(x)\big)
\end{aligned}$$

and

$$\begin{aligned}\psi'(y)^2|Q(\psi(y)) - \tilde{Q}_1(\psi(y))| &\leq 2\psi'(y)^2\big(e_{90}^-(\psi(y))e_{200}^-(4\psi(y))/2 + R_{90}(\psi(y))\big)\\ &\leq 2\psi'(y_2)^2\big(e_{90}^-(\psi(y_1))e_{200}^-(4\psi(y_1))/2 + R_{90}(\psi(y_2))\big)\end{aligned}$$

for all $y \in [y_1, y_2] \subseteq I_1$. From Lemma 5.7 on I_1 with $N = 10$ we conclude

$$\psi'(y)^2|Q(\psi(y)) - \tilde{Q}_1(\psi(y))| < 6 \cdot 10^{-6}$$

for all $y \in I_1$.

It remains to show that $\psi'(y)^2 Q(\psi(y))$ is small for $y \in I_2$. Differentiating

$$\begin{aligned}\frac{d}{dy}(\psi'(y)^2 Q(\psi(y))) &= 3^{1/4}\frac{d}{dy}\left(\psi'(y)^2\cosh(2\psi(y))^{-1/2}\right)\\ &= 3^{1/4}\left(2\psi''(y)\psi'(y)\cosh(2\psi(y))^{-1/2} - \psi'(y)^3\cosh(2\psi(y))^{-3/2}\sinh(2\psi(y))\right)\\ &< 3^{1/4}\left(2\psi''(y)\psi'(y) - \psi'(y)^3\right)\cosh(2\psi(y))^{-1/2}\\ &= 3^{1/4}\left(\frac{2y(1+y^2)(3+y^2)(1-y^2) - (1+y^2)^3}{(1-y^2)^6}\right)\cosh(2\psi(y))^{-1/2}\end{aligned}$$

and observing

$$2y(1+y^2)(3+y^2)(1-y^2) - (1+y^2)^3 \leq 16(1-y^2) - (1+y^2)^3 < 0$$

for all $y \in [\frac{98}{100}, 1]$, we conclude that $\psi'(y)^2 Q(\psi(y))$ is decreasing for $y \in [\frac{98}{100}, 1]$ (and obviously positive). Finally, using $Q(x) < 2e_{100}^-(x)$ and evaluating $2(\psi')^2(e_{100}^- \circ \psi)$ at $y = \frac{98}{100}$, we conclude

$$\psi'(y)^2 Q(\psi(y)) < 6 \cdot 10^{-5}$$

for all $y \in I_2$. □

Approximation of V_1

We rewrite

$$\begin{aligned} V_1(x) &= -\frac{100}{3}x\sinh(2x)\cosh(2x)^{-3} - \frac{1}{9}\cosh\left(\tfrac{9x}{10}\right)^{-2} \\ &= -\frac{100}{3}x\left(\frac{e^{2x}-e^{-2x}}{2}\right)\left(\frac{e^{2x}+e^{-2x}}{2}\right)^{-3} - \frac{1}{9}\left(\frac{e^{\frac{9x}{10}}+e^{-\frac{9x}{10}}}{2}\right)^{-2} \\ &= -\frac{400}{3}xe^{-4x}(1-e^{-4x})(1+e^{-4x})^{-3} - \frac{4}{9}e^{-\frac{9x}{5}}\left(1+e^{-\frac{9x}{5}}\right)^{-2} \end{aligned}$$

and set

$$\begin{aligned} \tilde{V}_{1,0}(x) &:= -\frac{400}{3}xe^-_{60}(4x)(1-e^-_{60}(4x))(1+e^-_{60}(4x))^{-3} - \frac{4}{9}e^-_{30}\left(\tfrac{9x}{5}\right)\left(1+e^-_{30}\left(\tfrac{9x}{5}\right)\right)^{-2}, \\ \tilde{V}_{1,1}(x) &:= -\frac{400}{3}xe^-_{140}(4x) - \frac{4}{9}e^-_{64}\left(\tfrac{9x}{5}\right), \\ \tilde{V}_{1,2}(x) &:= 0, \end{aligned}$$

and

$$J_0 := \left[0, \frac{88}{100}\right], \qquad J_1 := \left[\frac{88}{100}, \frac{95}{100}\right], \qquad J_2 := \left[\frac{95}{100}, 1\right].$$

Remark. Observing that $\psi(\frac{88}{100}) < 4$ and $\psi(\frac{95}{100}) < 10$ and evaluating

$$e^-_{57}\left(4\psi\left(\tfrac{88}{100}\right)\right) > 0 \qquad e^-_{27}\left(\tfrac{9}{5}\psi\left(\tfrac{88}{100}\right)\right) > 0, \quad e^-_{137}\left(4\psi\left(\tfrac{95}{100}\right)\right) > 0, \qquad e^-_{61}\left(\tfrac{9}{5}\psi\left(\tfrac{95}{100}\right)\right) > 0$$

we see that all functions e^-_N appearing in $\tilde{V}_{1,j}$ satisfy (5.11) on the interval J_j.

Lemma 5.9. *The approximations $\tilde{V}_{1,0}$, $\tilde{V}_{1,1}$ and $\tilde{V}_{1,2}$ satisfy the following estimates:*

$$\begin{aligned} &\|(\psi')^2(V_1 - \tilde{V}_{1,0}) \circ \psi\|_{L^\infty(J_0)} < 2 \cdot 10^{-5}, \\ &\|(\psi')^2(V_1 - \tilde{V}_{1,1}) \circ \psi\|_{L^\infty(J_1)} < 10^{-3}, \\ &\|(\psi')^2(V_1 - \tilde{V}_{1,2}) \circ \psi\|_{L^\infty(J_2)} < 5 \cdot 10^{-4}. \end{aligned}$$

Proof. We have

$$|\tilde{V}_{1,0}(x) - V_1(x)| \le \frac{400}{3}xA_0(x) + \frac{4}{9}B_0(x)$$

with

$$A_0(x) = \left| e_{60}^-(4x)(1-e_{60}^-(4x))(1+e_{60}(4x))^{-3} - e^{-4x}(1-e^{-4x})(1+e^{-4x})^{-3} \right| \le R_{60}(4x)$$
$$B_0(x) = \left| e_{30}^-\left(\tfrac{9x}{5}\right)\left(1+e_{30}^-\left(\tfrac{9x}{5}\right)\right)^{-2} - e^{-\frac{9x}{5}}(1+e^{-\frac{9x}{5}})^{-2} \right| \le R_{30}\left(\tfrac{9x}{5}\right)$$

by the mean value-theorem and hence

$$|\tilde{V}_{1,0}(x) - V_1(x)| \le \frac{400}{3} x R_{60}(4x) + \frac{4}{9} R_{30}\left(\tfrac{9x}{5}\right)$$

and

$$\psi'(y)^2 \left|\tilde{V}_{1,0}(\psi(y)) - V_1(\psi(y))\right| \le \psi'(y_2)^2 \left(\frac{400}{3}\psi(y_2) R_{60}(4\psi(y_2)) + \frac{4}{9} R_{30}\left(\tfrac{9}{5}\psi(y_2)\right) \right)$$

for all $y \in [y_1, y_2] \subseteq J_0$.

From Lemma 5.7 on J_0 with $N = 880$ we conclude

$$\psi'(y)^2 |V_1(\psi(y)) - \tilde{V}_{1,0}(\psi(y))| < 2 \cdot 10^{-5}$$

for all $y \in J_0$.

Similarly we estimate

$$|\tilde{V}_{1,1}(x) - V_1(x)| \le \frac{400}{3} x A_1(x) + \frac{4}{9} B_1(x)$$

with

$$A_1(x) = \left| e^{-4x}(1-e^{-4x})(1+e^{-4x})^{-3} - e_{140}^-(4x) \right| \le R_{140}(4x) + 4e_{140}^-(4x)^2$$
$$B_1(x) = \left| e^{-\frac{9x}{5}} \left(1+e^{-\frac{9x}{5}}\right)^{-2} - e_{64}^-\left(\tfrac{9x}{5}\right) \right| \le R_{64}\left(\tfrac{9x}{5}\right) + 2e_{64}^-\left(\tfrac{9x}{5}\right)^2$$

and hence

$$|\tilde{V}_{1,1}(x) - V_1(x)| \le \frac{400}{3} x \left(R_{140}(4x) + 4e_{140}^-(4x)^2 \right) + \frac{4}{9} \left(R_{64}\left(\tfrac{9x}{5}\right) + 2e_{64}^-\left(\tfrac{9x}{5}\right)^2 \right)$$

and

$$\psi'(y)^2 \left|\tilde{V}_{1,1}(\psi(y)) - V_1(\psi(y))\right| \le \psi'(y_2)^2 \Big(\frac{400}{3}\psi(y_2) \left(R_{140}(4\psi(y_2)) + 4e_{140}^-(4\psi(y_1))^2 \right) + \frac{4}{9} \left(R_{64}(\tfrac{9}{5}\psi(y_2)) + 2e_{64}^-(\tfrac{9}{5}\psi(y_1))^2 \right) \Big)$$

for all $y \in [y_1, y_2] \subseteq J_1$.

From Lemma 5.7 on J_1 with $N = 70$ we conclude

$$\psi'(y)^2|V_1(\psi(y)) - \tilde{V}_{1,1}(\psi(y))| < 10^{-3}$$

for all $y \in J_1$.

It remains to show that $\psi'(y)^2 V_1(\psi(y))$ is small for $y \in [\frac{95}{100}, 1]$:

Using that $\sinh(x)/\cosh(x) < 1$, we have

$$|\psi'(y)^2 V_1(\psi(y))| < \psi'(y)^2 \left(\frac{100}{3}\psi(y)\cosh(2\psi(y))^{-2} + \frac{1}{9}\cosh(\tfrac{9}{10}\psi(y))^{-2} \right).$$

We show that this dominating function is decreasing for $y \in \left[\frac{95}{100}, 1\right]$. By differentiating

$$\begin{aligned}
&\frac{d}{dy}\left(\psi'(y)^2 \left(\frac{100}{3}\psi(y)\cosh(2\psi(y))^{-2} + \frac{1}{9}\cosh(\tfrac{9}{10}\psi(y))^{-2} \right) \right) \\
=&\frac{100}{3}\frac{d}{dy}\left(\psi'(y)^2\psi(y)\cosh(2\psi(y))^{-2} \right) + \frac{1}{9}\frac{d}{dy}\left(\psi'(y)^2\cosh(\tfrac{9}{10}\psi(y))^{-2} \right)
\end{aligned}$$

and observing

$$\begin{aligned}
&\frac{d}{dy}\left(\psi'(y)^2\psi(y)\cosh(2\psi(y))^{-2} \right) \\
&= \left(2\psi''(y)\psi'(y)\psi(y) + \psi'(y)^3 \right)\cosh(2\psi(y))^{-2} - 2\psi'(y)^2\psi(y)\cosh(2\psi(y))^{-3}\sinh(2\psi(y))2\psi'(y) \\
&< \left(2\psi''(y)\psi'(y)\psi(y) + \psi'(y)^3 - 2\psi'(y)^3\psi(y) \right)\cosh(2\psi(y))^{-2} \\
&= \left(\frac{2y^2(1+y^2)(3+y^2)(1-y^2) + (1+y^2)^3(1-y^2) - y(1+y^2)^3}{(1-y^2)^7} \right)\cosh(2\psi(y))^{-2} \\
&\leq \left(\frac{30(1-y^2) - y(1+y^2)^3}{(1-y^2)^7} \right)\cosh(2\psi(y))^{-2} < 0 \text{ for all } y \in \left[\tfrac{95}{100}, 1\right]
\end{aligned}$$

and

$$\begin{aligned}
&\frac{d}{dy}\left(\psi'(y)^2\cosh(\tfrac{9}{10}\psi(y))^{-2}\right)\\
&\quad= 2\psi''(y)\psi'(y)\cosh(\tfrac{9}{10}\psi(y))^{-2} - 2\psi'(y)^2\cosh(\tfrac{9}{10}\psi(y))^{-3}\sinh(\tfrac{9}{10}\psi(y))\frac{9}{10}\psi'(y)\\
&\quad< \left(2\psi''(y)\psi'(y) - \frac{9}{5}\psi'(y)^3\right)\cosh(\tfrac{9}{10}\psi(y))^{-2}\\
&\quad= \left(\frac{10y(1+y^2)(3+y^2)(1-y^2) - 9(1+y^2)^3}{5(1-y^2)^6}\right)\cosh(\tfrac{9}{10}\psi(y))^{-2}\\
&\quad\leq \left(\frac{80(1-y^2) - 9(1+y^2)^3}{5(1-y^2)^6}\right)\cosh(\tfrac{9}{10}\psi(y))^{-2} < 0 \text{ for all } y\in\left[\tfrac{95}{100},1\right]
\end{aligned}$$

it suffices to show that the dominating function is small at $y=\frac{95}{100}$ to deduce smallness for all $y\in[\frac{95}{100},1]$.

We have

$$\psi'(y)^2\left(\frac{100}{3}\psi(y)\cosh(2\psi(y))^{-2} + \frac{4}{9}\cosh(\tfrac{9}{10}\psi(y))^{-2}\right) < \psi'(y)^2\left(\frac{400}{3}\psi(y)e^-_{200}(4\psi(y)) + \frac{4}{9}e^-_{200}(\tfrac{9}{5}\psi(y))\right)$$

and evaluating the right hand side at $y=\frac{95}{100}$ gives

$$|\psi'(y)^2 V_1(\psi(y))| < 5\cdot 10^{-4}$$

for all $y\in J_2$. □

Further estimates for $\tilde{Q}_i$

In this Section we will derive bounds on norms of the form

$$\left\|\left((\psi')^l(\tilde{Q}_i\circ\psi)\right)^{(k)}\right\|_{L^\infty(I_i)}$$

with $l,k\in\{0,1,2\}$, $i=0,1$. For that aim we will make maximum use of underlying monotonic properties. More specifically we decompose the functions involved into a difference of positive functions, which again consist of monotonic factors. This will allow us to estimate second derivatives by Lemma 5.7. The first derivatives and functions themselves can then be estimated by Lemma 5.6.

To avoid evaluation of the factor $C=3^{1/4}2^{1/2}$ and the square root occuring in $\tilde{Q}_0$ and its derivatives, we will omit them when estimating second derivative and replace them by a rational constant and a rational function for the remaining estimates.
Moreover by scaling $\tilde{Q}_0$, $\tilde{Q}_0'$ and $\tilde{Q}_0''$ by the same positive factor, we can pull this factor out of estimates.

Lemma 5.10. *Let*

$$C_- := \frac{4190166673}{2251313558} - 10^{-9}, \qquad C_+ := \frac{4190166673}{2251313558} + 10^{-9}.$$

Then

$$C_- < C < C_+$$

for $C = 3^{1/4}2^{1/2}$ *as defined in (5.15).*

Proof. Denoting

$$\frac{4190166673}{2251313558} = \frac{110033}{83607}\frac{114243}{80782} =: C_1 \cdot C_2$$

we have

$$\left|3 - C_1^4\right| < 2 \cdot 10^{-10}, \qquad \left|2 - C_2^2\right| < 2 \cdot 10^{-10}$$

and hence, by the mean-value theorem

$$\left|3^{1/4} - C_1\right| < \frac{10^{-10}}{2}, \qquad \left|2^{1/2} - C_2\right| < 10^{-10}.$$

Consequently

$$|3^{1/4}2^{1/2} - C_1C_2| \le C_2|3^{1/4} - C_1| + 3^{1/4}|2^{1/2} - C_2| < \left(\frac{3}{2} \cdot \frac{1}{2} + \frac{3}{2}\right) 10^{-10} < 10^{-9},$$

which gives

$$C_- < 3^{1/4}2^{1/2} < C_+.$$

□

Definition 5.11. (Decomposition of $\tilde{Q}_0^{(k)}$ into monotonous, non-negative components)
We define

$$\begin{aligned}
(\tilde{Q}_0)^+(x_1, x_2) &:= C_+ e_{22}^-(x_1), \\
(\tilde{Q}_0{}')^+(x_1, x_2) &:= 2\ C_+ e_{22}^-(x_1) e_{55}^-(4x_1)(1 + e_{56}^-(4x_2))^{-1}, \\
(\tilde{Q}_0{}')^-(x_1, x_2) &:= C_+ e_{21}^-(x_1), \\
(\tilde{Q}_0{}'')^+(x_1, x_2) &:= C_+ \left(e_{20}^-(x_1) + 12 e_{22}^-(x_1)(e_{55}^-(4x_1))^2(1 + e_{56}^-(4x_2))^{-2}\right), \\
(\tilde{Q}_0{}'')^-(x_1, x_2) &:= C_+ \left(1 + e_{56}^-(4x_2)\right)^{-1} \left(8 e_{22}^-(x_1) e_{54}^-(4x_1) + 4 e_{21}^-(x_1) e_{55}^-(4x_1)\right),
\end{aligned}$$

such that

$$(\tilde{Q}_0)^+,\ (\tilde{Q}_0')^\pm,\ (\tilde{Q}_0'')^\pm \ge 0,$$

$$(\tilde{Q}_0)^-(x_2,x_1) \le (\tilde{Q}_0)^-(x,x) \le (\tilde{Q}_0)^-(x_1,x_2),$$
$$(\tilde{Q}_0')^{\pm}(x_2,x_1) \le (\tilde{Q}_0')^{\pm}(x,x) \le (\tilde{Q}_0')^{\pm}(x_1,x_2),$$
$$(\tilde{Q}_0'')^{\pm}(x_2,x_1) \le (\tilde{Q}_0'')^{\pm}(x,x) \le (\tilde{Q}_0'')^{\pm}(x_1,x_2)$$

and

$$\tilde{Q}_0(x) = \frac{C}{C_+}(1+e_{56}^-(4x))^{-1/2}(\tilde{Q}_0)^+(x,x),$$
$$\tilde{Q}_0'(x) = \frac{C}{C_+}(1+e_{56}^-(4x))^{-1/2}\bigg((\tilde{Q}_0')^+(x,x) - (\tilde{Q}_0')^-(x,x)\bigg),$$
$$\tilde{Q}_0''(x) = \frac{C}{C_+}(1+e_{56}^-(4x))^{-1/2}\bigg((\tilde{Q}_0'')^+(x,x) - (\tilde{Q}_0'')^-(x,x)\bigg)$$

for all $x_1 \le x \le x_2$ *in* $\psi(I_0)$.

Lemma 5.12. *Let $F(y) = (F_0(y), F_1(y), F_2(y))$ with non-negative, increasing functions F_0, F_1, F_2 and $y \in [y_1, y_2] \subseteq I_0$. Then*

$$\begin{aligned}
&\left|F_0(y)\tilde{Q}_0(\psi(y)) + F_1(y)\tilde{Q}_0'(\psi(y)) + F_2(y)\tilde{Q}_0''(\psi(y))\right| \\
\leq &\max\left\{\left|F_0(y_2)(\tilde{Q}_0)^+(\psi(y_1),\psi(y_2)) + F_1(y_2)(\tilde{Q}_0')^+(\psi(y_1),\psi(y_2)) + F_2(y_2)(\tilde{Q}_0'')^+(\psi(y_1),\psi(y_2))\right.\right. \\
&\qquad \left. - F_1(y_1)(\tilde{Q}_0')^-(\psi(y_2),\psi(y_1)) - F_2(y_1)(\tilde{Q}_0'')^-(\psi(y_2),\psi(y_1))\right|, \\
&\qquad \left|F_0(y_1)(\tilde{Q}_0)^+(\psi(y_2),\psi(y_1)) + F_1(y_1)(\tilde{Q}_0')^+(\psi(y_2),\psi(y_1)) + F_2(y_1)(\tilde{Q}_0'')^+(\psi(y_2),\psi(y_1))\right. \\
&\qquad \left.\left. - F_1(y_2)(\tilde{Q}_0')^-(\psi(y_1),\psi(y_2)) - F_2(y_2)(\tilde{Q}_0'')^-(\psi(y_1),\psi(y_2))\right|\right\} =: F_{dom,\tilde{Q}_0}(y_1, y_2).
\end{aligned}$$

In particular

$$\|F_0(\tilde{Q}_0 \circ \psi) + F_1(\tilde{Q}_0' \circ \psi) + F_2(\tilde{Q}_0'' \circ \psi)\|_{L^\infty([a,b])} \leq \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{Q}_0}\left(a + i \cdot \frac{b-a}{N}, a + (i+1) \cdot \frac{b-a}{N}\right)\right\}$$

for all $[a, b] \subseteq I_0$, $N > 1$.

Proof. This follows from

$$\begin{aligned}
&\left|F_0(y)\tilde{Q}_0(\psi(y)) + F_1(y)\tilde{Q}_0'(\psi(y)) + F_2(y)\tilde{Q}_0''(\psi(y))\right| \\
=&\frac{C}{C_+}(1 + e_{56}^-(4\psi(y))^{-1/2}\left|F_0(y)(\tilde{Q}_0')^+(\psi(y),\psi(y)) + F_1(y)(\tilde{Q}_0')^+(\psi(y),\psi(y)) + F_2(y)(\tilde{Q}_0'')^+(\psi(y),\psi(y))\right. \\
&\qquad \left. - F_1(y)(\tilde{Q}_0')^-(\psi(y),\psi(y)) - F_2(y)(\tilde{Q}_0'')^-(\psi(y),\psi(y))\right| \\
\leq&\left|F_0(y)(\tilde{Q}_0')^+(\psi(y),\psi(y)) + F_1(y)(\tilde{Q}_0')^+(\psi(y),\psi(y)) + F_2(y)(\tilde{Q}_0'')^+(\psi(y),\psi(y))\right. \\
&\left. - F_1(y)(\tilde{Q}_0')^-(\psi(y),\psi(y)) - F_2(y)(\tilde{Q}_0'')^-(\psi(y),\psi(y))\right|,
\end{aligned}$$

Definition 5.11 and Lemma 5.7. □

The analogue for $\tilde{Q}_1$ is immediate:

Lemma 5.13. *Let $F(y) = (F_0(y), F_1(y), F_2(y))$ with non-negative, increasing functions F_0, F_1, F_2 and $y \in [y_1, y_2] \subseteq I_1$. Then*

$$\begin{aligned}
&\left|F_0(y)\tilde{Q}_1(\psi(y)) + F_1(y)\tilde{Q}_1'(\psi(y)) + F_2(y)\tilde{Q}_1''(\psi(y))\right| \\
\leq & C_+ \max\left\{\left|F_0(y_2)e_{90}^-(\psi(y_1)) + F_2(y_2)e_{88}^-(\psi(y_1)) - F_1(y_1)e_{89}^-(\psi(y_2))\right|,\right. \\
&\left.\left|F_0(y_1)e_{90}^-(\psi(y_2)) + F_2(y_1)e_{88}^-(\psi(y_2)) - F_1(y_2)e_{89}^-(\psi(y_1))\right|\right\} =: F_{dom,\tilde{Q}_1}(y_1, y_2).
\end{aligned}$$

In particular

$$\|F_0(\tilde{Q}_1 \circ \psi) + F_1(\tilde{Q}_1' \circ \psi) + F_2(\tilde{Q}_1'' \circ \psi)\|_{L^\infty([a,b])} \leq \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{Q}_1}\left(a + i \cdot \frac{b-a}{N}, a + (i+1) \cdot \frac{b-a}{N}\right)\right\}$$

for all $[a, b] \subseteq I_1$, $N > 1$.

The following definition allows to estimate $\tilde{Q}_0$ and $\tilde{Q}_0'$ avoiding the constant C and square roots.

Definition 5.14. (Estimates for $\tilde{Q}_0$ and $\tilde{Q}_0'$ in rational expressions)
We define

$$\begin{aligned}
\tilde{Q}_{0,+}(x) &:= C_+\left[(1 + e_{56}^-(4x))^{-1/2,50} + R_{50}^{sr}(e_{56}^-(4x))\right]e_{22}^-(x), \\
\tilde{Q}_{0,+}'(x) &:= C_+\left[(1 + e_{56}^-(4x))^{-1/2,50} + R_{50}^{sr}(e_{56}^-(4x))\right](1 + e_{56}^-(4x))^{-1}\left[2e_{22}^-(x)e_{55}^-(4x) - e_{21}^-(x)(1 + e_{56}^-(4x))\right] \\
\tilde{Q}_{0,-}(x) &:= C_-\left[(1 + e_{56}^-(4x))^{-1/2,50} - R_{50}^{sr}(e_{56}^-(4x))\right]e_{22}^-(x), \\
\tilde{Q}_{0,-}'(x) &:= C_-\left[(1 + e_{56}^-(4x))^{-1/2,50} - R_{50}^{sr}(e_{56}^-(4x))\right](1 + e_{56}^-(4x))^{-1}\left[2e_{22}^-(x)e_{55}^-(4x) - e_{21}^-(x)(1 + e_{56}^-(4x))\right],
\end{aligned}$$

where R_N^{sr} and $(1 + .\,)^{-1/2,N}$ are given by (5.12) and (5.14), such that by Lemma 5.10 and (5.13)

$$\left|\tilde{Q}_{0,-}\right| \leq \left|\tilde{Q}_0\right| \leq \left|\tilde{Q}_{0,+}\right| \quad \text{and} \quad \left|\tilde{Q}_{0,-}'\right| \leq \left|\tilde{Q}_0'\right| \leq \left|\tilde{Q}_{0,+}'\right|.$$

Lemma 5.15. *The functions $(\tilde{Q}_i \circ \psi)(\psi')^2$ obey the following bounds:*

$$\left\|\left((\psi')^2(\tilde{Q}_0 \circ \psi)\right)''\right\|_{L^\infty(I_0)} < 25000, \qquad \left\|\left((\psi')^2(\tilde{Q}_1 \circ \psi)\right)''\right\|_{L^\infty(I_1)} < 43000.$$

Proof. We denote

$$\frac{d^2}{dy^2}\big(\psi'(y)^2 f(\psi(y))\big) = F_{2,0}(y)f(\psi(y)) + F_{2,1}(y)f'(\psi(y)) + F_{2,2}(y)f''(\psi(y))$$

with

$$F_{2,0}(y) := 2\psi'(y)\psi'''(y) + 2\psi''(y)^2, \qquad F_{2,1}(y) := 5\psi'(y)^2\psi''(y), \qquad F_{2,2}(y) := \psi'(y)^4. \tag{5.16}$$

Applying Lemma 5.12 on I_0 with $N = 880$ and Lemma 5.13 on I_1 with $N = 1000$ for $F = (F_{2,0}, F_{2,1}, F_{2,2})$ gives the claimed bounds. □

Lemma 5.16. *The functions $\psi' \cdot (\tilde{Q}_i \circ \psi)$ obey the following bounds:*

$$\|\psi'(\tilde{Q}_0 \circ \psi)\|_{L^\infty(I_0)} < \frac{28}{10}, \qquad \Big\|\big(\psi'(\tilde{Q}_0 \circ \psi)\big)'\Big\|_{L^\infty(I_0)} < 25, \qquad \Big\|\big(\psi'(\tilde{Q}_0 \circ \psi)\big)''\Big\|_{L^\infty(I_0)} < 350$$

and

$$\|\psi'(\tilde{Q}_1 \circ \psi)\|_{L^\infty(I_1)} < \frac{14}{10}, \qquad \Big\|\big(\psi'(\tilde{Q}_1 \circ \psi)\big)'\Big\|_{L^\infty(I_1)} < 26, \qquad \Big\|\big(\psi'(\tilde{Q}_1 \circ \psi)\big)''\Big\|_{L^\infty(I_1)} < 630.$$

Proof. We denote

$$\frac{d^2}{dy^2}\big(\psi'(y) f(\psi(y))\big) = G_{2,0}(y)f(\psi(y)) + G_{2,1}(y)f'(\psi(y)) + G_{2,2}(y)f''(\psi(y))$$

with

$$G_{2,0}(y) := \psi'''(y), \qquad G_{2,1}(y) := 3\psi'(y)\psi''(y), \qquad G_{2,2}(y) = \psi'(y)^3. \tag{5.17}$$

Applying Lemma 5.12 on I_0 with $N = 880$ and Lemma 5.13 on I_1 with $N = 1000$ for $F = (G_{2,0}, G_{2,1}, G_{2,2})$ gives

$$\Big\|\big(\psi'(\tilde{Q}_0 \circ \psi)\big)''\Big\|_{L^\infty(I_0)} < 350, \qquad \Big\|\big(\psi'(\tilde{Q}_1 \circ \psi)\big)''\Big\|_{L^\infty(I_1)} < 630.$$

From

$$\begin{aligned}\Big|\frac{d}{dy}\big(\psi'(y)\tilde{Q}_0(\psi(y))\big)\Big| &\le \big|\psi''(y)\tilde{Q}_{0,+}(\psi(y)) + \psi'(y)^2\tilde{Q}'_{0,+}(\psi(y))\big| \\ \big|\psi'(y)\tilde{Q}_0(\psi(y))\big| &\le \big|\psi'(y)\tilde{Q}_{0,+}(\psi(y))\big|\end{aligned}$$

and Lemma 5.6 on I_0 with $N = 880$ we infer

$$\left|\frac{d}{dy}\big(\psi'(y)\tilde{Q}_0(\psi(y))\big)\right| \leq 24 + \frac{350}{1000} < 25,$$
$$\left|\psi'(y)\tilde{Q}_0(\psi(y))\right| \leq \frac{274}{100} + \frac{25}{1000} < \frac{28}{10}$$

for all $y \in I_0$ and from

$$\left|\frac{d}{dy}\big(\psi'(y)\tilde{Q}_1(\psi(y))\big)\right| \leq C_+ \left|\psi''(y)e_{90}^-(\psi(y)) - \psi'(y)^2 e_{89}^-(\psi(y))\right|$$
$$\left|\psi'(y)\tilde{Q}_1(\psi(y))\right| \leq C_+ \left|\psi'(y)e_{90}^-(\psi(y))\right|$$

and Lemma 5.6 on I_1 with $N = 100$

$$\left|\frac{d}{dy}\big(\psi'(y)\tilde{Q}_1(\psi(y))\big)\right| \leq 25 + \frac{630}{1000} < 26,$$
$$\left|\psi'(y)\tilde{Q}_1(\psi(y))|\right| \leq \frac{132}{100} + \frac{26}{1000} < \frac{14}{10}$$

for all $y \in I_1$. □

Lemma 5.17. *The functions $(\tilde{Q}_i \circ \psi)$ obey the following bounds:*

$$\|\tilde{Q}_0 \circ \psi\|_{L^\infty(I_0)} < \frac{14}{10}, \qquad \left\|\big(\tilde{Q}_0 \circ \psi\big)'\right\|_{L^\infty(I_0)} < \frac{28}{10}, \qquad \left\|\big(\tilde{Q}_0 \circ \psi\big)''\right\|_{L^\infty(I_0)} < 27$$

and

$$\|\tilde{Q}_1 \circ \psi\|_{L^\infty(I_1)} < \frac{4}{100}, \qquad \left\|\big(\tilde{Q}_1 \circ \psi\big)'\right\|_{L^\infty(I_1)} < \frac{14}{10}, \qquad \left\|\big(\tilde{Q}_1 \circ \psi\big)''\right\|_{L^\infty(I_1)} < 28.$$

Moreover

$$\|Q \circ \psi\|_{L^\infty(I_0)} \leq \frac{141}{100}, \qquad \|Q \circ \psi\|_{L^\infty(I_1)} \leq \frac{41}{100}, \qquad \|Q \circ \psi\|_{L^\infty(I_2)} \leq 6 \cdot 10^{-5}.$$

Proof. Observing

$$\frac{d^2}{dy^2} f(\psi(y)) = \psi''(y) f'(\psi(y)) + \psi'(y)^2 f''(\psi(y))$$

and applying Lemma 5.12 on I_0 with $N = 880$ and Lemma 5.13 on I_1 with $N = 1000$ for $F = (0, \psi''(y), \psi'(y)^2)$ gives

$$\left\|\big(\tilde{Q}_0 \circ \psi\big)''\right\|_{L^\infty(I_0)} < 27, \qquad \left\|\big(\tilde{Q}_1 \circ \psi\big)''\right\|_{L^\infty(I_1)} < 28.$$

From

$$\begin{aligned}\left|\frac{d}{dy}\big(\tilde{Q}_0(\psi(y))\big)\right| &\leq \left|\psi'(y)\tilde{Q}'_{0,+}(\psi(y))\right|,\\ \left|\tilde{Q}_0(\psi(y))\right| &\leq \left|\tilde{Q}_{0,+}(\psi(y))\right|\end{aligned}$$

and Lemma 5.6 on I_0 with $N = 880$ we infer

$$\begin{aligned}\left|\frac{d}{dy}\big(\tilde{Q}_0(\psi(y))\big)\right| &\leq \frac{274}{100} + \frac{27}{1000} < \frac{28}{10},\\ \left|\tilde{Q}_0(\psi(y))\right| &\leq \frac{132}{100} + \frac{28}{10000} < \frac{14}{10}\end{aligned}$$

for all $y \in I_0$ and from

$$\begin{aligned}\left|\frac{d}{dy}\big(\tilde{Q}_1(\psi(y))\big)\right| &\leq C_+ \left|\psi'(y)e^-_{89}(\psi(y))\right|\\ \left|\tilde{Q}_1(\psi(y))\right| &\leq C_+ \left|e^-_{90}(\psi(y))\right|\end{aligned}$$

and Lemma 5.6 on I_1 with $N = 100$

$$\begin{aligned}\left|\frac{d}{dy}\big(\tilde{Q}_1(\psi(y))\big)\right| &\leq \frac{132}{100} + \frac{28}{1000} < \frac{14}{10},\\ \left|\tilde{Q}_1(\psi(y))\right|| &\leq \frac{38}{1000} + 14 \cdot 10^{-4} < \frac{4}{100}\end{aligned}$$

for all $y \in I_1$.

Finally, using the rough bounds

$$\begin{aligned}\|Q \circ \psi\|_{L^\infty(I_i)} &\leq \|\tilde{Q}_{i,i} \circ \psi\|_{L^\infty(I_i)} + \|\left(Q - \tilde{Q}_i\right) \circ \psi\|_{L^\infty(I_i)}\\ &\leq \|\tilde{Q}_i \circ \psi\|_{L^\infty(I_i)} + \|(\psi')^2\left(Q - \tilde{Q}_i\right) \circ \psi\|_{L^\infty(I_i)},\end{aligned}$$

we obtain from Lemma 5.8

$$\begin{aligned}\|Q \circ \psi\|_{L^\infty(I_0)} &\leq \frac{14}{10} + 4 \cdot 10^{-6} < \frac{141}{100},\\ \|Q \circ \psi\|_{L^\infty(I_1)} &\leq \frac{4}{100} + 6 \cdot 10^{-6} < \frac{41}{100},\\ \|Q \circ \psi\|_{L^\infty(I_2)} &\leq 6 \cdot 10^{-5}.\end{aligned}$$

□

Further estimates for $\tilde{V}_{1,j}$

Definition 5.18. (Decomposition of $\tilde{V}_{1,0}^{(k)}$ into monotonous, non-negative components)
We define

$$
\begin{aligned}
(\tilde{V}_{1,0})^-(x_1,x_2) :=& \frac{400}{3} x_2 e_{60}^-(4x_1)(1-e_{60}(4x_2))(1+e_{60}^-(4x_2))^{-3} + \frac{4}{9} e_{30}^-(\tfrac{9x_1}{5})(1+e_{30}^-(\tfrac{9x_2}{5}))^{-2},\\
(\tilde{V}'_{1,0})^+(x_1,x_2) :=& \frac{400}{3} 4x_2 \left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)\left(e_{60}^-(4x_1)^2+1\right) + \frac{4}{5}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-3} e_{29}^-(\tfrac{9x_1}{5}),\\
(\tilde{V}'_{1,0})^-(x_1,x_2) :=& \frac{400}{3}\Big[16x_2\left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)e_{60}^-(4x_1) + e_{60}^-(4x_1)\left(1-e_{60}^-(4x_2)\right)\left(1+e_{60}^-(4x_2)\right)^{-3}\Big]\\
&+ \frac{4}{5}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-3} e_{29}^-(\tfrac{9x_1}{5})e_{30}^-(\tfrac{9x_1}{5}),\\
(\tilde{V}''_{1,0})^+(x_1,x_2) :=& \frac{400}{3}\Big[32x_2\left(1+e_{60}^-(4x_2)\right)^{-5}\left[2\left(e_{60}^-(4x_1)+1\right)e_{58}^-(4x_1)e_{60}^-(4x_1) + e_{59}^-(4x_1)^2\left(e_{60}^-(4x_1)^2+4\right)\right]\\
&\quad + 8\left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)\left(e_{60}^-(4x_1)^2+1\right)\Big]\\
&+ \frac{36}{25}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-4}\left[e_{30}^-(\tfrac{9x_1}{5})^2 e_{28}^-(\tfrac{9x_1}{5}) + 4e_{29}^-(\tfrac{9x_1}{5})^2\right],\\
(\tilde{V}''_{1,0})^-(x_1,x_2) :=& \frac{400}{3}\Big[16x_2\left(1+e_{60}^-(4x_2)\right)^{-5}\left[\left(e_{60}^-(4x_1)+1\right)\left(e_{60}^-(4x_1)^2+1\right)e_{58}^-(4x_1) + 14e_{59}^-(4x_1)^2 e_{60}^-(4x_1)\right]\\
&\quad + 32\left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)e_{60}^-(4x_1)\Big]\\
&+ \frac{36}{25}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-4}\left[e_{28}^-(\tfrac{9x_1}{5}) + 2e_{30}^-(\tfrac{9x_1}{5})e_{29}^-(\tfrac{9x_1}{5})^2\right]
\end{aligned}
$$

such that

$$(\tilde{V}_{1,0})^-,\ (\tilde{V}'_{1,0})^\pm,\ (\tilde{V}''_{1,0})^\pm \geq 0,$$

$$
\begin{aligned}
(\tilde{V}_{1,0})^-(x_2,x_1) \leq (\tilde{V}_{1,0})^-(x,x) \leq (\tilde{V}_{1,0})^-(x_1,x_2),\\
(\tilde{V}'_{1,0})^\pm(x_2,x_1) \leq (\tilde{V}'_{1,0})^\pm(x,x) \leq (\tilde{V}'_{1,0})^\pm(x_1,x_2),\\
(\tilde{V}''_{1,0})^\pm(x_2,x_1) \leq (\tilde{V}''_{1,0})^\pm(x,x) \leq (\tilde{V}''_{1,0})^\pm(x_1,x_2)
\end{aligned}
$$

and

$$\tilde{V}_{1,0}(x) = -(\tilde{V}_{1,0})^-(x,x), \qquad \tilde{V}'_{1,0}(x) = (\tilde{V}'_{1,0})^+(x,x) - (\tilde{V}'_{1,0})^-(x,x), \qquad \tilde{V}''_{1,0}(x) = (\tilde{V}''_{1,0})^+(x,x) - (\tilde{V}''_{1,0})^-(x,x)$$

for all $x_1 \leq x \leq x_2$ in $\psi(J_0)$.

Lemma 5.19. *Let $F(y) = (F_0(y), F_1(y), F_2(y))$ with non-negative, increasing functions F_0, F_1, F_2 and $y \in [y_1, y_2] \subseteq J_0$. Then*

$$\begin{aligned}
&\left|F_0(y)\tilde{V}_{1,0}(\psi(y)) + F_1(y)\tilde{V}'_{1,0}(\psi(y)) + F_2(y)\tilde{V}''_{1,0}(\psi(y))\right| \\
\leq \max\Bigg\{&\Big|F_1(y_2)(\tilde{V}'_{1,0})^+(\psi(y_1),\psi(y_2)) + F_2(y_2)(\tilde{V}''_{1,0})^+(\psi(y_1),\psi(y_2)) - F_0(y_1)(\tilde{V}_{1,0})^-(\psi(y_2),\psi(y_1)) \\
&\quad - F_1(y_1)(\tilde{V}'_{1,0})^-(\psi(y_2),\psi(y_1)) - F_2(y_1)(\tilde{V}''_{1,0})^-(\psi(y_2),\psi(y_1))\Big|, \\
&\Big|F_1(y_1)(\tilde{V}'_{1,0})^+(\psi(y_2),\psi(y_1)) + F_2(y_1)(\tilde{V}''_{1,0})^+(\psi(y_2),\psi(y_1)) - F_0(y_2)(\tilde{V}_{1,0})^-(\psi(y_1),\psi(y_2)) \\
&\quad - F_1(y_2)(\tilde{V}'_{1,0})^-(\psi(y_1),\psi(y_2)) - F_2(y_2)(\tilde{V}''_{1,0})^-(\psi(y_1),\psi(y_2))\Big|\Bigg\} =: F_{dom,\tilde{V}_{1,0}}(y_1, y_2).
\end{aligned}$$

In particular

$$\|F_0(\tilde{V}_{1,0}\circ\psi) + (F_1\tilde{V}'_{1,0}\circ\psi) + F_2(\tilde{V}''_{1,0}\circ\psi)\|_{L^\infty([a,b])} \leq \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{V}_{1,0}}\left(a + i\cdot\frac{b-a}{N}, a + (i+1)\cdot\frac{b-a}{N}\right)\right\}$$

for all $[a,b] \subseteq J_0$, $N > 1$.

Proof. This follows directly from

$$\begin{aligned}
&|F_0(y)\tilde{V}_{1,0}(\psi(y)) + F_1(y)\tilde{V}'_{1,0}(\psi(y)) + F_2(y)\tilde{V}''_{1,0}(\psi(y))| \\
=&|F_1(y)(\tilde{V}'_{1,0})^+(\psi(y),\psi(y)) + F_2(y)(\tilde{V}''_{1,0})^+(\psi(y),\psi(y)) \\
&- F_0(\tilde{V}_{1,0})^-(\psi(y),\psi(y)) - F_1(y)(\tilde{V}'_{1,0})^-(\psi(y),\psi(y)) - F_2(y)(\tilde{V}''_{1,0})^-(\psi(y),\psi(y))|,
\end{aligned}$$

Definition 5.18 and Lemma 5.7. □

Definition 5.20. (Decomposition of $\tilde{V}_{1,1}^{(k)}$ into monotonous, non-negative components)
We define

$$\begin{aligned}
(\tilde{V}_{1,1})^-(x_1,x_2) :=& \frac{400}{3}x_2 e^-_{140}(4x_1) + \frac{4}{9}e^-_{64}(\tfrac{9x_1}{5}),\\
(\tilde{V}'_{1,1})^+(x_1,x_2) :=& \frac{1600}{3}x_2 e^-_{139}(4x_1) + \frac{4}{5}e^-_{63}(\tfrac{9x_1}{5}),\\
(\tilde{V}'_{1,1})^-(x_1,x_2) :=& \frac{400}{3}e^-_{140}(4x_1),\\
(\tilde{V}''_{1,1})^+(x_1,x_2) :=& \frac{3200}{3}e^-_{139}(4x_1),\\
(\tilde{V}''_{1,1})^-(x_1,x_2) :=& \frac{6400}{3}x_2 e^-_{138}(4x_1) + \frac{36}{25}e^-_{62}(\tfrac{9x_1}{5})
\end{aligned}$$

such that

$$(\tilde{V}_{1,1})^-,\ (\tilde{V}'_{1,1})^\pm,\ (\tilde{V}''_{1,1})^\pm \geq 0,$$

$$\begin{aligned}
(\tilde{V}_{1,1})^-(x_2,x_1) \leq (\tilde{V}_{1,1})^-(x,x) \leq (\tilde{V}_{1,1})^-(x_1,x_2),\\
(\tilde{V}'_{1,1})^\pm(x_2,x_1) \leq (\tilde{V}'_{1,1})^\pm(x,x) \leq (\tilde{V}'_{1,1})^\pm(x_1,x_2),\\
(\tilde{V}''_{1,1})^\pm(x_2,x_1) \leq (\tilde{V}''_{1,1})^\pm(x,x) \leq (\tilde{V}''_{1,1})^\pm(x_1,x_2)
\end{aligned}$$

and

$$\tilde{V}_{1,1}(x) = -(\tilde{V}_{1,1})^-(x,x), \quad \tilde{V}'_{1,1}(x) = (\tilde{V}'_{1,1})^+(x,x) - (\tilde{V}'_{1,1})^-(x,x), \quad \tilde{V}''_{1,1}(x) = (\tilde{V}''_{1,1})^+(x,x) - (\tilde{V}''_{1,1})^-(x,x)$$

for all $x_1 \leq x \leq x_2$ in $\psi(J_1)$.

Lemma 5.21. *Let $F(y) = (F_0(y), F_1(y), F_2(y))$ with non-negative, increasing functions F_0, F_1, F_2 and $y \in [y_1, y_2] \subseteq J_1$. Then*

$$
\begin{aligned}
&\left|F_0(y)\tilde{V}_{1,1}(\psi(y)) + F_1(y)\tilde{V}'_{1,1}(\psi(y)) + F_2(y)\tilde{V}''_{1,1}(\psi(y))\right| \\
&\leq \max\Bigg\{\Bigg|F_1(y_2)(\tilde{V}'_{1,1})^+(\psi(y_1),\psi(y_2)) + F_2(y_2)(\tilde{V}''_{1,1})^+(\psi(y_1),\psi(y_2)) \\
&\qquad - F_0(y_1)(\tilde{V}_{1,1})^-(\psi(y_2),\psi(y_1)) - F_1(y_1)(\tilde{V}'_{1,1})^-(\psi(y_2),\psi(y_1)) - F_2(y_1)(\tilde{V}''_{1,1})^-(\psi(y_2),\psi(y_1))\Bigg|, \\
&\qquad \Bigg|F_1(y_1)(\tilde{V}'_{1,1})^+(\psi(y_2),\psi(y_1)) + F_2(y_1)(\tilde{V}''_{1,1})^+(\psi(y_2),\psi(y_1)) \\
&\qquad - F_0(y_2)(\tilde{V}_{1,1})^-(\psi(y_1),\psi(y_2)) - F_1(y_2)(\tilde{V}'_{1,1})^-(\psi(y_1),\psi(y_2)) - F_2(y_2)(\tilde{V}''_{1,1})^-(\psi(y_1),\psi(y_2))\Bigg|\Bigg\} \\
&=: F_{dom,\tilde{V}_{1,1}}(y_1,y_2).
\end{aligned}
$$

In particular

$$
\|F_0(\tilde{V}_{1,1}\circ\psi) + F_1(\tilde{V}'_{1,1}\circ\psi) + F_2(\tilde{V}''_{1,1}\circ\psi)\|_{L^\infty([a,b])} \leq \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{V}_{1,1}}\left(a + i\cdot\frac{b-a}{N}, a + (i+1)\cdot\frac{b-a}{N}\right)\right\}
$$

for all $[a,b]\subseteq J_1$, $N>1$.

Proof. Analogous to the proof of Lemma 5.19. □

Lemma 5.22. *The functions* $(\psi')^2(\tilde{V}_{1,j}\circ\psi)$ *obey the following bounds:*

$$
\|(\psi')^2(\tilde{V}_{1,0}\circ\psi)\|_{L^\infty(J_0)} < 32, \qquad \left\|\left((\psi')^2(\tilde{V}_{1,0}\circ\psi)\right)'\right\|_{L^\infty(J_0)} < 200, \qquad \left\|\left((\psi')^2(\tilde{V}_{1,0}\circ\psi)\right)''\right\|_{L^\infty(J_0)} < 4050
$$

and

$$
\|(\psi')^2(\tilde{V}_{1,1}\circ\psi)\|_{L^\infty(J_1)} < \frac{7}{10}, \qquad \left\|\left((\psi')^2(\tilde{V}_{1,1}\circ\psi)\right)'\right\|_{L^\infty(J_1)} < 27, \qquad \left\|\left((\psi')^2(\tilde{V}_{1,1}\circ\psi)\right)''\right\|_{L^\infty(J_1)} < 1550.
$$

Proof. Applying Lemma 5.19 on J_0 with $N=880$ and Lemma 5.21 on J_1 with $N=70$ for $F=(F_{2,0},F_{2,1},F_{2,2})$ as defined in (5.16) gives

$$
\left\|\left((\psi')^2(\tilde{V}_{1,0}\circ\psi)\right)''\right\|_{L^\infty(J_0)} < 4050, \qquad \left\|\left((\psi')^2(\tilde{V}_{1,1}\circ\psi)\right)''\right\|_{L^\infty(J_1)} < 1550.
$$

From Lemma 5.6 on J_0 with $N = 880$ we infer

$$\Big|\frac{d}{dy}\big(\psi'(y)^2\tilde{V}_{1,0}(\psi(y))\big)\Big| = \big|2\psi'(y)\psi''(y)\tilde{V}_{1,0}(\psi(y)) + \psi'(y)^3\tilde{V}'_{1,0}(\psi(y))\big| \le 195 + \frac{4050}{1000} < 200,$$
$$\big|\psi'(y)^2\tilde{V}_{1,0}(\psi(y))\big| \le 31 + \frac{200}{1000} < 32,$$

and on J_1 with $N = 70$

$$\Big|\frac{d}{dy}\big(\psi'(y)^2\tilde{V}_{1,1}(\psi(y))\big)\Big| = \big|2\psi'(y)\psi''(y)\tilde{V}_{1,1}(\psi(y)) + \psi'(y)^3\tilde{V}'_{1,1}(\psi(y))\big| \le 25 + \frac{1550}{1000} < 27,$$
$$\big|\psi'(y)^2\tilde{V}_{1,0}(\psi(y))\big| \le \frac{6}{10} + \frac{27}{1000} < \frac{7}{10}.$$

□

Lemma 5.23. *The functions $(\tilde{V}_{1,j} \circ \psi)$ obey the following bounds:*

$$\|\tilde{V}_{1,0} \circ \psi\|_{L^\infty(J_0)} < 11, \qquad \big\|\big(\tilde{V}_{1,0} \circ \psi\big)'\big\|_{L^\infty(J_0)} < 24, \qquad \big\|\big(\tilde{V}_{1,0} \circ \psi\big)''\big\|_{L^\infty(J_0)} < 203$$

and

$$\|\tilde{V}_{1,1} \circ \psi\|_{L^\infty(J_1)} < 6 \cdot 10^{-4}, \qquad \big\|\big(\tilde{V}_{1,1} \circ \psi\big)'\big\|_{L^\infty(J_1)} < \frac{4}{100}, \qquad \big\|\big(\tilde{V}_{1,1} \circ \psi\big)''\big\|_{L^\infty(J_1)} < 3.$$

Proof. Applying Lemma 5.19 on J_0 with $N = 880$ and Lemma 5.21 on J_1 with $N = 70$ for $F = (0, \psi'', (\psi')^2)$ gives

$$\big\|\big(\tilde{V}_{1,0} \circ \psi\big)''\big\|_{L^\infty(J_0)} < 203, \qquad \big\|\big(\tilde{V}_{1,1} \circ \psi\big)''\big\|_{L^\infty(J_1)} < 3.$$

From Lemma 5.6 on J_0 with $N = 880$ we infer

$$\Big|\frac{d}{dy}\big(\tilde{V}_{1,0}(\psi(y))\big)\Big| = |\psi'(y)\tilde{V}'_{1,0}(\psi(y))| \le \frac{231}{10} + \frac{203}{1000} < 24,$$
$$\big|\tilde{V}_{1,0}(\psi(y))\big| \le \frac{11}{2} + \frac{24}{1000} < 11,$$

and on J_1 with $N = 70$

$$\Big|\frac{d}{dy}\big(\psi'(y)\tilde{V}_{1,1}(\psi(y))\big)\Big| = |\psi'(y)\tilde{V}'_{1,1}(\psi(y))| \le \frac{37}{1000} + \frac{3}{1000} = \frac{4}{100},$$
$$\big|\tilde{V}_{1,0}(\psi(y))\big| \le 5 \cdot 10^{-4} + 4 \cdot 10^{-5} < 6 \cdot 10^{-4}.$$

□

5.3 Smallness of $\mathcal{R}(g_1)$

Proposition 5.24. *The function g_1 satifies*

$$\|\mathcal{R}(g_1)\|_{L^\infty} < \frac{6}{1000}$$

Proof. Recall

$$\mathcal{R}(g_1) = -g_1'' + \frac{\psi''}{\psi'} g_1' + (\psi')^2 \big(V_1 \circ \psi\big) g_1 - (\psi')^2 \big(Q \circ \psi\big)$$

with

$$\frac{\psi''(y)}{\psi'(y)} = \frac{2y(y^2+3)}{(1+y^2)(1-y^2)}.$$

By construction g_1 satisfies the boundary condition $g_1'(1) = 0$, and hence

$$h(y) := \frac{2y(y^2+3)g_1'(y)}{1-y^2}$$

is a polynomial of degree atmost 110.

We rewrite

$$\mathcal{R}(g_1)(y) = -g_1''(y) + \frac{h(y)}{1+y^2} + \psi'(y)^2 V_1(\psi(y)) g_1(y) - \psi'(y)^2 Q(\psi(y))$$

and set

$$\tilde{\mathcal{R}}(g_1)_{i,j}(y) = -g_1''(y) + \frac{h(y)}{1+y^2} + \psi'(y)^2 \tilde{V}_{1,j}(\psi(y)) g_1(y) - \psi'(y)^2 \tilde{Q}_i(\psi(y)),$$

such that $\tilde{\mathcal{R}}(g_1)_{i,j} \in C^\infty(I_i \cap J_j)$.

In order to obtain a bound on

$$\begin{aligned}
\tilde{\mathcal{R}}(g_1)_{i,j}''(y) = &-g_1^{(4)}(y) + \frac{h''(y)}{1+y^2} + \frac{h(y)(6y^2-2)}{(1+y^2)^3} - \frac{h'(y)4y}{(1+y^2)^2} \\
&+ \left((\psi')^2(\tilde{V}_{1,j} \circ \psi)\right)''(y) g_1(y) + \left((\psi')^2(\tilde{V}_{1,j} \circ \psi)\right)(y) g_1''(y) + 2\left((\psi')^2(\tilde{V}_{1,j} \circ \psi)\right)'(y) g_1'(y) \\
&- \left((\psi')^2(\tilde{Q}_i \circ \psi)\right)''(y)
\end{aligned}$$

we estimate

$$\begin{aligned}
\|\tilde{\mathcal{R}}(g_1)_{i,j}''\|_{L^\infty(I_1 \cap J_j)} \leq &\|g_1^{(4)}\|_{L^\infty}\| + \|h''\|_{L^\infty} + 4\|h\|_{L^\infty} + 4\|h'\|_{L^\infty} \\
&+ \| \left((\psi')^2(\tilde{V}_{1,j} \circ \psi)\right)'' \|_{L^\infty} \cdot \|g_1\|_{L^\infty} + \|(\psi')^2(\tilde{V}_{1,j} \circ \psi)\|_{L^\infty} \|g_1''\|_{L^\infty} \\
&+ 2\| \left((\psi')^2(\tilde{V}_{1,j} \circ \psi)\right)' \|_{L^\infty} \cdot \|g_1'\|_{L^\infty} + \| \left((\psi')^2(\tilde{Q}_i \circ \psi)\right)'' \|_{L^\infty}.
\end{aligned}$$

From Lemma 5.5 we infer

$$\|h\|_{L^\infty} < 64, \qquad \|h'\|_{L^\infty} < 891, \qquad \|h''\|_{L^\infty} < 42600$$

and

$$\|g_1^{(4)}\|_{L^\infty} < 45800,$$

and from Lemma 5.6 on $[0,1]$ with $N = 1000$

$$\begin{aligned} \|g_1'''\|_{L^\infty} &\le 591 + \frac{45800}{1000} < 640, \\ \|g_1''\|_{L^\infty} &\le \frac{261}{10} + \frac{640}{1000} < 27, \\ \|g_1'\|_{L^\infty} &\le \frac{284}{100} + \frac{27}{1000} < \frac{29}{10}, \\ \|g_1\|_{L^\infty} &\le \frac{512}{1000} + \frac{29}{10000} < \frac{52}{100}, \end{aligned} \tag{5.18}$$

which gives

$$\begin{aligned} \|\tilde{\mathcal{R}}(g_1)''_{i,j}\|_{L^\infty(I_1\cap J_j)} \le 45800 + 42600 + 4\cdot 64 + 4\cdot 891 + \|\left((\psi')^2(\tilde V_{1,j}\circ\psi)\right)''\|_{L^\infty(J_j)}\cdot\frac{52}{100} + \|(\psi')^2(\tilde V_{1,j}\circ\psi)\|_{L^\infty(J_j)}\cdot 27 \\ + 2\|\left((\psi')^2(\tilde V_{1,j}\circ\psi)\right)'\|_{L^\infty(J_j)}\cdot\frac{29}{10} + \|\left((\psi')^2(\tilde Q_i\circ\psi)\right)''\|_{L^\infty(I_i)}, \end{aligned}$$

hence by Lemmas 5.22 and 5.15

$$\begin{aligned} \|\tilde{\mathcal{R}}(g_1)''_{0,0}\|_{L^\infty(I_0\cap J_0)} &< 122000 \\ \|\tilde{\mathcal{R}}(g_1)''_{1,1}\|_{L^\infty(I_1\cap J_1)} &< 136000 \\ \|\tilde{\mathcal{R}}(g_1)''_{1,2}\|_{L^\infty(I_1\cap J_2)} &< 136000 \\ \|\tilde{\mathcal{R}}(g_1)''_{2,2}\|_{L^\infty(I_1\cap J_1)} &\le 92220. \end{aligned}$$

Now consider

$$\begin{aligned} \tilde{\mathcal{R}}(g_1)'_{i,j}(y) = -g_1^{(3)}(y) + \frac{h'(y)}{1+y^2} - \frac{2y}{(1+y^2)^2}h(y) + \left((\psi')^2(\tilde V_{1,j}\circ\psi)\right)'(y)g_1(y) \\ + \left((\psi')^2(\tilde V_{1,j}\circ\psi)\right)(y)g_1'(y) - \left((\psi')^2(\tilde Q_i\circ\psi)\right)'(y) \end{aligned}$$

with

$$\left((\psi')^2(\tilde Q_i\circ\psi)\right)'(y) = 2\psi'(y)\psi''(y)\tilde Q_i(\psi(y)) + \psi'(y)^3\tilde Q_i'(\psi(y)).$$

We estimate

$$\begin{aligned}\left|\tilde{\mathcal{R}}(g_1)'_{i,j}(y)\right| \leq \max\Big\{\Big| &- g_1^{(3)}(y) + \frac{h'(y)}{1+y^2} - \frac{2y}{(1+y^2)^2}h(y) + \big((\psi')^2(\tilde{V}_{1,j}\circ\psi)\big)'(y)g_1(y)\\ &+ \big((\psi')^2(\tilde{V}_{1,j}\circ\psi)\big)(y)g_1'(y) - \big[2\psi'(y)\psi''(y)\tilde{Q}_{i,+}(\psi(y)) + \psi'(y)^3\tilde{Q}'_{i,+}(\psi(y))\big]\Big|,\\ \Big| &- g_1^{(3)}(y) + \frac{h'(y)}{1+y^2} - \frac{2y}{(1+y^2)^2}h(y) + \big((\psi')^2(\tilde{V}_{1,j}\circ\psi)\big)'(y)g_1(y)\\ &+ \big((\psi')^2(\tilde{V}_{1,j}\circ\psi)\big)(y)g_1'(y) - \big[2\psi'(y)\psi''(y)\tilde{Q}_{i,-}(\psi(y)) + \psi'(y)^3\tilde{Q}'_{i,-}(\psi(y))\big]\Big|\Big\}.\end{aligned}$$

for all $y \in I_i$ with $\tilde{Q}_{i,\pm}$, $\tilde{Q}'_{i,\pm}$ as in Definition 5.14.
From Lemma 5.6 on $I_i \cap J_j$ with $N = 8800, 700, 300, 2000$ we infer

$$\begin{aligned}\|\tilde{\mathcal{R}}(g_1)'_{0,0}\|_{L^\infty(I_0\cap J_0)} &< \frac{6}{1000} + \frac{122}{10} < 13,\\ \|\tilde{\mathcal{R}}(g_1)'_{1,1}\|_{L^\infty(I_1\cap J_1)} &< \frac{28}{1000} + \frac{136}{10} < 14,\\ \|\tilde{\mathcal{R}}(g_1)'_{1,2}\|_{L^\infty(I_1\cap J_2)} &< \frac{48}{1000} + \frac{136}{10} < 14,\\ \|\tilde{\mathcal{R}}(g_1)'_{2,2}\|_{L^\infty(I_2\cap J_2)} &< 17 + 9222\cdot 10^{-4} < 18.\end{aligned}$$

Analogously we estimate

$$\begin{aligned}\left|\tilde{\mathcal{R}}(g_1)_{i,j}(y)\right| \leq \max\Big\{\Big| &- g_1''(y) + \frac{h(y)}{1+y^2} + \psi'(y)^2\tilde{V}_{1,j}(\psi(y))g_1(y) - \psi'(y)^2\tilde{Q}_{i,+}(\psi(y))\Big|,\\ \Big| &- g_1''(y) + \frac{h(y)}{1+y^2} + \psi'(y)^2\tilde{V}_{1,j}(\psi(y))g_1(y) - \psi'(y)^2\tilde{Q}_{i,-}(\psi(y))\Big|\Big\}\end{aligned}$$

and from Lemma 5.6 on $I_i \cap J_j$ with $N = 8800, 700, 300, 2000$ we infer

$$\begin{aligned}\|\tilde{\mathcal{R}}(g_1)_{0,0}\|_{L^\infty(I_0\cap J_0)} &< \frac{2}{1000} + 13\cdot 10^{-4} = \frac{4}{1000},\\ \|\tilde{\mathcal{R}}(g_1)_{1,1}\|_{L^\infty(I_1\cap J_1)} &< 4\cdot 10^{-4} + 14\cdot 10^{-4} < \frac{2}{1000},\\ \|\tilde{\mathcal{R}}(g_1)_{1,2}\|_{L^\infty(I_1\cap J_2)} &< 2\cdot 10^{-4} + 14\cdot 10^{-4} < \frac{2}{1000},\\ \|\tilde{\mathcal{R}}(g_1)_{2,2}\|_{L^\infty(I_2\cap J_2)} &< 48\cdot 10^{-4} + 18\cdot 10^{-5} < \frac{5}{1000}.\end{aligned}$$

Finally, from

$$\|\mathcal{R}(g_1) - \tilde{\mathcal{R}}(g_1)_{i,j}\|_{L^\infty(I_i\cap J_j)} \leq \|g_1\|_{L^\infty}\|(\psi')^2\big(V_1\circ\psi - \tilde{V}_{1,j}\circ\psi\big)\|_{L^\infty(J_j)} + \|(\psi')^2\big(Q\circ\psi - \tilde{Q}_i\circ\psi\big)\|_{L^\infty(I_i)}$$

we conclude

$$\begin{aligned}
\|\mathcal{R}(g_1) - \tilde{\mathcal{R}}(g_1)_{0,0}\|_{L^\infty(I_0\cap J_0)} &< 2\cdot 10^{-5},\\
\|\mathcal{R}(g_1) - \tilde{\mathcal{R}}(g_1)_{1,1}\|_{L^\infty(I_1\cap J_1)} &< 6\cdot 10^{-4},\\
\|\mathcal{R}(g_1) - \tilde{\mathcal{R}}(g_1)_{1,2}\|_{L^\infty(I_1\cap J_2)} &< 3\cdot 10^{-4},\\
\|\mathcal{R}(g_1) - \tilde{\mathcal{R}}(g_1)_{2,2}\|_{L^\infty(I_2\cap J_2)} &< 4\cdot 10^{-4}
\end{aligned}$$

and

$$\left\|\mathcal{R}(g_1)\right\|_{L^\infty} < 54\cdot 10^{-4}.$$

□

5.4 Approximation of $\mathcal{L}_{c,1}$

Consider the solutions of the homogeneous problem $\mathcal{L}_1 f = 0$:

$$\begin{aligned}
f_1(x) &= x + \int_x^\infty \int_s^\infty V_1(y) f_1(y) dy ds = x + \int_x^\infty (y-x) V_1(y) f_1(y) dy = x + \int_x^\infty K(x,y) f_1(y) dy,\\
f_2(x) &= 1 + \int_x^\infty \int_s^\infty V_1(y) f_1(y) dy ds = 1 + \int_x^\infty (y-x) V_1(y) f_1(y) dy = 1 + \int_x^\infty K(x,y) f_1(y) dy
\end{aligned}$$

with $K(x,y) = (y-x)V(y)$. From the exponential decay of V_1 is easily follows that K satisfies the assumption of Theorem 4.21 for any $a \in \mathbb{R}$ and hence f_1 and f_2 exist by the Volterra iteration. Moreover from their asymptotic behaviour at ∞ we infer that f_1 and f_2 are linearly independent. In particular, any solution of $\mathcal{L}_1 f = 0$ can grow atmost linearly at ∞.
Taking $v_+ = f_2$ and similarly constructing v_- such that $\mathcal{L}_1 v_- = 0$ and $v_-(x) \to 1$ as $x \to -\infty$, we obtain a fundamental system $\{v_+, v_-\}$ of $\mathcal{L}_1$ with

$$v_+(x) \to \begin{cases} 1, & x \to \infty \\ x, & x \to -\infty \end{cases} \qquad v_-(x) \to \begin{cases} x, & x \to \infty \\ 1, & x \to -\infty. \end{cases}$$

and similarly to Theorem 4.21, the inverse $\mathcal{L}_1^{-1}$ is given by the Green function corresponding to $\{v_+, v_-\}$. Moreover, since $\{v_+, v_-\}$ are bounded at $\pm\infty$ respectively, $\mathcal{L}_1^{-1}$ maps $L^\infty(\mathbb{R})$ to $L^\infty(\mathbb{R})$.

Consequently, translating the boundary conditions for the fundamental system on $\mathbb{R}$ to $(-1,1)$, the fundamental system of $\mathcal{L}_{c,1}$ is given by $\{u_+, u_-\}$, where $u_\pm$ are solutions of $\mathcal{L}_{c,1} u = 0$ with

$$u_+(y) \to \begin{cases} 1, & y \to 1 \\ \frac{y}{1-y^2}, & y \to -1 \end{cases} \qquad u_-(y) \to \begin{cases} \frac{y}{1-y^2}, & y \to 1 \\ 1, & y \to -1. \end{cases}$$

We define

$$w_+(y) := (1+y)u_+(y), \qquad\qquad w_-(y) := (1-y)u_-(y),$$

for which the boundary conditions translate to

$$\begin{cases} w_+(1) &= 2, \\ w'_+(1) &= 1, \end{cases} \qquad\qquad \begin{cases} w_-(-1) &= 2, \\ w'_-(-1) &= -1. \end{cases} \tag{5.19}$$

Next, we approximate $u_\pm$, $w_\pm$ and by a slight abuse of notation we will refer to these approximations as $u_\pm$ and $w_\pm$.

Using the ansatz

$$w_+(y) = \sum_{n=0}^{N} a_n^+ T_n(y), \qquad\qquad w_-(y) = \sum_{n=0}^{N} a_n^- T_n(y)$$

and implementing the boundary conditions (5.19) gives

$$a_0^+ = 1 + \sum_{n=2}^{N} a_n^+ (T'_n(1) - 1), \qquad\qquad a_1^+ = 1 - \sum_{n=2}^{N} a_n^+ T'_n(1),$$

$$a_0^- = 1 - \sum_{n=2}^{N} a_n^- (T_n(-1) + T'_n(-1)), \qquad\qquad a_1^- = -1 - \sum_{n=2}^{N} a_n^- T'_n(-1),$$

and hence

$$u_+(y) = 1 + \sum_{n=2}^{N} a_n^+ \Phi_n^+(y), \qquad\qquad u_-(y) = 1 + \sum_{n=2}^{N} a_n^- \Phi_n^-(y),$$

with

$$\Phi_n^+(y) = \big[(T'_n(1) - 1) - T'_n(1)y + T_n(y)\big]/(1+y), \qquad\qquad \Phi_n^-(y) = \big[-T_n(-1) - T'_n(1)(1+y) + T_n(y)\big]/(1-y).$$

Numerically solving

$$\mathcal{L}_{1,c}\left(1 + \sum_{n=2}^{N} a_n^+ \Phi_n^+\right)(y_i) = 0, \qquad\qquad \mathcal{L}_{1,c}\left(1 + \sum_{n=2}^{N} a_n^- \Phi_n^-\right)(y_i) = 0$$

with $y_i = \cos(\frac{\pi i}{N})$, $i = 1, ..., N-1$, $N = 40$ and rationalizing the obtained coefficients gives $(a_n^\pm)_{n=2}^{40} \subset \mathbb{Q}$ listed in Appendix F, Tables 2 and 3.

Remark. Note that by looking at the coefficients of $w_\pm$ we obviously have $w_+(y) = -w_-(-y)$, which comes as no surprise since both V_1 and Q are even.

Now $u_\pm$ are only approximations of the fundamental system of $\mathcal{L}_{1,c}$. In order to compare $\mathcal{L}_{1,c}$ to the unique operator corresponding to $\{u_+, u_-\}$ we define:

Definition 5.25.

$$\tilde{\mathcal{L}}_{1,c} f := -f'' + \tilde{p} f' + \tilde{q} f,$$

with

$$\tilde{p} := \frac{u_+ u_-'' - u_+'' u_-}{W}, \qquad \tilde{q} := \frac{u_+'' u_-' - u_+' u_-''}{W}$$

and

$$W := W(u_+, u_-) = u_+ u_-' - u_- u_+'.$$

First note that by construction

$$\tilde{\mathcal{L}}_{1,c} u_\pm = 0$$

and setting

$$W_0(y) := 2w_+(y)w_-(y) + (1-y^2)W(w_+, w_-)(y)$$

we have

$$\begin{aligned} W(y) &= W\left(\frac{1}{1+y}, \frac{1}{1-y}\right) w_+(y)w_-(y) + W(w_+, w_-)(y)\frac{1}{1-y^2} \\ &= \frac{2w_+(y)w_-(y)}{(1-y^2)^2} + \frac{W(w_+, w_-)(y)}{1-y^2} = \frac{W_0(y)}{(1-y^2)^2} \end{aligned}$$

and both W and W_0 are even functions.
Moreover W_0 is a polynomial of degree atmost 81 and by re-expanding W_0 in Chebychev polynomials we infer from Lemma 5.5

$$\|W_0\|_{L^\infty} < 4, \qquad \|W_0'\|_{L^\infty} < 4,$$

and from Lemma 5.6 on $[0,1]$ with $N = 100$

$$\min_{[-1,1]} |W_0| \geq \frac{19}{20} - \frac{4}{100} \geq \frac{18}{20},$$

in particular W_0 has no zeros in $[-1,1]$.

Writing $\mathcal{L}_{1,c}$ as in (5.5) as $\mathcal{L}_{1,c} f = -f'' + pf' + qf$ with $p = \frac{\psi''}{\psi'} = \frac{2y(y^2+3)}{(1+y^2)(1-y^2)}$, $q = (\psi')^2 (V_1 \circ \psi)$, we see that the comparison of $\mathcal{L}_{1,c}$ to $\tilde{\mathcal{L}}_{1,c}$ reduces to comparing p and q to $\tilde{p}$ and $\tilde{q}$.

Lemma 5.26. *$\tilde{p}$ and $\tilde{q}$ satisfy*

$$\|\tilde{p}-p\|_{L^\infty} < 6\cdot 10^{-4}, \qquad \|\tilde{q}-q\|_{L^\infty} < \frac{15}{1000},$$

where

$$p = \frac{\psi''}{\psi'} = \frac{2y(y^2+3)}{(1+y^2)(1-y^2)}, \qquad q = (\psi')^2(V_1\circ\psi).$$

Proof. We have

$$u_+(y)u_-''(y) - u_+''(y)u_-(y) = \frac{8yw_+(y)w_-(y)}{(1-y^2)^3} + \frac{P_1(y)}{(1-y^2)^2}$$

with

$$P_1(y) := 2\Big[w_+'(y)w_-(y) + w_+(y)w_-'(y) + yW(w_+(y),w_-(y))\Big] - (1-y^2)\Big[w_+''(y)w_-(y) - w_+(y)w_-''(y)\Big],$$

and hence

$$\tilde{p}(y) = \frac{8yw_+(y)w_-(y)}{(1-y^2)W_0(y)} + \frac{P_1(y)}{W_0(y)}$$

and

$$\tilde{p}(y) - p(y) = \frac{P_1(y)}{W_0(y)} - \frac{P_2(y)}{(1+y^2)W_0(y)}$$

with

$$P_2(y) := 4yw_+(y)w_-(y) + 2y(y^2+3)W(w_+(y),w_-(y)).$$

P_1 and P_2 are polynomials of degree atmost 80 and 82 respectively and we define

$$P_3(y) := (1+y^2)P_1(y) - P_2(y), \qquad P_4(y) := (1+y^2)W_0(y)$$

such that

$$\tilde{p}(y) - p(y) = \frac{P_3(y)}{P_4(y)}$$

and P_3 and P_4 are polynomials of degree atmost 82 and 83 respectively.
Re-expanding both P_3 and P_4 in Chebychev polynomials, we infer from Lemma 5.5

$$\|P_3\|_{L^\infty} < \frac{1}{1000}, \qquad \|P_4'\|_{L^\infty} < 16,$$

and from Lemma 5.6 on $[0,1]$ with $N = 100$

$$\min_{[-1,1]} |P_4| > \frac{19}{10} - \frac{16}{100} > \frac{17}{10},$$

from which we conclude

$$\|\tilde{p}-p\|_{L^\infty} \leq \frac{\|P_3\|_{L^\infty}}{\min_{[-1,1]}|P_4|} < \frac{1}{1000}\cdot\frac{10}{17} < 6\cdot 10^{-4}.$$

For the second estimate we write

$$u_+''(y)u_-'(y) - u_+'(y)u_-''(y) = \frac{P_5(y)}{(1-y^2)^2} + \frac{4P_6(y)}{(1-y^2)^3}$$

where

$$P_5(y) = (1-y^2)\Big[w_+''(y)w_-'(y) - w_+'(y)w_-''(y)\Big] - (1-y)w_+(y)w_-''(y) + (1+y)w_+''(y)w_-(y) - 4w_+'(y)w_-'(y),$$
$$P_6(y) = (1-y)w_+(y)w_-'(y) - (1+y)w_+'(y)w_-(y) + w_+(y)w_-(y)$$

are polynomials of degree atmost 79 and 80 respectively.
Moreover from the boundary conditions (5.19) we deduce that $\frac{P_6}{1-(.)^2}$ is a polynomial and define

$$P_7(y) := P_5(y) + \frac{4P_6(y)}{1-y^2}$$

which is a polynomial of degree atmost 79 and

$$\tilde{q} = \frac{P_7}{W_0}.$$

Re-expanding the polynomial $P_7'W_0 - P_7W_0'$ of degree atmost 159 in Chebychev polynomials, we infer from Lemma 5.5

$$\|P_7'W_0 - P_7W_0'\|_{L^\infty} < 2130,$$

which gives

$$\|\tilde{q}'\|_{L^\infty} \leq \frac{\|P_7'W_0 - P_7W_0'\|_{L^\infty}}{\min_{[-1,1]}|W_0|^2} \leq \frac{2130}{(\frac{18}{10})^2} < 658$$

and from

$$\Big\|\big(\tilde{q} - (\psi')^2(\tilde{V}_{1,j}\circ\psi)\big)'\Big\|_{L^\infty(J_j)} \leq \|\tilde{q}'\|_{L^\infty} + \Big\|\big((\psi')^2(\tilde{V}_{1,j}\circ\psi)\big)'\Big\|_{L^\infty(J_j)}$$

and Lemma 5.22 we infer

$$\Big\|\big(\tilde{q} - (\psi')^2(\tilde{V}_{1,0}\circ\psi)\big)'\Big\|_{L^\infty(J_0)} \leq 858,$$
$$\Big\|\big(\tilde{q} - (\psi')^2(\tilde{V}_{1,1}\circ\psi)\big)'\Big\|_{L^\infty(J_1)} \leq 685,$$
$$\Big\|\big(\tilde{q} - (\psi')^2(\tilde{V}_{1,2}\circ\psi)\big)'\Big\|_{L^\infty(J_2)} \leq 658.$$

Lemma 5.6 on $J_0, ..., J_2$ with $N = 88000,\ 7000,\ 5000$ gives

$$\begin{aligned}
\|\tilde{q} - (\psi')^2(\tilde{V}_{1,0} \circ \psi)\|_{L^\infty(J_0)} &< \frac{5}{1000} + 858 \cdot 10^{-5} < \frac{14}{1000}, \\
\|\tilde{q} - (\psi')^2(\tilde{V}_{1,1} \circ \psi)\|_{L^\infty(J_1)} &< \frac{6}{1000} + 685 \cdot 10^{-5} < \frac{13}{1000}, \\
\|\tilde{q} - (\psi')^2(\tilde{V}_{1,2} \circ \psi)\|_{L^\infty(J_2)} &< \frac{7}{1000} + 658 \cdot 10^{-5} < \frac{14}{1000}
\end{aligned}$$

and finally from Lemma 5.9 we conclude

$$\|\tilde{q} - q\|_{L^\infty} \leq \frac{14}{1000} + \max_{j=0,\dots,2} \|(\psi')^2(V_1 - \tilde{V}_{1,j}) \circ \psi\|_{L^\infty(J_j)} < \frac{15}{1000}.$$

□

The inverse of the operator $\tilde{\mathcal{L}}_{1,c}$ can now be constructed from the Green function corresponding to the fundamental system $\{u_+, u_-\}$:

Definition 5.27. *The Green function of $\tilde{\mathcal{L}}_{1,c}$ is given by*

$$G(y,s) := \frac{1}{W(s)} \begin{cases} u_+(s)u_-(y), & s \geq y, \\ u_+(y)u_-(s), & s \leq y. \end{cases}$$

The unique solution of $\tilde{\mathcal{L}}_{1,c}u = f \in L^\infty(-1,1)$ is given by

$$u(y) = \tilde{\mathcal{L}}_{1,c}^{-1} f(y) := \int_{-1}^{1} G(y,s)f(s)ds$$

and $\tilde{\mathcal{L}}_{1,c}^{-1} f \in L^\infty(-1,1)$ for all $f \in L^\infty(-1,1)$.

Lemma 5.28. *Let $f \in L^\infty(-1,1)$. Then*

$$\|\tilde{\mathcal{L}}_{1,c}^{-1} f\|_{W^{1,\infty}} \leq \frac{87}{10} \|f\|_{L^\infty}.$$

Proof. By Definition 5.27

$$\begin{aligned}\tilde{\mathcal{L}}_{1,c}^{-1}f(y) &= u_-(y)\int_y^1 \frac{u_+(s)}{W(s)}f(s)ds + u_+(y)\int_{-1}^y \frac{u_-(s)}{W(s)}f(s)ds \\ &= \frac{w_-(y)}{1-y}\int_y^1 \frac{w_+(s)}{1+s}\frac{(1-s^2)^2}{W_0(s)}f(s)ds + \frac{w_+(y)}{1+y}\int_{-1}^y \frac{w_-(s)}{1-s}\frac{(1-s^2)^2}{W_0(s)}f(s)ds \\ &= w_-(y)\int_y^1 \frac{w_+(s)}{W_0(s)}\frac{(1-s^2)(1-s)}{1-y}f(s)ds + w_+(y)\int_{-1}^y \frac{w_-(s)}{W_0(s)}\frac{(1-s^2)(1+s)}{1+y}f(s)ds\end{aligned}$$

Reexpanding $w\pm$ in Chebychev polynomials we infer

$$\|w'_\pm\|_{L^\infty} < 9$$

from Lemma 5.5, and Lemma 5.6 on $[-1,1]$ with $N = 2000$ gives

$$\|w_\pm\|_{L^\infty} \leq 2 + \frac{9}{1000} \leq \frac{201}{100},$$

hence

$$\left\|\frac{w_\pm}{W_0}\right\|_{L^\infty} \leq \frac{\|w_\pm\|_{L^\infty}}{\min_{[-1,1]}|W_0|} < \frac{201}{100}\cdot\frac{10}{18} < \frac{1117}{1000}$$

and

$$\|\tilde{\mathcal{L}}_{1,c}^{-1}f\|_{L^\infty} \leq \|f\|_{L^\infty}\|w_\pm\|_{L^\infty}\left\|\frac{w_\pm}{W_0}\right\|_{L^\infty}\int_{-1}^1 |1-s^2|ds < \|f\|_{L^\infty}\frac{201}{100}\frac{1117}{1000}\frac{4}{3} < 3\|f\|_{L^\infty}.$$

Similarly we have

$$\begin{aligned}(\tilde{\mathcal{L}}_{1,c}^{-1}f)'(y) &= u'_-(y)\int_y^1 \frac{u_+(s)}{W(s)}f(s)ds + u'_+(y)\int_{-1}^y \frac{u_-(s)}{W(s)}f(s)ds \\ &= \frac{w_-(y)+w'_-(y)(1-y)}{(1-y)^2}\int_y^1 \frac{w_+(s)}{1+s}\frac{(1-s^2)^2}{W_0(s)}f(s)ds \\ &+ \frac{w'_+(y)(1+y)-w_+(y)}{(1+y)^2}\int_{-1}^y \frac{w_-(s)}{1-s}\frac{(1-s^2)^2}{W_0(s)}f(s)ds \\ &= (w_-(y)(1+y)+w'_-(y)(1-y^2))\int_y^1 \frac{w_+(s)}{W_0(s)}\frac{(1-s^2)(1-s)}{(1-y^2)(1-y)}f(s)ds \\ &+ (w'_+(y)(1-y^2)-w_+(y)(1-y))\int_{-1}^y \frac{w_-(s)}{W_0(s)}\frac{(1-s^2)(1+s)}{(1-y^2)(1+y)}f(s)ds.\end{aligned}$$

Reexpanding the polynomial

$$P_8(y) := \Big(w_-(1+.)+w'_-(1-(.)^2)\Big)(y) = -\Big(w'_+(1-(.)^2)-w_+(1-.)\Big)(-y)$$

of degree atmost 41 in Chebychev polynomials we infer from Lemma 5.5

$$\|P_8'\|_{L^\infty} < 129$$

and from Lemma 5.6 on $[-1,1]$ with $N = 3000$

$$\|P_8\|_{L^\infty} < \frac{35}{10} + \frac{129}{1500} < \frac{36}{10}.$$

We conclude

$$\|(\tilde{\mathcal{L}}_{1,c}^{-1} f)'\|_{L^\infty} \leq \|f\|_{L^\infty} \|P_8\|_{L^\infty} \left\| \frac{w_\pm}{W_0} \right\|_{L^\infty} \int_{-1}^{1} ds < \frac{81}{10} \|f\|_{L^\infty}$$

and

$$\|\tilde{\mathcal{L}}_{1,c}^{-1} f\|_{W^{1,\infty}} = \left(\|\tilde{\mathcal{L}}_{1,c}^{-1} f\|_{L^\infty}^2 + \|(\tilde{\mathcal{L}}_{1,c}^{-1} f)'\|_{L^\infty}^2 \right)^{1/2} < \left(9\|f\|_{L^\infty}^2 + \left(\frac{81}{10}\right)^2 \|f\|_{L^\infty}^2 \right)^{1/2} < \frac{87}{10} \|f\|_{L^\infty}$$

□

5.5 The contraction argument

Recall from (5.9)

$$\mathcal{K}(u) = -\tilde{\mathcal{L}}_{c,1}^{-1} \mathcal{R}(g_1) + \tilde{\mathcal{L}}_{c,1}^{-1} (\tilde{\mathcal{L}}_{c,1} - \mathcal{L}_{c,1}) u.$$

Proposition 5.29. *Let $X := \{u \in C^1[-1,1] : \|u\|_{W^{1,\infty}} < \frac{1}{18}\}$. Then $\mathcal{K}$ has a unique fixed point in X. In particular there exists some $\delta_1 \in W^{1,\infty}$ with*

$$\|\delta_1\|_{W^{1,\infty}} < \frac{1}{18}$$

such that $\mathcal{R}(g_1 + \delta_1) = 0$, which proves the existence of ϕ_1.

Proof. From Proposition 5.24 and Lemma 5.26 and 5.28 we have

$$\begin{aligned}\|\mathcal{K}(u)\|_{W^{1,\infty}} &\leq \frac{87}{10}\bigg(\|\mathcal{R}(g_1)\|_{L^\infty} + \|\tilde{\mathcal{L}}_{c,1}u - \mathcal{L}_{c,1}u\|_{L^\infty}\bigg)\\ &\leq \frac{87}{10}\bigg(\|\mathcal{R}(g_1)\|_{L^\infty} + \|\tilde{p}-p\|_{L^\infty}\|u'\|_{L^\infty} + \|\tilde{q}-q\|_{L^\infty}\|u\|_{L^\infty}\bigg)\\ &\leq \frac{87}{10}\bigg(54\cdot 10^{-4} + 6\cdot 10^{-4}\cdot\frac{1}{18} + \frac{15}{1000}\frac{1}{18}\bigg) < \frac{1}{18}.\end{aligned}$$

which gives $\mathcal{K}(u) \in X$ for all $u \in X$.
Moreover,

$$\begin{aligned}\|\mathcal{K}(u) - \mathcal{K}(v)\|_{W^{1,\infty}} &\leq \frac{87}{10}\big\|\big(\tilde{\mathcal{L}}_{c,1} - \mathcal{L}_{c,1}\big)(u-v)\big\|_{L^\infty}\\ &\leq \frac{87}{10}\bigg(\|\tilde{p}-p\|_{L^\infty}\|u'-v'\|_{L^\infty} + \|\tilde{q}-q\|_{L^\infty}\|u-v\|_{L^\infty}\bigg)\\ &\leq \frac{87}{10}\bigg(6\cdot 10^{-4} + \frac{15}{1000}\bigg)\|u-v\|_{W^{1,\infty}} < \frac{14}{100}\|u-v\|_{W^{1,\infty}}\end{aligned}$$

for all $u, v \in X$.
We conclude that $\mathcal{K}$ is a contraction on X and the claim follows from the completeness of $W^{1,\infty}$. □

Corollary 5.30. *There exists a unique regular function $\phi_1 \in L^\infty(\mathbb{R})$ such that*

$$\mathcal{L}_1\phi_1 = Q \qquad \textit{and} \qquad \phi_1' \in L^2(\mathbb{R}).$$

Proof. From the exponential decay of Q and V_1 and $\mathcal{L}_1\phi_1 = -\phi_1'' + V_1\phi = Q$ we infer

$$\int(\phi_1')^2 = -\int \phi_1''\phi_1 = \int Q\phi_1 - \int V_1\phi_1^2 < \infty.$$

□

5.6 The positivity estimate

It remains to show

$$-\big(\phi_1\big|Q\big)\left(1-\bar{H}_1(Q,Q)\frac{\big(\phi_1\big|Q\big)}{\big(Q\big|Q\big)^2}\right)>0$$

where

$$\bar{H}_1(Q,Q)=\big(-Q''+V_1Q\big|Q\big)=\big(Q'\big|Q'\big)+\big(V_1Q\big|Q\big).$$

Lemma 5.31.

$$\big(Q\big|Q\big)^2=\frac{3\pi^2}{4},\qquad\qquad \big(Q'\big|Q'\big)=\frac{\sqrt{3}\pi}{4}$$

Proof. This statement follows from simple computations:

$$\big(Q\big|Q\big)=3^{1/2}\int_{-\infty}^{\infty}\frac{1}{\cosh(2x)}dx=2\cdot 3^{1/2}\int_{-\infty}^{\infty}\frac{1}{\cosh(u)}du=2\cdot 3^{1/2}\int_{-\infty}^{\infty}\operatorname{sech}(u)du=\frac{3^{1/2}\pi}{2}.$$

For the second claim note that

$$Q'(x)=3^{1/4}\frac{\sinh(2x)}{\cosh(2x)^{3/2}}$$

and

$$\begin{aligned}\big(Q'\big|Q'\big)&=3^{1/2}\int_{-\infty}^{\infty}\sinh(2x)^2\cosh(2x)^{-3}dx=\frac{3^{1/2}}{2}\int_{-\infty}^{\infty}\frac{\sinh(u)^2}{\cosh(u)^2}\frac{1}{\cosh(u)}du\\&=\frac{3^{1/2}}{2}\int_{-\infty}^{\infty}\tanh(u)^2\operatorname{sech}(u)du=\frac{3^{1/2}}{2}\int_{-\infty}^{\infty}(1-\operatorname{sech}(u)^2)\operatorname{sech}(u)du\\&=\frac{3^{1/2}}{2}\left(\int_{-\infty}^{\infty}\operatorname{sech}(u)du-\int_{-\infty}^{\infty}\operatorname{sech}(u)^3du\right)=\frac{3^{1/2}}{4}\int_{-\infty}^{\infty}\operatorname{sech}(u)du=\frac{3^{1/2}\pi}{4},\end{aligned}$$

where for the last equality we used

$$\int_{-\infty}^{\infty}\operatorname{sech}(u)^3du=\frac{\operatorname{sech}(u)\tanh(u)}{2}\bigg|_{-\infty}^{\infty}+\frac{1}{2}\int_{-\infty}^{\infty}\operatorname{sech}(u)du=\frac{1}{2}\int_{-\infty}^{\infty}\operatorname{sech}(u)du.$$

□

Lemma 5.32. *The function Q satisfies the following integral bounds.*

$$\int_{I_0}Q(\psi(y))\psi'(y)dy\leq\frac{17}{10},\qquad\int_{I_1}Q(\psi(y))\psi'(y)dy\leq\frac{38}{1000},\qquad\int_{I_2}Q(\psi(y))\psi'(y)dy\leq 2\cdot 10^{-6}.$$

Proof. We have

$$\int_{I_1} Q(\psi(y))\psi'(y)dy = \int_{I_i} \tilde{Q}_i(\psi(y))\psi'(y)dy + \int_{I_i} \left(Q(\psi(y)) - \tilde{Q}_i(\psi(y))\right)\psi'(y)dy$$

with

$$\left|\int_{I_i} \left(Q(\psi(y) - \tilde{Q}_i(\psi(y))\right)\psi'(y)dy\right| \leq |I_i| \cdot \left\|\psi'(Q - \tilde{Q}_i) \circ \psi\right\|_{L^\infty(I_i)} \leq |I_i| \cdot \left\|(\psi')^2(Q - \tilde{Q}_i) \circ \psi\right\|_{L^\infty(I_i)}$$

and hence by Lemma 5.8

$$\begin{aligned}
\left|\int_{I_0} \left(Q(\psi(y) - \tilde{Q}_0(\psi(y))\right)\psi'(y)dy\right| &\leq \frac{88}{100} \cdot 4 \cdot 10^{-4} < 4 \cdot 10^{-6}, \\
\left|\int_{I_1} \left(Q(\psi(y) - \tilde{Q}_1(\psi(y))\right)\psi'(y)dy\right| &\leq \frac{1}{10} \cdot 6 \cdot 10^{-6} = 6 \cdot 10^{-7}, \\
\left|\int_{I_2} \left(Q(\psi(y) - \tilde{Q}_2(\psi(y))\right)\psi'(y)dy\right| &\leq \frac{2}{100} \cdot 6 \cdot 10^{-5} < 2 \cdot 10^{-6}.
\end{aligned}$$

Consider the *trapezoidal rule*

$$\int_a^b F(y)dy = \frac{b-a}{2N} \sum_{n=0}^{N-1} \left(F\left(a + i \cdot \frac{b-a}{N}\right) + F\left(a + (i+1) \cdot \frac{b-a}{N}\right)\right) + R_{F,[a,b],N}$$

with

$$|R_{F,[a,b],N}| \leq \frac{(b-a)^3}{12N^2} \|F''\|_{L^\infty}.$$

Applying the trapezoidal rule on I_0 and I_1 with $N = 880$ and 100 gives

$$\begin{aligned}
\int_{I_0} \tilde{Q}_0(\psi(y))\psi'(y)dy &\leq \frac{1688}{1000} + \left(\frac{88}{100}\right)^3 \frac{1}{12 \cdot (880)^2} \cdot 350 < \frac{169}{100}, \\
\int_{I_1} \tilde{Q}_1(\psi(y))\psi'(y)dy &\leq 377 \cdot 10^{-4} + \left(\frac{1}{10}\right)^3 \frac{1}{12 \cdot (100)^2} \cdot 630 < 377 \cdot 10^{-4}
\end{aligned}$$

where we replaced $\tilde{Q}_0$ by $\tilde{Q}_{0,+}$ for the evaluation of $\tilde{Q}_0$ and C by C_+ for the evaluation of $\tilde{Q}_1$ and used Lemma 5.16 for the bounds on the second derivatives of the integrands.

We conclude

$$\int_{I_0} Q(\psi(y))\psi'(y)dy \leq \frac{169}{100} + 4 \cdot 10^{-6} \leq \frac{17}{10},$$
$$\int_{I_1} Q(\psi(y))\psi'(y)dy \leq 377 \cdot 10^{-4} + 6 \cdot 10^{-7} \leq \frac{38}{1000},$$
$$\int_{I_2} Q(\psi(y))\psi'(y)dy \leq 2 \cdot 10^{-6}.$$

□

Lemma 5.33.

$$0 > \big(\phi_1\big|Q\big) > -\frac{111}{100}.$$

Proof. We write

$$\begin{aligned}\big(\phi_1\big|Q\big) &= 2\int_0^1 \phi_1(\psi(y))Q(\psi(y))\psi'(y)dy \\ &= 2\sum_{i=0}^{2}\int_{I_i} g_1(y)\tilde{Q}_i(\psi(y))\psi'(y)dy + 2\sum_{i=0}^{2}\int_{I_i}\Big(\phi_1(\psi(y))Q(\psi(y)) - g_1(y)\tilde{Q}_i(\psi(y))\Big)\psi'(y)dy\end{aligned}$$

with

$$\begin{aligned}&\left|\int_{I_i}\Big(\phi_1(\psi(y))Q(\psi(y)) - g_1(y)\tilde{Q}_i(\psi(y))\Big)\psi'(y)dy\right| \\ \leq &\int_{I_i}\Big(|Q(y)|\cdot|\phi_1(\psi(y)) - g_1(y)| + |g_1(y)|\cdot|Q(\psi(y) - \tilde{Q}_i(\psi(y)|\Big)\psi'(y)dy \\ \leq &\|\delta_1\|_{L^\infty}\int_{I_i}|Q(\psi(y))|\psi'(y)dy + |I_i|\cdot\|g_1\|_{L^\infty}\cdot\|(\psi')(Q-\tilde{Q}_i)\circ\psi\|_{L^\infty(I_i)} \\ \leq &\|\delta_1\|_{L^\infty}\int_{I_i}Q(\psi(y))\psi'(y)dy + |I_i|\cdot\|g_1\|_{L^\infty}\cdot\|(\psi')^2(Q-\tilde{Q}_i)\circ\psi\|_{L^\infty(I_i)}\end{aligned}$$

and hence by Lemmas 5.8, 5.32, Proposition 5.29 and (5.18)

$$\left|\int_{I_0}\Big(\phi_1(\psi(y))Q(\psi(y)) - g_1(y)\tilde{Q}_0(\psi(y))\Big)\psi'(y)dy\right| < \frac{95}{1000},$$
$$\left|\int_{I_1}\Big(\phi_1(\psi(y))Q(\psi(y)) - g_1(y)\tilde{Q}_1(\psi(y))\Big)\psi'(y)dy\right| < \frac{3}{1000},$$
$$\left|\int_{I_0}\Big(\phi_1(\psi(y))Q(\psi(y)) - g_1(y)\tilde{Q}_2(\psi(y))\Big)\psi'(y)dy\right| < 10^{-6}.$$

From

$$\left\|\left(\psi' g_1(\tilde{Q}_i\circ\psi)\right)''\right\|_{L^\infty(I_i)} \le \left\|\left(\psi'(\tilde{Q}_i\circ\psi)\right)''\right\|_{L^\infty(I_i)}\cdot\|g_1\|_{L^\infty} + \left\|\psi'(\tilde{Q}_i\circ\psi)\right\|_{L^\infty(I_i)}\cdot\|g_1''\|_{L^\infty} + 2\left\|\left(\psi'(\tilde{Q}_i\circ\psi)\right)'\right\|_{L^\infty(I_i)}\cdot\|g_1'\|_{L^\infty},$$

Lemma 6.9 and (6.6) we infer

$$\left\|\left(\psi' g_1(\tilde{Q}_0\circ\psi)\right)''\right\|_{L^\infty(I_0)} < 403, \qquad \left\|\left(\psi' g_1(\tilde{Q}_1\circ\psi)\right)''\right\|_{L^\infty(I_1)} < 520.$$

We bound the integrands $g_1(y)\tilde{Q}_i(\psi(y))\psi'(y)$ for the evaluation of the trapezoidal rule by

$$g_1(y)\tilde{Q}_0(\psi(y))\psi'(y) \le \max\left\{g_1(y)\tilde{Q}_{0,-}(\psi(y))\psi'(y),\ g_1(y)\tilde{Q}_{0,+}(\psi(y))\psi'(y)\right\},$$
$$g_1(y)\tilde{Q}_0(\psi(y))\psi'(y) \ge \min\left\{g_1(y)\tilde{Q}_{0,-}(\psi(y))\psi'(y),\ g_1(y)\tilde{Q}_{0,+}(\psi(y))\psi'(y)\right\}$$

and

$$g_1(y)\tilde{Q}_1(\psi(y))\psi'(y) \le \max\left\{g_1(y)\frac{C_+}{C}\tilde{Q}_1(\psi(y))\psi'(y), g_1(y)\frac{C_-}{C}\tilde{Q}_1(\psi(y))\psi'(y)\right\},$$
$$g_1(y)\tilde{Q}_1(\psi(y))\psi'(y) \ge \min\left\{g_1(y)\frac{C_+}{C}\tilde{Q}_1(\psi(y))\psi'(y), g_1(y)\frac{C_-}{C}\tilde{Q}_1(\psi(y))\psi'(y)\right\}$$

and the trapezoidal rule on I_0 and I_1 with $N = 880$ and $N = 100$ gives

$$\int_{I_0} g_1(y)\tilde{Q}_0(\psi(y))\psi'(y)dy \le -\frac{464}{1000} + \left(\frac{88}{100}\right)^3\frac{1}{12\cdot(880)^2}\cdot 403 < -\frac{463}{1000},$$
$$\int_{I_0} g_1(y)\tilde{Q}_0(\psi(y))\psi'(y)dy \ge -\frac{465}{1000} - \left(\frac{88}{100}\right)^3\frac{1}{12\cdot(880)^2}\cdot 403 > -\frac{466}{1000},$$
$$\int_{I_1} g_1(y)\tilde{Q}_1(\psi(y))\psi'(y)dy \le \frac{15}{1000} + \left(\frac{1}{10}\right)^3\frac{1}{12\cdot(100)^2}\cdot 520 < \frac{16}{1000},$$
$$\int_{I_1} g_1(y)\tilde{Q}_1(\psi(y))\psi'(y)dy \ge \frac{14}{1000} - \left(\frac{1}{10}\right)^3\frac{1}{12\cdot(100)^2}\cdot 520 > \frac{13}{1000},$$

and hence

$$\begin{aligned}\big(\phi_1\big|Q\big) &\leq 2\cdot\left(-\frac{447}{1000}\right)+2\cdot\left(\frac{95}{1000}+\frac{3}{1000}+10^{-6}\right)<-\frac{69}{100},\\ \big(\phi_1\big|Q\big) &\geq 2\cdot\left(-\frac{453}{1000}\right)-2\cdot\left(\frac{95}{1000}+\frac{3}{1000}+10^{-6}\right)>-\frac{111}{100},\end{aligned}$$

□

Lemma 5.34.

$$-\frac{645}{100}<\bar{H}_1(Q,Q)<0.$$

Proof. We have

$$\begin{aligned}\big(V_1Q\big|Q\big) =&2\int_0^1 V_1(\psi(y))Q(\psi(y))^2\psi'(y)dy=2\sum_{i,j=0}^{2}\int_{I_i\cap J_j}V(\psi(y))Q(\psi(y))^2\psi'(y)dy\\ =&2\sum_{i,j=0}^{2}\int_{I_i\cap J_j}\tilde{V}_{1,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\psi'(y)dy\\ &+2\sum_{i,j=0}^{2}\int_{I_i\cap J_j}\Big(V_1(\psi(y))Q(\psi(y))^2-\tilde{V}_{1,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\Big)\psi'(y)dy\end{aligned}$$

with

$$\begin{aligned}&\left|\int_{I_i\cap J_j}\Big(V_1(\psi(y))Q(\psi(y))^2-\tilde{V}_{1,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\Big)\psi'(y)dy\right|\\ \leq&\int_{I_i\cap J_j}\Big(\big|V_1(\psi(y))-\tilde{V}_{1,j}(\psi(y))\big|\cdot|Q(\psi(y))|^2+\big|\tilde{V}_{1,j}(\psi(y))\big|\cdot\big|Q(\psi(y))^2-\tilde{Q}_i(\psi(y))^2\big|\Big)\psi'(y)\,dy\\ \leq&|I_i\cap J_j|\cdot\Big(\big\|(\psi')^2\left(V_1-\tilde{V}_{1,j}\right)\circ\psi\big\|_{L^\infty(J_j)}\cdot\|Q\circ\psi\|^2_{L^\infty(I_i)}+\big\|\tilde{V}_{1,j}\circ\psi\big\|_{L^\infty(J_j)}\cdot\big\|(\psi')^2\left(Q^2-\tilde{Q}_i^2\right)\circ\psi\big\|_{L^\infty(I_i)}\Big)\end{aligned}$$

and by the mean-value theorem

$$\big\|(\psi')^2\left(Q^2-\tilde{Q}_i^2\right)\circ\psi\big\|_{L^\infty(I_i)}\leq 2\cdot\max\Big\{\|Q\circ\psi\|_{L^\infty(I_i)},\ \big\|\tilde{Q}\circ\psi\big\|_{L^\infty(I_i)}\Big\}\cdot\big\|(\psi')^2\left(Q-\tilde{Q}_i\right)\circ\psi\big\|_{L^\infty(I_i)}$$

which gives

$$\left|2\sum_{i,j=0}^{2}\int_{I_i\cap J_j}\Big(V_1(\psi(y))Q(\psi(y))^2-\tilde{V}_{1,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\Big)\psi'(y)dy\right|<6\cdot10^{-4}$$

by Lemmas 5.8, 5.17, 5.9 and 5.23.

In order to estimate the integrals $\int_{I_i\cap J_j}\tilde V_{1,j}(\psi(y))\tilde Q_i(\psi(y))^2\psi'(y)dy$ by the trapezoidal rule, we estimate the second derivatives of the integrands by

$$\begin{aligned}
&\left\|\left(\psi'\left(\left(\tilde V_{1,j}\cdot\tilde Q_i^2\right)\circ\psi\right)\right)''\right\|_{L^\infty(I_i\cap J_j)}\\
\le&\left\|\left(\left(\tilde V_{1,j}\cdot\tilde Q_i\right)\circ\psi\right)''\right\|_{L^\infty(I_i\cap J_j)}\cdot\left\|\psi'\left(\tilde Q_i\circ\psi\right)\right\|_{L^\infty(I_i)}+\left\|\left(\tilde V_{1,j}\cdot\tilde Q_i\right)\circ\psi\right\|_{L^\infty(I_i\cap J_j)}\left\|\left(\psi'\left(\tilde Q_i\circ\psi\right)\right)''\right\|_{L^\infty(I_i)}\\
&+2\cdot\left\|\left(\left(\tilde V_{1,j}\cdot\tilde Q_i\right)\circ\psi\right)'\right\|_{L^\infty(I_i\cap J_j)}\cdot\left\|\left(\psi'\left(\tilde Q_i\circ\psi\right)\right)'\right\|_{L^\infty(I_i)}\\
\le&\Bigg(\left\|\left(\tilde V_{1,j}\circ\psi\right)''\right\|_{L^\infty(J_j)}\left\|\tilde Q_i\circ\psi\right\|_{L^\infty(I_i)}+\left\|\tilde V_{1,j}\circ\psi\right\|_{L^\infty(J_j)}\left\|\left(\tilde Q_i\circ\psi\right)''\right\|_{L^\infty(I_i)}\\
&\quad+2\left\|\left(\tilde V_{1,j}\circ\psi\right)'\right\|_{L^\infty(J_j)}\cdot\left\|\left(\tilde Q_i\circ\psi\right)'\right\|_{L^\infty(I_i)}\Bigg)\cdot\left\|\psi'\left(\tilde Q_i\circ\psi\right)\right\|_{L^\infty(I_i)}\\
&+\left\|\tilde V_{1,j}\circ\psi\right\|_{L^\infty(J_j)}\cdot\left\|\tilde Q_i\circ\psi\right\|_{L^\infty(I_i)}\cdot\left\|\left(\psi'\left(\tilde Q_i\circ\psi\right)\right)''\right\|_{L^\infty(I_i)}\\
&+2\cdot\left(\left\|\left(\tilde V_{1,j}\circ\psi\right)'\right\|_{L^\infty(J_j)}\cdot\left\|\tilde Q_i\circ\psi\right\|_{L^\infty(I_i)}+\left\|\tilde V_{1,j}\circ\psi\right\|_{L^\infty(J_j)}\cdot\left\|\left(\tilde Q_i\circ\psi\right)'\right\|_{L^\infty(I_i)}\right)\cdot\left\|\left(\psi'\left(\tilde Q_i\circ\psi\right)\right)'\right\|_{L^\infty(I_i)}
\end{aligned}$$

which by Lemmas 5.16, 5.17 and 5.23 gives

$$\left\|\left(\psi'\left(\left(V_{1,0}\cdot Q_0^2\right)\circ\psi\right)\right)''\right\|_{L^\infty(I_0\cap J_0)}<11000,\qquad\left\|\left(\psi'\left(\left(V_{1,1}\cdot Q_1^2\right)\circ\psi\right)\right)''\right\|_{L^\infty(I_1\cap J_1)}<\frac12.$$

Replacing the constant C^2 in $\tilde Q_i$ by C_-^2 for the evaluation of the trapezoidal rule on $I_0\cap J_0$ and $I_1\cap J_1$ with $N=880$ and $N=70$ gives

$$\begin{aligned}
0>\int_{I_0\cap J_0}\tilde V_{1,0}(\psi(y))\tilde Q_0(\psi(y))^2\psi'(y)dy>-\frac{3894}{1000}-\left(\frac{88}{100}\right)^3\cdot\frac{1}{12\cdot(880)^2}\cdot11000>-\frac{39}{10},\\
0>\int_{I_1\cap J_1}\tilde V_{1,1}(\psi(y))\tilde Q_1(\psi(y))^2\psi'(y)dy>-2\cdot10^{-7}-\left(\frac{7}{100}\right)^3\cdot\frac{1}{12\cdot(70)^2}\cdot\frac12>-3\cdot10^{-7}.
\end{aligned}$$

We conclude

$$0>\left(V_1Q\middle|Q\right)>2\cdot\left(-\frac{39}{10}-3\cdot10^{-7}\right)-6\cdot10^{-4}>-\frac{7801}{1000}.$$

Recall from the proof of Proposition 4.32 that $\bar H_1(Q,Q)<H_1(Q,Q)<0$ and hence by Lemma 5.31

$$0>\bar H_1(Q,Q)=\left(Q'\middle|Q'\right)+\left(V_1Q\middle|Q\right)>\frac{\sqrt3\pi}{4}-\frac{7801}{1000}>-\frac{645}{100}.$$

□

Finally, using Lemma 5.31, 5.34 and 5.33 we compute

$$1 - \bar{H}_1(Q,Q)\frac{\big(\phi_1\big|Q\big)}{\big(Q\big|Q\big)^2} \geq 1 - \frac{111}{100}\cdot\frac{645}{100}\cdot\frac{4}{3\pi^2} > \frac{3}{100}$$

and hence

$$-\big(\phi_1\big|Q\big)\left(1 - \bar{H}_1(Q,Q)\frac{\big(\phi_1\big|Q\big)}{\big(Q\big|Q\big)^2}\right) > 0,$$

which concludes the proof of the positivity estimate (5.3).

6 Proof of Theorem 4.33 ii)

As in Section 5 we denote the operator $\bar{\mathcal{L}}_2$ from Theorem 4.33 ii) as $\mathcal{L}_2$ and restate the claim:

Let

$$\begin{aligned} Q_3(x) :=& 3^{1/4}\cosh(2x)^{-1/2}\left(\frac{5}{8} - 2x\tanh(2x) + \frac{x^2}{2}\left(3\tanh(2x)^2 - 2\right)\right), \\ V_2(x) :=& \frac{20}{9}xQ^3(x)Q'(x) - \frac{1}{9}\cosh(\tfrac{9x}{10})^{-2} \end{aligned}$$

and

$$\mathcal{L}_2 f = -f'' + V_2 f, \qquad\qquad \bar{H}_2(f,f) = \big(\mathcal{L}_2 f \big| f\big).$$

Then there exists a unique regular function $\phi_2 \in L^\infty$ such that

$$\mathcal{L}_2\phi_2 = Q_3. \tag{6.1}$$

Moreover

$$\phi_2' \in L^2 \tag{6.2}$$

and

$$-\big(\phi_2\big|Q_3\big)\left(1 - \bar{H}_2(Q,Q)\frac{\big(\phi_2\big|Q_3\big)}{\big(Q\big|Q_3\big)^2}\right) > 0. \tag{6.3}$$

As in Section 5, the compactification

$$\begin{aligned} \Phi_2 &:= \phi_2 \circ \psi, \\ \mathcal{L}_{c,2} f &:= -f'' + \frac{\psi''}{\psi'}f' + (\psi')^2\big(V_2 \circ \psi\big)f \end{aligned}$$

and

$$\mathcal{R}(\Phi_2) := \mathcal{L}_{c,2}\Phi_2 - (\psi')^2\big(Q_3 \circ \psi\big)$$

makes (6.1) on $\mathbb{R}$ equivalent to

$$\mathcal{R}(\Phi_2) = 0. \tag{6.4}$$

The exponential decay of Q_3 and V_2 leads to the same boundary conditions for g_2 and hence by using the same ansatz and basis functions as in (5.7) we numerically solve the problem

$$\mathcal{R}\Big(\sum_{n=0}^{N-2} a_n \Psi_n\Big)(y_i) = 0$$

with $y_i = 1 - (\frac{i}{N+3})^2$, $i = 5, ..., N+3$ and $N = 120$.

Rationalizing the obtained coefficients gives $(a_n)_{n=0}^{118} \subset \mathbb{Q}$ listed in Appendix F, Table 4, and we obtain a polynomial g_2 of degree 240.

6.1 Approximation of Q_3 and V_2

Approximation of Q_3

We rewrite

$$\begin{aligned}
Q_3(x) &= Ce^{-x}(1+e^{-4x})^{-1/2}\left(\frac{5}{8} - 2x\,\frac{e^{2x}-e^{-2x}}{e^{2x}+e^{-2x}} + \frac{x^2}{2}\left(3\,\left(\frac{e^{2x}-e^{-2x}}{e^{2x}+e^{-2x}}\right)^2 - 2\right)\right)\\
&= Ce^{-x}(1+e^{-4x})^{-1/2}\left(\frac{5}{8} - 2x\,\frac{1-e^{-4x}}{1+e^{-4x}} + \frac{x^2}{2}\left(3\,\left(\frac{1-e^{-4x}}{1+e^{-4x}}\right)^2 - 2\right)\right)\\
&= Ce^{-x}(1+e^{-4x})^{-1/2}\left(\frac{5}{8} - 2x\left(\frac{2}{1+e^{-4x}} - 1\right) + \frac{x^2}{2}\left(3\,\left(\frac{2}{1+e^{-4x}} - 1\right)^2 - 2\right)\right)
\end{aligned}$$

and define the following approximations for Q_3

$$\begin{aligned}
\tilde{Q}_{3,0}(x) &:= Ce_{22}^{-}(x)(1+e_{56}^{-}(4x))^{-1/2}\left(\frac{5}{8} - 2x\;t(x) + \frac{x^2}{2}\left(3\;t(x)^2 - 2\right)\right) = \tilde{Q}_0(x)T(x),\\
\tilde{Q}_{3,1}(x) &:= Ce_{118}^{-}(x)\left(\frac{5}{8} - 2x + \frac{x^2}{2}\right),\\
\tilde{Q}_{3,2}(x) &:= 0
\end{aligned}$$

with

$$\begin{aligned}
t(x) &:= \frac{2}{1+e_{56}^{-}(4x)} - 1,\\
T(x) &:= \frac{5}{8} - 2x\;t(x) + \frac{x^2}{2}\left(3\;t(x)^2 - 2\right)
\end{aligned}$$

and

$$\mathcal{I}_0 := \left[0, \frac{88}{100}\right], \qquad \mathcal{I}_1 := \left[\frac{88}{100}, \frac{985}{1000}\right], \qquad \mathcal{I}_2 := \left[\frac{985}{1000}, 1\right].$$

Remark. Observing that $\psi(\frac{88}{100}) < 4$ and $\psi(\frac{985}{1000}) < 34$ and evaluating

$$e_{19}^{-}\left(\psi\left(\tfrac{88}{100}\right)\right) > 0 \qquad e_{53}^{-}(4\psi\left(\tfrac{88}{100}\right)) > 0, \qquad e_{115}^{-}(\psi\left(\tfrac{985}{1000}\right)) > 0$$

we see that all functions e_N^- appearing in $\tilde{Q}_{3,i}$ satisfy (5.11) on the interval $\mathcal{I}_i$.

Lemma 6.1. *The approximations $\tilde{Q}_{3,0}$, $\tilde{Q}_{3,1}$ and $\tilde{Q}_{3,2}$ satisfy the following estimates:*

$$\begin{aligned}
\|(\psi')^2(Q_3-\tilde{Q}_{3,0})\circ\psi\|_{L^\infty(\mathcal{I}_0)} &< 2\cdot 10^{-4},\\
\|(\psi')^2(Q_3-\tilde{Q}_{3,1})\circ\psi\|_{L^\infty(\mathcal{I}_1)} &< 10^{-3},\\
\|(\psi')^2(Q_3-\tilde{Q}_{3,2})\circ\psi\|_{L^\infty(\mathcal{I}_2)} &< 3\cdot 10^{-5}.
\end{aligned}$$

Proof. By the mean-value theorem we have

$$\begin{aligned}
\left|\left(\frac{2}{1+e^{-4x}}-1\right)-t(x)\right| &= \left|\frac{2}{1+e^{-4x}}-\frac{2}{1+e_{56}^-(4x)}\right| \le 2R_{56}(4x),\\
\left|\left(\frac{2}{1+e^{-4x}}-1\right)^2-t(x)^2\right| &= \left|\left(\frac{2}{1+e^{-4x}}-1\right)^2-\left(\frac{2}{1+e_{56}^-(4x)}-1\right)^2\right| \le 4R_{56}(4x),
\end{aligned} \tag{6.5}$$

and using the bound on $|Q(x)-\tilde{Q}_0(x)|$ from the proof of Lemma 5.8 and $|T(x)|\le\frac{5}{8}+2x+x^2$ we obtain

$$\begin{aligned}
|Q_3(x)-\tilde{Q}_{3,0}(x)| &\le |Q(x)|\left|\left(\frac{5}{8}-2x\left(\frac{2}{1+e^{-4x}}-1\right)+\frac{x^2}{2}\left(3\left(\frac{2}{1-e^{-4x}}-1\right)^2-2\right)\right)-T(x)\right| + \left|Q(x)-\tilde{Q}_0(x)\right||T(x)|\\
&\le 2e^{-x}\left(4xR_{56}(4x)+6x^2R_{56}(4x)\right)+2\left(e_{22}^-(x)R_{56}(4x)/2+R_{22}(x)\right)\left(\frac{5}{8}+2x+x^2\right)\\
&\le 2e_{100}^-(x)\left(4xR_{56}(4x)+6x^2R_{56}(4x)\right)+2\left(e_{22}^-(x)R_{56}(4x)/2+R_{22}(x)\right)\left(\frac{5}{8}+2x+x^2\right)
\end{aligned}$$

and hence

$$\begin{aligned}
\psi'(y)^2|Q_3(\psi(y))-\tilde{Q}_{3,0}(\psi(y))| \le\ & 2\psi'(y_2)^2\Big(e_{100}^-(\psi(y_1))\left(4\psi(y_2)R_{56}(4\psi(y_2))+6x^2R_{56}(\psi(y_2))\right)\\
&+2\left(e_{22}^-(\psi(y_1))R_{56}(4\psi(y_2))/2+R_{22}(\psi(y_2))\right)\left(\frac{5}{8}+2\psi(y_2)+\psi(y_2)^2\right)\Big)
\end{aligned}$$

for all $y\in[y_1,y_2]\subseteq\mathcal{I}_0$. From Lemma 5.7 on $\mathcal{I}_0$ with $N=88$ we conclude

$$\psi'(y)^2|Q_3(\psi(y))-\tilde{Q}_{3,0}(\psi(y))|<2\cdot 10^{-4}$$

for all $y\in\mathcal{I}_0$.

Observing that $|\frac{5}{8} - 2x + \frac{x^2}{2}| < \frac{5}{8} + x^2$ for $x \geq \psi(\frac{88}{100}) > 3$,

$$\left|1 - \frac{1-e^{-4x}}{1+e^{-4x}}\right| \leq 2e^{-4x}, \qquad \left|1 - \left(\frac{1-e^{-4x}}{1+e^{-4x}}\right)^2\right| \leq 4e^{-4x}$$

and

$$\left|e^{-x}(1+e^{-4x})^{-1/2} - e^{-}_{118}(x)\right| \leq R_{118}(x) + e^{-4x}e^{-}_{118}(x)/2$$

by the mean value theorem, we estimate

$$\begin{aligned}
|Q_3(x) - \tilde{Q}_{3,1}(x)| &\leq 2\Bigg(\left|e^{-x}(1+e^{-4x})^{-1/2} - e^{-}_{118}(x)\right| \left(\frac{5}{8} + x^2\right) + e^{-x}\left(2x\left|1 - \frac{1-e^{-4x}}{1+e^{-4x}}\right| + \frac{3x^2}{2}\left|1 - \left(\frac{1-e^{-4x}}{1+e^{-4x}}\right)^2\right|\right)\Bigg) \\
&\leq 2\Bigg(\left(R_{118}(x) + e^{-4x}e^{-}_{118}(x)/2\right)\left(\frac{5}{8} + x^2\right) + e^{-x}\left(4xe^{-4x} + 6x^2e^{-4x}\right)\Bigg) \\
&\leq 2\Bigg(\left(R_{118}(x) + e^{-}_{500}(4x)e^{-}_{118}(x)/2\right)\left(\frac{5}{8} + x^2\right) + e^{-}_{500}(x)e^{-}_{500}(4x)\left(4x + 6x^2\right)\Bigg)
\end{aligned}$$

and

$$\begin{aligned}
\psi'(y)^2|Q_3(\psi(y)) - \tilde{Q}_{3,1}(\psi(y))| \leq & 2\psi'(y)^2\Bigg(\left(R_{118}(\psi(y_2)) + e^{-}_{500}(4\psi(y_1))e^{-}_{118}(\psi(y_1))/2\right)\left(\frac{5}{8} + \psi(y_2)^2\right) \\
& + e^{-}_{500}(\psi(y_1))e^{-}_{500}(4\psi(y_1))\left(4\psi(y_2) + 6\psi(y_2)^2\right)\Bigg)
\end{aligned}$$

for all $y \in [y_1, y_2] \subseteq \mathcal{I}_1$. From Lemma 5.7 on $\mathcal{I}_1$ with $N = 105$ we conclude

$$\psi'(y)^2|Q_3(\psi(y)) - \tilde{Q}_{3,1}(\psi(y))| < 10^{-3}$$

for all $y \in \mathcal{I}_1$.

It remains to show that $\psi'(y)^2 Q_3(\psi(y))$ is small for $y \in \mathcal{I}_2$.

Observe that for $x \geq \psi(\frac{985}{1000}) > 33$ we have

$$3\tanh(2x)^2 - 2 > \frac{1}{2}$$

and hence

$$\frac{x^2}{2}\left(3\tanh(2x)^2 - 2\right) - 2x\tanh(2x) > 0$$

which gives

$$|Q_3(x)| < 2e^{-x}\left(\frac{5}{8} + \frac{x^2}{2}\right)$$

for $x \in \psi(\mathcal{I}_2)$ and

$$|\psi'(y)^2 Q_3(\psi(y))| < 2\psi'(y)^2 e^{-\psi(y)} \left(\frac{5}{8} + \frac{\psi(y)^2}{2}\right)$$

for $y \in \mathcal{I}_2$.

We differentiate

$$\begin{aligned}\frac{d}{dy}\left(\psi'(y)^2 e^{-\psi(y)} \left(\frac{5}{8} + \frac{\psi(y)^2}{2}\right)\right) &= \psi'(y) e^{-\psi(y)} \left(2\psi''(y) \left(\frac{5}{8} + \frac{\psi(y)^2}{2}\right) - \psi'(y)^2 \left(\frac{5}{8} + \frac{\psi(y)^2}{2}\right) + \psi'(y)^2 \psi(y)\right) \\ &= \psi'(y) e^{-\psi(y)} \frac{(-5 + 68 - 4y^2 - 104y^3 + 2y^4 + 80y^5 - 4y^6 - 24y^7 - 5y^8 - 20y^9)}{8(1+y^2)^6} < 0\end{aligned}$$

for all $y \geq \frac{985}{1000}$ and hence by evaluating

$$2\psi'(y)^2 e^{-\psi} \left(\frac{5}{8} + \frac{\psi^2}{2}\right) \leq 2\psi'(y)^2 e_{500}^-(\psi) \left(\frac{5}{8} + \frac{\psi^2}{2}\right)$$

at $y = \frac{985}{1000}$, we conclude

$$\psi'(y)^2 |Q_3(\psi(y)) - \tilde{Q}_{3,2}(\psi(y))| < 3 \cdot 10^{-5}$$

for all $y \in \mathcal{I}_2$. □

Approximation of V_2

Since V_2 differs from V_1 by only a factor of $\frac{1}{5}$ in the first term, all methods involved are essentially the same as for V_1 and we will omit details refering to Section 5.2.

$$\begin{aligned}\tilde{V}_{2,0}(x) &:= -\frac{80}{3} x e_{60}^-(4x)(1 - e_{60}^-(4x))(1 + e_{60}^-(4x))^{-3} - \frac{4}{9} e_{30}^-(\tfrac{9x}{5})(1 + e_{30}^-(\tfrac{9x}{5}))^{-2}, \\ \tilde{V}_{2,1}(x) &:= -\frac{80}{3} x e_{140}^-(4x) - \frac{4}{9} e_{64}^-(\tfrac{9x}{5}), \\ \tilde{V}_{2,2}(x) &:= 0,\end{aligned}$$

and

$$\mathcal{J}_0 := \left[0, \frac{88}{100}\right], \qquad \mathcal{J}_1 := \left[\frac{88}{100}, \frac{95}{100}\right], \qquad \mathcal{J}_2 := \left[\frac{95}{100}, 1\right].$$

Lemma 6.2. *The approximations $\tilde{V}_{2,0}$, $\tilde{V}_{2,1}$ and $\tilde{V}_{2,2}$ satisfy the following estimates:*

$$\begin{aligned}
\|(\psi')^2(V_2 - \tilde{V}_{2,0}) \circ \psi\|_{L^\infty(\mathcal{J}_0)} &< 2 \cdot 10^{-5}, \\
\|(\psi')^2(V_2 - \tilde{V}_{2,1}) \circ \psi\|_{L^\infty(\mathcal{J}_1)} &< 10^{-3}, \\
\|(\psi')^2(V_2 - \tilde{V}_{2,2}) \circ \psi\|_{L^\infty(\mathcal{J}_2)} &< 5 \cdot 10^{-4}.
\end{aligned}$$

Proof. From the proof of Lemma 5.9 it is obvious that the estimates for $\|(\psi')^2(V_1 - \tilde{V}_{1,j}) \circ \psi\|_{L^\infty(\mathcal{J}_j)}$ are upper bounds for $\|(\psi')^2(V_2 - \tilde{V}_{2,j}) \circ \psi\|_{L^\infty(\mathcal{J}_j)}$. □

Further estimates for $\tilde{Q}_{3,i}$

Definition 6.3. (Decomposition of $\tilde{Q}_{3,0}^{(k)}$ into monotonous, non-negative components)
We define

$$\begin{aligned}
(t)^+(x_1, x_2) &:= 2(1 + e_{56}^-(4x_2))^{-1} - 1, \\
(t')^+(x_1, x_2) &:= 8e_{55}^-(4x_1)(1 + e_{56}^-(4x_2))^{-2}, \\
(t'')^+(x_1, x_2) &:= 64e_{55}^-(4x_1)^2(1 + e_{56}^-(4x_2))^{-3}, \\
(t'')^-(x_1, x_2) &:= 32e_{54}^-(4x_1)(1 + e_{56}^-(4x_2))^{-2}
\end{aligned}$$

such that

$$(t^{(k)})^\pm \geq 0, \qquad (t^{(k)})^\pm(x_2, x_1) \leq (t^{(k)})^\pm(x, x) \leq (t^{(k)})^\pm(x_1, x_2)$$

and

$$t(x) = (t)^+(x, x), \qquad t'(x) = (t')^+(x, x), \qquad t''(x) = (t'')^+(x, x) - (t'')^-(x, x)$$

for all $x_1 \le x \le x_2$ in $\psi(\mathcal{I}_0)$,

$$(T)^+(x_1,x_2) := \frac{5}{8} + \frac{3x_2^2}{2}(t)^+(x_1,x_2)^2,$$

$$(T)^-(x_1,x_2) := 2x_2\ (t)^+(x_1,x_2) + x_2^2,$$

$$(T')^+(x_1,x_2) := 3x_2\ (t)^+(x_1,x_2)^2 + 3x_2^2\ (t)^+(x_1,x_2)(t')^+(x_1,x_2),$$

$$(T')^-(x_1,x_2) := 2(t)^+(x_1,x_2) + 2x_2\ (t')^+(x_1,x_2) + 2x_2,$$

$$\begin{aligned}(T'')^+(x_1,x_2) := {}& 3(t)^+(x_1,x_2)^2 + 12x_2\ (t)^+(x_1,x_2)(t')^+(x_1,x_2)\\ &+ 3x_2^2(t)^+(x_1,x_2)\ (t'')^+(x_1,x_2) + 3x_2^2\ (t')^+(x_1,x_2)^2 + 2x_2\ (t'')^-(x_1,x_2),\end{aligned}$$

$$(T'')^-(x_1,x_2) := 3x_2^2(t)^+(x_1,x_2)(t'')^-(x_1,x_2) + 4(t')^+(x_1,x_2) + 2x_2(t'')^+(x_1,x_2) + 2$$

such that

$$(T^{(k)})^\pm \ge 0, \qquad (T^{(k)})^\pm(x_2,x_1) \le (T^{(k)})^\pm(x,x) \le (T^{(k)})^\pm(x_1,x_2)$$

and

$$(T^{(k)})(x) = (T^{(k)})^+(x,x) - (T^{(k)})^-(x,x)$$

for all $x_1 \le x \le x_2$ in $\psi(\mathcal{I}_0)$, and

$$(\tilde{Q}_{3,0})^+(x_1,x_2) := (\tilde{Q}_0)^+(x_1,x_2)\ (T)^+(x_1,x_2),$$

$$(\tilde{Q}_{3,0})^-(x_1,x_2) := (\tilde{Q}_0)^+(x_1,x_2)\ (T)^-(x_1,x_2),$$

$$(\tilde{Q}'_{3,0})^+(x_1,x_2) := (\tilde{Q}'_0)^+(x_1,x_2)\ (T)^+(x_1,x_2) + (\tilde{Q}'_0)^-(x_1,x_2)\ (T)^-(x_1,x_2) + (\tilde{Q}_0)^+(x_1,x_2)\ (T')^+(x_1,x_2),$$

$$(\tilde{Q}'_{3,0})^-(x_1,x_2) := (\tilde{Q}'_0)^-(x_1,x_2)\ (T)^+(x_1,x_2) + (\tilde{Q}'_0)^+(x_1,x_2)\ (T)^-(x_1,x_2) + (\tilde{Q}_0)^+(x_1,x_2)\ (T')^-(x_1,x_2) \quad ,$$

$$\begin{aligned}(\tilde{Q}''_{3,0})^+(x_1,x_2) := {}& (\tilde{Q}''_0)^+(x_1,x_2)(T)^+(x_1,x_2) + (\tilde{Q}''_0)^-(x_1,x_2)(T)^-(x_1,x_2) + (\tilde{Q}_0)^+(x_1,x_2)(T'')^+(x_1,x_2)\\ &+ 2(\tilde{Q}'_0)^+(x_1,x_2)(T')^+(x_1,x_2) + 2(\tilde{Q}'_0)^-(x_1,x_2)(T')^-(x_1,x_2),\end{aligned}$$

$$\begin{aligned}(\tilde{Q}''_{3,0})^-(x_1,x_2) := {}& (\tilde{Q}''_0)^-(x_1,x_2)(T)^+(x_1,x_2) + (\tilde{Q}''_0)^+(x_1,x_2)(T)^-(x_1,x_2) + (\tilde{Q}_0)^+(x_1,x_2)(T'')^-(x_1,x_2)\\ &+ 2(\tilde{Q}'_0)^-(x_1,x_2)(T')^+(x_1,x_2) + 2(\tilde{Q}'_0)^+(x_1,x_2)(T')^-(x_1,x_2)\end{aligned}$$

with $(\tilde{Q}_0^{(k)})^\pm$ as in (5.11), such that

$$(\tilde{Q}_{3,0}^{(k)})^\pm \ge 0, \qquad (\tilde{Q}_{3,0}^{(k)})^\pm(x_2,x_1) \le (\tilde{Q}_{3,0}^{(k)})^\pm(x,x) \le (\tilde{Q}_{3,0}^{(k)})^-(x_1,x_2)$$

and

$$\tilde{Q}_{3,0}^{(k)}(x) = \frac{C}{C_+}(1+e_{56}^-(4x))^{-1/2}\Big((\tilde{Q}_{3,0}^{(k)})^+(x,x) - (\tilde{Q}_{3,0}^{(k)})^-(x,x)\Big)$$

for all $x_1 \le x \le x_2$ *in* $\psi(\mathcal{I}_0)$ *and* $0 \le k \le 2$.

Lemma 6.4. *Let* $F(y) = (F_0(y), F_1(y), F_2(y))$ *with non-negative, increasing functions* F_0, F_1, F_2 *and* $y \in [y_1, y_2] \subseteq \mathcal{I}_0$. *Then*

$$\begin{aligned}
&\big|F_0(y)\tilde{Q}_{3,0}(\psi(y)) + F_1(y)\tilde{Q}'_{3,0}(\psi(y)) + F_2(y)\tilde{Q}''_{3,0}(\psi(y))\big| \\
\le &\max\Bigg\{\Big|F_0(y_2)(\tilde{Q}_{3,0})^+(\psi(y_1),\psi(y_2)) + F_1(y_2)(\tilde{Q}'_{3,0})^+(\psi(y_1),\psi(y_2)) + F_2(y_2)(\tilde{Q}''_{3,0})^+(\psi(y_1),\psi(y_2)) \\
&\quad - F_0(y_1)(\tilde{Q}_{3,0})^+(\psi(y_2),\psi(y_1)) - F_1(y_1)(\tilde{Q}'_{3,0})^-(\psi(y_2),\psi(y_1)) - F_2(y_1)(\tilde{Q}''_{3,0})^-(\psi(y_2),\psi(y_1))\Big|, \\
&\quad \Big|F_0(y_1)(\tilde{Q}_{3,0})^+(\psi(y_2),\psi(y_1)) + F_1(y_1)(\tilde{Q}'_{3,0})^+(\psi(y_2),\psi(y_1)) + F_2(y_1)(\tilde{Q}''_{3,0})^+(\psi(y_2),\psi(y_1)) \\
&\quad - F_0(y_2)(\tilde{Q}_{3,0})^+(\psi(y_1),\psi(y_2)) - F_1(y_2)(\tilde{Q}'_{3,0})^-(\psi(y_1),\psi(y_2)) - F_2(y_2)(\tilde{Q}''_{3,0})^-(\psi(y_1),\psi(y_2))\Big|\Bigg\} \\
=: &\, F_{dom,\tilde{Q}_{3,0}}(y_1,y_2).
\end{aligned}$$

In particular

$$\|F_0(\tilde{Q}_{3,0}\circ\psi) + F_1(\tilde{Q}'_{3,0}\circ\psi) + F_2(\tilde{Q}''_{3,0}\circ\psi)\|_{L^\infty([a,b])} \le \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{Q}_{3,0}}\left(a + i\cdot\frac{b-a}{N}, a + (i+1)\cdot\frac{b-a}{N}\right)\right\}$$

for all $[a,b] \subseteq \mathcal{I}_0$, $N > 1$.

Proof. Analogous to the proof of Lemma 5.12. □

Definition 6.5. (Decomposition of $\tilde{Q}_{3,1}^{(k)}$ into monotonous, non-negative components)
We define

$$\begin{aligned}
(\tilde{Q}_{3,1})^+(x_1,x_2) &:= C_+ e_{118}^-(x_1)\left(\tfrac{5}{8} + \tfrac{1}{2}x_2^2\right), \\
(\tilde{Q}_{3,1})^-(x_1,x_2) &:= 2C_+ x_2 e_{118}^-(x_1), \\
(\tilde{Q}'_{3,1})^+(x_1,x_2) &:= C_+ x_2\left(e_{118}^-(x_1) + 2e_{117}^-(x_1)\right), \\
(\tilde{Q}'_{3,1})^-(x_1,x_2) &:= C_+\big(2e_{118}^-(x_1) + e_{117}^-(x_1)\left(\tfrac{1}{2}x_2^2 + \tfrac{5}{8}\right)\big), \\
(\tilde{Q}''_{3,1})^+(x_1,x_2) &:= C_+\big(e_{116}^-(x_1)\left(\tfrac{5}{8} + \tfrac{1}{2}x_2^2\right) + 4e_{117}^-(x_1) + e_{118}^-(x_1)\big), \\
(\tilde{Q}''_{3,1})^-(x_1,x_2) &:= 2C_+ x_2\left(e_{116}^-(x_1) + e_{117}^-(x_1)\right)
\end{aligned}$$

such that

$$(\tilde{Q}_{3,1}^{(k)})^{\pm} \geq 0, \qquad (\tilde{Q}_{3,1}^{(k)})^{\pm}(x_2, x_1) \leq (\tilde{Q}_{3,1}^{(k)})^{\pm}(x, x) \leq (\tilde{Q}_{3,1}^{(k)})^{\pm}(x_1, x_2)$$

and

$$\begin{aligned}
\tilde{Q}_{3,1}(x) &= \frac{C}{C_+}\Big((\tilde{Q}_{3,1})^+(x,x) - (\tilde{Q}_{3,1})^-(x,x)\Big),\\
\tilde{Q}'_{3,1}(x) &= \frac{C}{C_+}\Big((\tilde{Q}'_{3,1})^+(x,x) - (\tilde{Q}'_{3,1})^-(x,x)\Big),\\
\tilde{Q}''_{3,1}(x) &= \frac{C}{C_+}\Big((\tilde{Q}''_{3,1})^+(x,x) - (\tilde{Q}''_{3,1})^-(x,x)\Big)
\end{aligned}$$

for all $x_1 \leq x \leq x_2$ in $\psi(\mathcal{I}_1)$.

Lemma 6.6. *Let $F(y) = (F_0(y), F_1(y), F_2(y))$ with non-negative, increasing functions F_0, F_1, F_2 and $y \in [y_1, y_2] \subseteq \mathcal{I}_1$. Then*

$$\begin{aligned}
&\big|F_0(y)\tilde{Q}_{3,1}(\psi(y)) + F_1(y)\tilde{Q}'_{3,1}(\psi(y)) + F_2(y)\tilde{Q}''_{3,1}(\psi(y))\big|\\
\leq &\max\Bigg\{\Big|F_0(y_2)(\tilde{Q}_{3,1})^+(\psi(y_1),\psi(y_2)) + F_1(y_2)(\tilde{Q}'_{3,1})^+(\psi(y_1),\psi(y_2)) + F_2(y_2)(\tilde{Q}''_{3,1})^+(\psi(y_1),\psi(y_2))\\
&\qquad - F_0(y_1)(\tilde{Q}_{3,1})^-(\psi(y_2),\psi(y_1)) - F_1(y_1)(\tilde{Q}'_{3,1})^-(\psi(y_2),\psi(y_1)) - F_2(y_1)(\tilde{Q}''_{3,1})^-(\psi(y_2),\psi(y_1))\Big|,\\
&\qquad \Big|F_0(y_1)(\tilde{Q}_{3,1})^+(\psi(y_2),\psi(y_1)) + F_1(y_1)(\tilde{Q}'_{3,1})^+(\psi(y_2),\psi(y_1)) + F_2(y_1)(\tilde{Q}''_{3,1})^+(\psi(y_2),\psi(y_1))\\
&\qquad - F_0(y_1)(\tilde{Q}_{3,1})^-(\psi(y_1),\psi(y_2)) - F_1(y_2)(\tilde{Q}'_{3,1})^-(\psi(y_1),\psi(y_2)) - F_2(y_2)(\tilde{Q}''_{3,1})^-(\psi(y_1),\psi(y_2))\Big|\Bigg\}\\
=: &\, F_{dom,\tilde{Q}_{3,1}}(y_1, y_2).
\end{aligned}$$

In particular

$$\|F_0(\tilde{Q}_{3,1}\circ\psi) + F_1(\tilde{Q}'_{3,1}\circ\psi) + F_2(\tilde{Q}''_{3,1}\circ\psi)\|_{L^\infty([a,b])} \leq \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{Q}_{3,1}}\left(a + i\cdot\frac{b-a}{N}, a + (i+1)\cdot\frac{b-a}{N}\right)\right\}$$

for all $[a,b] \subseteq \mathcal{I}_1$, $N > 1$.

Definition 6.7. (Estimates for $\tilde{Q}_{3,0}$, $\tilde{Q}'_{3,0}$ and $\tilde{Q}_{3,1}$, $\tilde{Q}'_{3,1}$ in rational expressions)
We define

$$\begin{aligned}
\tilde{Q}_{3,0,+}(x) &:= \tilde{Q}_{0,+}(x)T(x),\\
\tilde{Q}'_{3,0,+}(x) &:= \tilde{Q}_{0,+}(x)T'(x) + \tilde{Q}'_{0,+}(x)T(x),\\
\tilde{Q}_{3,0,-}(x) &:= \tilde{Q}_{0,-}(x)T(x),\\
\tilde{Q}'_{3,0,-}(x) &:= \tilde{Q}_{0,-}(x)T'(x) + \tilde{Q}'_{0,-}(x)T(x),
\end{aligned}$$

and

$$\begin{aligned}
\tilde{Q}_{3,1,\pm}(x) &:= C^{\pm}e^{-}_{118}(x)\left(\tfrac{5}{8} + \tfrac{x^2}{2} - 2x\right),\\
\tilde{Q}'_{3,1,\pm}(x) &:= C^{\pm}\big(e^{-}_{118}(x)\,(x-2) - e^{-}_{117}(x)\left(\tfrac{5}{8} + \tfrac{x^2}{2} - 2x\right)\big)
\end{aligned}$$

with $\tilde{Q}_{0,+}$, $\tilde{Q}'_{0,+}$ as in Definition 5.14, such that

$$\left|\tilde{Q}_{3,i,-}\right| \le \left|\tilde{Q}_{3,i}\right| \le \left|\tilde{Q}_{3,i,+}\right|, \qquad \left|\tilde{Q}'_{3,i,-}\right| \le \left|\tilde{Q}'_{3,i}\right| \le \left|\tilde{Q}'_{3,i,+}\right|.$$

Lemma 6.8. *The functions $(\tilde{Q}_{3,i}\circ\psi)(\psi')^2$ obey the following bounds:*

$$\left\|\big((\psi')^2(\tilde{Q}_{3,0}\circ\psi)\big)''\right\|_{L^\infty(\mathcal{I}_0)} < 183000, \qquad \left\|\big((\psi')^2(\tilde{Q}_{3,1}\circ\psi)\big)''\right\|_{L^\infty(\mathcal{I}_1)} < 615000.$$

Proof. Applying Lemma 6.4 on $\mathcal{I}_0$ with $N = 8800$ and Lemma 6.6 on $\mathcal{I}_1$ with $N = 10500$ for $F = (F_{2,0}, F_{2,1}, F_{2,2})$ as in Definition 5.16 gives the claimed bounds. □

Lemma 6.9. *The functions $\psi'\cdot(\tilde{Q}_{3,i}\circ\psi)$ obey the following bounds:*

$$\|\psi'(\tilde{Q}_{3,0}\circ\psi)\|_{L^\infty(\mathcal{I}_0)} < \frac{39}{10}, \qquad \left\|\big(\psi'(\tilde{Q}_{3,0}\circ\psi)\big)'\right\|_{L^\infty(\mathcal{I}_0)} < 81, \qquad \left\|\big(\psi'(\tilde{Q}_{3,0}\circ\psi)\big)''\right\|_{L^\infty(\mathcal{I}_0)} < 1800$$

and

$$\|\psi'(\tilde{Q}_{3,1}\circ\psi)\|_{L^\infty(\mathcal{I}_1)} < \frac{26}{10}, \qquad \left\|\big(\psi'(\tilde{Q}_{3,1}\circ\psi)\big)'\right\|_{L^\infty(\mathcal{I}_1)} < 85, \qquad \left\|\big(\psi'(\tilde{Q}_{3,1}\circ\psi)\big)''\right\|_{L^\infty(\mathcal{I}_1)} < 6000.$$

Proof. Applying Lemma 6.4 on $\mathcal{I}_0$ with $N = 8800$ and Lemma 6.6 on $\mathcal{I}_1$ with $N = 1050$ for $F = (G_{2,0}, G_{2,1}, G_{2,2})$

as defined in (5.17) gives

$$\left\|\left(\psi'(\tilde{Q}_{3,0}\circ\psi)\right)''\right\|_{L^\infty(\mathcal{I}_0)}<1800,\qquad \left\|\left(\psi'(\tilde{Q}_{3,1}\circ\psi)\right)''\right\|_{L^\infty(\mathcal{I}_1)}<6000.$$

From

$$\begin{aligned}\left|\frac{d}{dy}\left(\psi'(y)\tilde{Q}_{3,i}(\psi(y))\right)\right|&\le\left|\psi''(y)\tilde{Q}_{3,i,+}(\psi(y))+\psi'(y)^2\tilde{Q}'_{3,i,+}(\psi(y))\right|,\\ \left|\psi'(y)\tilde{Q}_{3,i}(\psi(y))\right|&\le\left|\psi'(y)\tilde{Q}_{3,i,+}(\psi(y))\right|\end{aligned}$$

and Lemma 5.6 on $\mathcal{I}_0$ with $N=880$ we infer

$$\begin{aligned}\left|\frac{d}{dy}\left(\psi'(y)\tilde{Q}_{3,0}(\psi(y))\right)\right|&\le 77+\frac{1800}{1000}<81,\\ \left|\psi'(y)\tilde{Q}_{3,0}(\psi(y))\right|&\le\frac{38}{10}+\frac{81}{1000}<\frac{39}{10}\end{aligned}$$

for all $y\in\mathcal{I}_0$ and on $\mathcal{I}_1$ with $N=105$

$$\begin{aligned}\left|\frac{d}{dy}\left(\psi'(y)\tilde{Q}_{3,1}(\psi(y))\right)\right|&\le 79+\frac{6000}{1000}=85,\\ \left|\psi'(y)\tilde{Q}_{3,1}(\psi(y))\right|&\le\frac{25}{10}+\frac{85}{1000}<\frac{26}{10}\end{aligned}$$

for all $y\in\mathcal{I}_1$. □

Lemma 6.10. *The functions $(\tilde{Q}_{3,i}\circ\psi)$ obey the following bounds:*

$$\|\tilde{Q}_{3,0}\circ\psi\|_{L^\infty(\mathcal{I}_0)}<\frac{84}{100},\qquad \left\|\left(\tilde{Q}_{3,0}\circ\psi\right)'\right\|_{L^\infty(\mathcal{I}_0)}<\frac{43}{10},\qquad \left\|\left(\tilde{Q}_{3,0}\circ\psi\right)''\right\|_{L^\infty(\mathcal{I}_0)}<100$$

and

$$\|\tilde{Q}_{3,1}\circ\psi\|_{L^\infty(\mathcal{I}_1)}<\frac{43}{1000},\qquad \left\|\left(\tilde{Q}_{3,1}\circ\psi\right)'\right\|_{L^\infty(\mathcal{I}_1)}<\frac{21}{10},\qquad \left\|\left(\tilde{Q}_{3,1}\circ\psi\right)''\right\|_{L^\infty(\mathcal{I}_1)}<92.$$

Proof. Applying Lemma 6.4 on $\mathcal{I}_0$ with $N=8800$ and Lemma 6.6 on $\mathcal{I}_1$ with $N=1050$ for $F=(0,\psi'',(\psi')^2)$ gives

$$\left\|\left(\tilde{Q}_{3,0}\circ\psi\right)''\right\|_{L^\infty(\mathcal{I}_0)}<100,\qquad \left\|\left(\tilde{Q}_{3,1}\circ\psi\right)''\right\|_{L^\infty(\mathcal{I}_1)}<92.$$

From

$$\left|\frac{d}{dy}\tilde{Q}_{3,i}(\psi(y))\right| \leq \left|\psi'(y)\tilde{Q}'_{3,i,+}(\psi(y))\right|,$$
$$\left|\tilde{Q}_{3,i}(\psi(y))\right| \leq \left|\tilde{Q}_{3,i,+}(\psi(y))\right|$$

and Lemma 5.6 on $\mathcal{I}_0$ with $N = 880$ we conclude

$$\left|\frac{d}{dy}\tilde{Q}_{3,0}(\psi(y))\right| \leq \frac{42}{10} + \frac{100}{1000} < \frac{43}{10},$$
$$\left|\tilde{Q}_{3,0}(\psi(y))\right| \leq \frac{83}{100} + \frac{43}{10000} < \frac{84}{100}$$

for all $y \in \mathcal{I}_0$ and on $\mathcal{I}_1$ with $N = 105$

$$\left|\frac{d}{dy}\tilde{Q}_{3,1}(\psi(y))\right| \leq 2 + \frac{92}{1000} < \frac{21}{10},$$
$$\left|\tilde{Q}_{3,1}(\psi(y))\right| \leq \frac{4}{100} + \frac{21}{10000} < \frac{43}{1000}$$

for all $y \in \mathcal{I}_1$.

□

Further estimates for $\tilde{V}_{2,j}$

Definition 6.11. (Decomposition of $\tilde{V}_{2,0}^{(k)}$ into monotonous, non-negative components)
We define

$$
\begin{aligned}
(\tilde{V}_{2,0})^-(x_1,x_2) :=& \frac{80}{3} x_2 e_{60}^-(4x_1)(1-e_{60}(4x_2))(1+e_{60}^-(4x_2))^{-3} + \frac{4}{9} e_{30}^-(\tfrac{9x_1}{5})(1+e_{30}^-(\tfrac{9x_2}{5}))^{-2},\\
(\tilde{V}'_{2,0})^+(x_1,x_2) :=& \frac{80}{3} 4x_2 \left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)\left(e_{60}^-(4x_1)^2+1\right) + \frac{4}{5}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-3} e_{29}^-(\tfrac{9x_1}{5}),\\
(\tilde{V}'_{2,0})^-(x_1,x_2) :=& \frac{80}{3}\Bigg(16x_2\left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)e_{60}^-(4x_1) + e_{60}^-(4x_1)\left(1-e_{60}^-(4x_2)\right)\left(1+e_{60}^-(4x_2)\right)^{-3}\Bigg)\\
&+ \frac{4}{5}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-3} e_{29}^-(\tfrac{9x_1}{5})e_{30}^-(\tfrac{9x_1}{5}),\\
(\tilde{V}''_{2,0})^+(x_1,x_2) :=& \frac{80}{3}\Bigg(32x_2\left(1+e_{60}^-(4x_2)\right)^{-5}\left[2\left(e_{60}^-(4x_1)+1\right)e_{58}^-(4x_1)e_{60}^-(4x_1) + e_{59}^-(4x_1)^2\left(e_{60}^-(4x_1)^2+4\right)\right]\\
&\quad + 8\left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)\left(e_{60}^-(4x_1)^2+1\right)\Bigg)\\
&+ \frac{36}{25}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-4}\left(e_{30}^-(\tfrac{9x_1}{5})^2 e_{28}^-(\tfrac{9x_1}{5}) + 4e_{29}^-(\tfrac{9x_1}{5})^2\right),\\
(\tilde{V}''_{2,0})^-(x_1,x_2) :=& \frac{80}{3}\Bigg(16x_2\left(1+e_{60}^-(4x_2)\right)^{-5}\left[\left(e_{60}^-(4x_1)+1\right)\left(e_{60}^-(4x_1)^2+1\right)e_{58}^-(4x_1) + 14e_{59}^-(4x_1)^2 e_{60}^-(4x_1)\right]\\
&\quad + 32\left(1+e_{60}^-(4x_2)\right)^{-4} e_{59}^-(4x_1)e_{60}^-(4x_1)\Bigg)\\
&+ \frac{36}{25}\left(1+e_{30}^-(\tfrac{9x_2}{5})\right)^{-4}\left(e_{28}^-(\tfrac{9x_1}{5}) + 2e_{30}^-(\tfrac{9x_1}{5})e_{29}^-(\tfrac{9x_1}{5})^2\right)
\end{aligned}
$$

such that

$$(\tilde{V}_{2,0})^-,\ (\tilde{V}'_{2,0})^\pm,\ (\tilde{V}''_{2,0})^\pm \geq 0,$$

$$
\begin{aligned}
(\tilde{V}_{2,0})^-(x_2,x_1) \leq (\tilde{V}_{2,0})^-(x,x) \leq (\tilde{V}_{2,0})^-(x_1,x_2),\\
(\tilde{V}'_{2,0})^\pm(x_2,x_1) \leq (\tilde{V}'_{2,0})^\pm(x,x) \leq (\tilde{V}'_{2,0})^\pm(x_1,x_2),\\
(\tilde{V}''_{2,0})^\pm(x_2,x_1) \leq (\tilde{V}''_{2,0})^\pm(x,x) \leq (\tilde{V}''_{2,0})^\pm(x_1,x_2)
\end{aligned}
$$

and

$$\tilde{V}_{2,0}(x) = -(\tilde{V}_{2,0})^-(x,x), \qquad \tilde{V}'_{2,0}(x) = (\tilde{V}'_{2,0})^+(x,x) - (\tilde{V}'_{2,0})^-(x,x), \qquad \tilde{V}''_{2,0}(x) = (\tilde{V}''_{2,0})^+(x,x) - (\tilde{V}''_{2,0})^-(x,x)$$

for all $x_1 \leq x \leq x_2$ in $\psi(\mathcal{J}_0)$.

Lemma 6.12. *Let $F(y) = (F_0(y), F_1(y), F_2(y))$ with non-negative, increasing functions F_0, F_1, F_2 and $y \in [y_1, y_2] \subseteq \mathcal{J}_0$. Then*

$$\begin{aligned}
&\left|F_0(y)\tilde{V}_{2,0}(\psi(y)) + F_1(y)\tilde{V}'_{2,0}(\psi(y)) + F_2(y)\tilde{V}''_{2,0}(\psi(y))\right| \\
\leq &\max\Bigg\{\Bigg|F_1(y_2)(\tilde{V}'_{2,0})^+(\psi(y_1),\psi(y_2)) + F_2(y_2)(\tilde{V}''_{2,0})^+(\psi(y_1),\psi(y_2)) \\
&\quad - F_0(y_1)(\tilde{V}_{2,0})^-(\psi(y_2),\psi(y_1)) - F_1(y_1)(\tilde{V}'_{2,0})^-(\psi(y_2),\psi(y_1)) - F_2(y_1)(\tilde{V}''_{2,0})^-(\psi(y_2),\psi(y_1))\Bigg|, \\
&\quad \Bigg|F_1(y_1)(\tilde{V}'_{2,0})^+(\psi(y_2),\psi(y_1)) + F_2(y_1)(\tilde{V}''_{2,0})^+(\psi(y_2),\psi(y_1)) \\
&\quad - F_0(y_2)(\tilde{V}_{2,0})^-(\psi(y_1),\psi(y_2)) - F_1(y_2)(\tilde{V}'_{2,0})^-(\psi(y_1),\psi(y_2)) - F_2(y_2)(\tilde{V}''_{2,0})^-(\psi(y_1),\psi(y_2))\Bigg|\Bigg\} \\
=: &\, F_{dom,\tilde{V}_{2,0}}(y_1, y_2).
\end{aligned}$$

In particular

$$\|F_0(\tilde{V}_{2,0}\circ\psi) + F_1(\tilde{V}'_{2,0}\circ\psi) + F_2(\tilde{V}''_{2,0}\circ\psi)\|_{L^\infty([a,b])} \leq \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{V}_{2,0}}\left(a + i\cdot\frac{b-a}{N}, a + (i+1)\cdot\frac{b-a}{N}\right)\right\}$$

for all $[a,b] \subseteq \mathcal{J}_0$, $N > 1$.

Definition 6.13. (Decomposition of $\tilde{V}^{(k)}_{2,1}$ into monotonous, non-negative components)
We define

$$\begin{aligned}
(\tilde{V}_{2,1})^-(x_1,x_2) :=& \frac{80}{3}x_2 e^-_{140}(4x_1) + \frac{4}{9}e^-_{64}(\tfrac{9x_1}{5}), \\
(\tilde{V}'_{2,1})^+(x_1,x_2) :=& \frac{320}{3}x_2 e^-_{139}(4x_1) + \frac{4}{5}e^-_{63}(\tfrac{9x_1}{5}), \\
(\tilde{V}'_{2,1})^-(x_1,x_2) :=& \frac{80}{3}e^-_{140}(4x_1), \\
(\tilde{V}''_{2,1})^+(x_1,x_2) :=& \frac{640}{3}e^-_{139}(4x_1), \\
(\tilde{V}''_{2,1})^-(x_1,x_2) :=& \frac{1280}{3}x_2 e^-_{138}(4x_1) + \frac{36}{25}e^-_{62}(\tfrac{9x_1}{5})
\end{aligned}$$

such that

$$(\tilde{V}_{2,1})^-,\ (\tilde{V}'_{2,1})^\pm,\ (\tilde{V}''_{2,1})^\pm \geq 0,$$

$$
\begin{aligned}
(\tilde{V}_{2,1})^-(x_2,x_1) &\le (\tilde{V}_{2,1})^-(x,x) \le (\tilde{V}_{2,1})^-(x_1,x_2),\\
(\tilde{V}'_{2,1})^\pm(x_2,x_1) &\le (\tilde{V}'_{2,1})^\pm(x,x) \le (\tilde{V}'_{2,1})^\pm(x_1,x_2),\\
(\tilde{V}''_{2,1})^\pm(x_2,x_1) &\le (\tilde{V}''_{2,1})^\pm(x,x) \le (\tilde{V}''_{2,1})^\pm(x_1,x_2)
\end{aligned}
$$

and

$$
\tilde{V}_{2,1}(x) = -(\tilde{V}_{2,1})^-(x,x), \qquad \tilde{V}'_{2,1}(x) = (\tilde{V}'_{2,1})^+(x,x) - (\tilde{V}'_{2,1})^-(x,x), \qquad \tilde{V}''_{2,1}(x) = (\tilde{V}''_{2,1})^+(x,x) - (\tilde{V}''_{2,1})^-(x,x)
$$

for all $x_1 \le x \le x_2$ in $\psi(\mathcal{J}_1)$.

Lemma 6.14. *Let $F(y) = (F_0(y), F_1(y), F_2(y))$ with non-negative, increasing functions F_0, F_1, F_2 and $y \in [y_1, y_2] \subseteq \mathcal{J}_1$. Then*

$$
\begin{aligned}
&\left|F_0(y)\tilde{V}_{2,1}(\psi(y)) + F_1(y)\tilde{V}'_{2,1}(\psi(y)) + F_2(y)\tilde{V}''_{2,1}(\psi(y))\right|\\
\le &\max\Bigg\{\Bigg|F_1(y_2)(\tilde{V}'_{2,1})^+(\psi(y_1),\psi(y_2)) + F_2(y_2)(\tilde{V}''_{2,1})^+(\psi(y_1),\psi(y_2))\\
&\qquad - F_0(y_1)(\tilde{V}_{2,1})^-(\psi(y_2),\psi(y_1)) - F_1(y_1)(\tilde{V}'_{2,1})^-(\psi(y_2),\psi(y_1)) - F_2(y_1)(\tilde{V}''_{2,1})^-(\psi(y_2),\psi(y_1))\Bigg|,\\
&\qquad \Bigg|F_1(y_1)(\tilde{V}'_{2,1})^+(\psi(y_2),\psi(y_1)) + F_2(y_1)(\tilde{V}''_{2,1})^+(\psi(y_2),\psi(y_1))\\
&\qquad - F_0(y_2)(\tilde{V}_{2,1})^-(\psi(y_1),\psi(y_2)) - F_1(y_2)(\tilde{V}'_{2,1})^-(\psi(y_1),\psi(y_2)) - F_2(y_2)(\tilde{V}''_{2,1})^-(\psi(y_1),\psi(y_2))\Bigg|\Bigg\}\\
=: &\, F_{dom,\tilde{V}_{2,1}}(y_1,y_2).
\end{aligned}
$$

In particular

$$
\|F_0(\tilde{V}_{2,1}\circ\psi) + F_1(\tilde{V}'_{2,1}\circ\psi) + F_2(\tilde{V}''_{2,1}\circ\psi)\|_{L^\infty([a,b])} \le \max_{i=0,\dots,N-1}\left\{F_{dom,\tilde{V}_{2,1}}\left(a + i\cdot\frac{b-a}{N}, a + (i+1)\cdot\frac{b-a}{N}\right)\right\}
$$

for all $[a,b] \subseteq \mathcal{J}_1$, $N > 1$.

Lemma 6.15. *The functions $(\psi')^2(\tilde{V}_{2,j}\circ\psi)$ obey the following bounds:*

$$
\|(\psi')^2(\tilde{V}_{2,0}\circ\psi)\|_{L^\infty(\mathcal{J}_0)} < 7, \qquad \left\|\left((\psi')^2(\tilde{V}_{2,0}\circ\psi)\right)'\right\|_{L^\infty(\mathcal{J}_0)} < 40, \qquad \left\|\left((\psi')^2(\tilde{V}_{2,0}\circ\psi)\right)''\right\|_{L^\infty(\mathcal{J}_0)} < 760
$$

and

$$\|(\psi')^2(\tilde{V}_{2,1}\circ\psi)\|_{L^\infty(\mathcal{J}_1)} < \frac{6}{100}, \qquad \Big\|\big((\psi')^2(\tilde{V}_{2,1}\circ\psi)\big)'\Big\|_{L^\infty(\mathcal{J}_1)} < 17, \qquad \Big\|\big((\psi')^2(\tilde{V}_{2,1}\circ\psi)\big)''\Big\|_{L^\infty(\mathcal{J}_1)} < 670.$$

Proof. Applying Lemma 6.12 on $\mathcal{J}_0$ with $N = 880$ and Lemma 6.14 on $\mathcal{J}_1$ with $N = 70$ for $F = (F_{2,0}, F_{2,1}, F_{2,2})$ as defined in (5.16) gives

$$\Big\|\big((\psi')^2(\tilde{V}_{2,0}\circ\psi)\big)''\Big\|_{L^\infty(\mathcal{J}_0)} < 760, \qquad \Big\|\big((\psi')^2(\tilde{V}_{2,1}\circ\psi)\big)''\Big\|_{L^\infty(\mathcal{J}_1)} < 670.$$

From Lemma 5.6 on $\mathcal{J}_0$ with $N = 880$ we infer

$$\begin{aligned}\Big|\frac{d}{dy}\big(\psi'(y)^2\tilde{V}_{2,0}(\psi(y))\big)\Big| &= \big|2\psi'(y)\psi''(y)\tilde{V}_{2,0}(\psi(y)) + \psi'(y)^3\tilde{V}'_{2,0}(\psi(y))\big| \le 39 + \frac{760}{1000} < 40,\\ \big|\psi'(y)^2\tilde{V}_{2,0}(\psi(y))\big| &\le \frac{67}{10} + \frac{40}{1000} < 7,\end{aligned}$$

and on $\mathcal{J}_1$ with $N = 70$

$$\begin{aligned}\Big|\frac{d}{dy}\big(\psi'(y)^2\tilde{V}_{2,1}(\psi(y))\big)\Big| &= \big|2\psi'(y)\psi''(y)\tilde{V}_{2,1}(\psi(y)) + \psi'(y)^3\tilde{V}'_{2,1}(\psi(y))\big| \le \frac{1632}{100} + \frac{670}{1000} < 17,\\ \big|\psi'(y)^2\tilde{V}_{2,0}(\psi(y))\big| &\le \frac{51}{100} + \frac{17}{1000} < \frac{6}{100}.\end{aligned}$$

□

Lemma 6.16. *The functions $(\tilde{V}_{2,j}\circ\psi)$ obey the following bounds:*

$$\|\tilde{V}_{2,0}\circ\psi\|_{L^\infty(\mathcal{J}_0)} < \frac{12}{10}, \qquad \Big\|\big(\tilde{V}_{2,0}\circ\psi\big)'\Big\|_{L^\infty(\mathcal{J}_0)} < 5, \qquad \Big\|\big(\tilde{V}_{2,0}\circ\psi\big)''\Big\|_{L^\infty(\mathcal{J}_0)} < 42$$

and

$$\|\tilde{V}_{2,1}\circ\psi\|_{L^\infty(\mathcal{J}_1)} < 6\cdot 10^{-4}, \qquad \Big\|\big(\tilde{V}_{2,1}\circ\psi\big)'\Big\|_{L^\infty(\mathcal{J}_1)} < \frac{3}{100}, \qquad \Big\|\big(\tilde{V}_{2,1}\circ\psi\big)''\Big\|_{L^\infty(\mathcal{J}_1)} < \frac{16}{10}.$$

Moreover

$$\|V_2\circ\psi\|_{L^\infty(\mathcal{J}_0)} \le \frac{121}{100}, \qquad \|V_2\circ\psi\|_{L^\infty(\mathcal{J}_1)} \le 16\cdot 10^{-4}, \qquad \|V_2\circ\psi\|_{L^\infty(\mathcal{J}_2)} \le 5\cdot 10^{-4}$$

Proof. Applying Lemma 6.12 on $\mathcal{J}_0$ with $N = 880$ and Lemma 6.14 on $\mathcal{J}_1$ with $N = 70$ for $F = (0, \psi'', (\psi')^2)$ gives

$$\Big\|\big(\tilde{V}_{2,0}\circ\psi\big)''\Big\|_{L^\infty(\mathcal{J}_0)} < 42, \qquad \Big\|\big(\tilde{V}_{2,1}\circ\psi\big)''\Big\|_{L^\infty(\mathcal{J}_1)} < \frac{16}{10}.$$

From Lemma 5.6 on $\mathcal{J}_0$ with $N = 880$ we infer

$$\begin{aligned}\left|\frac{d}{dy}\big(\tilde{V}_{2,0}(\psi(y))\big)\right| &= \left|\psi'(y)\tilde{V}'_{2,0}(\psi(y))\right| \leq \frac{48}{10} + \frac{42}{1000} < 5,\\ \left|\tilde{V}_{2,0}(\psi(y))\right| &\leq \frac{116}{100} + \frac{5}{1000} < \frac{12}{10},\end{aligned}$$

and on $\mathcal{J}_1$ with $N = 70$

$$\begin{aligned}\left|\frac{d}{dy}\big(\psi'(y)\tilde{V}_{2,1}(\psi(y))\big)\right| &= \left|\psi'(y)\tilde{V}'_{2,1}(\psi(y))\right| \leq \frac{28}{1000} + 16\cdot 10^{-4} < \frac{3}{100},\\ \left|\tilde{V}_{2,0}(\psi(y))\right| &\leq 5\cdot 10^{-4} + 3\cdot 10^{-5} < 6\cdot 10^{-4}.\end{aligned}$$

Using the rough bounds

$$\begin{aligned}\|V_2\circ\psi\|_{L^\infty(\mathcal{J}_J)} &\leq \|\tilde{V}_{2,j}\circ\psi\|_{L^\infty(\mathcal{J}_J)} + \|\left(V_2 - \tilde{V}_{2,j}\right)\circ\psi\|_{L^\infty(\mathcal{J}_J)}\\ &\leq \|\tilde{V}_{2,j}\circ\psi\|_{L^\infty(\mathcal{J}_J)} + \|(\psi')^2\left(V_2 - \tilde{V}_{2,j}\right)\circ\psi\|_{L^\infty(I_i)},\end{aligned}$$

we obtain

$$\begin{aligned}\|V_2\circ\psi\|_{L^\infty(\mathcal{J}_0)} &\leq \frac{12}{10} + 2\cdot 10^{-5} < \frac{121}{100},\\ \|V_2\circ\psi\|_{L^\infty(\mathcal{J}_1)} &\leq 6\cdot 10^{-4} + 10^{-3} < 17\cdot 10^{-4},\\ \|V_2\circ\psi\|_{L^\infty(\mathcal{J}_2)} &\leq 5\cdot 10^{-4}.\end{aligned}$$

□

6.2 Smallness of $\mathcal{R}(g_2)$

Proposition 6.17. *The function g_2 satifies*

$$\|\mathcal{R}(g_2)\|_{L^\infty} < 86\cdot 10^{-4}$$

Proof. As in the proof of Proposition 5.24 we define

$$h(y) := \frac{2y(y^2+3)g_2'(y)}{1-y^2}$$

which is a polynomial of degree atmost 240, such that

$$\mathcal{R}(g_2)(y) = -g_2''(y) + \frac{h(y)}{1+y^2} + \psi'(y)^2 V_2(\psi(y))g_2(y) - \psi'(y)^2 Q_3(\psi(y))$$

and we set

$$\tilde{\mathcal{R}}(g_2)_{i,j}(y) = -g_2''(y) + \frac{h(y)}{1+y^2} + \psi'(y)^2 \tilde{V}_{2,j}(\psi(y)) g_2(y) - \psi'(y)^2 \tilde{Q}_{3,i}(\psi(y)),$$

such that $\tilde{\mathcal{R}}(g_2)_{i,j} \in C^\infty(\mathcal{I}_i \cap \mathcal{J}_j)$ and

$$\begin{aligned}\tilde{\mathcal{R}}(g_2)''_{i,j}(y) = &-g_2^{(4)}(y) + \frac{h''(y)}{1+y^2} + \frac{h(y)(6y^2-2)}{(1+y^2)^3} - \frac{h'(y)4y}{(1+y^2)^2} + \left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)''(y) g_2(y) \\ &+ \left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)(y) g_2''(y) + 2\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)'(y) g_2'(y) - \left((\psi')^2(\tilde{Q}_{3,i}\circ\psi)\right)''(y)\end{aligned}$$

with

$$\begin{aligned}\|\tilde{\mathcal{R}}(g_2)''_{i,j}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_j)} \le &\|g_2^{(4)}\|_{L^\infty}\| + \|h''\|_{L^\infty} + 4\|h\|_{L^\infty} + 4\|h'\|_{L^\infty} \\ &+ \| \left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)''\|_{L^\infty(\mathcal{J}_j)} \cdot \|g_2\|_{L^\infty} + \|(\psi')^2(\tilde{V}_{2,j}\circ\psi)\|_{L^\infty(\mathcal{J}_j)}\|g_2''\|_{L^\infty} \\ &+ 2\| \left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)'\|_{L^\infty(\mathcal{J}_j)} \cdot \|g_2'\|_{L^\infty} + \| \left((\psi')^2(\tilde{Q}_{3,i}\circ\psi)\right)''\|_{L^\infty(\mathcal{I}_i)}.\end{aligned}$$

Re-expanding h''' and $g_2^{(5)}$ in Chebychev polynomials we infer from Lemma 5.5

$$\|h'''\|_{L^\infty} < 77 \cdot 10^7, \qquad\qquad \|g_2^{(5)}\|_{L^\infty} < 77 \cdot 10^7$$

and from Lemma 5.6 on $[0,1]$ with $N = 10000$

$$\begin{aligned}\|h''\|_{L^\infty} &\le 335 \cdot 10^3 + 77 \cdot 10^3 \le 402 \cdot 10^3, \\ \|g_2^{(4)}\|_{L^\infty} &\le 448 \cdot 10^3 + 77 \cdot 10^3 \le 525 \cdot 10^3.\end{aligned}$$

From Lemma 5.6 on $[0,1]$ with $N = 1000$ we infer

$$\begin{aligned}\|g_2^{(3)}\|_{L^\infty} &\le 5900 + 402 = 6302, \\ \|g_2''\|_{L^\infty} &\le 129 + \frac{6302}{1000} < 136, \\ \|g_2'\|_{L^\infty} &\le 5 + \frac{136}{1000} < \frac{52}{10}, \\ \|g_2\|_{L^\infty} &\le \frac{911}{1000} + \frac{52}{10000} < \frac{92}{100},\end{aligned} \tag{6.6}$$

and

$$\begin{aligned}\|h'\|_{L^\infty} &\le 6110 + 402 < 6520, \\ \|h\|_{L^\infty} &\le 198 + \frac{6520}{1000} < 205,\end{aligned}$$

which gives

$$\begin{aligned}\|\tilde{\mathcal{R}}(g_2)''_{i,j}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_j)} &\le 525\cdot 10^3+402\cdot 10^3+4\cdot 205+4\cdot 6520+\|\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)''\|_{L^\infty(\mathcal{J}_j)}\cdot\frac{92}{100}\\ &+\|(\psi')^2(\tilde{V}_{2,j}\circ\psi)\|_{L^\infty(\mathcal{J}_j)}\cdot 136+2\|\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)'\|_{L^\infty(\mathcal{J}_j)}\cdot\frac{52}{10}\\ &+\|\left((\psi')^2(\tilde{Q}_{3,i}\circ\psi)\right)''\|_{L^\infty(\mathcal{I}_i)}\end{aligned}$$

and hence by Lemmas 6.15 and 6.8

$$\begin{aligned}\|\tilde{\mathcal{R}}(g_2)''_{0,0}\|_{L^\infty(\mathcal{I}_0\cap\mathcal{J}_0)} &\le 954\cdot 10^3+17\cdot\frac{92}{100}+7\cdot 136+2\cdot 40\cdot\frac{52}{10}+183000<114\cdot 10^4\\ \|\tilde{\mathcal{R}}(g_2)''_{1,1}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_1)} &\le 954\cdot 10^3+670\cdot\frac{92}{100}+\frac{6}{100}\cdot 136+2\cdot 760\cdot\frac{52}{10}+615000<158\cdot 10^4\\ \|\tilde{\mathcal{R}}(g_2)''_{1,2}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_2)} &\le 954\cdot 10^3+615000<157\cdot 10^4\\ \|\tilde{\mathcal{R}}(g_2)''_{2,2}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_1)} &\le 954\cdot 10^3.\end{aligned}$$

From

$$\begin{aligned}\left|\tilde{\mathcal{R}}(g_2)'_{i,j}(y)\right| \le \max\Bigg\{\Bigg| &-g_2^{(3)}(y)+\frac{h'(y)}{1+y^2}-\frac{2y}{(1+y^2)^2}h(y)+\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)'(y)g_2(y)\\ &+\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)(y)g_2'(y)-\left[2\psi'(y)\psi''(y)\tilde{Q}_{3,i,+}(\psi(y))+\psi'(y)^3\tilde{Q}'_{3,i,+}(\psi(y))\right]\Bigg|,\\ \Bigg| &-g_2^{(3)}(y)+\frac{h'(y)}{1+y^2}-\frac{2y}{(1+y^2)^2}h(y)+\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)'(y)g_2(y)\\ &+\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)(y)g_2'(y)-\left[2\psi'(y)\psi''(y)\tilde{Q}_{3,i,-}(\psi(y))+\psi'(y)^3\tilde{Q}'_{3,i,-}(\psi(y))\right]\Bigg|\Bigg\}\end{aligned}$$

with $\tilde{Q}^{(k)}_{3,i,\pm}$ as in Definition 6.7 and Lemma 5.6 on $[0,\frac{15}{100}]$, $[\frac{15}{100},\frac{88}{100}]$, $\mathcal{I}_1\cap\mathcal{J}_1$, $\mathcal{I}_1\cap\mathcal{J}_2$ and $\mathcal{I}_2\cap\mathcal{J}_2$ with $N=15000,7300,700,350,150$ we infer

$$\begin{aligned}\|\tilde{\mathcal{R}}(g_2)'_{0,0}\|_{L^\infty([0,\frac{15}{100}])} &< \frac{16}{10}+\frac{114}{10}<12,\\ \|\tilde{\mathcal{R}}(g_2)'_{0,0}\|_{L^\infty([\frac{15}{100},\frac{88}{100}])} &< \frac{9}{10}+114<115,\\ \|\tilde{\mathcal{R}}(g_2)'_{1,1}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_1)} &< \frac{1}{10}+158<159,\\ \|\tilde{\mathcal{R}}(g_2)'_{1,2}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_2)} &< \frac{8}{100}+157<158,\\ \|\tilde{\mathcal{R}}(g_2)'_{2,2}\|_{L^\infty(\mathcal{I}_2\cap\mathcal{J}_2)} &< 40+\frac{954}{10}<136.\end{aligned}$$

Analogously we estimate

$$\begin{aligned}\left|\tilde{\mathcal{R}}(g_2)_{i,j}(y)\right| \leq \max\Big\{&\Big| -g_2''(y)+\frac{h(y)}{1+y^2}+\psi'(y)^2\tilde{V}_{2,j}(\psi(y))g_2(y)-\psi'(y)^2\tilde{Q}_{3,i,+}(\psi(y))\Big|,\\ &\Big| -g_2''(y)+\frac{h(y)}{1+y^2}+\psi'(y)^2\tilde{V}_{2,j}(\psi(y))g_2(y)-\psi'(y)^2\tilde{Q}_{3,i,-}(\psi(y))\Big|\Big\}\end{aligned}$$

and from Lemma 5.6 on $[0,\frac{15}{100}]$, $[\frac{15}{100},\frac{88}{100}]$, $\mathcal{I}_1\cap\mathcal{J}_1$, $\mathcal{I}_1\cap\mathcal{J}_2$ and $\mathcal{I}_2\cap\mathcal{J}_2$ with $N=15000,73000,7000,3500,1500$ we infer

$$\begin{aligned}\|\tilde{\mathcal{R}}(g_2)_{0,0}\|_{L^\infty([0,\frac{15}{100}])} &< 79\cdot 10^{-4}+12\cdot 10^{-5}<802\cdot 10^{-5},\\ \|\tilde{\mathcal{R}}(g_2)_{0,0}\|_{L^\infty([\frac{15}{100},\frac{88}{100}])} &< 43\cdot 10^{-4}+115\cdot 10^{-5}<6\cdot 10^{-3},\\ \|\tilde{\mathcal{R}}(g_2)_{1,1}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_1)} &< 9\cdot 10^{-4}+159\cdot 10^{-5}<25\cdot 10^{-4},\\ \|\tilde{\mathcal{R}}(g_2)_{1,2}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_2)} &< 3\cdot 10^{-4}+158\cdot 10^{-5}<19\cdot 10^{-4},\\ \|\tilde{\mathcal{R}}(g_2)_{2,2}\|_{L^\infty(\mathcal{I}_2\cap\mathcal{J}_2)} &< 43\cdot 10^{-4}+136\cdot 10^{-5}<57\cdot 10^{-4}.\end{aligned}$$

Finally, from

$$\|\mathcal{R}(g_2)-\tilde{\mathcal{R}}(g_2)_{i,j}\|_{L^\infty(\mathcal{I}_i\cap\mathcal{J}_j)}\leq\|g_2\|_{L^\infty}\|(\psi')^2\big(V_2\circ\psi-\tilde{V}_{2,j}\circ\psi\big)\|_{L^\infty(\mathcal{J}_j)}+\|(\psi')^2\big(Q_3\circ\psi-\tilde{Q}_{3,i}\circ\psi\big)\|_{L^\infty(\mathcal{I}_i)}$$

we conclude

$$\begin{aligned}\|\mathcal{R}(g_2)-\tilde{\mathcal{R}}(g_2)_{0,0}\|_{L^\infty(\mathcal{I}_0\cap\mathcal{J}_0)} &\leq \frac{92}{100}\cdot 2\cdot 10^{-5}+2\cdot 10^{-4}<3\cdot 10^{-4},\\ \|\mathcal{R}(g_2)-\tilde{\mathcal{R}}(g_2)_{1,1}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_1)} &\leq \frac{92}{100}\cdot 10^{-3}+10^{-3}<2\cdot 10^{-3},\\ \|\mathcal{R}(g_2)-\tilde{\mathcal{R}}(g_2)_{1,2}\|_{L^\infty(\mathcal{I}_1\cap\mathcal{J}_2)} &\leq \frac{92}{100}\cdot 5\cdot 10^{-4}+10^{-3}<2\cdot 10^{-3},\\ \|\mathcal{R}(g_2)-\tilde{\mathcal{R}}(g_2)_{2,2}\|_{L^\infty(\mathcal{I}_2\cap\mathcal{J}_2)} &\leq \frac{92}{100}\cdot 5\cdot 10^{-4}+3\cdot 10^{-5}<5\cdot 10^{-4},\end{aligned}$$

and

$$\big\|\mathcal{R}(g_2)\big\|_{L^\infty}<84\cdot 10^{-4}.$$

□

6.3 Approximation of $\mathcal{L}_{c,2}$

Analogously to Section 5.4 we approximate the fundamental system of $\mathcal{L}_{c,2}$ by $\{u_+, u_-\}$ with

$$w_+(y) := (1+y)u_+(y), \qquad w_-(y) := (1-y)u_-(y).$$

The rationalized coefficients $(a_n^{\pm})_{n=2}^{40} \subset \mathbb{Q}$ are listed in Appendix F, Tables 5 and 6.

Definition 6.18. *We define*

$$\tilde{\mathcal{L}}_{2,c} f := -f'' + \tilde{p} f' + \tilde{q} f,$$

with

$$\tilde{p} := \frac{u_+ u_-'' - u_+'' u_-}{W}, \qquad \tilde{q} := \frac{u_+'' u_-' - u_+' u_-''}{W}$$

and

$$W := W(u_+, u_-) = u_+ u_-' - u_- u_+',$$
$$W_0(y) := 2w_+(y)w_-(y) + (1-y^2)W(w_+, w_-)(y).$$

Re-expanding the a polynomial W_0 of degree atmost 81 in Chebychev polynomials, Lemma 5.5 yields

$$\|W_0\|_{L^\infty} < \frac{13}{10}, \qquad \|W_0'\|_{L^\infty} < \frac{13}{10}$$

and from Lemma 5.6 on $[0,1]$ with $N = 100$ we obtain

$$\min_{[-1,1]} |W_0| \geq \frac{635}{1000} - \frac{13}{1000} \geq \frac{62}{100}.$$

In particular W_0 has no zeros in $[-1,1]$.

Lemma 6.19. *$\tilde{p}$ and $\tilde{q}$ satisfy*

$$\|\tilde{p} - p\|_{L^\infty} < 6 \cdot 10^{-4}, \qquad \|\tilde{q} - q\|_{L^\infty} < 5 \cdot 10^{-3},$$

where

$$p = \frac{\psi''}{\psi'} = \frac{2y(y^2+3)}{(1+y^2)(1-y^2)}, \qquad q = (\psi')^2 (V_2 \circ \psi).$$

Proof. We define

$$P_1(y) := 2\Big[w'_+(y)w_-(y) + w_+(y)w'_-(y) + yW(w_+(y), w_-(y))\Big] - (1-y^2)\Big[w''_+(y)w_-(y) - w_+(y)w''_-(y)\Big],$$
$$P_2(y) := 4yw_+(y)w_-(y) + 2y(y^2+3)W(w_+(y), w_-(y))$$

which are polynomials of degree atmost 80 and 82 respectively and

$$P_3(y) := (1+y^2)P_1(y) - P_2(y), \qquad P_4(y) := (1+y^2)W_0(y)$$

such that

$$\tilde{p}(y) - p(y) = \frac{P_3(y)}{P_4(y)}$$

and P_3 and P_4 are polynomials of degree atmost 82 and 83 respectively.
Lemma 5.5 yields

$$\|P_3\|_{L^\infty} < 3 \cdot 10^{-4}, \qquad \|P'_4\|_{L^\infty} < \frac{51}{10},$$

and Lemma 5.6 on $[0,1]$ with $N = 100$ gives

$$\min_{[-1,1]} |P_4| > \frac{63}{100} - \frac{51}{1000} > \frac{55}{100},$$

from which we conclude

$$\|\tilde{p} - p\|_{L^\infty} < 6 \cdot 10^{-4}.$$

For the second estimate we define

$$P_5(y) = (1-y^2)\Big[w''_+(y)w'_-(y) - w'_+(y)w''_-(y)\Big] - (1-y)w_+(y)w''_-(y) + (1+y)w''_+(y)w_-(y) - 4w'_+(y)w'_-(y),$$
$$P_6(y) = (1-y)w_+(y)w'_-(y) - (1+y)w'_+(y)w_-(y) + w_+(y)w_-(y)$$

which are polynomials of degree atmost 79 and 80 respectively and

$$P_7(y) := P_5(y) + \frac{4P_6(y)}{1-y^2}$$

such that

$$\tilde{q} = \frac{P_7}{W_0}$$

and P_7 is a polynomial of degree atmost 79.
Applying Lemma 5.5 to the polynomial $P'_7W_0 - P_7W'_0$ of degree atmost 159 we infer

$$\|P'_7W_0 - P_7W'_0\|_{L^\infty} < 51,$$

which gives

$$\|\tilde{q}'\|_{L^\infty} \leq \frac{\|P_7'W_0 - P_7W_0'\|_{L^\infty}}{\min_{[-1,1]}|W_0|^2} \leq \frac{51}{(\frac{62}{100})^2} < 133$$

and from

$$\left\|\left(\tilde{q} - (\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)'\right\|_{L^\infty(\mathcal{J}_j)} \leq \|\tilde{q}'\|_{L^\infty} + \left\|\left((\psi')^2(\tilde{V}_{2,j}\circ\psi)\right)'\right\|_{L^\infty(\mathcal{J}_j)}$$

and Lemma 6.15 we infer

$$\begin{aligned}
\left\|\left(\tilde{q} - (\psi')^2(\tilde{V}_{2,0}\circ\psi)\right)'\right\|_{L^\infty(\mathcal{J}_0)} &\leq 173,\\
\left\|\left(\tilde{q} - (\psi')^2(\tilde{V}_{2,1}\circ\psi)\right)'\right\|_{L^\infty(\mathcal{J}_1)} &\leq 150,\\
\left\|\left(\tilde{q} - (\psi')^2(\tilde{V}_{2,2}\circ\psi)\right)'\right\|_{L^\infty(\mathcal{J}_2)} &\leq 133.
\end{aligned}$$

Lemma 5.6 on $\mathcal{J}_0, ..., \mathcal{J}_2$ with $N = 88000,\ 7000,\ 5000$ gives

$$\begin{aligned}
\|\tilde{q} - (\psi')^2(\tilde{V}_{2,0}\circ\psi)\|_{L^\infty(\mathcal{J}_0)} &< 18\cdot 10^{-4} + 173\cdot 10^{-5} = 355\cdot 10^{-5},\\
\|\tilde{q} - (\psi')^2(\tilde{V}_{2,1}\circ\psi)\|_{L^\infty(\mathcal{J}_1)} &< 24\cdot 10^{-4} + 150\cdot 10^{-5} = 290\cdot 10^{-5},\\
\|\tilde{q} - (\psi')^2(\tilde{V}_{2,2}\circ\psi)\|_{L^\infty(\mathcal{J}_2)} &< 15\cdot 10^{-4} + 133\cdot 10^{-5} = 18\cdot 10^{-4}
\end{aligned}$$

and finally with Lemma 5.9 we conclude

$$\|\tilde{q} - q\|_{L^\infty} \leq 4\cdot 10^{-3} + \max_{j=0,\dots,2}\|(\psi')^2(V_2 - \tilde{V}_{2,j})\circ\psi\|_{L^\infty(\mathcal{J}_j)} < 5\cdot 10^{-3}.$$

□

Definition 6.20. *The Green function of $\tilde{\mathcal{L}}_{2,c}$ is given by*

$$G(y,s) := \frac{1}{W(s)}\begin{cases} u_+(s)u_-(y), & s \geq y,\\ u_+(y)u_-(s), & s \leq y.\end{cases}$$

The unique solution of $\tilde{\mathcal{L}}_{2,c}u = f \in L^\infty(-1,1)$ is given by

$$u(y) = \tilde{\mathcal{L}}_{2,c}^{-1}f(y) := \int_{-1}^{1} G(y,s)f(s)ds$$

and $\tilde{\mathcal{L}}_{2,c}^{-1} f \in L^\infty(-1,1)$ *for all* $f \in L^\infty(-1,1)$.

Lemma 6.21. *Let* $f \in L^\infty(-1,1)$. *Then*

$$\|\tilde{\mathcal{L}}_{2,c}^{-1} f\|_{W^{1,\infty}} \leq \frac{68}{10} \|f\|_{L^\infty}.$$

Proof. From Lemma 5.5 infer

$$\|w_\pm''\|_{L^\infty} < \frac{78}{10}$$

and from Lemma 5.6 on $[-1,1]$ with $N = 2000$

$$\|w_\pm'\|_{L^\infty} \leq \frac{22}{10} + 78 \cdot 10^{-4} < \frac{23}{10},$$
$$\|w_\pm\|_{L^\infty} \leq 2 + 23 \cdot 10^{-4} < \frac{201}{100},$$

which gives

$$\left\| \left(\frac{w_\pm}{W_0} \right)' \right\|_{L^\infty} \leq \frac{\|w_\pm'\|_{L^\infty} \|W_0\|_{L^\infty} + \|w_\pm\|_{L^\infty} \|W_0'\|_{L^\infty}}{\min_{[-1,1]} |W_0|^2} \leq \frac{\frac{23}{10}\frac{13}{10} + 2 \cdot \frac{13}{10}}{\left(\frac{62}{100}\right)^2} < 15.$$

Lemma 5.6 on $[-1,1]$ with $N = 2000$ gives

$$\left\| \frac{w_\pm}{W_0} \right\|_{L^\infty} \leq \frac{176}{100} + \frac{15}{1000} < \frac{178}{100}$$

and we conclude

$$\|\tilde{\mathcal{L}}_{2,c}^{-1} f\|_{L^\infty} \leq \|f\|_{L^\infty} \|w_\pm\|_{L^\infty} \left\| \frac{w_\pm}{W_0} \right\|_{L^\infty} \int_{-1}^{1} |1 - s^2| ds < \|f\|_{L^\infty} \frac{201}{100} \frac{178}{100} \frac{4}{3} < \frac{48}{10} \|f\|_{L^\infty}.$$

Applying Lemma 5.5 to the polynomial

$$P_8(y) := \Big(w_-(1 + .) + w_-'(1 - (.)^2) \Big)(y) = -\Big(w_+'(1 - (.)^2) - w_+(1 - .) \Big)(-y)$$

of degree atmost 41 we infer

$$\|P_8'\|_{L^\infty} < 24$$

and from Lemma 5.6 on $[-1,1]$ with $N = 3000$

$$\|P_8\|_{L^\infty} < \frac{12}{10} + \frac{24}{1500} < \frac{13}{10}.$$

We conclude

$$\|(\tilde{\mathcal{L}}_{2,c}^{-1}f)'\|_{L^\infty} \leq \|f\|_{L^\infty}\|P_8\|_{L^\infty}\left\|\frac{w_\pm}{W_0}\right\|_{L^\infty}\int_{-1}^{1} ds \leq \|f\|_{L^\infty}\frac{13}{10}\frac{178}{100}\cdot 2 < \frac{47}{10}\|f\|_{L^\infty}$$

and

$$\|\tilde{\mathcal{L}}_{1,c}^{-1}f\|_{W^{1,\infty}} = \left(\|\tilde{\mathcal{L}}_{1,c}^{-1}f\|_{L^\infty}^2 + \|(\tilde{\mathcal{L}}_{1,c}^{-1}f)'\|_{L^\infty}^2\right)^{1/2} < \left(\left(\frac{48}{10}\right)^2\|f\|_{L^\infty}^2 + \left(\frac{47}{10}\right)^2\|f\|_{L^\infty}^2\right)^{1/2} < \frac{68}{10}\|f\|_{L^\infty}$$

□

6.4 The contraction argument

Lemma 6.22. *Let $X := \{u \in C^1[-1,1] : \|u\|_{W^{1,\infty}} < \frac{1}{16}\}$. Then $\mathcal{K}$ has a unique fixed point in X. In particular there exists some $\delta_2 \in W^{1,\infty}$ with*

$$\|\delta_2\|_{W^{1,\infty}} < \frac{1}{16}$$

such that $\mathcal{R}(g_2+\delta_2) = 0$, which proves the existence of ϕ_2.

Proof. From Proposition 6.17 and Lemma 6.19 and 6.21 we have

$$\begin{aligned}
\|\mathcal{K}(u)\|_{W^{1,\infty}} &\leq \frac{68}{10}\left(\|\mathcal{R}(g_1)\|_{L^\infty} + \|\tilde{\mathcal{L}}_{c,2}u - \mathcal{L}_{c,2}u\|_{L^\infty}\right)\\
&\leq \frac{68}{10}\left(\|\mathcal{R}(g_2)\|_{L^\infty} + \|\tilde{p}-p\|_{L^\infty}\|u'\|_{L^\infty} + \|\tilde{q}-q\|_{L^\infty}\|u\|_{L^\infty}\right)\\
&\leq \frac{68}{10}\left(84\cdot 10^{-4} + 6\cdot 10^{-4}\frac{1}{16} + \frac{5}{1000}\frac{1}{16}\right) < \frac{1}{16}.
\end{aligned}$$

which gives $\mathcal{K}(u) \in X$ for all $u \in X$.
Moreover,

$$\begin{aligned}
\|\mathcal{K}(u) - \mathcal{K}(v)\|_{W^{1,\infty}} &\leq \frac{68}{10}\left\|\left(\tilde{\mathcal{L}}_{c,2} - \mathcal{L}_{c,2}\right)(u-v)\right\|_{L^\infty}\\
&\leq \frac{68}{10}\left[\|\tilde{p}-p\|_{L^\infty}\|u'-v'\|_{L^\infty} + \|\tilde{q}-q\|_{L^\infty}\|u-v\|_{L^\infty}\right]\\
&\leq \frac{68}{10}\left(6\cdot 10^{-4} + \frac{5}{1000}\right)\|u-v\|_{W^{1,\infty}} < \frac{4}{100}\|u-v\|_{W^{1,\infty}}
\end{aligned}$$

for all $u, v \in X$. □

Corollary 6.23. *There exists a unique regular function $\phi_2 \in L^\infty(\mathbb{R})$ such that*

$$\mathcal{L}_2\phi_2 = Q_3 \qquad \text{and} \qquad \phi_2' \in L^2(\mathbb{R}).$$

Proof. From the exponential decay of Q_3 and V_2 and $\mathcal{L}_2\phi_2 = -\phi_2'' + V_2\phi_2 = Q_3$ we infer

$$\int (\phi_2')^2 = -\int \phi_2''\phi_2 = \int Q_3\phi_2 - \int V_2\phi_2^2 < \infty.$$

□

6.5 The positivity estimate

Lemma 6.24. *The function Q_3 satisfies the following integral bounds.*

$$\int_{\mathcal{I}_0} |Q_3(\psi(y))|\psi'(y)dy \le \frac{12}{10}, \qquad \int_{\mathcal{I}_1} |Q_3(\psi(y))|\psi'(y)dy \le \frac{13}{100}, \qquad \int_{\mathcal{I}_2} |Q_3(\psi(y))|\psi'(y)dy \le 5\cdot 10^{-7}.$$

Proof. We have

$$\int_{\mathcal{I}_1} |Q_3(\psi(y))|\psi'(y)dy \le \int_{\mathcal{I}_i} |\tilde{Q}_{3,i}(\psi(y))|\psi'(y)dy + \int_{\mathcal{I}_i} |Q_3(\psi(y)) - \tilde{Q}_{3_i}(\psi(y))|\psi'(y)dy$$

with

$$\int_{\mathcal{I}_i} |Q_3(\psi(y) - \tilde{Q}_{3_i}(\psi(y))|\psi'(y)dy \le |\mathcal{I}_i|\cdot \left\|\psi'(Q_3 - \tilde{Q}_{3,i})\circ\psi\right\|_{L^\infty(\mathcal{I}_i)} \le |\mathcal{I}_i|\cdot \left\|(\psi')^2(Q_3 - \tilde{Q}_{3,i})\circ\psi\right\|_{L^\infty(\mathcal{I}_i)}$$

and hence

$$\begin{aligned}
\int_{\mathcal{I}_0} |Q_3(\psi(y) - \tilde{Q}_{3,0}(\psi(y))|\psi'(y)dy &\le \frac{88}{100}\cdot 2\cdot 10^{-4} < 2\cdot 10^{-4},\\
\int_{\mathcal{I}_1} |Q_3(\psi(y) - \tilde{Q}_{3,1}(\psi(y))|\psi'(y)dy &\le \frac{105}{1000}\cdot 10^{-3} < 2\cdot 10^{-4},\\
\int_{\mathcal{I}_2} |Q_3(\psi(y) - \tilde{Q}_{3,2}(\psi(y))|\psi'(y)dy &\le \frac{15}{1000}\cdot 3\cdot 10^{-5} < 5\cdot 10^{-7}.
\end{aligned}$$

The trapezoidal rule on $\mathcal{I}_0$ and $\mathcal{I}_1$ with $N = 880$ and 105 gives

$$\int_{\mathcal{I}_0} |\tilde{Q}_{3,0}(\psi(y))|\psi'(y)dy \leq \frac{1192}{1000} + \left(\frac{88}{100}\right)^3 \frac{1}{12 \cdot (880)^2} \cdot 1800 < \frac{1193}{1000},$$
$$\int_{\mathcal{I}_1} |\tilde{Q}_{3,1}(\psi(y))|\psi'(y)dy \leq \frac{126}{1000} + \left(\frac{105}{1000}\right)^3 \frac{1}{12 \cdot (105)^2} \cdot 6000 < \frac{127}{1000}$$

where we replaced $\tilde{Q}_{3,0}$ and $\tilde{Q}_{3,1}$ by $\tilde{Q}_{3,0,+}$ and $\tilde{Q}_{3,1,+}$ as in Definition 6.7 for the evaluation and used Lemma 6.9 for the bounds on the second derivatives of the integrands.

We conclude

$$\int_{\mathcal{I}_0} |Q_3(\psi(y))|\psi'(y)dy \leq \frac{1193}{1000} + 2 \cdot 10^{-4} \leq \frac{12}{10},$$
$$\int_{\mathcal{I}_1} |Q_3(\psi(y))|\psi'(y)dy \leq \frac{127}{1000} + 2 \cdot 10^{-4} \leq \frac{13}{100},$$
$$\int_{\mathcal{I}_2} |Q_3(\psi(y))|\psi'(y)dy \leq 5 \cdot 10^{-7}.$$

□

Lemma 6.25.

$$-\frac{417}{1000} < \big(\phi_2\big|Q_3\big) < -\frac{63}{1000}$$

Proof. We write

$$\begin{aligned}\big(\phi_2\big|Q_3\big) &= 2\int_0^1 \phi_2(\psi(y))Q_3(\psi(y))\psi'(y)dy \\ &= 2\sum_{i=0}^{2}\int_{\mathcal{I}_i} g_2(y)\tilde{Q}_{3,i}(\psi(y))\psi'(y)dy + 2\sum_{i=0}^{2}\int_{\mathcal{I}_i}\Big(\phi_2(\psi(y))Q_3(\psi(y)) - g_2(y)\tilde{Q}_{3,i}(\psi(y))\Big)\psi'(y)dy\end{aligned}$$

with

$$\begin{aligned}&\left|\int_{\mathcal{I}_i}\Big(\phi_2(\psi(y))Q_3(\psi(y)) - g_2(y)\tilde{Q}_{3,i}(\psi(y))\Big)\psi'(y)dy\right| \\ \leq &\int_{\mathcal{I}_i}\Big(|Q_3(y)| \cdot |\phi_2(\psi(y)) - g_2(y)| + |g_2(y)| \cdot |Q_3(\psi(y) - \tilde{Q}_{3,i}(\psi(y)|\Big)\psi'(y)dy \\ \leq &\|\delta_2\|_{L^\infty}\int_{\mathcal{I}_i} |Q_3(\psi(y))|\psi'(y)dy + |\mathcal{I}_i| \cdot \|g_2\|_{L^\infty} \cdot \|(\psi')(Q_3 - \tilde{Q}_{3,i}) \circ \psi\|_{L^\infty(\mathcal{I}_i)} \\ \leq &\|\delta_2\|_{L^\infty}\int_{\mathcal{I}_i} |Q_3(\psi(y))|\psi'(y)dy + |\mathcal{I}_i| \cdot \|g_2\|_{L^\infty} \cdot \|(\psi')^2(Q_3 - \tilde{Q}_{3,i}) \circ \psi\|_{L^\infty(\mathcal{I}_i)}\end{aligned}$$

and hence by Lemmas 6.1, 6.24, Proposition 6.22 and (6.6)

$$\left|\int_{\mathcal{I}_0}\Big(\phi_2(\psi(y))Q_3(\psi(y))-g_2(y)\tilde{Q}_{3,0}(\psi(y))\Big)\psi'(y)dy\right|\le\frac{1}{16}\frac{12}{10}+\frac{88}{100}\cdot\frac{92}{100}\cdot 2\cdot 10^{-4}<\frac{76}{1000},$$
$$\left|\int_{\mathcal{I}_1}\Big(\phi_2(\psi(y))Q_3(\psi(y))-g_2(y)\tilde{Q}_{3,1}(\psi(y))\Big)\psi'(y)dy\right|\le\frac{1}{16}\frac{13}{100}+\frac{105}{1000}\cdot\frac{92}{100}\cdot 10^{-3}<\frac{9}{1000},$$
$$\left|\int_{\mathcal{I}_0}\Big(\phi_2(\psi(y))Q_3(\psi(y))-g_2(y)\tilde{Q}_{3,0}(\psi(y))\Big)\psi'(y)dy\right|\le\frac{1}{16}\cdot 5\cdot 10^{-7}+\frac{15}{1000}\cdot\frac{92}{100}\cdot 3\cdot 10^{-5}<10^{-6}.$$

From

$$\begin{aligned}\Big\|\big(\psi' g_2(\tilde{Q}_{3,i}\circ\psi)\big)''\Big\|_{L^\infty(\mathcal{I}_i)}\le&\Big\|\big(\psi'(\tilde{Q}_{3,i}\circ\psi)\big)''\Big\|_{L^\infty(\mathcal{I}_i)}\cdot\|g_2\|_{L^\infty}+\big\|\psi'(\tilde{Q}_{3,i}\circ\psi)\big\|_{L^\infty(\mathcal{I}_i)}\cdot\|g_2''\|_{L^\infty}\\&+2\Big\|\big(\psi'(\tilde{Q}_{3,i}\circ\psi)\big)'\Big\|_{L^\infty(\mathcal{I}_i)}\cdot\|g_2'\|_{L^\infty},\end{aligned}$$

Lemma 6.9 and (6.6) we infer

$$\Big\|\big(\psi' g_2(\tilde{Q}_{3,0}\circ\psi)\big)''\Big\|_{L^\infty(\mathcal{I}_0)}\le 1800\cdot\frac{92}{100}+\frac{39}{10}\cdot 136+2\cdot 81\cdot\frac{52}{10}<3030,$$
$$\Big\|\big(\psi' g_2(\tilde{Q}_{3,1}\circ\psi)\big)''\Big\|_{L^\infty(\mathcal{I}_1)}\le 6000\cdot\frac{92}{100}+\frac{26}{10}\cdot 136+2\cdot 85\cdot\frac{52}{10}<6760.$$

We bound the integrands $g_2(y)\tilde{Q}_{3,i}(\psi(y))\psi'(y)$ for the evaluation of the trapezoidal rule by

$$g_2(y)\tilde{Q}_{3,0}(\psi(y))\psi'(y)\le\max\Big\{g_2(y)\tilde{Q}_{3,0,-}(\psi(y))\psi'(y),\ g_2(y)\tilde{Q}_{3,0,+}(\psi(y))\psi'(y)\Big\},$$
$$g_2(y)\tilde{Q}_{3,0}(\psi(y))\psi'(y)\ge\min\Big\{g_2(y)\tilde{Q}_{3,0,-}(\psi(y))\psi'(y),\ g_2(y)\tilde{Q}_{3,0,+}(\psi(y))\psi'(y)\Big\}$$

and

$$g_2(y)\tilde{Q}_{3,1}(\psi(y))\psi'(y)\le\max\Big\{g_2(y)\tilde{Q}_{3,1,+}(\psi(y))\psi'(y),g_2(y)\tilde{Q}_{3,1,-}(\psi(y))\psi'(y)\Big\},$$
$$g_2(y)\tilde{Q}_{3,1}(\psi(y))\psi'(y)\ge\min\Big\{g_2(y)\tilde{Q}_{3,1,+}(\psi(y))\psi'(y),g_2(y)\tilde{Q}_{3,1,-}(\psi(y))\psi'(y)\Big\}$$

and the trapezoidal rule on $\mathcal{I}_0$ and $\mathcal{I}_1$ with $N = 880$ and $N = 105$ gives

$$\begin{aligned}
\int_{\mathcal{I}_0} g_2(y)\tilde{Q}_{3,0}(\psi(y))\psi'(y)dy &\leq -\frac{182}{1000} + \left(\frac{88}{100}\right)^3 \frac{1}{12\cdot(880)^2}\cdot 3030 < -\frac{181}{1000},\\
\int_{\mathcal{I}_0} g_2(y)\tilde{Q}_{3,0}(\psi(y))\psi'(y)dy &\geq -\frac{183}{1000} - \left(\frac{88}{100}\right)^3 \frac{1}{12\cdot(880)^2}\cdot 3030 > -\frac{184}{1000},\\
\int_{\mathcal{I}_1} g_2(y)\tilde{Q}_{3,1}(\psi(y))\psi'(y)dy &\leq \frac{63}{1000} + \left(\frac{105}{1000}\right)^3 \frac{1}{12\cdot(105)^2}\cdot 6760 < \frac{64}{1000},\\
\int_{\mathcal{I}_1} g_2(y)\tilde{Q}_{3,1}(\psi(y))\psi'(y)dy &\geq \frac{62}{1000} - \left(\frac{105}{1000}\right)^3 \frac{1}{12\cdot(105)^2}\cdot 6760 > \frac{61}{1000},
\end{aligned}$$

and hence

$$\begin{aligned}
\big(\phi_2\big|Q_3\big) &\leq 2\cdot\left(-\frac{117}{1000}\right) + 2\cdot\left(\frac{76}{1000}+\frac{9}{1000}+10^{-6}\right) < -\frac{63}{1000},\\
\big(\phi_2\big|Q_3\big) &\geq 2\cdot\left(-\frac{123}{1000}\right) - 2\cdot\left(\frac{76}{1000}+\frac{9}{1000}+10^{-6}\right) > -\frac{417}{1000},
\end{aligned}$$

□

Lemma 6.26.

$$0 > \bar{H}_2(Q,Q) > -\frac{39}{100}$$

Proof. We write

$$\begin{aligned}
(V_2Q\big|Q) &= 2\int_0^1 V_2(\psi(y))Q(\psi(y))^2\psi'(y)dy\\
&= 2\sum_{i,j=0}^{2}\int_{I_i\cap\mathcal{J}_j} \tilde{V}_{2,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\psi'(y)dy\\
&+ 2\sum_{i,j=0}^{2}\int_{I_i\cap\mathcal{J}_j} \left(V_2(\psi(y))Q(\psi(y))^2 - \tilde{V}_{2,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\right)\psi'(y)dy
\end{aligned}$$

with

$$\begin{aligned}
&\left|\int_{I_i\cap\mathcal{J}_j}\left(V_2(\psi(y))Q(\psi(y))^2-\tilde{V}_{2,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\right)\psi'(y)\,dy\right|\\
\leq&\int_{I_i\cap\mathcal{J}_j}\Big(\left|V_2(\psi(y))-\tilde{V}_{2,j}(\psi(y))\right|\cdot\left|Q(\psi(y))\right|^2+\left|\tilde{V}_{2,j}(\psi(y))\right|\cdot\left|Q(\psi(y))^2-\tilde{Q}_i(\psi(y))^2\right|\Big)\psi'(y)\,dy\\
\leq&|I_i\cap\mathcal{J}_j|\Big[\left\|(\psi')^2\left(V_2-\tilde{V}_{2,j}\right)\circ\psi\right\|_{L^\infty(\mathcal{J}_j)}\cdot\|Q\circ\psi\|^2_{L^\infty(I_i)}+\left\|\tilde{V}_{2,j}\circ\psi\right\|_{L^\infty(\mathcal{J}_j)}\cdot\left\|(\psi')^2\left(Q^2-\tilde{Q}_i^2\right)\circ\psi\right\|_{L^\infty(I_i)}\Big]
\end{aligned}$$

and by the mean-value theorem

$$\left\|(\psi')^2\left(Q^2-\tilde{Q}_i^2\right)\circ\psi\right\|_{L^\infty(I_i)}\leq 2\cdot\max\left\{\|Q\circ\psi\|_{L^\infty(I_i)},\ \left\|\tilde{Q}\circ\psi\right\|_{L^\infty(I_i)}\right\}\cdot\left\|(\psi')^2\left(Q-\tilde{Q}_i\right)\circ\psi\right\|_{L^\infty(I_i)}$$

which gives

$$\left|2\sum_{i,j=0}^{2}\int_{I_i\cap\mathcal{J}_j}\left[V_2(\psi(y))Q(\psi(y))^2-\tilde{V}_{2,j}(\psi(y))\tilde{Q}_i(\psi(y))^2\right]\psi'(y)dy\right|<4\cdot10^{-4}$$

by Lemmas 5.8, 5.17, 6.2 and 6.16.

The second derivatives of the integrands can be estimated by

$$\begin{aligned}
&\left\|\left(\psi'\left(\left(V_{2,j}\cdot Q_i^2\right)\circ\psi\right)\right)''\right\|_{L^\infty(I_i\cap\mathcal{J}_j)}\\
\leq&\left\|\left((V_{2,j}\cdot Q_i)\circ\psi\right)''\right\|_{L^\infty(I_i\cap\mathcal{J}_j)}\cdot\left\|\psi'\left(Q_i\circ\psi\right)\right\|_{L^\infty(I_i)}+\left\|(V_{2,j}\cdot Q_i)\circ\psi\right\|_{L^\infty(I_i\cap\mathcal{J}_j)}\left\|\left(\psi'\left(Q_i\circ\psi\right)\right)''\right\|_{L^\infty(I_i)}\\
&+2\cdot\left\|\left((V_{2,j}\cdot Q_i)\circ\psi\right)'\right\|_{L^\infty(I_i\cap\mathcal{J}_j)}\cdot\left\|\left(\psi'\left(Q_i\circ\psi\right)\right)'\right\|_{L^\infty(I_i)}\\
\leq&\Big[\left\|(V_{2,j}\circ\psi)''\right\|_{L^\infty(\mathcal{J}_j)}\|Q_i\circ\psi\|_{L^\infty(I_i)}+\|V_{2,j}\circ\psi\|_{L^\infty(\mathcal{J}_j)}\left\|(Q_i\circ\psi)''\right\|_{L^\infty(I_i)}\\
&\quad+2\left\|(V_{2,j}\circ\psi)'\right\|_{L^\infty(\mathcal{J}_j)}\cdot\left\|(Q_i\circ\psi)'\right\|_{L^\infty(I_i)}\Big]\cdot\left\|\psi'\left(Q_i\circ\psi\right)\right\|_{L^\infty(I_i)}\\
&+\|V_{2,j}\circ\psi\|_{L^\infty(\mathcal{J}_j)}\cdot\|Q_i\circ\psi\|_{L^\infty(I_i)}\cdot\left\|\left(\psi'\left(Q_i\circ\psi\right)\right)''\right\|_{L^\infty(I_i)}\\
&+2\cdot\left[\left\|(V_{2,j}\circ\psi)'\right\|_{L^\infty(\mathcal{J}_j)}\cdot\|Q_i\circ\psi\|_{L^\infty(I_i)}+\|V_{2,j}\circ\psi\|_{L^\infty(\mathcal{J}_j)}\cdot\left\|(Q_i\circ\psi)'\right\|_{L^\infty(I_i)}\right]\cdot\left\|\left(\psi'\left(Q_i\circ\psi\right)\right)'\right\|_{L^\infty(I_i)}
\end{aligned}$$

which by Lemmas 5.16, 5.17 and 6.16 gives

$$\left\|\left(\psi'\left(\left(V_{2,0}\cdot Q_0^2\right)\circ\psi\right)\right)''\right\|_{L^\infty(I_0\cap\mathcal{J}_0)}<1500,\qquad\left\|\left(\psi'\left(\left(V_{2,1}\cdot Q_1^2\right)\circ\psi\right)\right)''\right\|_{L^\infty(I_1\cap\mathcal{J}_1)}<1.$$

Recall from the proof of Proposition 4.32 that $\bar{H}_2(Q,Q) < H_2(Q,Q) = 0$.
Replacing the constant C^2 in $\tilde{Q}_i$ by C_-^2 for the evaluation of the trapezoidal rule on $I_0 \cap \mathcal{J}_0$ and $I_1 \cap \mathcal{J}_1$ with $N = 880$ and $N = 70$ gives

$$0 > \int_{I_0 \cap \mathcal{J}_0} \tilde{V}_{2,0}(\psi(y))\tilde{Q}_0(\psi(y))^2\psi'(y)dy > -\frac{870}{1000} - \left(\frac{88}{100}\right)^3 \cdot \frac{1}{12 \cdot (880)^2} \cdot 1500 > -\frac{871}{1000},$$
$$0 > \int_{I_1 \cap \mathcal{J}_1} \tilde{V}_{2,1}(\psi(y))\tilde{Q}_1(\psi(y))^2\psi'(y)dy > -2 \cdot 10^{-7} - \left(\frac{7}{100}\right)^3 \cdot \frac{1}{12 \cdot (70)^2} \cdot 1 > -3 \cdot 10^{-7}.$$

We conclude

$$0 > \big(V_2 Q\big|Q\big) > 2 \cdot \left(-\frac{871}{1000} - 3 \cdot 10^{-7}\right) - 4 \cdot 10^{-4} > -\frac{175}{100}$$

and hence by Lemma 5.31

$$0 > \bar{H}_2(Q,Q) = \big(Q'\big|Q'\big) + \big(V_2 Q\big|Q\big) > \frac{\sqrt{3}\pi}{4} - \frac{175}{100} > -\frac{39}{100}.$$

□

Lemma 6.27.

$$\big(Q\big|Q_3\big) < -\frac{41}{100}$$

Proof. We write

$$\begin{aligned}\big(Q\big|Q_3\big) &= 2\int_0^1 Q(\psi(y))Q_3(\psi(y))\psi'(y)dy = 2\sum_{i,k=0}^{2}\int_{I_i\cap\mathcal{I}_k} Q(\psi(y))Q_3(\psi(y))\psi'(y)dy \\ &= 2\sum_{i,k=0}^{2}\int_{I_i\cap\mathcal{I}_k} \tilde{Q}_i(\psi(y))\tilde{Q}_{3,k}(\psi(y))\psi'(y)dy + 2\sum_{i,k=0}^{2}\int_{I_i\cap\mathcal{I}_k}\Big(Q_i(\psi(y))Q_3(\psi(y)) - \tilde{Q}_i(\psi(y))\tilde{Q}_{3,k}(\psi(y))\Big)\psi'(y)dy\end{aligned}$$

with

$$\begin{aligned}&\left|\int_{I_i\cap\mathcal{I}_k}\Big(Q_i(\psi(y))Q_3(\psi(y)) - \tilde{Q}_i(\psi(y))\tilde{Q}_{3,k}(\psi(y))\Big)\psi'(y)dy\right| \\ \le&\int_{I_i\cap\mathcal{I}_k}\Big(|Q(\psi(y))|\cdot|Q_3(\psi(y)) - \tilde{Q}_{3,k}(\psi(y))| + |\tilde{Q}_{3,k}(\psi(y)|\cdot|Q(\psi(y)) - \tilde{Q}_i(\psi(y))\Big)\psi'(y)dy \\ \le&|I_i\cap\mathcal{I}_k|\cdot\Big(\|Q\circ\psi\|_{L^\infty(I_i)}\cdot\big\|(\psi')^2(Q_3-\tilde{Q}_{3,k})\circ\psi\big\|_{L^\infty(\mathcal{I}_k)} + \big\|\tilde{Q}_{3,k}\circ\psi\big\|_{L^\infty(\mathcal{I}_k)}\cdot\big\|(\psi')^2\left(Q-\tilde{Q}_i\right)\circ\psi\big\|_{L^\infty(I_i)}\Big)\end{aligned}$$

and hence

$$\left|2\sum_{i,k=0}^{2}\int_{I_i\cap\mathcal{I}_k}\Big(Q_i(\psi(y))Q_3(\psi(y))-\tilde{Q}_i(\psi(y))\tilde{Q}_{3,k}(\psi(y))\Big)\psi'(y)dy\right|<\frac{1}{1000}$$

by Lemmas 5.8, 5.17, 6.1 and 6.10.

The second derivatives of the integrands can be estimated by

$$\begin{aligned}\Big\|\big(\psi'(\tilde{Q}_i\cdot\tilde{Q}_{3,k}\circ\psi)\big)''\Big\|_{L^\infty(I_i\cap\mathcal{I}_k)}&\le\|\psi'(\tilde{Q}_i\circ\psi)\|_{L^\infty(I_i)}\Big\|\big(\tilde{Q}_{3,i}\circ\psi\big)''\Big\|_{L^\infty(\mathcal{I}_k)}+\Big\|\big(\psi'(\tilde{Q}_i\circ\psi)\big)''\Big\|_{L^\infty(I_i)}\|(\tilde{Q}_{3,i}\circ\psi)\|_{L^\infty(I_i)}\\&\quad+2\Big\|\big(\tilde{Q}_i\circ\psi)\big)'\Big\|_{L^\infty(I_i)}\cdot\Big\|\big(\psi'(\tilde{Q}_{3,k}\circ\psi)\big)'\Big\|_{L^\infty(\mathcal{I}_k)}\end{aligned}$$

which by Lemmas 5.16 and 6.10 gives

$$\begin{aligned}\Big\|\big(\psi'(\tilde{Q}_0\cdot\tilde{Q}_{3,0}\circ\psi)\big)''\Big\|_{L^\infty(I_0\cap\mathcal{I}_0)}&<600,\\\Big\|\big(\psi'(\tilde{Q}_1\cdot\tilde{Q}_{3,1}\circ\psi)\big)''\Big\|_{L^\infty(I_1\cap\mathcal{I}_1)}&<170.\end{aligned}$$

We are interested in a lower bound on $|(Q,Q_3)|$ and therefore replace the appearing constant C^2 by C_-^2 in $\tilde{Q}_0\cdot\tilde{Q}_{3,0}$ and C_+^2 in $\tilde{Q}_1\cdot\tilde{Q}_{3,1}$ for the evaluation of the trapezoidal rule, which on $I_0\cap\mathcal{I}_0$ and $I_1\cap\mathcal{I}_1$ with $N=880$ and $N=100$ gives

$$\begin{aligned}\int_{I_0\cap\mathcal{I}_0}\tilde{Q}_0(\psi(y))\tilde{Q}_{3,0}(\psi(y))\psi'(y)dy&<-\frac{21}{100}+\left(\frac{88}{100}\right)^3\cdot\frac{1}{12\cdot(880)^2}\cdot600<-\frac{209}{1000},\\\int_{I_1\cap\mathcal{I}_1}\tilde{Q}_1(\psi(y))\tilde{Q}_{3,1}(\psi(y)\psi'(y)dy&<12\cdot10^{-4}+\left(\frac{1}{10}\right)^3\cdot\frac{1}{12\cdot(100)^2}\cdot170<13\cdot10^{-4}.\end{aligned}$$

We conclude

$$(Q|Q_3)<2\cdot\left(-\frac{209}{1000}+13\cdot10^{-4}\right)+\frac{1}{1000}<-\frac{41}{100}.$$

□

Finally from Lemmas 6.25, 6.26 and 6.27 we obtain

$$0<\bar{H}_2(Q,Q)\frac{(\phi_2|Q)}{(Q|Q_3)^2}<\frac{39}{100}\frac{417}{1000}\left(\frac{100}{41}\right)^2<\frac{97}{100}$$

and hence

$$-\big(\phi_2\big|Q_3\big)\left(1-\bar{H}_2(Q,Q)\frac{\big(\phi_2\big|Q\big)}{\big(Q\big|Q_3\big)^2}\right)>0,$$

which concludes the proof of the positivity estimate (6.3).

A Sobolev Spaces

We define for $f \in \mathcal{S}(\mathbb{R}^d)$ and $s > -\frac{d}{2}$ the *L^2-based homogeneous Sobolev norm*

$$\|f\|_{\dot{H}^s(\mathbb{R}^d)} \coloneqq \|\mathcal{F}^{-1}(|.|^s \mathcal{F}(f))\|_{L^2(\mathbb{R}^d)}$$

and the *L^2-based homogeneous Sobolev space* $\dot{H}^s(\mathbb{R}^d)$ as the completion of $\mathcal{S}(\mathbb{R}^d)$ with respect to $\|.\|_{\dot{H}^s(\mathbb{R}^d)}$.

As a generalization, the *L^p-based homogeneous Sobolev norm* for $f \in \mathcal{S}(\mathbb{R}^d)$, $s \geq 0$ and $p \in [1, \infty]$ is defined as

$$\|f\|_{\dot{W}^{s,p}(\mathbb{R}^d)} \coloneqq \|\mathcal{F}^{-1}(|.|^s \mathcal{F}(f))\|_{L^p(\mathbb{R}^d)}.$$

The *L^p-based inhomogeneous Sobolev norm* for $f \in \mathcal{S}(\mathbb{R}^d)$, $s \geq 0$ and $p \in [1, \infty]$ is defined as

$$\|f\|_{W^{s,p}(\mathbb{R}^d)} \coloneqq \|f\|_{\dot{W}^{s,p}(\mathbb{R}^d)} + \|f\|_{L^p(\mathbb{R}^d)}$$

and analogously to the homogeneous case we define $\|.\|_{H^s(\mathbb{R}^d)} \coloneqq \|.\|_{W^{s,2}(\mathbb{R}^d)}$.

The term *homogeneous* refers to the following scaling property:
For $\lambda > 0$ and $f \in \mathcal{S}(\mathbb{R}^d)$ let $f_\lambda(x) \coloneqq f\left(\frac{x}{\lambda}\right)$, then

$$\|f_\lambda\|_{\dot{W}^{s,p}(\mathbb{R}^d)} = \lambda^{\frac{d}{p}-s} \|f\|_{\dot{W}^{s,p}(\mathbb{R}^d)}.$$

Moreover, note that while the homogeneous norm measures the derivatives of order s, the inhomogeneous norm measures all derivatives up to order s. In particular for $s \in \mathbb{N}_0$

$$\|f\|_{\dot{W}^{s,p}(\mathbb{R}^d)} \simeq \sum_{\alpha \in \mathbb{N}_0,\ |\alpha| = s} \|\partial^\alpha f\|_{L^p(\mathbb{R}^d)} \quad \text{and} \quad \|f\|_{W^{s,p}(\mathbb{R}^d)} \simeq \sum_{\alpha \in \mathbb{N}_0,\ |\alpha| \leq s} \|\partial^\alpha f\|_{L^p(\mathbb{R}^d)}.$$

B Littlewood-Paley decomposition

The idea of Littlewood-Paley decomposition is to decompose a function into frequency localized pieces by mapping it to the frequency space via Fourier transformation, localize it to a given frequency by some smooth function of compact support and then mapping it back via Inverse Fourier transform.

Lemma B.1. *There exists a radial function $\psi \in C_c^\infty(\mathbb{R}^d) \setminus \{0\}$, $\psi \geq 0$ such that*

$$\sum_{N\in\mathbb{N}} \psi(2^{-N}x) = 1 \ \forall x \in \mathbb{R}^d \setminus \{0\}$$

This is achieved by taking a smooth radial bump function

$$\chi(x) = \begin{cases} 1, & |x| \leq 1 \\ smooth, & 1 \leq |x| \leq 2 \\ 0, & |x| > 2 \end{cases}$$

and

$$\psi(x) \coloneqq \chi(x) - \chi(2x).$$

Denote $\psi_N(x) \coloneqq \psi(2^{-N}x)$, then $x \in \operatorname{supp}(\psi_N) \Leftrightarrow |x| \simeq 2^N$,
and for $N \in \mathbb{Z}$, $f \in \mathcal{S}(\mathbb{R}^d)$ we define

$$P_N(f) \coloneqq \mathcal{F}(\psi_N \mathcal{F}^{-1} f).$$

such that by dominated convergence

$$\sum_{N\in\mathbb{N}} P_N(f)(x) = f(x).$$

Moreoever

$$\|f\|_{\dot{H}^s(\mathbb{R}^d)} \simeq \sum_{N\in\mathbb{Z}} 2^{2Ns} \|P_N f\|_{L^2(\mathbb{R}^d)}, \tag{B.1}$$

which is known as the *Littlewood-Paley characterization of Sobolev spaces.*

Proposition B.2. (Bernstein inequalities)
For all $f \in \mathcal{S}(\mathbb{R}^d)$, $s \in \mathbb{R}$, $N \in \mathbb{N}$ and $1 \leq p \leq q \leq \infty$:

- $\|P_N |\nabla|^s f\|_{L^p(\mathbb{R}^d)} \simeq 2^{Ns} \|P_N f\|_{L^p(\mathbb{R}^d)}$
- $\|P_N f\|_{L^q(\mathbb{R}^d)} \lesssim 2^{N(\frac{d}{p} - \frac{d}{q})} \|P_N f\|_{L^p(\mathbb{R}^d)}$

Lemma B.3. *Let $f \in H^1(\mathbb{R}^d)$ with $\|f\|_{L^2(\mathbb{R}^d)} = \|\nabla f\|_{L^2(\mathbb{R}^d)} = 1$.*
Then $\sum_{N\in\mathbb{N}} \|P_N f\|_{L^{p+1}(\mathbb{R}^d)}$ is absolutely convergent for all $p \in (1, \infty]$.

Proof. From Proposition B.2 we have

$$\|P_N f\|_{L^{p+1}(\mathbb{R}^d)} \lesssim 2^{N(\frac{d}{2}-\frac{d}{p+1})}\|P_N f\|_{L^2(\mathbb{R}^d)},$$

$$\|P_N f\|_{L^2(\mathbb{R}^d)} \lesssim 2^{-N}\|P_N|\nabla|f\|_{L^2(\mathbb{R}^d)} \lesssim 2^{-N}\|\nabla f\|_{L^2(\mathbb{R}^d)} = 2^{-N},$$

and from (B.1)

$$\|P_N f\|_{L^2(\mathbb{R}^d)} \lesssim \|f\|_{L^2(\mathbb{R}^d)} = 1,$$

which gives

$$\sum_{N\in\mathbb{N}} \|P_N f\|_{L^{p+1}(\mathbb{R}^d)} \lesssim \sum_{N\in\mathbb{N}} 2^{N(\frac{d}{2}-\frac{d}{p+1})} \min\{1, 2^{-N}\}$$

where $p > 1$ ensures $\theta \coloneqq \frac{d}{2} - \frac{d}{p+1} > 0$ and absolute convergence follows from the geometric series. □

C Euler-Lagrange equations

We follow [12].

Let $\Omega \subseteq \mathbb{R}^d$, $F \in C^2(\mathbb{C}^2 \times \mathbb{R}^d)$ and

$$I[u] \coloneqq \int_\Omega F(u, \nabla u, x) dx$$

be a functional on

$$\mathcal{A} \coloneqq \{u \in C^1(\Omega, \mathbb{C}) : \ u\big|_{\partial\Omega} = 0\}.$$

The aim is to find a function u_0 which minimizes I among all $u \in \mathcal{A}$.

Remark. A simple interpretation of this problem in dimension $d = 1$ would be to regard all trajectories u parametrized by x in the $x - u$-plane which connect the boundary points of Ω and to look for a *geodesic* u_0, a trajectory of shortest length or minimal cost with respect to the function F.

If u_0 minimizes I, then I must be stationary at u_0, i.e. the infinitesimal variation δI of I with respect to u must vanish:

$$0 = \delta I[x]\big|_{u=u_0} = \int_\Omega \left(\partial_u F(u, \nabla u, x)\big|_{\substack{u=u_0 \\ \nabla u = \nabla u_0}} \delta u(x) + \partial_{\nabla u} F(u, \nabla u, x)\big|_{\substack{u=u_0 \\ \nabla u = \nabla u_0}} \nabla_x . \delta u(x) \right) dx$$

By partial integration we have

$$0 = \delta I[x]\big|_{u=u_0} = \int_\Omega \left(\partial_u F(u, \nabla u, x)\big|_{\substack{u=u_0 \\ \nabla u = \nabla u_0}} - \nabla_x . \partial_{\nabla u} F(u, \nabla u, x)\big|_{\substack{u=u_0 \\ \nabla u = \nabla u_0}} \right) \delta u(x) dx$$

and since $\delta u(x)$ can be chosen arbitrary for any x

$$\partial_u F(u, \nabla u, x)\big|_{u=u_0} = \nabla_x . \partial_{\nabla u} F(u, \nabla u, x)\big|_{u=u_0}.$$

This is known as the *Euler-Lagrange equations* for a minimizing function u_0 of I.
Moreover, functional derivatives obey the standard product rule for derivatives.

D Self-adjoint operators on Hilbert spaces

Let A be a self-adjoint operator on some Hilbert space $\mathcal{H}$ and denote the set of linear operators on $\mathcal{H}$ by $L(\mathcal{H})$. We recall some basic facts and refer to [16] for details:

Let

- P_A be the unique projection-valued measure on $\mathbb{R}$ such that $A = \int_{\mathbb{R}} \lambda dP_A(\lambda)$,
- $\Phi_A : \mathcal{B}(\mathbb{R}) \to L(\mathcal{H})$, $f \mapsto \int_{\mathbb{R}} f(\lambda) dP_A(\lambda) = f(A)$ be the functional calculus of A,
- $\phi, \psi \in \mathcal{H}$ and $\mu_{\phi,\psi}$ be the corresponding spectral measure such that $\langle \phi, f(A)\psi \rangle = \int_R f(\lambda) d\mu_{\phi,\psi}(\lambda)$, $\mu_\psi = \mu_{\psi,\psi}$
- $\mathcal{H}_\psi$ denote the closed subspace $\{f(A)\psi : \ f \in L^2(\mathbb{R}, d\mu_\psi)\}$ of $\mathcal{H}$.

Definition D.1. (Discrete and essential spectrum of a self-adjoint operator)
Let

$$\sigma(A) \coloneqq \{\lambda \in \mathbb{R} : \ P_A((\lambda - \varepsilon, \lambda + \varepsilon)) \neq 0 \ \forall \varepsilon > 0\} \subseteq \mathbb{R}$$

be the spectrum of A and

$$\mathrm{Res}(A) \coloneqq \mathbb{C} \setminus \sigma(A)$$

be the resolvent set of A. We call

$$\sigma_{\mathrm{d}} \coloneqq \{\lambda \in \mathbb{R} : \ \lambda \textit{ is an isolated eigenvalue of } A \textit{ of finite multiplicity}\}$$

the discrete spectrum of A and

$$\sigma_{\mathrm{ess}}(A) \coloneqq \sigma(A) \setminus \sigma_{\mathrm{d}}(A)$$

the essential spectrum of A, which consists of accumulation points of the spectrum plus isolated eigenvalues of infinite multiplicity. Moreover $\sigma_{\mathrm{ess}}(A)$ is closed.

Lemma D.2. (Existence of a maximal spectral measure)
There exists a maximal spectral measure μ for A, i.e. a spectral measure μ such that $\mu_\psi << \mu$ for all $\psi \in \mathcal{H}$. In particular

$$\sigma(A) = \sigma(\mu) = \{\lambda \in \mathbb{R} : \ \mu((\lambda - \varepsilon, \lambda + \varepsilon)) > 0 \textit{ for all } \varepsilon > 0\}.$$

This allows us to describe the spectrum of A in terms of continuity of a maximal spectral measure μ. Recall that we can uniquely decompose

$$\mu = \mu_{\mathrm{ac}} + \mu_{\mathrm{s}}$$

with μ_{ac} is absolutely continuous with respect to Lebesgue measure and μ_{s} singular with respect to Lebesgue measure and

$$\mu_{\mathrm{s}} = \mu_{\mathrm{sc}} + \mu_{\mathrm{pp}}$$

where μ_{sc} is continuous on $\mathbb{R}$ and μ_{pp} is a step function.

Definition D.3. *We call*

$$\sigma_{\mathrm{ac}}(A) \coloneqq \sigma(\mu_{\mathrm{ac}}), \qquad \sigma_{\mathrm{sc}}(A) \coloneqq \sigma(\mu_{\mathrm{sc}}), \qquad \sigma_{\mathrm{pp}}(A) \coloneqq \sigma(\mu_{\mathrm{pp}})$$

the absolutely continuous, the singular continuous and the pure point spectrum of A.

The set

$$\sigma_p(A) \coloneqq \{\lambda \in \mathbb{R} : \ \lambda \text{ is an eigenvalue of } A\} = \{\lambda \in \mathbb{R} : \ \mu \text{ is discontinuous at } \lambda\}$$

is called the point spectrum or set of eigenvalues of A, which contains the discrete spectrum $\sigma_{\mathrm{d}}(A)$ such as isolated eigenvalues of infinite multiplicity and accumulation points of eigenvalues.

Moreover, the closure of the point spectrum $\overline{\sigma_p(A)}$ coincides with the pure point spectrum $\sigma_{\mathrm{pp}}(A)$.

Definition D.4. (Quadratic form)
The quadratic form corresponding to A is given by

$$q_A(\psi) \coloneqq \int_{\mathbb{R}} \lambda \mu_\psi(\lambda) = \langle \psi, A\psi \rangle, \qquad \mathbf{D}(q_A) \coloneqq \{\psi \in \mathcal{H} : \ \int_{\mathbb{R}} |\lambda| d\mu_\psi(\lambda) < \infty\},$$

where $\mathbf{D}(q_A)$ is called the form domain of A.

Theorem D.5. (Spectral Mapping Theorem, multiplication version)
There exists a countable spectral basis,
i.e. a sequence $\{\psi_n\}_n$ with $\|\psi_n\| = 1$, $\mathcal{H}_{\psi_n} \perp \mathcal{H}_{\psi_k}$ for $n \neq k$ and $\mathcal{H} = \oplus_n \mathcal{H}_{\psi_n}$,
and a unitary operator $U = \oplus_n U_{\psi_n} : \mathcal{H} \to \oplus_n L^2(\mathbb{R}, d\mu_{\psi_n})$ such that $Uf(A) = M_f U$ for every Borel-measurable function f on $\mathbb{R}$, where M_f denotes the multiplication operator by f.

E Chebychev polynomials

The *Chebychev polynomials* defined by

$$T_n(\cos(\theta)) \coloneqq \cos(n\theta) \qquad \textit{(Chebychev polynomials of first kind)},$$
$$U_n(\cos(\theta)) \coloneqq \frac{\sin((n+1)\theta)}{\sin(\theta)} \qquad \textit{(Chebychev polynomials of } 2^{nd} \textit{ kind)}$$

form a complete polynomial on $[-1, 1]$.
Let us focus on the Chebychev polynomials of first kind, used in the proof of Theorem 4.33:

From trigonometric identities we have

$$\begin{aligned} \cos(0) &= 1, \\ \cos(\theta) &= T_1(\theta), \\ \cos(2\theta) &= 2\cos(\theta)^2 - 1 = T_2(\theta), \\ \cos(3\theta) &= 4\cos(\theta)^3 - 3\cos(\theta) = T_3(\theta), \\ &\vdots \end{aligned} \qquad \Longrightarrow \qquad \begin{aligned} T_0(x) &= 1, \\ T_1(x) &= x, \\ T_2(x) &= 2x^2 - 1, \\ T_3(x) &= 4x^3 - 3x, \\ &\vdots \end{aligned}$$

From an approximation theory point of view, Chebychev polynomials have the advantage that the error of an order N approximation of an analytic function on $[-1, 1]$ decreases exponentially in N. In fact, a Chebychev series is just a Fourier-Cosine series in disguise, since

$$f(x) = \sum_{n=0}^{\infty} a_n T_n(x) \qquad \xleftrightarrow{x \,\mapsto \cos(\theta)} \qquad f(\cos(\theta)) = \sum_{n=0}^{\infty} a_n \cos(n\theta)).$$

While the individual terms of a Fourier series, by periodicity, automatically satisfy given boundary conditions, it is still easy to implement boundary conditions for Chebychev polynomials by changing to suitable basis functions as we did in Sections 5 and 6. The main reason for choosing a Chebychev approximation over a Fourier approximation, despite dealing with even/periodic functions on $[-1, 1]$, is to avoid transcendental functions.
We refer to [1] for details.

F Coefficient tables

n	0	1	2	3	4	5	6	7
a_n	$\frac{-127417}{2284380}$	$\frac{3175219}{5947565}$	$\frac{54009}{3628382}$	$\frac{-313677}{2569037}$	$\frac{11320}{2531529}$	$\frac{82381}{4632215}$	$\frac{8521}{5195918}$	$\frac{2150}{3626729}$
n	8	9	10	11	12	13	14	15
a_n	$\frac{61}{559854}$	$\frac{-2647}{2799878}$	$\frac{-1283}{1914313}$	$\frac{-445}{4776544}$	$\frac{846}{6060013}$	$\frac{379}{2750598}$	$\frac{209}{2883415}$	$\frac{71}{4145819}$
n	16	17	18	19	20	21	22	23
a_n	$\frac{-55}{5038118}$	$\frac{-56}{3191591}$	$\frac{-22}{1622717}$	$\frac{-24}{3515321}$	$\frac{-6}{4422853}$	$\frac{12}{7421387}$	$\frac{11}{4561849}$	$\frac{9}{4658824}$
n	24	25	26	27	28	29	30	31
a_n	$\frac{1}{963497}$	$\frac{1}{3788261}$	$\frac{-1}{5255869}$	$\frac{-1}{2899110}$	$\frac{-1}{3232751}$	$\frac{-1}{5102458}$	$\frac{-1}{12402248}$	$\frac{1}{3798255627}$
n	32	33	34	35	36	37	38	39
a_n	$\frac{1}{24437990}$	$\frac{1}{20247538}$	$\frac{1}{24861118}$	$\frac{1}{41910031}$	$\frac{1}{104954716}$	$\frac{-1}{777110184}$	$\frac{-1}{176686297}$	$\frac{-1}{130965769}$
n	40	41	42	43	44	45	46	47
a_n	$\frac{-1}{186545992}$	$\frac{-1}{231399568}$	$\frac{-1}{1023867773}$	$\frac{-1}{1461679003}$	$\frac{1}{749220108}$	$\frac{1}{1429083896}$	$\frac{1}{898580281}$	$\frac{1}{1150752017}$
n	48	49	50	51	52	53		
a_n	$\frac{-1}{9662677202}$	$\frac{1}{1174658503}$	$\frac{-1}{1119506863}$	$\frac{1}{1596316017}$	$\frac{-1}{1428969364}$	$\frac{1}{7629617650}$		

Table 1: Table of coefficients a_n for g_1

n	2	3	4	5	6	7	8	9
a_n^+	$\frac{62516}{56795}$	$\frac{-3443}{16182}$	$\frac{-15843}{77263}$	$\frac{-1007}{21768}$	$\frac{-1298}{33953}$	$\frac{335}{7099}$	$\frac{1541}{26409}$	$\frac{-137}{33477}$
n	10	11	12	13	14	15	16	17
a_n^+	$\frac{-526}{47741}$	$\frac{-174}{22091}$	$\frac{-251}{26905}$	$\frac{60}{31609}$	$\frac{319}{86050}$	$\frac{13}{10817}$	$\frac{47}{34878}$	$\frac{-11}{32444}$
n	18	19	20	21	22	23	24	25
a_n^+	$\frac{-16}{23705}$	$\frac{-6}{30017}$	$\frac{-7}{28769}$	$\frac{1}{41309}$	$\frac{1}{14242}$	$\frac{1}{29847}$	$\frac{2}{38437}$	$\frac{1}{118902}$
n	26	27	28	29	30	31	32	33
a_n^+	$\frac{1}{121669}$	$\frac{-1}{391833}$	$\frac{-1}{138738}$	$\frac{-1}{255278}$	$\frac{-1}{146591}$	$\frac{-1}{687991}$	$\frac{-1}{657613}$	$\frac{1}{1979293}$
n	34	35	36	37	38	39	40	
a_n^+	$\frac{1}{682036}$	$\frac{1}{1305396}$	$\frac{1}{811882}$	$\frac{1}{4704965}$	$\frac{1}{200724713}$	$\frac{-1}{3730255}$	$\frac{-1}{3749935}$	

Table 2: Coefficients a_n^+ for w_+ of the operator $\mathcal{L}_{1,c}$

n	2	3	4	5	6	7	8
a_n^-	$\frac{62516}{56795}$	$\frac{3443}{16182}$	$\frac{-15843}{77263}$	$\frac{1007}{21768}$	$\frac{-1298}{33953}$	$\frac{-335}{7099}$	$\frac{1541}{26409}$
n	9	10	11	12	13	14	15
a_n^-	$\frac{137}{33477}$	$\frac{-526}{47741}$	$\frac{174}{22091}$	$\frac{-251}{26905}$	$\frac{-60}{31609}$	$\frac{319}{86050}$	$\frac{-13}{10817}$
n	16	17	18	19	20	21	22
a_n^-	$\frac{47}{34878}$	$\frac{11}{32444}$	$\frac{-16}{23705}$	$\frac{6}{30017}$	$\frac{-7}{28769}$	$\frac{-1}{41309}$	$\frac{1}{14242}$
n	23	24	25	26	27	28	29
a_n^-	$\frac{-1}{29847}$	$\frac{2}{38437}$	$\frac{-1}{118902}$	$\frac{1}{121669}$	$\frac{1}{391833}$	$\frac{-1}{138738}$	$\frac{1}{255277}$
n	30	31	32	33	34	35	36
a_n^-	$\frac{-1}{146591}$	$\frac{1}{687991}$	$\frac{-1}{657613}$	$\frac{-1}{1979293}$	$\frac{1}{682036}$	$\frac{-1}{1305396}$	$\frac{1}{811882}$
n	37	38	39	40			
a_n^-	$\frac{-1}{4704962}$	$\frac{1}{200717985}$	$\frac{1}{3730258}$	$\frac{-1}{3749936}$			

Table 3: Coefficients a_n^- for w_- of the operator $\mathcal{L}_{1,c}$

n	0	1	2	3	4	5	6	7
a_n	$\frac{3057947}{5149984}$	$\frac{-560468}{2926017}$	$\frac{555463}{2414423}$	$\frac{108165}{1332413}$	$\frac{-258701}{3982156}$	$\frac{-187869}{3305963}$	$\frac{-50765}{4602801}$	$\frac{7582}{581015}$
n	8	9	10	11	12	13	14	15
a_n	$\frac{28443}{1926251}$	$\frac{16607}{2348410}$	$\frac{-210}{2099353}$	$\frac{-12719}{3977811}$	$\frac{-5451}{1819340}$	$\frac{-14087}{9463755}$	$\frac{-734}{6122245}$	$\frac{2096}{3660951}$
n	16	17	18	19	20	21	22	23
a_n	$\frac{3901}{5903745}$	$\frac{1191}{2737913}$	$\frac{228}{1481249}$	$\frac{-75}{1727618}$	$\frac{-242}{1925727}$	$\frac{-247}{2029698}$	$\frac{-303}{3943481}$	$\frac{-13}{473690}$
n	24	25	26	27	28	29	30	31
a_n	$\frac{32}{4382505}$	$\frac{230}{9991221}$	$\frac{24}{1004449}$	$\frac{101}{5992591}$	$\frac{33}{4167475}$	$\frac{3}{4069691}$	$\frac{-10}{2977617}$	$\frac{-9}{1953280}$
n	32	33	34	35	36	37	38	39
a_n	$\frac{-32}{8048373}$	$\frac{-14}{5569467}$	$\frac{-3}{2962310}$	$\frac{1}{10404223}$	$\frac{2}{2900835}$	$\frac{4}{4753783}$	$\frac{3}{4230950}$	$\frac{1}{2205507}$
n	40	41	42	43	44	45	46	47
a_n	$\frac{1}{5162703}$	$\frac{-1}{398618662}$	$\frac{-1}{8716103}$	$\frac{-1}{6602839}$	$\frac{-1}{7305761}$	$\frac{-1}{10420905}$	$\frac{-1}{19955312}$	$\frac{-1}{86906636}$
n	48	49	50	51	52	53	54	55
a_n	$\frac{1}{74325145}$	$\frac{1}{39270247}$	$\frac{1}{37615488}$	$\frac{1}{45898496}$	$\frac{1}{72267468}$	$\frac{1}{153045540}$	$\frac{1}{2866041410}$	$\frac{-1}{335813134}$
n	56	57	58	59	60	61	62	63
a_n	$\frac{-1}{205911985}$	$\frac{-1}{224059828}$	$\frac{-1}{256933874}$	$\frac{-1}{467177014}$	$\frac{-1}{754368719}$	$\frac{1}{5788651424}$	$\frac{1}{4105990847}$	$\frac{1}{882557051}$
n	64	65	66	67	68	69	70	71
a_n	$\frac{1}{2110021797}$	$\frac{1}{930919993}$	$\frac{1}{51687779654}$	$\frac{1}{1367489807}$	$\frac{-1}{1994690970}$	$\frac{1}{1782892689}$	$\frac{-1}{1179482381}$	$\frac{1}{1502906635}$
n	72	73	74	75	76	77	78	79
a_n	$\frac{-1}{938445455}$	$\frac{1}{1028946431}$	$\frac{-1}{772657506}$	$\frac{1}{714144826}$	$\frac{-1}{606009315}$	$\frac{1}{517153258}$	$\frac{-1}{454297801}$	$\frac{1}{382565452}$
n	80	81	82	83	84	85	86	87
a_n	$\frac{-1}{334768183}$	$\frac{1}{284940123}$	$\frac{-1}{247516840}$	$\frac{1}{213584097}$	$\frac{-1}{185778281}$	$\frac{1}{162485095}$	$\frac{-1}{142890747}$	$\frac{1}{127035905}$
n	88	89	90	91	92	93	94	95
a_n	$\frac{-1}{113927095}$	$\frac{1}{103642993}$	$\frac{-1}{95659607}$	$\frac{1}{89977221}$	$\frac{-1}{86531021}$	$\frac{1}{85501352}$	$\frac{-1}{87435252}$	$\frac{1}{93401490}$
n	96	97	98	99	100	101	102	103
a_n	$\frac{-1}{106015030}$	$\frac{1}{131668031}$	$\frac{-1}{192139867}$	$\frac{1}{426319358}$	$\frac{1}{1186676000}$	$\frac{-1}{240832788}$	$\frac{1}{136368077}$	$\frac{-1}{98884847}$
n	104	105	106	107	108	109	110	111
a_n	$\frac{1}{81706109}$	$\frac{-1}{73978942}$	$\frac{1}{72195937}$	$\frac{-1}{75404149}$	$\frac{1}{84085497}$	$\frac{-1}{100184227}$	$\frac{1}{127885910}$	$\frac{-1}{175753062}$
n	112	113	114	115	116	117	118	
a_n	$\frac{1}{261763015}$	$\frac{-1}{426431192}$	$\frac{1}{768872892}$	$\frac{-1}{1560067213}$	$\frac{1}{3641816109}$	$\frac{-1}{10122637386}$	$\frac{1}{35268403948}$	

Table 4: Coefficients a_n for g_2

n	2	3	4	5	6	7	8	9
a_n^+	$\frac{3587}{17075}$	$\frac{-745}{13489}$	$\frac{-1178}{21833}$	$\frac{-743}{30422}$	$\frac{58}{9915}$	$\frac{587}{38332}$	$\frac{213}{40426}$	$\frac{-9}{49022}$
n	10	11	12	13	14	15	16	17
a_n^+	$\frac{-80}{42241}$	$\frac{-27}{12517}$	$\frac{-19}{38445}$	$\frac{5}{21076}$	$\frac{28}{93073}$	$\frac{3}{10408}$	$\frac{2}{30993}$	$\frac{-1}{31133}$
n	18	19	20	21	22	23	24	25
a_n^+	$\frac{-1}{23118}$	$\frac{-1}{21473}$	$\frac{-1}{64664}$	$\frac{-1}{1652738}$	$\frac{1}{168001}$	$\frac{1}{97613}$	$\frac{1}{177689}$	$\frac{1}{270261}$
n	26	27	28	29	30	31	32	33
a_n^+	$\frac{1}{2205525}$	$\frac{-1}{626133}$	$\frac{-1}{617642}$	$\frac{-1}{488021}$	$\frac{-1}{1001008}$	$\frac{-1}{1777864}$	$\frac{1}{142602543}$	$\frac{1}{2492035}$
n	34	35	36	37	38	39	40	
a_n^+	$\frac{1}{2770245}$	$\frac{1}{2259306}$	$\frac{1}{4734297}$	$\frac{1}{9558129}$	$\frac{-1}{29939258}$	$\frac{-1}{6532083}$	$\frac{-1}{14493211}$	

Table 5: Coefficients a_n^+ for w_+ of the operator $\mathcal{L}_{2,c}$

n	2	3	4	5	6	7	8	9
a_n^-	$\frac{3587}{17075}$	$\frac{745}{13489}$	$\frac{-1178}{21833}$	$\frac{743}{30422}$	$\frac{58}{9915}$	$\frac{-587}{38332}$	$\frac{213}{40426}$	$\frac{9}{49022}$
n	10	11	12	13	14	15	16	17
a_n^-	$\frac{-80}{42241}$	$\frac{27}{12517}$	$\frac{-19}{38445}$	$\frac{-5}{21076}$	$\frac{28}{93073}$	$\frac{-3}{10408}$	$\frac{2}{30993}$	$\frac{1}{31133}$
n	18	19	20	21	22	23	24	25
a_n^-	$\frac{-1}{23118}$	$\frac{1}{21473}$	$\frac{-1}{64664}$	$\frac{1}{1652738}$	$\frac{1}{168001}$	$\frac{-1}{97613}$	$\frac{1}{177689}$	$\frac{-1}{270261}$
n	26	27	28	29	30	31	32	33
a_n^-	$\frac{1}{2205525}$	$\frac{1}{626133}$	$\frac{-1}{617642}$	$\frac{1}{488021}$	$\frac{-1}{1001008}$	$\frac{1}{1777863}$	$\frac{1}{142603040}$	$\frac{-1}{2492036}$
n	34	35	36	37	38	39	40	
a_n^-	$\frac{1}{2770245}$	$\frac{-1}{2259306}$	$\frac{1}{4734296}$	$\frac{-1}{9558125}$	$\frac{-1}{29939302}$	$\frac{1}{6532085}$	$\frac{-1}{14493216}$	

Table 6: Coefficients a_n^- for w_- of the operator $\mathcal{L}_{2,c}$

References

[1] John P. Boyd. *Chebyshev and Fourier spectral methods*. Second. Dover Publications, Inc., Mineola, NY, 2001, pp. xvi+668.

[2] Matthew Creek et al. "Linear stability of the skyrmion". *Int. Math. Res. Not. IMRN* 2017. 8. Pp. 2497–2537. URL: https://doi.org/10.1093/imrn/rnw114.

[3] Roland Donninger and Birgit Schörkhuber. "Self-similar Blowup for the cubic Schrödinger Equation". *preprint arXiv: 2406.16597* 2024.

[4] Gadi Fibich, Frank Merle, and Pierre Raphaël. "Proof of a spectral property related to the singularity formation for the L^2 critical nonlinear Schrödinger equation". *Phys. D* 2006. 2201. Pp. 1–13. URL: https://doi.org/10.1016/j.physd.2006.06.010.

[5] J. Ginibre and G. Velo. "On a class of nonlinear Schrödinger equations. I. The Cauchy problem, general case". *J. Functional Analysis* 1979. 321. Pp. 1–32. URL: https://doi.org/10.1016/0022-1236(79)90076-4.

[6] Brian C. Hall. *Quantum theory for mathematicians*. Vol. 267. Graduate Texts in Mathematics. Springer, New York, 2013, pp. xvi+554. URL: https://doi.org/10.1007/978-1-4614-7116-5.

[7] Man Kam Kwong. "Uniqueness of positive solutions of $\Delta u - u + u^p = 0$ in $\mathbf{R}^n$". *Arch. Rational Mech. Anal.* 1989. 1053. Pp. 243–266. URL: https://doi.org/10.1007/BF00251502.

[8] Yvan Martel and Frank Merle. "A Liouville theorem for the critical generalized Korteweg-de Vries equation". *J. Math. Pures Appl. (9)* 2000. 794. Pp. 339–425. URL: https://doi.org/10.1016/S0021-7824(00)00159-8.

[9] Kevin McLeod. "Uniqueness of positive radial solutions of $\Delta u + f(u) = 0$ in $\mathbf{R}^n$. II". *Trans. Amer. Math. Soc.* 1993. 3392. Pp. 495–505. URL: https://doi.org/10.2307/2154282.

[10] Frank Merle and Pierre Raphael. "The blow-up dynamic and upper bound on the blow-up rate for critical nonlinear Schrödinger equation". *Ann. of Math. (2)* 2005. 1611. Pp. 157–222. URL: https://doi.org/10.4007/annals.2005.161.157.

[11] Galina Perelman. "On the blow up phenomenon for the critical nonlinear Schrödinger equation in 1D". In: *Séminaire: Équations aux Dérivées Partielles, 1999–2000*. Sémin. Équ. Dériv. Partielles. École Polytech., Palaiseau, 2000, Exp. No. III, 16.

[12] Robin Santra. *Einführung in den Lagrange- und Hamilton-Formalismus*. Springer Spektrum, 2022.

[13] Wilhelm Schlag, Avy Soffer, and Wolfgang Staubach. "Decay for the wave and Schrödinger evolutions on manifolds with conical ends. I". *Trans. Amer. Math. Soc.* 2010. 3621. Pp. 19–52. URL: https://doi.org/10.1090/S0002-9947-09-04690-X.

[14] Catherine Sulem and Pierre-Louis Sulem. *The nonlinear Schrödinger equation*. Vol. 139. Applied Mathematical Sciences. Self-focusing and wave collapse. Springer-Verlag, New York, 1999, pp. xvi+350.

[15] Terence Tao. *Nonlinear dispersive equations*. Vol. 106. CBMS Regional Conference Series in Mathematics. Local and global analysis. Conference Board of the Mathematical Sciences, Washington, DC; by the American Mathematical Society, Providence, RI, 2006, pp. xvi+373. URL: https://doi.org/10.1090/cbms/106.

[16] Gerald Teschl. *Mathematical methods in quantum mechanics*. Second. Vol. 157. Graduate Studies in Mathematics. With applications to Schrödinger operators. American Mathematical Society, Providence, RI, 2014, pp. xiv+358. URL: https://doi.org/10.1090/gsm/157.

[17] Michael I. Weinstein. "Modulational stability of ground states of nonlinear Schrödinger equations". *SIAM J. Math. Anal.* 1985. 163. Pp. 472–491. URL: https://doi.org/10.1137/0516034.

[18] Michael I. Weinstein. "Nonlinear Schrödinger equations and sharp interpolation estimates". *Comm. Math. Phys.* 1982/83. 874. Pp. 567–576. URL: http://projecteuclid.org/euclid.cmp/1103922134.

[19] Kai Yang, Svetlana Roudenko, and Yanxiang Zhao. "Blow-up dynamics and spectral property in the L^2-critical nonlinear Schrödinger equation in high dimensions". *Nonlinearity* 2018. 319. Pp. 4354–4392. URL: https://doi.org/10.1088/1361-6544/aacc41.