Chebyshev spectral and pseudo-spectral methods in unbounded domains

by

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Preface

The work described in this dissertation was carried out in the School of Mathematics, Satistics and Computer Science at University of KwaZulu-Natal, Durban, from July 2014 to July 2015, under the supervision of Dr S.K. Shindin and Dr N. Parumasur.

This study represents original work by the author and has not otherwise been submitted in any form for any degree or diploma to any other tertiary institution. Where use has been made of the work of others, it is duly acknowledged in the text.

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Above all, I thank God for being beside me every step of the way and for giving me good health, guidance and strength to this stage.

Abstract

Chebyshev type spectral methods are widely used in numerical simulations of PDEs posed in unbounded domains. Such methods have a number of important computational advantages. In particular, they admit very efficient practical implementation. However, the stability and convergence analysis of these methods require deep understanding of approximation properties of the underlying functional basis. In this project, we deal with Chebyshev spectral and pseudo-spectral methods in unbounded domains. The first part of the project deals with theoretical analysis of Chebyshev-type spectral projection and interpolation operators in Bessel potential spaces. In the second part, we provide rigorous analyses of Chebyshev-type pseudo-spectral (collocation) scheme applied to the nonlinear Schrödinger equation. The project is concluded with several numerical experiments.

Contents

Introduction

Spectral methods were first developed by Steven Orzag in 1969 through a long series of papers. These methods belong to a class of techniques that are used in applied mathematics and scientific computing to numerically solve specific differential equations. To construct these methods, we first write the solution of the differential equation as a sum of specific "basis functions." Then, we specifically choose the coefficients in the sum, so that they satisfy the differential equation as well as possible.

Spectral methods can be applied to solve PDEs, ODEs and eigenvalue problems that involve differential equations. Spectral methods are implemented by using either collocation or by using a Galerkin or Tau approach [Fun92, Boy00, Tre00, CQHZ06, HGG07, STW11]. These methods are computationally less expensive than other methods. However, they become less accurate when problems with complex geometries and discontinuous coefficients are involved.

Pseudo-spectral methods are closely aligned to spectral methods, but contain an additional pseudo-spectral basis. Using these methods, we can approximate a function as a weighted sum of smooth basis functions. These basis functions are often chosen to be Chebyshev or Legendre polynomials [Fun92, Boy00, Tre00, CQHZ06, HGG07, SP10, STW11, JBS14].

In this thesis, we deal specifically with Chebyshev spectral and pseudo-spectral methods in unbounded domains. Such methods have a number of important computational advantages. In particular, they allow very efficient practical implementation. However, the stability and convergence analysis of these methods requires deep understanding of approximation properties of the underlying functional basis.

The project is organized as follows: Chapter 1 contains results related to the Fourier transform, fractional calculus and some basic theory of function spaces. In Chapter 2, we define the algebraically mapped Chebyshev basis and establish its connection with Laguerre functions. The main results of our research are presented in Chapter 3. In this Chapter, we provide approximation and interpolation estimates in $L^2(\mathbb{R})$ and $H^{2,\alpha}(\mathbb{R})$ settings. These results form a foundation for the theory of Chebyshev-type spectral and pseudo-spectral (collocation) schemes. In Chapter 4, we apply Chebyshev-type pseudo-spectral method to the classical nonlinear Schrödinger equation and conclude this chapter by adding several numerical experiments.

Chapter 1

Preliminaries

In the thesis, we shall study Chebyshev type pseudo-spectral methods for differential equations posed in the real line. An analysis of such methods is based on approximative properties of the algebraically mapped Chebyshev basis. As we shall see later, these properties are controlled by two parameters — the regularity and decay rate at infinity of functions $f(x)$ being approximated. In the thesis, we work mainly in Hilbert space settings. In that case, both properties can be naturally described in terms of Fourier images of $f(x)$. Below, we list several results related to the Fourier transform, fractional calculus and some basic theory of function spaces. These results are used extensively in Chapter 3.

1.1 The Fourier transform

The (normalized) Fourier transform and its inverse, when applied to $f \in L^p(\mathbb{R})$, with $1 \le p \le 2$, are given by (see, for instance, [SS03])

$$\mathcal{F}[f](s) = \hat{f}(s) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-isx} f(x)dx, \tag{1.1.1a}$$

$$\mathcal{F}^{-1}[\hat{f}](x) = f(x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{isx} \hat{f}(s)ds. \tag{1.1.1b}$$

When $1 < p \le 2$ both integrals are understood in the principle value sense. From standard theory [SS03] it is known that

$$\langle f, g\rangle = \langle \hat{f}, \hat{g}\rangle \quad \text{and in particular} \quad \|f\|_{L^2(\mathbb{R})} = \|\hat{f}\|_{L^2(\mathbb{R})}, \tag{1.1.2a}$$

$$\mathcal{F}[fg](s) = [\hat{f} * \hat{g}](s) = \int_{\mathbb{R}} \hat{f}(s-t)\hat{g}(t)dt, \tag{1.1.2b}$$

$$\mathcal{F}^{-1}[\hat{f}\hat{g}](x) = [f * g](x) = \int_{\mathbb{R}} f(x-y)g(y)dy, \tag{1.1.2c}$$

$$\mathcal{F}[f'](s) = is\hat{f}(s) = is\mathcal{F}[f](s), \tag{1.1.2d}$$

$$\mathcal{F}^{-1}[\hat{f}'](x) = -ixf(x) = -ix\mathcal{F}^{-1}[\hat{f}](x). \tag{1.1.2e}$$

Formula (1.1.2) (known as *Parseval's identity*) indicates that the Lebesgue space $L^2(\mathbb{R})$ and its Fourier image $\mathcal{F}[L^2(\mathbb{R})]$ are isometrically isomorphic. Formulas (1.1.2b)-(1.1.2e) hold for all sufficiently smooth functions and can be obtained directly from (1.1.1), see [SS03].

1.2 Fractional integrals and derivatives

There are several possible ways of measuring regularity of functions. The simplest one is to use classical derivatives. However, in many applications, this approach is very limited. Below, we employ the measure of regularity based on the use of Bessel fractional integrals. This approach is commonly used in the theory of partial differential equations and in analysis, see [SW71, SKM93, AF03, Bre11, Gra14] and references therein.

1.2.1 The Bessel fractional integrals

In terms of Fourier images, the left (right) Bessel fractional integrals (denoted by $J_{\pm}^{\alpha,\ell}$, respectively) of order $\alpha > 0$, are given by

$$J_{\pm}^{\alpha,\ell}[f](x) = \frac{1}{\sqrt{2\pi}}\mathcal{F}^{-1}[(\ell \pm is)^{-\alpha}\hat{f}](x), \tag{1.2.1}$$

where $\ell > 0$.

Lemma 1.2.1 (see [SKM93])**.** *The left (right) Bessel fractional integrals can be realized as the Fourier convolution*

$$J_{\pm}^{\alpha,\ell}[f](x) = \frac{1}{\Gamma(\alpha)}\left[x_{\pm}^{\alpha-1}e^{\pm\ell x} * f\right](x), \tag{1.2.2}$$

where

$$x_{+}^{\alpha-1} = \begin{cases} x^{\alpha-1}, & x \geq 0, \\ 0, & x < 0, \end{cases} \qquad x_{-}^{\alpha-1} = \begin{cases} 0, & x > 0, \\ (-x)^{\alpha-1}, & x \leq 0, \end{cases}$$

are cut-off functions.

Proof. From (1.1.2c) it follows that

$$J_{\pm}^{\alpha,\ell}[f](x) = \frac{1}{\sqrt{2\pi}}\left[\mathcal{F}^{-1}[(\ell \pm is)^{-\alpha}] * f\right](x).$$

We have

$$\mathcal{F}^{-1}[(\ell \pm is)^{-\alpha}](x) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \frac{e^{isx}}{(\ell \pm is)^{\alpha}}ds,$$

where z^{α} is understood in the sense of the principal value. Making the substitution $z = \ell \pm is$ and using the fact that z^{α} is analytic everywhere outside the region $\{\mathrm{Re}z \leq 0, \mathrm{Im}z = 0\}$, we infer:

$$\mathcal{F}^{-1}[(\ell \pm is)^{-\alpha}](x) = i\frac{e^{\mp\ell x}}{\sqrt{2\pi}}\int_{\gamma} \frac{e^{\pm zx}}{z^{\alpha}}dz,$$

where γ is a contour that goes around the line $\{\mathrm{Re}z \leq 0, \mathrm{Im}z = 0\}$ in the counterclockwise direction. Hence, making one more substitution $u = \pm xz$ to obtain

$$\mathcal{F}^{-1}[(\ell \pm is)^{-\alpha}](x) = i\frac{x_{\pm}^{\alpha-1}e^{\mp\ell x}}{\sqrt{2\pi}} \int_{\gamma} \frac{e^z}{z^\alpha} dz.$$

Since, $\dfrac{e^z}{z^\alpha}$ is analytic in the region $\{\mathrm{Re}z \leq \ell\}/\{\mathrm{Re}z \leq 0, \mathrm{Im}z = 0\}$ and since contour integrals over arcs

$$|z-\ell| \leq R, \quad \arg z \in \left(\arctan\frac{\sqrt{R^2-\ell^2}}{\ell}, \frac{\pi}{2}\right) \cup \left(-\frac{\pi}{2}, -\arctan\frac{\sqrt{R^2-\ell^2}}{\ell}\right)$$

vanish as R approaches infinity, we deform contour γ into a contour γ_1 that goes around negative part of real axis in counterclockwise direction and apply Hankels formula for $\dfrac{1}{\Gamma(z)}$. This gives

$$\mathcal{F}^{-1}[(\ell \pm is)^{-\alpha}](x) = i\frac{x_{\pm}^{\alpha-1}e^{\mp\ell x}}{\sqrt{2\pi}} \int_{\gamma_1} \frac{e^z}{z^\alpha} dz = \frac{\sqrt{2\pi}}{\Gamma(\alpha)} x_{\pm}^{\alpha-1} e^{\mp\ell x}.$$

The last formula completes the proof. □

The main properties of Bessel's fractional integrals are listed below:

Lemma 1.2.2 (see [SKM93])**.** *The Bessel fractional integrals on the line satisfy:*

$$\int_{\mathbb{R}} f J_{\pm}^{\alpha}[g] dx = \int_{\mathbb{R}} J_{\pm}^{\alpha}[f] g dx, \tag{1.2.3a}$$

$$J_{\pm}^{\alpha} J_{\pm}^{\beta}[f] = J_{\pm}^{\alpha+\beta}[f], \tag{1.2.3b}$$

provided that integrals that appear on the left and right-hand sides of each formula exist. Identity (1.2.3a) *is known as the* formula of fractional integration by parts*. Formula* (1.2.3b) *indicates that the Bessel fractional integrals on the line satisfy the* semigroup property*.*

Proof. To prove(1.2.3a), we change the order of integration:

$$\begin{aligned}
\int_{\mathbb{R}} f J_{\pm}^{\alpha}[g] dx &= \int_{\mathbb{R}} f(x) \frac{dx}{\Gamma(\alpha)} \int_{\mathbb{R}} g(x-y) y_{\pm}^{\alpha-1} e^{\mp \ell y} dy \\
&= \int_{\mathbb{R}} f(x) \frac{dx}{\Gamma(\alpha)} \int_{\mathbb{R}} g(y)(x-y)_{\pm}^{\alpha-1} e^{\mp \ell (x-y)} dy \\
&= \int_{\mathbb{R}} g(y) \frac{dy}{\Gamma(\alpha)} \int_{\mathbb{R}} f(x)(x-y)_{\pm}^{\alpha-1} e^{\mp \ell (x-y)} dx \\
&= \int_{\mathbb{R}} g(y) \frac{dy}{\Gamma(\alpha)} \int_{\mathbb{R}} f(y-x) x_{\mp}^{\alpha-1} e^{\pm \ell y} dx = \int_{\mathbb{R}} J_{\mp}^{\alpha}[f] g dx.
\end{aligned}$$

The semigroup property (1.2.3b) is obtained in the same way:

$$\begin{aligned}
J_{\pm}^{\alpha} J_{\pm}^{\beta}[f](x) = &= \frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(\beta)} \int_{\mathbb{R}} y_{\pm}^{\alpha-1} e^{\mp \ell y} dy \int_{\mathbb{R}} z_{\pm}^{\beta-1} e^{\mp \ell z} f(x-y-z) dz \\
&= \frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(\beta)} \int_{\mathbb{R}} y_{\pm}^{\alpha-1} e^{\mp \ell y} dy \int_{\mathbb{R}} (z-y)_{\pm}^{\beta-1} e^{\mp \ell (z-y)} f(x-z) dz \\
&= \frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(\beta)} \int_{\mathbb{R}} f(x-z) e^{\mp \ell z} dz \int_{\mathbb{R}} y_{\pm}^{\alpha-1} (z-y)_{\pm}^{\beta-1} dy \\
&= \frac{1}{\Gamma(\alpha)} \frac{1}{\Gamma(\beta)} \int_{\mathbb{R}} f(x-z) z_{\pm}^{\alpha+\beta-1} e^{\mp \ell z} dz \int_{0}^{1} t^{\alpha-1} (1-t)^{\beta-1} dt \\
&= \frac{1}{\Gamma(\alpha+\beta)} \int_{\mathbb{R}} f(x-z) z_{\pm}^{\alpha+\beta-1} e^{\mp \ell z} dz = J_{\pm}^{\alpha+\beta}[f](x).
\end{aligned}$$

□

1.2.2 The Bessel fractional derivatives

It is not difficult to see that operators $J_{\pm}^{\alpha}$, $\alpha > 0$ are invertible. In terms of Fourier images, the inverse is given by formula (1.2.1) with negative exponent $-\alpha$. However, in some calculations, it is convenient to use the representation of $J_{\pm}^{-\alpha}$ in terms of the original function f. The explicit construction is provided below.

To begin, we assume that $0 < \alpha < 1$. For sufficiently regular functions, the *left (right) Bessel fractional derivatives* on the real line are defined as follows:

$$\begin{aligned} J_{\pm}^{-\alpha}[f](x) &= e^{\mp\ell x}\frac{d}{dx}[e^{\pm\ell x}J_{\pm}^{1-\alpha}[f](x)] \\ &= \frac{e^{\mp\ell x}}{\Gamma(1-\alpha)}\frac{d}{dx}\int_{\mathbb{R}} f(x-y)y_{\pm}^{-\alpha}e^{\mp\ell(y-x)}dy. \end{aligned} \tag{1.2.4}$$

We observe that $J_{\pm}^{-\alpha}$, with $0<\alpha<1$, is the left inverse of $J_{\pm}^{\alpha}$ for smooth functions f. Furthermore, formula (1.2.4) can be rewritten in the equivalent form [SKM93]:

$$\begin{aligned} J_{\pm}^{-\alpha}[f](x) &= \frac{e^{\mp\ell x}}{\Gamma(1-\alpha)}\int_{\mathbb{R}}\frac{d}{dx}\Big[f(x-y)e^{\mp\ell(y-x)}\Big]y_{\pm}^{-\alpha}dy \\ &= \pm\frac{e^{\mp\ell x}\alpha}{\Gamma(1-\alpha)}\int_{\mathbb{R}}h(\pm y)\frac{d}{dx}\Big[f(x-y)e^{\mp\ell(y-x)}\Big]\int_{y}^{\pm\infty}z_{\pm}^{-1-\alpha}dzdy \\ &= \pm\frac{e^{\mp\ell x}\alpha}{\Gamma(1-\alpha)}\int_{\mathbb{R}}z_{\pm}^{-1-\alpha}\int_{0}^{z}\frac{d}{dx}\Big[f(x-y)e^{\mp\ell(y-x)}\Big]dydz \\ &= \pm\frac{e^{\mp\ell x}\alpha}{\Gamma(1-\alpha)}\int_{\mathbb{R}}z_{\pm}^{-1-\alpha}\Big[f(x-y)e^{\mp\ell(y-x)}\Big]_{y=z}^{y=0}dz, \end{aligned}$$

where $h(y)=\dfrac{y_+}{|y|}$ is the Heaviside function. Using the notation $\Delta_h^1[f](x)=f(x)-f(x-h)$, the last formula reads

$$J_{\pm}^{-\alpha}[f](x)=\pm\frac{e^{\mp\ell x}\alpha}{\Gamma(1-\alpha)}\int_{\mathbb{R}}\Delta_z^1[fe^{\pm\ell\cdot}](x)z_{\pm}^{-1-\alpha}dz. \tag{1.2.5}$$

We note that (1.2.5) makes sense for a wider class of functions as compared to (1.2.4). Formula (1.2.5) is known as the *Bessel-Marchaud fractional derivative* in the real line, see [SKM93].

In the remainder of this section, we show that formula (1.2.5) can be extended to all $\alpha>0$. For this, we employ the notion of finite differences of order n. Let f be analytic at x, then

$$f(x+h)=\sum_{n\geq 0}\frac{1}{n!}\Big(h\frac{d}{dx}\Big)^n f(x)=: e^{h\frac{d}{dx}}f(x),$$

at least formally. The *finite difference of order* n is given by the identity

$$\Delta_h^n[f](x)=\big(1-e^{-h\frac{d}{dx}}\big)^n f(x)=\sum_{m=0}^{n}\binom{n}{m}(-1)^m f(x-mh). \tag{1.2.6}$$

Using (1.2.6) we define

$$J_{\pm}^{-\alpha}[f](x) = \pm\frac{e^{\mp\ell x}}{\kappa(\alpha)}\int_{\mathbb{R}} \Delta_y^{\lfloor\alpha\rfloor+1}[fe^{\pm\ell\cdot}](x)y_{\pm}^{-1-\alpha}dy, \qquad (1.2.7)$$

where $\lfloor\alpha\rfloor$ denotes the largest positive integer that is smaller than or equal to α. We show below that the normalization coefficient $\kappa(\alpha)$ can be chosen so that $J_{\pm}^{-\alpha}J_{\pm}^{\alpha}[f] = f$ for all smooth functions f.

Lemma 1.2.3 (see [SKM93]). *For continuous functions with compact support, the operator $J_{\pm}^{-\alpha}$ is the left inverse of $J_{\pm}^{\alpha}$, provided that*

$$\kappa(\alpha) = \frac{1}{\Gamma(\alpha+1)}\int_0^\infty \Delta_1^{\lfloor\alpha\rfloor+1}[z_+^\alpha](z)\frac{dz}{z}. \qquad (1.2.8)$$

Proof. Let us evaluate the composition $J_{\pm}^{-\alpha}J_{\pm}^{\alpha}[f]$. For this, we introduce the truncated operator

$$J_{\pm,\varepsilon}^{-\alpha}[f](x) = \pm\frac{e^{\mp\ell x}}{\kappa(\alpha)}\int_{|y|\geq\varepsilon} \Delta_y^{\lfloor\alpha\rfloor+1}[fe^{\pm\ell\cdot}](x)y_{\pm}^{-1-\alpha}dy.$$

Then

$$\begin{aligned}
J_{\pm,\varepsilon}^{-\alpha}J_{\pm}^{\alpha}[f](x) &= \pm\frac{e^{\mp\ell x}}{\Gamma(\alpha)\kappa(\alpha)}\int_{|y|\geq\varepsilon}\sum_{m=0}^{\lfloor\alpha\rfloor+1}\binom{\lfloor\alpha\rfloor+1}{m}(-1)^m e^{\pm\ell(x-my)} \\
&\qquad \int_{\mathbb{R}} f(x-my-z)z_{\pm}^{\alpha-1}e^{\mp\ell z}y_{\pm}^{-\alpha-1}dzdy \\
&= \pm\frac{e^{\mp\ell x}}{\Gamma(\alpha)\kappa(\alpha)}\int_{|y|\geq\varepsilon}\sum_{m=0}^{\lfloor\alpha\rfloor+1}\binom{\lfloor\alpha\rfloor+1}{m}(-1)^m e^{\pm\ell(x-my)} \\
&\qquad \int_{\mathbb{R}} f(x-z)(z-my)_{\pm}^{\alpha-1}e^{\mp\ell(z-my)}y_{\pm}^{-\alpha-1}dzdy \\
&= \pm\frac{1}{\Gamma(\alpha)\kappa(\alpha)}\int_{|y|\geq\varepsilon}\int_{\mathbb{R}} f(x-z)e^{\mp\ell z}\Delta_y^{\lfloor\alpha\rfloor+1}[z_{\pm}^{\alpha-1}](z)y_{\pm}^{-\alpha-1}dzdy \\
&= \pm\frac{1}{\Gamma(\alpha)\kappa(\alpha)}\int_{\mathbb{R}} f(x-\varepsilon z)e^{\mp\ell\varepsilon z}\int_{|y|\geq1}\Delta_y^{\lfloor\alpha\rfloor+1}[z_{\pm}^{\alpha-1}](z)y_{\pm}^{-\alpha-1}dydz \\
&= \pm\frac{1}{\Gamma(\alpha)\kappa(\alpha)}\int_{\mathbb{R}} f(x-\varepsilon z)e^{\mp\ell\varepsilon z}z_{\pm}^{-1}\int_{|y|\geq1/|z|}\Delta_y^{\lfloor\alpha\rfloor+1}[z_{\pm}^{\alpha-1}](\pm1)y_{\pm}^{-\alpha-1}dydz \\
&= \frac{1}{\Gamma(\alpha)\kappa(\alpha)}\int_0^\infty f(x\pm\varepsilon z)e^{-\ell\varepsilon z}\int_0^z \Delta_1^{\lfloor\alpha\rfloor+1}[z_+^{\alpha-1}](y)dy\frac{dz}{z} \\
&= \frac{1}{\Gamma(\alpha+1)\kappa(\alpha)}\int_0^\infty f(x\pm\varepsilon z)e^{-\ell\varepsilon z}\Delta_1^{\lfloor\alpha\rfloor+1}[z_+^\alpha](z)\frac{dz}{z}.
\end{aligned}$$

Since

$$\frac{\Delta_1^{\lfloor\alpha\rfloor+1}[z_+^\alpha](z)}{z} = \begin{cases} \mathcal{O}(z^{\alpha-1}), & z \to 0, \\ \mathcal{O}(z^{\alpha-\lfloor\alpha\rfloor-2}), & z \to \infty, \end{cases}$$

we have

$$\int_0^\infty \left|\Delta_1^{\lfloor\alpha\rfloor+1}[z_+^\alpha](z)\right| \frac{dz}{z} < \infty.$$

This fact together with the assumption that f is continuous and has a compact support implies that

$$\lim_{\varepsilon\to 0^+} J_{\pm,\varepsilon}^{-\alpha} J_\pm^\alpha[f](x) = \frac{f(x)}{\Gamma(\alpha+1)\kappa(\alpha)} \int_0^\infty \Delta_1^{\lfloor\alpha\rfloor+1}[z_+^\alpha](z)\frac{dz}{z},$$

uniformly in ε. This completes the proof. $\square$

Two most commonly used properties of Bessel fractional derivatives are listed below.

Lemma 1.2.4 (see [SKM93]). *The Bessel fractional derivatives on the line satisfy:*

$$\int_{\mathbb{R}} f J_\pm^\alpha[g]dx = \int_{\mathbb{R}} J_\pm^\alpha[f]g dx, \;\; f, J_\pm^\alpha[f] \in L^p(\mathbb{R}), \;\; g, J_\pm^\alpha[g] \in L^{p'}(\mathbb{R}), \tag{1.2.9a}$$

$$J_\pm^{-\alpha} J_\pm^\alpha = I \quad \text{in the sense of } L^p(\mathbb{R}), \text{ with } 1 \le p < \infty. \tag{1.2.9b}$$

Proof. Formula (1.2.9a) is obtained by changing the order of integration exactly as in the proof of (1.2.3a). To prove (1.2.9b), we observe (see proof of Lemma 1.2.3) that for any $\varepsilon > 0$ and any $f \in L^p(\mathbb{R})$

$$J_{\pm,\varepsilon}^{-\alpha} J_\pm^\alpha[f](x) = \int_{\mathbb{R}} K_\pm^\alpha(z) f(x+\varepsilon z) e^{\mp\ell\varepsilon z} dz,$$

where

$$K_\pm^\alpha(x) = \frac{\Delta_1^{\lfloor\alpha\rfloor+1}[x_+^\alpha](\pm x)}{x\Gamma(\alpha+1)\kappa(\alpha)}, \qquad \int_{\mathbb{R}} K_\pm^\alpha(x)dx = 1, \qquad \int_{\mathbb{R}} |K_\pm^\alpha(x)|dx = c_\alpha < \infty.$$

Using these facts, we write

$$(J_{\pm,\varepsilon}^{-\alpha} J_\pm^\alpha - I)[f](x) = \int_{\mathbb{R}} [f(x+\varepsilon z)e^{\mp\ell\varepsilon z} - f(x)] K_\pm^\alpha(z) dz.$$

Taking $L^p(\mathbb{R})$ norm of both sides of the last identity and applying integral Minkowski's inequality, we infer

$$\|(J_{\pm,\varepsilon}^{-\alpha} J_{\pm}^{\alpha} - I)[f]\|_{L^p(\mathbb{R})} \leq \int_{\mathbb{R}} |K_{\pm}^{\alpha}(z)| \cdot \|f(\cdot + \varepsilon z)e^{\mp \ell \varepsilon z} - f(\cdot)\|_{L^p(\mathbb{R})} dz.$$

Since $\|f(\cdot + \varepsilon z)e^{\mp \ell \varepsilon z} - f(\cdot)\|_{L^p(\mathbb{R})} \to 0$ as $\varepsilon \to 0$, it follows that $J_{\pm}^{-\alpha} J_{\pm}^{\alpha}[f] = f$ in $L^p(\mathbb{R})$. $\square$

1.3 Weighted Bessel potential spaces in $\mathbb{R}$

As mentioned in the introduction, the approximative properties of the algebraically mapped Chebyshev basis are naturally described on the scale of weighted Bessel potential spaces. There are two equivalent ways to define such spaces. The classical approach consists in using the A. Calderon complex interpolation method and can be found in [BL76, AF03]. Alternatively, one can define the spaces by using the Fourier transform [SKM93]. We follow the latter approach specialized to the geometry of $\mathbb{R}$.

Let w be locally integrable function (a *weight*) in $\mathbb{R}$. We define two functional classes:

$$H_{w,\pm}^{2,\alpha}(\mathbb{R}) = \{f \in \mathcal{D}' | \|wJ_{\pm}^{-\alpha,\ell}[f]\|_{L^2(\mathbb{R})} < \infty\},$$
$$H_{2,\alpha}^{w,\pm}(\mathbb{R}) = \{f \in \mathcal{D}' | \|J_{\pm}^{-\alpha,\ell}[wf]\|_{L^2(\mathbb{R})} < \infty\},$$

where operators $J_{\pm}^{-\alpha,\ell}[f]$ are understood as the strong L^2 limits of the truncated operators $J_{\pm,\varepsilon}^{-\alpha}[f]$ as $\varepsilon \to 0^+$.

Remark 1.3.1. We note that $H_{2,\alpha}^{w,+}(\mathbb{R}) = H_{2,\alpha}^{w,-}(\mathbb{R})$. The identity follows immediately from the definition of the Bessel fractional integroderivatives. In the sequel, we deal with the power weights only. For such weights, the identity $H_{w,+}^{2,\alpha}(\mathbb{R}) = H_{w,-}^{2,\alpha}(\mathbb{R})$ is the consequence of formula (1.3.2) below.

This allow us to omit the sign $\pm$ in the above definition and use the right Bessel fractional integroderivatives only.

The functional classes $H^{2,\alpha}_w(\mathbb{R})$ and $H^w_{2,\alpha}(\mathbb{R})$, equipped with

$$\langle f, g\rangle_{H^{2,\alpha}_w} = \int_{\mathbb{R}} |w|^2 J_+^{-\alpha,\ell}[f]\overline{J_+^{-\alpha,\ell}[g]}dx, \quad \langle f, g\rangle_{H^w_{2,\alpha}} = \int_{\mathbb{R}} J_+^{-\alpha,\ell}[wf]\overline{J_+^{-\alpha,\ell}[wg]}dx,$$

are Hilbert spaces. We denote their induced norms by symbols $\|\cdot\|_{H^w_{2,\alpha}}$ and $\|\cdot\|_{H^{2,\alpha}_w}$, respectively. In the sequel, we deal with the power weights only, i.e. we use

$$w_\beta = (\ell \pm ix)^\beta, \quad \beta \in \mathbb{R}.$$

For such weights we abbreviate $H^{2,\alpha}_{w_\beta}(\mathbb{R}) = H^{2,\alpha}_\beta(\mathbb{R})$, $H^{w_\beta}_{2,\alpha}(\mathbb{R}) = H^\beta_{2,\alpha}(\mathbb{R})$ and $H^{2,\alpha}_{w_0}(\mathbb{R}) = H^{w_0}_{2,\alpha}(\mathbb{R}) = H^{2,\alpha}(\mathbb{R})$. The meaning of symbols α and β are straightforward. The parameter α controls the regularity of functions, while parameter β describes the growth/decay rate of functions at infinity.

The basic connections between the two Hilbert scales $H^{2,\alpha}_\beta(\mathbb{R})$ and $H^\beta_{2,\alpha}(\mathbb{R})$ are given by the identities

$$\begin{aligned} &\mathcal{F}[H^{2,\alpha}_\beta(\mathbb{R})] = H^\alpha_{2,\beta}(\mathbb{R}), \quad \mathcal{F}[H^\beta_{2,\alpha}(\mathbb{R})] = H^{2,\beta}_\alpha(\mathbb{R}), \\ &\mathcal{F}^{-1}[H^{2,\alpha}_\beta(\mathbb{R})] = H^\alpha_{2,\beta}(\mathbb{R}), \quad \mathcal{F}^{-1}[H^\beta_{2,\alpha}(\mathbb{R})] = H^{2,\beta}_\alpha(\mathbb{R}), \end{aligned} \tag{1.3.1}$$

which follow directly from the definition of Bessel's fractional integroderivatives (1.2.1), (1.2.7) and Lemmas 1.2.2 and 1.2.4. In what follows, we show that in fact

$$H^{2,\alpha}_\beta(\mathbb{R}) = H^\alpha_{2,\beta}(\mathbb{R}), \ \ \alpha \geq 0, \ \ \beta \in \mathbb{R}, \ \text{ with equivalent norms.} \tag{1.3.2}$$

The proof is lengthy and is based on a sequence of Lemmas.

Lemma 1.3.1. *Let $0 \leq \alpha < 1$, $\beta \in \mathbb{R}$ and f, g be two smooth functions. If $|g|$ is bounded away from zero and $e^{-cx}|f|(x) < \infty$ with some $c < \ell$, then*

$$J_+^{-\alpha,\ell}[gf](x) = gJ_+^{-\alpha,\ell}[f](x) + K_g^{\alpha,\ell}[gJ_+^{-\alpha,\ell}[f](x)], \tag{1.3.3a}$$

where

$$K_g^{\alpha,\ell}[f](x) = \int_{-\infty}^{x} f(y)\kappa_g^{\alpha,\ell}(x,y)dy, \tag{1.3.3b}$$

$$\kappa_g^{\alpha,\ell}(x,y) = \frac{e^{\ell(y-x)}}{\Gamma(\alpha)\Gamma(1-\alpha)} \int_y^x \frac{g'(s)}{g(y)} \frac{(s-y)^\alpha}{(x-s)^\alpha} \frac{ds}{x-y}. \tag{1.3.3c}$$

Proof. For $\alpha = 0$ or $g = 1$, the assertion is trivial. Therefore, we assume $0 < \alpha < 1$. We denote $\psi(x) = J_+^{-\alpha,\ell}[gf](x)$ and $\varphi(x) = gJ_+^{-\alpha,\ell}[f](x)$. Then

$$\psi(x) = \varphi(x) + K_g^{\alpha,\ell}[\varphi](x),$$

where $K_g^{\alpha,\ell}[\varphi](x) = \psi(x) - \varphi(x)$. Comparing definitions of $\psi(x)$ and $\varphi(x)$ and using formulas (1.2.2) and (1.2.7), it is not difficult to deduce

$$\begin{aligned}
K_g^{\alpha,\ell}[\varphi](x) &= J_+^{-\alpha,\ell}\left[gJ_+^{\alpha,\ell}[g^{-1}\varphi]\right](x) - gJ_+^{-\alpha,\ell}\left[J_+^{\alpha,\ell}[g^{-1}\varphi]\right](x) \\
&= \frac{\alpha e^{-\ell x}}{\Gamma(\alpha)\Gamma(1-\alpha)} \int_0^{+\infty} [g(x) - g(x-z)] \frac{dz}{z^{\alpha+1}} \\
&\qquad\qquad \int_{-\infty}^{x-z} (y-x+z)^{\alpha-1} \frac{\varphi(y)e^{\ell y}}{g(y)} dy \\
&= \int_{-\infty}^{x} \varphi(y) \left(\frac{e^{\ell(y-x)}}{\Gamma(\alpha)\Gamma(1-\alpha)} \int_y^x \frac{g'(s)}{g(y)} \frac{(s-y)^\alpha}{(x-s)^\alpha} \frac{ds}{x-y} \right) dy \\
&= \int_{-\infty}^{x} \varphi(y)\kappa_g^{\alpha,\ell}(x,y)dy.
\end{aligned}$$

□

Next, we let $g = w_\beta$ and estimate $K_g^{\alpha,\ell}[f]$. To simplify the notation, we abbreviate $K_{w_\beta}^{\alpha,\ell} = K_\beta^{\alpha,\ell}$.

Lemma 1.3.2. *The operator $K_\beta^{\alpha,\ell}$ obtained in Lemma 1.3.1 satisfies:*

$$\begin{aligned}
\left|K_\beta^{\alpha,\ell}[\varphi](x)\right| &\le \beta J_+^{1,\ell}[|w_{-1}\varphi|](x) \\
&\qquad + \beta|w_{\beta-1}|(x)h(x)J_+^{1,\ell}[h|w_{-\beta}\varphi| + h|w_{-\beta}\varphi_-|](x), \quad \beta > 0,
\end{aligned} \tag{1.3.4a}$$

$$
\begin{aligned}
\left|K_\beta^{\alpha,\ell}[\varphi](x)\right| \le\ & |\beta||w_{\beta-1}|(x) J_+^{1,\ell}[|w_{-\beta}\varphi|](x) \\
& + |\beta| h(x) J_+^{1,\ell}[h|w_{-1}\varphi| + h|w_{-1}\varphi_-|](x), \quad \beta < 0,
\end{aligned} \tag{1.3.4b}
$$

where $h(x) = \max\{0, x\}$ is the Heaviside function and $\varphi_-(x) = \varphi(-x)$.

Proof. (a) Assume initially that $x \le 0$. Then $|y| \ge |s| \ge |x|$ and

$$
\frac{|w'_\beta(s)|}{|w_\beta(y)|} \le \beta |w_{-1}|(y), \quad \beta > 0; \qquad \frac{|w'_\beta(s)|}{|w_\beta(y)|} \le |\beta| \frac{|w_{\beta-1}|(x)}{|w_\beta|(y)}, \quad \beta > 0.
$$

Making the substitution $s = (x-y)t + y$ in the remaining integral, we arrive at the estimate

$$
|\kappa_\beta^{\alpha,\ell}(x,y)| \le |\beta| e^{\ell(y-x)} \begin{cases} |w_{-1}|(y), & \text{if } \beta > 0, \\ \frac{|w_{\beta-1}|(x)}{|w_\beta|(y)}, & \text{if } \beta < 0, \end{cases} \quad y \le x \le 0.
$$

(b) Now, let $x > 0$. We have two sub-cases: $|y| < x$ and $y \le -x$. In the latter case, the same calculations as in part (a) of the proof yield

$$
|\kappa_\beta^{\alpha,\ell}(x,y)| \le |\beta| e^{\ell(y-x)} \begin{cases} |w_{-1}|(y), & \text{if } \beta > 0, \\ \frac{|w_{\beta-1}|(x)}{|w_\beta|(y)}, & \text{if } \beta < 0, \end{cases} \quad y \le -x \le 0.
$$

In the former case, we have

$$
\frac{|w'_\beta(s)|}{|w_\beta(y)|} \le \beta \frac{|w_{\beta-1}(x)|}{|w_\beta(y)|}, \quad \beta > 0, \qquad \frac{|w'_\beta(s)|}{|w_\beta(y)|} \le \beta |w_{-1}|(y), \quad \beta < 0.
$$

Combining all inequalities together, we arrive at

$$
|\kappa_\beta^{\alpha,\ell}(x,y)| \le \beta e^{\ell(y-x)} \begin{cases} |w_{-1}|(y), & \text{if } |y| \ge |x|, \\ \frac{|w_{\beta-1}|(x)}{|w_\beta|(y)}, & \text{if } |x| \ge |y|, \end{cases} \quad \beta > 0, \tag{1.3.5a}
$$

and

$$
|\kappa_\beta^{\alpha,\ell}(x,y)| \le |\beta| e^{\ell(y-x)} \begin{cases} \frac{|w_{\beta-1}|(x)}{|w_\beta|(y)}, & \text{if } |y| \ge |x|, \\ |w_{-1}|(x), & \text{if } |x| \ge |y|, \end{cases} \quad \beta < 0. \tag{1.3.5b}
$$

Estimates (1.3.4) follow directly from (1.3.5). $\square$

Lemma 1.3.3. *If $\beta \le \gamma$, then*

$$\|w_\beta J_+^{1,\ell}[f]\|_{L^2(\mathbb{R})} \le c\|w_\gamma f\|_{L^2(\mathbb{R})}, \tag{1.3.6}$$

with $c > 0$ that depends on β, γ and ℓ only.

Proof. (a) The inequality is a special case of the general Hardy-type inequality, see [KP03]. Estimate (1.3.6) holds if and only if

$$\begin{aligned} A &= \sup_{x\in\mathbb{R}} A(x) < \infty, \\ A(x) &= \int_x^\infty |w_{2\beta}|(y)e^{-2\ell y}dy \int_{-\infty}^x |w_{-2\gamma}|(y)e^{2\ell y}dy. \end{aligned}$$

Since both integrals $\int_0^\infty |w_{2\beta}|(y)e^{-2\ell y}dy$ and $\int_{-\infty}^0 |w_{2\gamma}|(y)e^{2\ell y}dy$ are finite, it follows that A is finite if and only if

$$\begin{aligned} A &= \max\left\{\sup_{x\in\mathbb{R}_+} A_{2\beta,-2\gamma}(x), \sup_{x\in\mathbb{R}_+} A_{-2\gamma,2\beta}(x)\right\} < \infty, \\ A_{a,b}(x) &= \int_x^\infty |w_a|(y)e^{-2\ell y}dy \int_0^x |w_b|(y)e^{2\ell y}dy := I_a^-(x)I_b^+(x), \quad a,b\in\mathbb{R}. \end{aligned}$$

Function $A_{a,b}(x)$ is smooth in $\mathbb{R}_+$ and bounded near $x = 0$ for all $a, b \in \mathbb{R}$. Hence, it suffices to show that $A_{a,b}(x)$ is uniformly bounded at infinity.

(b) We observe that

$$I_a^-(x) \le \frac{|w_a|(x)}{2\ell}e^{-2\ell x}, \quad I_b^+(x) \le \frac{|w_b|(x)}{2\ell}e^{-2\ell x},$$

provided that $a \le 0$, $b \ge 0$ and $x \ge 0$. It remains to estimate $I_a^-(x)$ and $I_b^+(x)$, when $a > 0$, $b < 0$ and $x > 0$ is large.

To estimate $I_a^-(x)$, $a > 0$, we observe that $x^a \le |w_a|(x) \le 2^{a/2}x^a$ for x large (say $x \ge \ell$). Consequently,

$$I_a^-(x) \le \frac{1}{\sqrt{2}(\sqrt{2}\ell)^{a+1}}\Gamma(a+1, 2\ell x),$$

where $\Gamma(\alpha, z) = \int_z^\infty y^{\alpha-1}e^{-y}dy$. Note that $\Gamma(\alpha, z) \le cz^{\alpha-1}e^{-z}$, with some absolute constant $c > 0$, see [GR07]. We conclude that

$$I_a^-(x) \le c_1|w_a|(x)e^{-2\ell x},$$

with constant $c_1 > 0$ that depends on a and ℓ only.

To estimate $I_b^+(x)$, $b < 0$, we proceed as follows

$$\begin{aligned}
I_b^+(x) &= |w_b|(x)\int_0^x e^{2\ell y}dy + |w_b|(x)\int_0^x \big(|w_{-b}|(x) - |w_{-b}|(y)\big)|w_b|(y)e^{2\ell y}dy \\
&\le \frac{1}{2\ell}|w_b|(x)e^{2\ell x} + 2|w_b|(x)\int_0^x |w_b|(y)e^{2\ell y}dy\int_y^x |w_{-b}|'(z)dz \\
&= \frac{1}{2\ell}|w_b|(x)e^{2\ell x} + 2|w_b|(x)\int_0^x |w_{-b}|'(z)dz\int_0^z |w_b|(y)e^{2\ell y}dy.
\end{aligned}$$

Observe that function $|w_b|(y)e^{2\ell y}$ either monotone increases in $\mathbb{R}_+$ or has a local minimum that depends on ℓ and b only. Therefore,

$$|w_b|(y)e^{2\ell y} \le c'|w_b|(z)e^{2\ell z},$$

for a constant $c' > 0$ and all $0 \le y \le z$. Using this fact and the elementary inequality $z|w_{-b}|'(z)|w_b|(z) \le |b|$, we infer

$$I_b^+(x) \le c_2|w_b|(x)e^{2\ell x},$$

with constant $c_2 > 0$ that depends on b and ℓ only.

(c) Combining all the inequalities together, we conclude that there exists a constant c that depends on a, b and ℓ so that

$$A_{a,b}(x) \le c|w_a|(x)|w_b|(x) = c|w_{a+b}|(x).$$

Elementary calculations show that $\sup_{x\in\mathbb{R}_+} A_{a,b}(x)$ is finite if and only if $a + b \le 0$. Returning to our original parameters β and γ we conclude that (1.3.6) holds if and only if $\beta \le \gamma$. $\square$

Using Lemmas 1.3.1-1.3.3, it is easy to obtain:

Theorem 1.3.4. *Assume that* $\alpha \geq 0$ *and* $\beta \in \mathbb{R}$. *Then*

$$\|f\|_{H^{\beta}_{2,\alpha}} \leq c\|f\|_{H^{2,\alpha}_{\beta}}, \tag{1.3.7}$$

with $c > 0$ *that does not depend on* f.

Proof. (a) To begin, we observe that for $\alpha = 0$ and/or $\beta = 0$, the assertion is trivial. We let $\varphi(x) = J_+^{-\alpha,\ell}[f](x)$, and assume $0 < \alpha < 1$ and $\beta \neq 0$. The Lemmas 1.3.1-1.3.2 imply that

$$\begin{aligned}\|f\|_{H^{\beta}_{2,\alpha}} &\leq \|f\|_{H^{2,\alpha}_{\beta}} + \|K^{\alpha,\ell}_{\beta}[w_\beta\varphi]\|_{L^2(\mathbb{R})} \\ &\leq \|f\|_{H^{2,\alpha}_{\beta}} + \beta\|J_+^{1,\ell}[|w_{\beta-1}\varphi|]\|_{L^2(\mathbb{R})} \\ &+ \beta\|w_{\beta-1}hJ_+^{1,\ell}[h|\varphi|]\|_{L^2(\mathbb{R})} + \|w_{\beta-1}hJ_+^{1,\ell}[h|\varphi_-|]\|_{L^2(\mathbb{R})},\end{aligned}$$

when $\beta > 0$, and

$$\begin{aligned}\|f\|_{H^{\beta}_{2,\alpha}} &\leq \|f\|_{H^{2,\alpha}_{\beta}} + \|K^{\alpha,\ell}_{\beta}[w_\beta\varphi]\|_{L^2(\mathbb{R})} \\ &\leq \|f\|_{H^{2,\alpha}_{\beta}} + |\beta|\|w_{\beta-1}J_+^{1,\ell}[|\varphi|]\|_{L^2(\mathbb{R})} \\ &+ |\beta|\|hJ_+^{1,\ell}[h|w_{\beta-1}\varphi|]\|_{L^2(\mathbb{R})} + \|hJ_+^{1,\ell}[h|w_{\beta-1}\varphi_-|]\|_{L^2(\mathbb{R})},\end{aligned}$$

when $\beta < 0$. The last two inequalities, combined with Lemma 1.3.3, settle (1.3.7) for $0 < \alpha < 1$ and $\beta \in \mathbb{R}$.

(b) Assume $n \in \mathbb{N}$. For regular functions, operators $J_\pm^{-n,\ell}$ can be realized as:

$$J_\pm^{-n,\ell}[f](x) = e^{\mp\ell x}\Big(\pm\frac{d}{dx}\Big)^n e^{\pm\ell x} f(x).$$

Therefore, for any two smooth functions f and g, we have

$$J_\pm^{-n,\ell}[fg](x) = \sum_{m=0}^{n}\binom{n}{m}(\pm 1)^{n-m} g^{(n-m)}(x) J_\pm^{-m,\ell}[f](x).$$

Now, let $\alpha \geq 1$. Any such number can be written as $\alpha = n + \gamma$, where $n \in \mathbb{N}$ and $0 \leq \gamma < 1$. Using this notation, the last formula and elementary properties of fractional derivatives, we infer:

$$J_{\pm}^{-\alpha,\ell}[w_\beta f](x) = \sum_{m=0}^{n} \binom{n}{m} (\pm 1)^{n-m} w_\beta^{(n-m)}(x) J_{\pm}^{-m-\gamma,\ell}[f](x).$$

Consequently,

$$\begin{aligned} \|f\|_{H^{\beta}_{2,\alpha}} &\leq \sum_{m=0}^{n} \binom{n}{m} \|J_{\pm}^{-\gamma,\ell}[w_\beta^{(n-m)} J_{+}^{-m,\ell}[f]]\|_{L^2(\mathbb{R})} \\ &\leq c \sum_{m=0}^{n} \binom{n}{m} \|J_{\pm}^{-m,\ell}[f]\|_{H^{\beta-n+m}_{2,\gamma}}. \end{aligned}$$

Since $0 \leq \gamma < 1$, we can apply (1.3.7) to obtain

$$\|f\|_{H^{\beta}_{2,\alpha}} \leq c \sum_{m=0}^{n} \binom{n}{m} \|f\|_{H^{2,m+\gamma}_{\beta-n+m}}.$$

In view of Lemma 1.3.3,

$$\|f\|_{H^{2,m+\gamma}_{\beta-n+m}} = \|w_{\beta-n+m} J_{+}^{n-m,\ell}[J_{+}^{-n-\gamma,\ell}[f]]\|_{L^2(\mathbb{R}_+)} \leq c\|f\|_{H^{2,n+\gamma}_{\beta}}$$

and (1.3.7) follows for all $\alpha \geq 1$. □

Corollary 1.3.1. *Equation* (1.3.2) *holds for all* $\alpha \geq 0$ *and* $\beta \in \mathbb{R}$.

Proof. Theorem (1.3.4) implies that $H^{2,\alpha}_{\beta}(\mathbb{R}) \subset H^{\beta}_{2,\alpha}(\mathbb{R})$. The converse embedding follows directly from identities (1.3.1). □

To conclude this section, we mention that unweighted Bessel potential spaces $H^{2,\alpha}$ are known to be Banach algebras (see [AF03]), i.e.

$$\|fg\|_{H^{2,\alpha}} \leq c_\alpha \|f\|_{H^{2,\alpha}} \|g\|_{H^{2,\alpha}}, \tag{1.3.8}$$

provided that $\alpha > \frac{1}{2}$. By (1.3.8) and Corollary 1.3.1, we have

$$\|fg\|_{H^{2,\alpha}_{\beta}} \leq c_\alpha \|f\|_{H^{2,\alpha}_{\frac{\beta}{2}}} \|g\|_{H^{2,\alpha}_{\frac{\beta}{2}}} \leq c_\alpha \|f\|_{H^{2,\alpha}_{\beta}} \|g\|_{H^{2,\alpha}_{\beta}}, \tag{1.3.9}$$

provided that $\alpha > \frac{1}{2}$ and $\beta \geq 0$. This fact will be used in Chapter 4. In the next chapter, we define the algebraically mapped Chebyshev basis and establish its connection with Laguerre functions.

Chapter 2

The algebraically mapped Chebyshev basis

In this chapter, we provide a review of several classical results related to Chebyshev polynomials $T_n(x)$. Then, we define the algebraically mapped Chebyshev basis and establish its connection with Laguerre functions. We conclude this chapter by listing several properties of the generalized Laguerre functions in the half line.

2.1 Chebyshev polynomials of the first kind and their properties

Chebyshev polynomials of the first kind were discovered by P.L. Chebyshev in [Che54] when solving the following extremal problem: *Find a monic polynomial of degree n that has the smallest possible magnitude in a fixed closed interval, say* $[-1, 1]$. He found that such polynomials are given explicitly by the formula

$$2^{1-n}\cos(n \arccos x), \quad x \in [-1, 1], \quad n \geq 0. \tag{2.1.1}$$

Nowadays, the renormalized version of monic polynomials (2.1.1), namely,

$$T_n(x) = \cos(n \arccos x), \quad x \in [-1, 1], \quad n \geq 0, \tag{2.1.2}$$

are known as Chebyshev polynomials of the first kind. Since the discovery of Chebyshev, polynomials $T_n(x)$ play an important role in many fields of pure and applied mathematics. In particular, the discovery itself was one of the sources for modern *constructive approximation theory*. In numerical mathematics, polynomials $T_n(x)$ are employed in two different contexts. In the first one, $T_n(x)$ are used in *optimization of computational processes*, for instance, in finding optimal parameters for iterative techniques or in optimizing stability of certain numerical schemes. In the second one, $T_n(x)$ are used in *approximating functions*, in particular, in signal processing and in numerical schemes for differential equations [Fun92, Boy00, Tre00, CQHZ06, HGG07, STW11]. Below, we provide a brief overview of a theory of Chebyshev polynomials.

2.1.1 Alternative definitions

There are several ways to define Chebyshev polynomials. First of all, they can be defined explicitly. The explicit formula is obtained by letting $x = \cos(\theta)$ in (2.1.2) and then expanding $\cos(n\theta)$:

$$T_n(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} C_n^{2k} x^{n-2k} (x^2 - 1)^k = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k x^{n-2k} \sum_{\ell=k}^{\lfloor n/2 \rfloor} C_n^{2k} C_\ell^k. \tag{2.1.3}$$

Alternatively, one can employ the Rodriguez formula:

$$T_n(x) = (-1)^n \frac{\sqrt{1-x^2}}{(2n-1)!} \frac{d^n}{dx^n} (1 - x^2)^{n - \frac{1}{2}}, \tag{2.1.4}$$

or the generating function:

$$\frac{1 - tx}{1 - 2tx + t^2} = \sum_{n=0}^{\infty} T_n(x) t^n. \tag{2.1.5}$$

Finally, they can be defined recursively:

$$T_0(x) = 1, \quad T_1(x) = x, \quad T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x), \quad n \geq 2. \quad (2.1.6)$$

The latter definition yields one more explicit formula:

$$T_n(x) = \frac{1}{2}\big[(x + \sqrt{x^2 - 1})^n + (x - \sqrt{x^2 - 1})^n\big]. \quad (2.1.7)$$

2.1.2 Identities

Chebyshev polynomials of the first kind satisfy an enormous amount of various identities (see [Sze67, PBM92, GR07]). We mention few, most commonly used. First of all, using the trigonometric representation (2.1.2), we infer

$$2T_n(x)T_m(x) = T_{n+m}(x) + T_{|n-m|}(x), \quad T_n(-x) = (-1)^n T_n(x), \quad (2.1.8a)$$

$$T_0(x) = T_1'(x), \quad 2T_n(x) = \frac{T_{n+1}'(x)}{n+1} - \frac{T_{n-1}'(x)}{n-1}, \quad (2.1.8b)$$

$$\sqrt{1-x^2}\frac{d}{dx}\left(\sqrt{1-x^2}\frac{dT_n(x)}{dx}\right) = -n^2 T_n(x). \quad (2.1.8c)$$

Further, from the same representation, it follows that

$$|T_n(x)| \leq 1 \text{ and } |T_n'(x)| \leq n^2, \quad x \in [-1, 1], \quad (2.1.9a)$$

$$T_n(\pm 1) = (\pm 1)^n \text{ and } T_n'(\pm 1) = (\pm 1)^{n+1} n^2, \quad (2.1.9b)$$

$$T_{2n}(0) = (-1)^n \text{ and } T_{2n+1}(0) = 0, \quad (2.1.9c)$$

$$T_{2n}'(0) = 0 \text{ and } T_{2n+1}'(0) = (-1)^n n. \quad (2.1.9d)$$

2.1.3 Extremal properties

We cite two extremal properties of Chebyshev polynomials. Both have fundamental consequences in constructive approximation theory and in numerical analysis.

Theorem 2.1.1 (see [Leb96]). *Monic Chebyshev polynomials of the first kind minimize the uniform norm in the interval* $[-1, 1]$. *That is, for any polynomial* $p_n(x)$ *of degree* n *we have*

$$\max_{x\in[-1,1]} |p_n(x)| \geq \max_{x\in[-1,1]} |2^{1-n}T_n(x)| = 2^{1-n}. \qquad (2.1.10)$$

Theorem 2.1.2 (see [Leb96]). *The derivative of Chebyshev polynomials of the first kind maximize the uniform norm in the interval* $[-1, 1]$. *That is, for any polynomial* $p_n(x)$ *of degree* n*, that satisfies* $\max_{x\in[-1,1]} |p_n(x)| \leq 1$*, the following inequality holds:*

$$\max_{x\in[-1,1,]} |p'_n(x)| \leq \max_{x\in[-1,1]} |T'_n(x)| = n^2. \qquad (2.1.11)$$

2.1.4 Approximative properties

Chebyshev polynomials of the first kind are particular instances of a more general class of *classical orthogonal polynomials* known as *Jacobi polynomials* [Sze67]. Polynomials $T_n(x)$ are orthogonal in $[-1, 1]$ with respect to the weight function $w(x) = (1 - x^2)^{-\frac{1}{2}}$:

$$\langle T_n, T_m\rangle_w = \int_{-1}^{1} \frac{T_n(x)T_m(x)}{\sqrt{1-x^2}}dx = \delta_{nm} \begin{cases} \pi, & \text{if } n = 0, \\ \dfrac{\pi}{2}, & \text{if } n > 0. \end{cases} \qquad (2.1.12)$$

It is known (see [Sze67]) that the Chebyshev basis $\{T_n(x)\}_{n\geq 0}$ is *complete* in the weighted Hilbert space $L^2_w([-1, 1])$. Consequently, any function $f \in L^2_w([-1, 1])$ can be represented by its convergent (in the sense of L^2) Chebyshev-Fourier series

$$f(x) = \sum_{n\geq 0} \frac{f_n}{\kappa_n} T_n(x), \quad f_n = \langle T_n, f\rangle_w, \quad \kappa_n = \begin{cases} \pi, & n = 0, \\ \frac{\pi}{2}, & n \geq 1. \end{cases} \qquad (2.1.13)$$

The latter formula indicates that the truncated Chebyshev-Fourier series can be used to approximate square integrable functions. This observation is widely used in practical computations. In particular, it is the origin of a large class of numerical schemes for differential equations known as *spectral schemes*.

2.2 Algebraically mapped Chebyshev polynomials

The set of Chebyshev polynomials $\{T_n(x)\}_{n\geq 0}$ provide a complete orthogonal basis in the Hilbert space $L^2_w([-1,1])$ with $w(x) = (1-x^2)^{-\frac{1}{2}}$ and, hence, can be used to approximate square integrable functions defined in $[-1,1]$. In our project, we deal with functions defined on the real line $\mathbb{R}$. Obviously we cannot use $T_n(x)$, $n \geq 0$, to approximate such functions directly. However, one can map the extended real line $\mathbb{R}$ one-to-one to $[-1,1]$ and then approximate the resulting composite function by Chebyshev polynomials. The quality of approximation depends on the particular map $\xi : \mathbb{R} \to [-1,1]$. Some analysis and applications of rational, exponential and trigonometric maps can be found in [AFR84, LP88, Boy90, FI92, Che93, YA96, BN98, Boy00].

In the project, we deal with rational maps (see [Boy00]). These are given by

$$\xi(x) = \frac{x}{\sqrt{\ell^2 + x^2}}, \quad \ell > 0, \tag{2.2.1}$$

where ℓ is a free parameter. In practical computations, ℓ is used to tune up the convergence speed.

The algebraically mapped Chebyshev basis reads

$$TB_n(x) = \frac{\sqrt{\ell}}{\sqrt{\ell^2 + x^2}} T_n\left(\frac{x}{\sqrt{\ell^2 + x^2}}\right), \quad n > 0, \quad \ell > 0. \tag{2.2.2}$$

It is easy to verify that the system $\{TB_n(x)\}_{n\geq 0}$ provides the complete orthogonal basis in the Hilbert space $L^2(\mathbb{R})$. Furthermore,

$$\langle TB_n, TB_m\rangle = \int_{\mathbb{R}} TB_n(x)TB_m(x)dx = \delta_{nm} \begin{cases} \pi, & \text{if } n = 0, \\ \frac{\pi}{2}, & \text{if } n > 0, \end{cases} \tag{2.2.3}$$

and any function $f \in L^2(\mathbb{R})$ can be represented by its convergent (in the sense of L^2) Chebyshev-Fourier series

$$f(x) = \sum_{n\geq 0} \frac{f_n}{\kappa_n} TB_n(x), \quad f_n = \langle TB_n, f\rangle, \quad \kappa_n = \begin{cases} \pi, & n = 0, \\ \frac{\pi}{2}, & n \geq 1. \end{cases} \tag{2.2.4}$$

In the next chapter, we provide a comprehensive study of the convergence of (2.2.4). Below, in this chapter, we provide several auxiliary results that are relevant for our study.

2.3 Generalized Laguerre functions and their properties

In the next section, we establish an important connection between generalized Laguerre functions and algebraically mapped Chebyshev polynomials. This will facilitate our error analysis in Chapter 3. Below, we briefly mention few properties of generalized Laguerre polynomials that are relevant for our study.

The generalized Laguerre functions are denoted by

$$\phi_n^{\alpha,\ell}(x) = e^{-\ell x} L_n^{(\alpha)}(2\ell x), \quad n \geq 0,$$

where $L_n^{(\alpha)}(x)$ are generalized Laguerre polynomials. The explicit formula can be obtained with the aid of the generating function [Sze67, GR07]

$$g(x,\xi) = \sum_{n\geq 0} \xi^n \phi_n^{\alpha,\ell}(x) = \frac{1}{(1-\xi)^{\alpha+1}} \exp\Big(-\ell s \frac{1+\xi}{1-\xi}\Big). \tag{2.3.1}$$

It is known that for $\alpha > -1$, the collection $\{\phi_n^{\alpha,\ell}\}_{n\geq 0}$ satisfies

$$\int_0^\infty x^\alpha \phi_n^{\alpha,\ell}(x)\phi_m^{\alpha,\ell}(x)dx = \frac{\Gamma(n+\alpha+1)}{(2\ell)^{\alpha+1}n!}\delta_{mn} \tag{2.3.2}$$

and provide a complete orthogonal basis in the weighted Hilbert space $L^2_{x^\alpha}(\mathbb{R}+)$, see [Sze67].

The generalized Laguerre function satisfy a number of important identities. In the sequel, we need only two [PBM92]

$$J_+^{\beta,\ell}[x_+^\alpha \phi_n^{\alpha,\ell}(x)] = \frac{\Gamma(\alpha+n+1)}{\Gamma(\alpha+\beta+n+1)} x_+^{\alpha+\beta}\phi_n^{\alpha+\beta,\ell}, \tag{2.3.3a}$$

$$J_-^{-\beta,\ell}[\phi_n^{\alpha,\ell}](x) = (2\ell)^\beta \phi_n^{\alpha+\beta,\ell}, \tag{2.3.3b}$$

where $x \geq 0$, $\alpha > -1$ and $\beta > 0$.

2.4 Fourier transform of the algebraically mapped Chebyshev basis

In this section, we derive a formula for the Fourier transforms of $TB_n(x)$.

Lemma 2.4.1. *The Fourier images of algebraically mapped Chebyshev polynomials are given by*

$$\widehat{TB}_{2n+1}(s) = -\operatorname{sgn}(s)\frac{\sqrt{\pi\ell}}{\sqrt{2}}\phi_n^{0,\ell}(|s|), \quad n \geq 0, \tag{2.4.1a}$$

$$\widehat{TB}_0(s) = 2\sqrt{\ell}K_0(\ell|s|), \tag{2.4.1b}$$

$$\widehat{TB}_{2n}(s) = \frac{\sqrt{2\pi\ell}}{2n}\left(J_-^{-1/2,\ell}J_+^{-1/2,\ell}\right)\left[|s|\phi_{n-1}^{1,\ell}(|s|)\right], \quad n \geq 1, \tag{2.4.1c}$$

where, $n \geq 0$, $\phi_n^{i,\ell}(x)$, $i = 0,1$, are Laguerre functions, $K_0(z)$ is the modified Bessel function and $J_-^{-1/2,\ell}$, $J_+^{-1/2,\ell}$ are the Bessel fractional derivatives defined in Section 1.2.

Proof. (a) We consider even and odd numbered functions separately. Consider first odd numbered functions. In view of (2.1.7), we have

$$TB_{2n+1}(x) = \frac{\sqrt{\ell}}{2}\left[\frac{(x+i\ell)^{2n+1}}{(x^2+\ell^2)^{n+1}} + \frac{(x-i\ell)^{2n+1}}{(x^2+\ell^2)^{n+1}}\right].$$

To facilitate our calculations, we introduce the generating function

$$g_o(x,\xi) = \sum_{n\geq 0} \xi^n TB_{2n+1}(x) = \frac{\sqrt{\ell}}{1-\xi}\frac{x}{x^2+\ell^2\frac{(1+\xi)^2}{(1-\xi)^2}}.$$

Now

$$\mathcal{F}[g_o](s,\xi) = \frac{\sqrt{\ell}}{(1-\xi)\sqrt{2\pi}}\int_{\mathbb{R}} \frac{e^{-isx}x}{x^2+\ell^2\frac{(1+\xi)^2}{(1-\xi)^2}}dx.$$

The last integral fell in the scope of Jordan's lemma and can be evaluated using methods of classical complex analysis [Mar65]:

$$F[g_o](s,\xi) = -\operatorname{sgn}(s)\frac{\sqrt{\pi\ell}}{\sqrt{2}}\frac{1}{1-\xi}\exp\Big(-\ell|s|\frac{1+\xi}{1-\xi}\Big).$$

By virtue of (2.3.1), we have (2.4.1a).

(b) Now, we turn to the even numbered functions. First, we consider

$$\mathcal{F}\left[\frac{1}{(\ell\pm ix)^{1/2}}\right](s) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \frac{e^{-isx}}{(\ell\pm ix)^{1/2}}dx,$$

where $(\cdot)^{1/2}$ represents the principal branch of the square root. We cut the complex plane along the line $Re(\ell \pm iz) \leq 0$ and replace the integral above with the contour integral that goes around the cut line to obtain

$$\mathcal{F}\left[\frac{1}{(\ell\pm ix)^{1/2}}\right](s) = -\sqrt{2}s_{\mp}^{-1/2}e^{\pm s\ell},$$

where $s_- = \max\{0,-s\}$ and $s_+ = \max\{0,s\}$ are cut-off functions. Using these formulas and properties of the Fourier transform, we infer

$$\begin{aligned}\widehat{TB_0}(s) = \mathcal{F}\left[\frac{\sqrt{\ell}}{\sqrt{x^2+\ell^2}}\right](s) &= -2\sqrt{\ell}(s_-^{-1/2}e^{s\ell}) * (s_+^{-1/2}e^{-s\ell}) \\ &= 2\sqrt{\ell}\int_1^\infty e^{-\ell|s|t}(t^2-1)^{-1/2}dt = 2\sqrt{\ell}K_0(\ell|s|),\end{aligned} \tag{2.4.2}$$

where $K_0(z)$ is the modified Bessel function.

To obtain (2.4.1c), we employ the generating function

$$g_e(x,\xi) = \frac{1}{2}TB_0(x) + \sum_{n\geq 1} \xi^n TB_{2n}(x) = \frac{\sqrt{\ell}}{2}\sqrt{x^2+\ell^2}\frac{1+\xi}{1-\xi}\frac{1}{x^2+\ell^2\frac{(1+\xi)^2}{(1-\xi)^2}},$$

the formula

$$\begin{aligned}\mathcal{F}\left[\frac{1}{x^2+\ell^2\frac{(1+\xi)^2}{(1-\xi)^2}}\right](s) &= \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \frac{e^{-isx}}{x^2+\ell^2\frac{(1+\xi)^2}{(1-\xi)^2}}ds \\ &= \frac{\sqrt{\pi}}{\sqrt{2}}\frac{1-\xi}{\ell(1+\xi)}\exp\Big(-\ell|s|\frac{1+\xi}{1-\xi}\Big),\end{aligned}$$

and results of Section 1.2. This gives

$$\mathcal{F}[g_e](s,\xi) = \frac{\sqrt{\pi}}{2\sqrt{2\ell}}\Big(J_-^{-1/2,\ell}J_+^{-1/2,\ell}\Big)\Big[e^{-\ell|s|}\exp\Big(-\frac{2\ell|s|\xi}{1-\xi}\Big)\Big].$$

The last identity, combined with the generating formula (2.3.1), yields (2.4.1c).

□

The next chapter conatins the main results of our research. In the next chapter, we provide approximation and interpolation estimates in $L^2(\mathbb{R})$ and $H^{2,\alpha}(\mathbb{R})$ settings.

Chapter 3

Approximation and interpolation estimates

In this chapter, we study the difference between the exact function f and its truncated Chebyshev-Fourier series (2.2.4). To aid our calculations, we introduce the following notation: the symbol $\mathbb{P}_N$ denotes the subspace of $L^2(\mathbb{R})$ spanned by $\{TB_n\}_{n=0}^N$; the symbol $\mathcal{P}_N : L^2(\mathbb{R}) \to \mathbb{P}_N$ denotes the orthogonal projector from $L^2(\mathbb{R})$ to $\mathbb{P}_N$. In coordinate form, the operator $\mathcal{P}_N[f]$ reads

$$\mathcal{P}_N[f](x) = \sum_{n=0}^{N} \frac{f_n}{\kappa_n} TB_n(x).$$

In this notation, we study

$$\|f - \mathcal{P}_N[f]\|_{H_\beta^{2,\alpha}} = \|(\mathcal{I} - \mathcal{P}_N)[f]\|_{H_\beta^{2,\alpha}},$$

where $\mathcal{I}$ is the identity operator.

3.1 Approximation estimates

3.1.1 $L^2(\mathbb{R})$ estimates

In this section, we study the approximation error in $L^2(\mathbb{R})$ settings. The main result of this section is the following:

Theorem 3.1.1. *Let $\alpha, N > 0$, then*

$$\|(\mathcal{I} - \mathcal{P}_N)[f]\|_{L^2(\mathbb{R})} \le c(\ell N)^{-\frac{\alpha}{2}} \|f\|_{H_\alpha^{2,\frac{\alpha}{2}}}, \tag{3.1.1}$$

where the positive constant c does not depend on f or N.

Proof. To begin, we observe that

$$\begin{aligned}
\|(\mathcal{I} - \mathcal{P}_N)[f]\|^2_{L^2(\mathbb{R})} &= \frac{1}{\pi} \sum_{n \ge N+1} |f_n|^2 \\
&= \frac{1}{\pi} \sum_{k \ge \lceil \frac{N}{2} \rceil} |f_{2k+1}|^2 + \frac{1}{\pi} \sum_{k \ge \lceil \frac{N+1}{2} \rceil} |f_{2k}|^2 := E_o + E_e.
\end{aligned}$$

We estimate E_o and E_e separately.

(a) First, we consider E_o. Using formula (2.4.1a), for the odd-indexed spectral coefficients, we have

$$\begin{aligned}
f_{2k+1} &= \langle TB_{2k+1}, f \rangle = \int_{\mathbb{R}} TB_{2k+1}(x) f(x) dx = \int_{\mathbb{R}} \widehat{TB}_{2k+1}(s) \hat{f}(s) ds \\
&= -\frac{\sqrt{\pi \ell}}{\sqrt{2}} \int_{\mathbb{R}} \operatorname{sgn}(s) \phi_k^{0,\ell}(|s|) \hat{f}(s) ds \\
&= \frac{\sqrt{\pi \ell}}{\sqrt{2}} \int_{\mathbb{R}_+} e^{-\ell s} \phi_k^{0,\ell}(s) \hat{f}(-s) ds - \frac{\sqrt{\pi \ell}}{\sqrt{2}} \int_{\mathbb{R}_+} \phi_k^{0,\ell}(s) \hat{f}(s) ds \\
&=: f^-_{2k+1} - f^+_{2k+1}.
\end{aligned}$$

In order to estimate f^+_{2k+1}, we let $\hat{f}(s) = J_-^{\alpha,\ell}[\varphi](s)$. Then, using fractional integration by parts and formula (2.3.3a), we arrive at

$$
\begin{aligned}
f_{2k+1}^{+} &= \frac{\sqrt{\pi\ell}}{\sqrt{2}\Gamma(\alpha)} \int_0^{+\infty} \varphi(s) e^{-\ell s} J_{+}^{\alpha,\ell}[\phi_k^{0,\ell}](s) ds \\
&= \frac{\sqrt{\pi\ell}k!}{\sqrt{2}\Gamma(\alpha+k+1)} \int_0^{+\infty} s^{\alpha} \phi_k^{\alpha,\ell}(s) \varphi(s) ds.
\end{aligned}
$$

Similarly, we let $\hat{f}(s) = J_{+}^{\alpha,\ell}[\psi](s)$ to obtain

$$
\begin{aligned}
f_{2k+1}^{-} &= \frac{\sqrt{\pi\ell}}{\sqrt{2}\Gamma(\alpha)} \int_0^{+\infty} \psi(-s) J_{+}^{\alpha,\ell}[\phi_k^{0,\ell}](s) ds \\
&= \frac{\sqrt{\pi\ell}k!}{\sqrt{2}\Gamma(\alpha+k+1)} \int_0^{+\infty} s^{\alpha} \phi_k^{\alpha,\ell}(s) \psi(-s) ds,
\end{aligned}
$$

and, hence,

$$
f_{2k+1} = \frac{\sqrt{\pi\ell}k!}{\sqrt{2}\Gamma(\alpha+k+1)} \int_0^{+\infty} s^{\alpha} \phi_k^{\alpha,\ell}(s) \big[\psi(-s) - \varphi(s)\big] ds.
$$

In view of formula (2.3.2) and the completeness of the orthogonal system $\{\phi_n^{\alpha,\ell}\}_{k\geq 0}$, we infer

$$
\begin{aligned}
E_o &= \frac{\ell}{2} \sum_{k\geq\lceil\frac{N}{2}\rceil} \frac{(k!)^2}{\Gamma^2(\alpha+k+1)} \left| \int_0^{+\infty} s^{\alpha} \phi_k^{\alpha,\ell}(s) [\varphi(s) - \psi(-s)] ds \right|^2 \\
&= \frac{1}{4(\ell N)^{\alpha}} \sum_{k\geq\lceil\frac{N}{2}\rceil} \frac{(2\ell)^{\alpha+1} k!}{\Gamma(\alpha+k+1)} \left| \int_0^{+\infty} s^{\alpha} \phi_k^{\alpha,\ell}(s) [\varphi(s) - \psi(-s)] ds \right|^2 \\
&\leq \frac{1}{4(\ell N)^{\alpha}} \int_{\mathbb{R}_+} (s^{\frac{\alpha}{2}}) \big|\varphi(s) - \psi(-s)\big|^2 ds \\
&\leq \frac{1}{4(\ell N)^{\alpha}} \big[\|w_{\frac{\alpha}{2}} \varphi\|_{L^2(\mathbb{R})} + \|w_{\frac{\alpha}{2}} \psi\|_{L^2(\mathbb{R})}\big]^2 \\
&= \frac{1}{4(\ell N)^{\alpha}} \big[\|w_{\frac{\alpha}{2}} J_{+}^{-\alpha,\ell}[\hat{f}]\|_{L^2(\mathbb{R})} + \|w_{\frac{\alpha}{2}} J_{-}^{-\alpha,\ell}[\hat{f}]\|_{L^2(\mathbb{R})}\big]^2.
\end{aligned}
$$

Using properties of the Fourier transform and results obtained in Section 1.3, we conclude that

$$
\|w_{\frac{\alpha}{2}} J_{\pm}^{-\alpha,\ell}[\hat{f}]\|_{L^2(\mathbb{R})} = \|f\|_{H^{\alpha}_{2,\frac{\alpha}{2}}} \leq c_1 \|f\|_{H^{2,\frac{\alpha}{2}}_{\alpha}},
$$

with some constant $c_1 > 0$ that does not depend on f. Hence,

$$E_o \leq \frac{c_1^2}{(\ell N)^\alpha} \|f\|^2_{H_\alpha^{2,\frac{\alpha}{2}}}. \tag{3.1.2}$$

(b) To estimate E_e, we employ (2.4.1c) and fractional integration by parts. This yields

$$\begin{aligned}
f_{2k} = \langle TB_{2k}, f \rangle &= \int_{\mathbb{R}} TB_{2k}(x) f(x) dx = \int_{\mathbb{R}} \widehat{TB}_{2k}(s) \hat{f}(s) ds \\
&= \frac{\sqrt{2\pi\ell}}{2k} \int_{\mathbb{R}} \left(J_-^{-\frac{1}{2},\ell} J_+^{-\frac{1}{2},\ell} \right) \big[|\cdot| \phi_{k-1}^{1,\ell}(|\cdot|) \big](s) \hat{f}(s) ds \\
&= \frac{\sqrt{2\pi\ell}}{2k} \int_{\mathbb{R}_+} s \phi_{k-1}^{1,\ell}(s) \hat{g}(-s) ds + \frac{\sqrt{2\pi\ell}}{2k} \int_{\mathbb{R}_+} s \phi_{k-1}^{1,\ell}(s) \hat{g}(s) ds \\
&=: f_{2k}^- + f_{2k}^+,
\end{aligned}$$

with $\hat{g}(s) = \left(J_-^{-\frac{1}{2},\ell} J_+^{-\frac{1}{2},\ell} \right) [\hat{f}](s)$. In the same way as above, we infer that

$$f_{2k} = \frac{\sqrt{2\pi\ell}(k-1)!}{2k\Gamma(\alpha+k)} \int_0^{+\infty} s^\alpha \phi_{k-1}^{\alpha,\ell}(s) \big[\psi(-s) + \varphi(s) \big] ds, \tag{3.1.3}$$

where $\hat{g}(s) = J_-^{\alpha-1,\ell}[\varphi](s) = J_+^{\alpha-1,\ell}[\psi](s)$. Using representation (3.1.3) and the same procedure as in part (a) of the proof, it is not difficult to verify that

$$E_e \leq \frac{c_2^2}{(\ell N)^{\alpha+2}} \|f\|^2_{H_\alpha^{2,\frac{\alpha}{2}}}, \tag{3.1.4}$$

with constant $c_2 > 0$ that does not depend on f and N. Inequalities (3.1.2) and (3.1.4), combined together, yield the result. □

3.1.2 $H^{2,\alpha}(\mathbb{R})$ estimates

In this section, we are dealing with general $H^{2,\alpha}(\mathbb{R})$ settings.

Theorem 3.1.2. *Let $0 < \alpha < \beta$ and $0 < N$, then*

$$\|(\mathcal{I} - \mathcal{P}_N)[f]\|_{H^{2,\alpha}} \leq c(\ell N)^{-(\beta-\alpha)} \|f\|_{H^{2,\beta}_{2\beta}}, \tag{3.1.5}$$

where the positive constant c does not depend on f or N.

Proof. (a) Consider $\|(\mathcal{I}-\mathcal{P}_N)[f]\|_{H^{2,\alpha}}$. Using properties of the Fourier transform, we infer

$$\|(\mathcal{I}-\mathcal{P}_N)[f]\|_{H^{2,\alpha}} = \|w_\alpha(\mathcal{I}-\hat{\mathcal{P}}_N)[\hat{f}]\|_{L^2(\mathbb{R})},$$

where

$$\hat{\mathcal{P}}_N[\hat{f}](s) = \sum_{n=0}^{N} \frac{f_n}{\kappa_n}\widehat{TB}_n(s).$$

Since $|w_\alpha| \le c[1+|s|^\alpha]$ for some $c>0$, it follows that

$$\|(\mathcal{I}-\mathcal{P}_N)[f]\|_{H^{2,\alpha}} \le c\|(\mathcal{I}-\mathcal{P}_N)[f]\|_{L^2(\mathbb{R})} + c\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}_N)[\hat{f}]\|_{L^2(\mathbb{R})}.$$

By Theorem 3.1.1, $\|(\mathcal{I}-\mathcal{P}_N)[f]\|_{L^2(\mathbb{R})} \le c(\ell N)^{-\beta}\|f\|_{H^{2,\beta}_{2\beta}}$. It remains to estimate the error $\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}_N)[\hat{f}]\|_{L^2(\mathbb{R})}$.

To aid our calculations, we write:

$$\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}_N)[\hat{f}]\|_{L^2(\mathbb{R})} \le \|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}^o_N)[\hat{f}]\|_{L^2(\mathbb{R})} + \|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}^e_N)[\hat{f}]\|_{L^2(\mathbb{R})},$$

where $\hat{\mathcal{P}}^o_N$ and $\hat{\mathcal{P}}^e_N$ are the orthogonal projectors onto the subspaces spanned by odd $\{\widehat{TB}_{2k+1}\}_{k=0}^{\lceil\frac{N-1}{2}\rceil}$ and even $\{\widehat{TB}_{2k}\}_{k=0}^{\lceil\frac{N}{2}\rceil}$ Chebyshev functions, respectively. We estimate the errors $\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}^o_N)[\hat{f}]\|_{L^2(\mathbb{R})}$ and $\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}^e_N)[\hat{f}]\|_{L^2(\mathbb{R})}$ separately.

(b) We start with the operator $\hat{\mathcal{P}}^o_N$. In view of the antisymmetry of $\widehat{TB}_{2k+1}$ (see formula (2.4.1a)), we have

$$\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}^o_N)[\hat{f}]\|_{L^2(\mathbb{R})} = 2\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}^o_N)[\hat{f}]\|_{L^2(\mathbb{R}_+)}.$$

By virtue of the embedding inequality, see [JBS14, formula (21a)], we obtain the estimate

$$\|s^\alpha(\mathcal{I}-\hat{\mathcal{P}}^o_N)[\hat{f}]\|_{L^2(\mathbb{R})} \le c\|s^\alpha J_-^{-2\alpha,\ell}(\mathcal{I}-\hat{\mathcal{P}}^o_N)[\hat{f}]\|_{L^2(\mathbb{R}+)},$$

with $c > 0$ independent on N or f. Taking into account formula (2.3.3b), we have

$$J_-^{-2\alpha,\ell}(\mathcal{I} - \hat{\mathcal{P}}_N^o)[\hat{f}](s) = \frac{(2\ell)^{2\alpha}}{\pi} \sum_{k \geq \lceil \frac{N}{2} \rceil} \phi_k^{2\alpha,\ell}(s) f_{2k+1}.$$

As in the proof of Theorem 3.1.1, for the Fourier-Chebyshev coefficient f_{2k+1}, we obtain

$$f_{2k+1} = \frac{\sqrt{\pi}\ell k!}{\sqrt{2}\Gamma(2\beta + k + 1)} \int_0^{+\infty} s^{2\beta} \phi_k^{2\beta,\ell}(s) \big[\psi(-s) - \varphi(s)\big] ds,$$

with $\hat{f}(s) = J_-^{2(\alpha+\beta),\ell}[\varphi](s) = J_+^{2(\alpha+\beta),\ell}[\psi](s)$, and then

$$\begin{aligned} \|s^\alpha(\mathcal{I} - \hat{\mathcal{P}}_N^o)[\hat{f}]\|_{L^2(\mathbb{R})} &\leq c(\ell N)^{\beta-\alpha} \big[\|w_\beta \varphi\|_{L^2(\mathbb{R})} + \|w_\beta \psi\|_{L^2(\mathbb{R})}\big] \\ &\leq c(\ell N)^{\beta-\alpha} \|\hat{f}\|_{H_\beta^{2,2\beta}} \leq c(\ell N)^{\beta-\alpha} \|f\|_{H_{2\beta}^{2,\beta}}. \end{aligned}$$

(c) The analysis of operator $\hat{\mathcal{P}}_N^e$ is similar and requires only minor adjustments. Lengthy but straightforward calculations yield

$$\|s^\alpha(\mathcal{I} - \hat{\mathcal{P}}_N^e)[\hat{f}]\|_{L^2(\mathbb{R})} \leq c(\ell N)^{\beta-\alpha} \|f\|_{H_{2\beta}^{2,\beta}},$$

and (3.1.5) follows. □

3.2 Interpolation estimates

The projection operator $\mathcal{P}_n$ considered in Section 3.1 is not useful in practical calculations as evaluating spectral coefficients f_n involves exact integration of f against TB_n over the real line. In realistic simulations, the integrals $\langle TB_n, f \rangle$ are calculated approximately with the aid of quadratures. In context of the real line, it is natural to use Gauss-Chebyshev quadratures.

The $N+1$-point Gauss-Chebyshev quadrature, applied to the exact spectral coefficient $f_n = \langle TB_n, f \rangle_{L^2(\mathbb{R})}$, reads

$$\bar{f}_n = \frac{\pi}{\ell(N+1)} \sum_{k=0}^{N} [\ell^2 + x_{k,N}^2] TB_n(x_{k,N}) f(x_{k,N}), \tag{3.2.1}$$

where

$$x_{k,N} = \ell \cot\Big(\frac{2k+1}{2(N+1)}\pi\Big), \qquad k = 0, 1, \dots, N,$$

are Gauss-Chebyshev nodes mapped from interval $(-1, 1)$ onto the real line. The approximate quantities $\bar{f}_n$ are often referenced as *pseudo-spectral coefficients*. In practice, we use $\bar{f}_n$ to approximate f by means of the operator

$$\mathcal{I}_N[f](x) = \sum_{k=0}^{N} \frac{\bar{f}_n}{\kappa_n} TB_n(x). \tag{3.2.2}$$

Lemma 3.2.1. *Operator $\mathcal{I}_N$ satisfies the following interpolation identity:*

$$\mathcal{I}_N[f](x_{k,N}) = f(x_{k,N}), \quad k = 0, 1, \dots, N. \tag{3.2.3}$$

Proof. Combining formulas (3.2.1) and (3.2.2) together, we arrive at

$$\mathcal{I}_N[f](x) = \sum_{k=0}^{N} f(x_{k,N}) K_N(x_{k,N}, x),$$

with

$$K_N(x, y) = \frac{\pi(\ell^2 + x^2)}{\ell(N+1)} \sum_{n=0}^{N} \frac{1}{\kappa_n} TB_n(x) TB_n(y).$$

By virtue of the classical Christoffel-Darboux summation formula [MM08], we obtain

$$K_N(x, y) = \frac{(\ell^2 + x^2)^{3/2}}{\ell(N+1)} \frac{TB_{N+1}(x) T_N(y) - T_N(x) T_{N+1}(y)}{x\sqrt{\ell^2 + y^2} - y\sqrt{\ell^2 + x^2}}.$$

It is easy to verify that

$$K_N(x_{k,N}, x_{m,N}) = \delta_{k,m}, \quad k, m = 0, 1, \dots, N.$$

Hence, (3.2.3) follows. □

In the remainder of this section, we study the behavior of the interpolation error $(\mathcal{I} - \mathcal{I}_N)[f]$ in $L^2(\mathbb{R})$ and $H^{2,\alpha}(\mathbb{R})$ settings. We observe that $\mathcal{I}_N \mathcal{P}_N =$

$\mathcal{P}_N$ as $\mathcal{I}_N$ is bijective when restricted to the finite dimensional space $\mathbb{P}_N$. Therefore,

$$
\begin{aligned}
(\mathcal{I}-\mathcal{I}_N)[f] &= (\mathcal{I}-\mathcal{P}_N+\mathcal{P}_N-\mathcal{I}_N)[f] \\
&= (\mathcal{I}-\mathcal{P}_N)[f]+(\mathcal{P}_N-\mathcal{I}_N)[f] \\
&= (\mathcal{I}-\mathcal{P}_N)[f]+(\mathcal{I}_N\mathcal{P}_N-\mathcal{I}_N)[f] \\
&= (\mathcal{I}-\mathcal{P}_N)[f]-\mathcal{I}_N(\mathcal{I}-\mathcal{P}_N)[f]
\end{aligned}
$$

and the interpolation error is controlled by the norm of the linear map $\mathcal{I}_N$. In the following subsection, we bound $\|\mathcal{I}_N\|_{L^2(\mathbb{R})}$. Such estimates are known as *stability estimates*.

3.2.1 $L^2(\mathbb{R})$ stability

To begin, we study the stability of the interpolation in $L^2(\mathbb{R})$.

Lemma 3.2.2. *Assume $\alpha > \frac{1}{2}$. Then*

$$\|\mathcal{I}_N[f]\|_{L^2(\mathbb{R})} \leq c_\alpha(N\ell)\|f\|_{H^{2,\alpha}}, \tag{3.2.4}$$

where $c_\alpha > 0$ does not depend on N or f.

Proof. (a) Taking into account that the Gauss-Chebyshev quadrature formula is exact for all $f \in \mathbb{P}_{2N+1}$ and using the interpolation property (3.2.3), we obtain

$$\|\mathcal{I}_N[f]\|^2_{L^2(\mathbb{R})} = \int_{\mathbb{R}} |\mathcal{I}_N[f]|^2 dx = \frac{\pi}{\ell(N+1)}\sum_{n=0}^{N}[\ell^2 + x^2_{k,N}]f^2(x_{n,N}).$$

Note that $H^{2,\alpha}(\mathbb{R}) = [W^{2,\lfloor\alpha\rfloor}(\mathbb{R}), W^{2,\lceil\alpha\rceil}(\mathbb{R})]_{\alpha-\lfloor\alpha\rfloor}$, where symbol $W^{2,n}(\mathbb{R})$ denotes the classical integer order Sobolev space and $[\cdot,\cdot]_\theta$ is the complex interpolation functor [Ada75, BL76]. In this context classical Sobolev embeddings apply and we have

$$\|f\|_\infty \leq c'_\alpha\|f\|_{H^{2,\alpha}},$$

provided that $\alpha > \frac{1}{2}$. Therefore,

$$\|\mathcal{I}_N[f]\|^2_{L^2(\mathbb{R})} \le \frac{c'_\alpha \pi}{\ell(N+1)} \Big(\sum_{n=0}^{N} [\ell^2 + x^2_{k,N+1}]\Big) \|f\|^2_{H^{2,\alpha}}$$
$$=: \frac{c'_\alpha \pi}{\ell(N+1)} S_N^2 \|f\|_{H^{2,\alpha}}.$$

It remains to evaluate S_N^2.

(b) Using explicit formula for the Gauss-Chebyshev nodes, we obtain

$$S_N^2 = \ell^2 \sum_{n=0}^{N} \frac{1}{\sin^2\Big(\frac{2k+1}{2(N+1)}\pi\Big)} = \ell^2 \sum_{n=0}^{N} \frac{\sin^2\Big((N+1)\frac{2k+1}{2(N+1)}\pi\Big)}{\sin^2\Big(\frac{2k+1}{2(N+1)}\pi\Big)}.$$

Note that $N+1$-point Gauss-Chebyshev quadrature is exact for all polynomials of degree $2N+1$. Consequently,

$$S_N^2 = \frac{(N+1)\ell^2}{\pi} \int_{-1}^{1} \frac{U_N^2(t)}{\sqrt{1-t^2}},$$

where $U_N(t) = \frac{\sin\big((n+1)\arccos t\big)}{\sin t}$ are Chebyshev polynomials of the second kind. Next, we make the substitution $t = \cos\theta$ and then integrate by parts to obtain

$$\int_{-1}^{1} \frac{U_N^2(t)}{\sqrt{1-t^2}} = \int_0^\pi \frac{\sin^2\Big((N+1)\theta\Big)}{\sin^2(\theta)} d\theta = -\int_0^\pi \sin^2\Big((N+1)\theta\Big) d\cot\theta$$
$$= (N+1)\int_0^\pi \cos\theta \frac{\sin\Big(2(N+1)\theta\Big)}{\sin\theta} d\theta = (N+1)\int_{-1}^{1} \frac{tU_{2N+1}(t)}{\sqrt{1-t^2}} dt.$$

With the aid of the identity $tU_n(t) = T_{n+1}(t) + U_{n-1}(t)$, the three term recurrence formula $U_{n+1}(t) = 2tU_n(t) - U_{n-2}(t)$ and the orthogonality of $T_n(t)$, we arrive at

$$\int_{-1}^{1} \frac{U_N^2(t)}{\sqrt{1-t^2}} dt = (N+1)\int_{-1}^{1} \frac{U_0(t)}{\sqrt{1-t^2}} dt = \pi(N+1).$$

Hence,

$$S_N^2 = \big(\ell(N+1)\big)^2$$

and (3.2.4) holds with $c_\alpha = 2\pi c'_\alpha$. □

3.2.2 An inverse inequality

The stability estimate in $H^{2,\alpha}(\mathbb{R})$ requires some additional work. Consider the linear space $\mathbb{P}_N$, equipped with the norms $\|\cdot\|_{L^2(\mathbb{R})}$ and $\|\cdot\|_{H^{2,\alpha}}$. Since $\mathbb{P}_N$ is finite dimensional, any two norms shall be equivalent. Therefore, there exists a constant (say $c(N,\alpha)$), such that

$$\|f\|_{H^{2,\alpha}} \leq c(N,\alpha)\|f\|_{L^2(\mathbb{R})},$$

for each $f \in \mathbb{P}_N$. Inequalities of this type are known as *inverse inequalities.* The main goal of this subsection is to derive an upper bound on the equivalence constant $c(N,\alpha)$.

Lemma 3.2.3. *Algebraically mapped Chebyshev polynomials satisfy:*

$$\frac{d^2}{dx^2}TB_0(x) = \frac{1}{(4\ell)^2}\Big[-6TB_4(x) + 8TB_2(x) - 2TB_0(x)\Big], \tag{3.2.5a}$$

$$\frac{d^2}{dx^2}TB_2(x) = \frac{1}{(4\ell)^2}\Big[-15TB_6(x) + 36TB_4(x) - 25TB_2(x) + 4TB_0(x)\Big], \tag{3.2.5b}$$

and

$$\begin{aligned}\frac{d^2}{dx^2}TB_n(x) = \frac{1}{(4\ell)^2}\Big[&-(n-1)(n-3)TB_{n-4}(x) + 4(n-1)^2TB_{n-2}(x)\\ &-(6n^2+2)TB_n(x)\\ &-(n+1)(n+3)TB_{n+4}(x) + 4(n+1)^2TB_{n+2}(x)\Big],\end{aligned} \tag{3.2.5c}$$

where $n \geq 0$, $n \neq 0, 2$ and $TB_n(x) = 0$, whenever $n < 0$.

Proof. Formula (3.2.5) is the straightforward consequence of (2.2.2) and identities (2.1.6) and (2.1.8c). □

Theorem 3.2.4. *Assume $f \in \mathbb{P}_N$ and $\alpha \geq 0$. Then*

$$\|f\|_{H^{2,\alpha}} \leq c_\alpha \Big(\frac{N}{\ell}\Big)^\alpha \|f\|_{L^2(\mathbb{R})}, \tag{3.2.6}$$

where c_α does not depend on N or f.

Proof. (a) To begin, we establish (3.2.6) with $\alpha = 2$. Consider $\mathbb{P}_N$, equipped with the norm $\|\cdot\|_{L^2(\mathbb{R})}$. Since, $\{TB_n\}_{n\geq 0}$ are orthogonal, the finite dimensional Euclidean space $\mathbb{P}_N$ is isometrically isomorphic to the standard real Euclidean space $\mathbb{R}^{N+1}$, equipped with the weighted norm

$$|x|_D^2 = \sum_{n=0}^{N} \frac{|x_n|^2}{\kappa_n}.$$

The norm $\|\cdot\|_{H^{2,\alpha}}$ is equal to one of the expressions $\|J_-^{-2,\ell}[\cdot]\|_{L^2(\mathbb{R})}$, $\|J_+^{-2,\ell}[\cdot]\|_{L^2(\mathbb{R})}$, or $\|(J_+^{-1,\ell}J_+^{-1,\ell})[\cdot]\|_{L^2(\mathbb{R})}$. Therefore, it is sufficient to consider the composite operator $J_+^{-1,\ell}J_+^{-1,\ell}$ only. Straightforward calculations show that $J_+^{-1,\ell}J_+^{-1,\ell}[\cdot] = \frac{d^2}{dx^2}[\cdot] - \ell^2\cdot$. By virtue of Lemma 3.2.3, the latter operator maps $\mathbb{P}_N$ into $\mathbb{P}_{N+4}$. Moving to the isometrically isomorphic spaces $\mathbb{R}^{N+1}$ and $\mathbb{R}^{N+5}$, we see that the operator $J_+^{-1,\ell}J_+^{-1,\ell}$ can be realized as ordinary matrix-vector multiplication. If we denote the matrix of the operator by $J_N \in \mathbb{R}^{(N+5)\times(N+1)}$, then

$$\|f\|_{H^{2,\alpha}} = |J_N x|_D \leq |J_N|_D |x|_D = |J_N|_D \|f\|_{L^2(\mathbb{R})},$$

where $x = (f_0, \dots, f_N)^T \in \mathbb{R}^{N+1}$ and $|J_N|_D = \sup_{x\in\mathbb{R}^{N+1}, |x|\neq 0} \frac{|J_N x|_D}{|x|_D}$ denotes the norm of matrix J_N subordinate to the weighted vector norm $|\cdot|_D$. It remains to estimate the norm of matrix J_N.

In view of formula (3.2.5), we can write

$$J_N = \bar{J}_N(I, O)^T,$$

where $I \in \mathbb{R}^{(N+1)\times(N+1)}$ is an identity matrix, $O \in \mathbb{R}^{(N+1)\times 4}$ is a zero matrix and $\bar{J}_N = (j_{n,k}) \in \mathbb{R}^{(N+5)\times(N+5)}$ is a five diagonal symmetric matrix, whose nonzero entries are given explicitly by

$$j_{n,n} = -\frac{6n^2 + 2 + \ell^4}{(4\ell)^2}, \quad j_{n,n+2} = \frac{4(n+1)^2}{(4\ell)^2}, \quad j_{n,n+4} = -\frac{(n+1)(n+3)}{(4\ell)^2}.$$

Let $\bar{J}_N^k \in \mathbb{R}^{(N+5)\times(N+5)}$ denote the matrix whose k-th diagonal is equal to the k-th diagonal of $\bar{J}_N$ and all other entries are zeros. Using this notation, and taking into account that $|J_N|_D = \sigma^{1/2}(DJ_N^T D^{-2} J_N D)$,[1] where $D^{-1} = \mathrm{diag}(\kappa_0, \dots, \kappa_N)$ and $\sigma(\cdot)$ is the spectral radius of a matrix, we obtain

$$|J_N|_D \le |\bar{J}_N|_D \le |\bar{J}_N^0|_D + 2|\bar{J}_N^2|_D + 2|\bar{J}_N^4|_D \le c_2\Big(\frac{N}{\ell}\Big)^2,$$

with some $c_2 > 0$ independent on N. This proves (3.2.6) with $\alpha = 2$.

(b) Using (3.2.6) with $\alpha = 2$, we show that in fact (3.2.6) holds with $0 \le \alpha < 2$. For this, we consider the operator $\mathcal{P}_N$. From part (a) of the proof, we know that

$$\|\mathcal{P}_N[f]\|_{H^{2,2}} \le c_2\Big(\frac{N}{\ell}\Big)^2 \|f\|_{L^2(\mathbb{R})},$$

and, in addition, $\|\mathcal{P}_N[f]\|_{L^2(\mathbb{R})} \le \|f\|_{L^2(\mathbb{R})}$. It is known that $H^{2,\alpha}$ are interpolation spaces, that is $H^{2,\alpha} = [L^2_{(\mathbb{R})}, H^{2,2}_{(\mathbb{R})}]_{\frac{\alpha}{2}}$, where $[\cdot,\cdot]_\theta$, $0 < \theta < 1$ is the complex interpolation functor of A. Calderon, see [Ada75, BL76]. This allows us to conclude that $\mathcal{P}_N$ is bounded from $L^2(\mathbb{R})$ to $H^{2,\alpha}(\mathbb{R})$ for all $0 < \alpha < 2$. Moreover, since the functor $[\cdot,\cdot]_\theta$ is exact[2], it follows that

$$\|\mathcal{P}_N[f]\|_{H^{2,\alpha}} \le c_\alpha\Big(\frac{N}{\ell}\Big)^\alpha \|f\|_{L^2(\mathbb{R})},$$

[1] This follows from the equation $|A|_D = |D^{-1}AD|$, where $|\cdot|$ is usual unweighted Euclidean norm in $\mathbb{R}^{N+1}$ and classical formula $|A| = \sigma^{1/2}(A^T A)$.

[2] That is for a compatible couple of Banach spaces $X_0 \subset X_1$ and a linear operator T that satisfies $\|T\|_{X_0}, \|T\|_{X_1} < \infty$, we have $\|T\|_{[X_0,X_1]_\theta} \le \|T\|_{X_0}^{1-\theta}\|T\|_{X_1}^{\theta}$, see [BL76].

with $c_\alpha > 0$ that does not depend on N or f.

(c) Parts (a) and (b) of the proof settle (3.2.6) for $0 \le \alpha \le 2$. To obtain (3.2.6) for all $0 \le \alpha$, we recall (see formula (1.2.3b)) that $J_\pm^{\alpha,\ell} J_\pm^{\beta,\ell}[f] = J_\pm^{\alpha+\beta,\ell}[f]$, for all $\alpha, \beta \in \mathbb{R}$ and all regular functions f that uniformly bounded for large values of $|x|$. $\square$

3.2.3 $H^{2,\alpha}(\mathbb{R})$ stability and error estimates

The stability and error estimates for $\mathcal{I}_N$ are immediate consequences of Lemma 3.2.2 and Theorem 3.2.4.

Corollary 3.2.1. *Assume $\alpha \ge 0$ and $\beta > \frac{1}{2}$. Then,*

$$\|\mathcal{I}_N[f]\|_{H^{2,\alpha}} \le c\ell^{-2\alpha}(\ell N)^{\alpha+1}\|f\|_{H^{2,\beta}}, \tag{3.2.7}$$

where $c > 0$ does not depend on N or f.

Proof. With the aid of Lemma 3.2.2 and Theorem 3.2.4, we obtain

$$\begin{aligned}\|\mathcal{I}_N[f]\|_{H^{2,\alpha}(\mathbb{R})} &\le c_\alpha \left(\frac{N}{\ell}\right)^\alpha \|\mathcal{I}_N[f]\|_{L^2(\mathbb{R})} \\ &\le c\ell^{-2\alpha}(\ell N)^{\alpha+1}\|f\|_{H^{2,\beta}}.\end{aligned}$$

$\square$

Combining our stability and approximation estimates, we arrive at

Corollary 3.2.2. *Let $0 \le \alpha$, $\frac{1}{2} < \gamma$ and $\max\{\alpha, \gamma\} < \beta$. Then,*

$$\|(\mathcal{I} - \mathcal{I}_N)[f]\|_{H^{2,\alpha}} \le c(1 + \ell^{-2\alpha})(\ell N)^{-(\beta-\alpha-\gamma-1)}\|f\|_{H^{2,\beta}_{2\beta}}, \tag{3.2.8}$$

where $c > 0$ does not depend on N or f.

Proof. We have:

$$
\begin{aligned}
\|(\mathcal{I}-\mathcal{I}_N)[f]\|_{H^{2,\alpha}} &\le \|(\mathcal{I}-\mathcal{P}_N)[f]\|_{H^{2,\alpha}} + \|\mathcal{I}_N(\mathcal{I}-\mathcal{P}_N)[f]\|_{H^{2,\alpha}} \\
&\le c'(\ell N)^{-(\beta-\alpha)}\|f\|_{H^{2,\beta}_{2\beta}} + c''\ell^{-2\alpha}(\ell N)^{\alpha+1}\|(\mathcal{I}-\mathcal{P}_N)[f]\|_{H^{2,\gamma}} \\
&\le c(1+\ell^{-2\alpha})(\ell N)^{-(\beta-\alpha-\gamma-1)}\|f\|_{H^{2,\beta}_{2\beta}},
\end{aligned}
$$

provided that $\alpha < \beta$ and $\gamma < \beta$. □

In the next and final chapter, we apply the Chebyshev-type pseudo-spectral method to the classical nonlinear Schrödinger equation and then conclude with several numerical experiments.

Chapter 4

Applications: the nonlinear Schrödinger equation

In this chapter, we study Chebyshev-type pseudo-spectral methods applied to differential equations posed on the real line. Rigorous mathematical analysis of any such scheme is based on approximation and interpolation estimates similar to those presented in Chapter 3. However, the concrete details strongly depend on a particular differential equation. To avoid abstract speculations, we apply the Chebyshev-type pseudo-spectral method to the classical nonlinear Schrödinger equation.

4.1 The nonlinear Schrödinger equation

4.1.1 Continuous problem

The nonlinear Schrödinger equation on the real line reads:

$$u_t = i\nabla\mathcal{H}(u) = iu_{xx} + 2i\nu|u|^2u, \quad u(x,0) = u_0(x), \tag{4.1.1a}$$

where $\nu \neq 0$. The problem (4.1.1) is Hamiltonian, with

$$\mathcal{H}(u) = \frac{1}{2}\int_{\mathbb{R}} (-|u_x|^2 + \nu|u|^4)dx \tag{4.1.1b}$$

and the zeroth order antisymmetric automorphism $\mathcal{J} = i$ of the Hilbert scale $H^{2,\alpha}(\mathbb{R})$, equipped with the real duality pairing

$$\langle u, v\rangle = \mathrm{Re}\int_{\mathbb{R}} u\bar{v}dx.$$

Equation (4.1.1a) is completely integrable. The exact solutions are obtained using the inverse scattering method, see [APT04] and references therein.

4.1.2 Spatial discretization

To obtain spatial semidiscretization of (4.1.1), we apply the Galerkin method. For this, we proceed as follows:

(a) We rewrite the original problem in the weak form. For this we view the solutions $u(\cdot, t)$ as maps form half line $t \in [0, \infty)$ into the Hilbert space $H^{2,1}(\mathbb{R})$. In these settings, the problem reads:

find $u \in C^{(1)}((0,\infty), H^{2,1}(\mathbb{R})) \cap C([0,\infty), H^{2,1}(\mathbb{R}))$ so that

$$\begin{cases} \langle u_t, \phi\rangle = -\langle iu_x, \phi_x\rangle + 2\nu\langle i|u|^2u, \phi\rangle, \quad \text{for all} \quad \phi \in H^{2,1}(\mathbb{R}), \\ u(0) = u_0. \end{cases} \tag{4.1.2}$$

(b) We approximate the exact solutions by the truncated Fourier-Chebyshev series:

$$\hat{u}(x,t) = \sum_{n=0}^{N} \frac{f_n(t)}{k_n} TB_n(x). \tag{4.1.3}$$

(c) For a fixed $N > 0$, we replace (4.1.2) with the following problem:

find $\hat{u} \in C^{(1)}((0,\infty), \mathbb{P}_N) \cap C([0,\infty), \mathbb{P}_N)$ so that

$$\begin{cases} \langle \hat{u}_t, \phi\rangle = -\langle i\hat{u}_x, \phi_x\rangle + 2\nu\langle i\mathcal{I}_N[|\hat{u}|^2\hat{u}], \phi\rangle, \quad \text{for all} \quad \phi \in \mathbb{P}_N, \\ \hat{u}(0) = \hat{u}_0 := \mathcal{I}_N[u_0]. \end{cases} \tag{4.1.4}$$

We observe that the semi-discrete problem (4.1.4) is again Hamiltonian, with the total energy given by

$$\hat{\mathcal{H}}(\hat{u}) = \frac{1}{2}\int_{\mathbb{R}} \big(-|\hat{u}_x|^2 + \nu \mathcal{I}_N[|\hat{u}|^2]^2\big)dx. \tag{4.1.5}$$

The semi-discrete problem (4.1.4) represents an $N+1$-dimensional system of ordinary differential equations (ODEs) for unknown spectral coefficients $f_n(t)$.

In the remainder of this chapter, we show that the numerical solution $\hat{u}$ converges to the exact one in finite time intervals. Our analysis follows the classical framework. First, we study stability of (4.1.4). Next, we show that results of Chapters 1 and 3 yield consistency of the scheme. Once these two basic facts are established, the convergence follows automatically.

4.2 Stability analysis

To begin we derive several a priori estimates:

Lemma 4.2.1. *The numerical solution $\hat{u}$ of* (4.1.4) *satisfies:*

$$\|\hat{u}(t)\|_{L^2(\mathbb{R})} = \|\hat{u}_0\|_{L^2(\mathbb{R})}, \quad \hat{\mathcal{H}}(\hat{u}(t)) = \hat{\mathcal{H}}(\hat{u}_0), \tag{4.2.1a}$$

$$\|\hat{u}_x(t)\|_{L^2(\mathbb{R})} \le c\big(\|\hat{u}_0\|_{L^2(\mathbb{R})}, \|\hat{u}_{0x}\|_{L^2(\mathbb{R})}\big), \tag{4.2.1b}$$

for all $t > 0$, where $c(x, y)$ is a bounded function of both arguments.

Proof. (a) We let $\phi = \hat{u}$ in (4.1.4). Since the automorphism $\mathcal{J} = i$ is antisymmetric and since the Gauss-Chebyshev quadrature is exact for $\phi \in \mathbb{P}_{2N+1}$, we obtain

$$\begin{aligned}
\langle \hat{u}_t, \hat{u}\rangle &= \frac{d}{dt}\|\hat{u}\|^2_{L^2(\mathbb{R})} \\
&= -\langle i\hat{u}_x, \hat{u}_x\rangle + 2\nu\langle i\mathcal{I}_N[|\hat{u}|^2\hat{u}], \hat{u}\rangle \\
&= -\langle i\hat{u}_x, \hat{u}_x\rangle + 2\nu\langle i\mathcal{I}_N[|\hat{u}|^2], \mathcal{I}_N[|\hat{u}|^2]\rangle = 0,
\end{aligned}$$

because $\langle iu, u\rangle = \mathrm{Re}\int_{\mathbb{R}} i|u|^2 dx = 0$ for any u. This gives us the first identity in (4.2.1a).

(b) Next, we let $\phi = iu_t$ in (4.1.4) to obtain

$$
\begin{aligned}
0 = \langle i\hat{u}_t, \hat{u}_t\rangle &= -\langle i\hat{u}_x, i\hat{u}_{xt}\rangle + 2\nu\langle i\mathcal{I}_N[|\hat{u}|^2\hat{u}], i\hat{u}_t\rangle \\
&= -\frac{d}{dt}\|\hat{u}_x\|^2_{L^2(\mathbb{R})} + \nu\big\langle \mathcal{I}_N[|\hat{u}|^2], \tfrac{\partial}{\partial t}\mathcal{I}_N[|\hat{u}|^2]\big\rangle \\
&= \frac{d}{dt}\Big(-\|\hat{u}_x\|^2_{L^2(\mathbb{R})} + \nu\|\mathcal{I}_N[|\hat{u}|^2]\|^2_{L^2(\mathbb{R})}\Big) = 2\frac{d}{dt}\hat{\mathcal{H}}(\hat{u}),
\end{aligned}
$$

which implies that the numerical Hamiltonian $\hat{\mathcal{H}}(\hat{u})$ is conserved.

(c) We estimate $\|u_x\|_{L^2(\mathbb{R})}$ and $\|\mathcal{I}_N[|\hat{u}|^2]\|_{L^2(\mathbb{R})}$. First, we observe that both $\hat{u}_x$ and $\mathcal{I}_N[|\hat{u}|^2]$ are individually bounded in $L^2(\mathbb{R})$, as $\hat{u}$ is an element of the finite dimensional space $\mathbb{P}_N$ for every fixed value of $t > 0$. Second, it is known that [Ada75]

$$
\|u\|^2_{L^\infty(\mathbb{R})} \leq 2\|u\|_{L^2(\mathbb{R})}\|u_x\|_{L^2(\mathbb{R})}. \tag{4.2.2}
$$

We employ this fact to obtain

$$
\begin{aligned}
\|\mathcal{I}_N[|\hat{u}|^2]\|^2_{L^2(\mathbb{R})} &= \frac{\pi}{\ell(N+1)}\sum_{n=0}^{N}\Big(\ell^2 + x^2_{k,N}\Big)|\hat{u}|^4(x_{k,N}) \\
&\leq \frac{2\pi}{\ell(N+1)}\sum_{n=0}^{N}\Big(\ell^2 + x^2_{k,N}\Big)|\hat{u}|^2(x_{k,N})\|\hat{u}\|_{L^2(\mathbb{R})}\|\hat{u}_x\|_{L^2(\mathbb{R})} \\
&= 2\|\hat{u}\|^3_{L^2(\mathbb{R})}\|\hat{u}_x\|_{L^2(\mathbb{R})}.
\end{aligned} \tag{4.2.3}
$$

To complete the proof, we consider two cases $\nu > 0$ and $\nu < 0$, separately. Case $\nu < 0$ is trivial, as inequality (4.2.3) yields (4.2.1b) with $c(x, y) = y^2 - 4\nu x^3 y$.

Now, let $\nu > 0$. By virtue of (4.2.3) and (4.2.1a),

$$
\|\hat{u}_x\|^2_{L^2(\mathbb{R})} - 4\nu\|\hat{u}_0\|^3_{L^2}\|\hat{u}_x\|_{L^2(\mathbb{R})} \leq -2\hat{\mathcal{H}}(\hat{u}_0),
$$

which implies that

$$\begin{aligned}\|\hat{u}_x\|_{L^2(\mathbb{R})} &\leq 2\nu\|\hat{u}_0\|^3_{L^2(\mathbb{R})} + \sqrt{4\nu^2\|\hat{u}_0\|^6_{L^2(\mathbb{R})} - 2\hat{\mathcal{H}}(\hat{u}_0)} \\ &= c\big(\|\hat{u}_0\|_{L^2(\mathbb{R})}, \|\hat{u}_{0x}\|_{L^2(\mathbb{R})}\big).\end{aligned}$$

Note, that function $c(x,y)$ is real and positive as

$$\begin{aligned}2\big|\hat{\mathcal{H}}(\hat{u}_0)\big| &\leq \|\hat{u}_{0x}\|^2_{L^2(\mathbb{R})} + 4\nu\|\hat{u}_0\|^3_{L^2(\mathbb{R})}\|\hat{u}_{0x}\|_{L^2(\mathbb{R})}, \\ 2\hat{\mathcal{H}}(\hat{u}_0) &\leq -\|\hat{u}_{0x}\|^2_{L^2(\mathbb{R})} + 4\nu\|\hat{u}_0\|^3_{L^2(\mathbb{R})}\|\hat{u}_{0x}\|_{L^2(\mathbb{R})} \leq 4\nu^2\|\hat{u}_0\|^6_{L^2(\mathbb{R})},\end{aligned}$$

by (4.2.3). The proof is complete. □

The following result shows that numerical scheme (4.1.4) is continuous with respect to input data, i.e. stable.

Lemma 4.2.2. *Let $\hat{u}^j$, $j = 0, 1$, be solutions of the following perturbed problems: find $\hat{u}^j \in C^{(1)}((0,\infty), \mathbb{P}_N) \cap C([0,\infty), \mathbb{P}_N)$ so that*

$$\begin{cases} \langle \hat{u}^j_t, \phi\rangle = -\langle i\hat{u}^j_x, \phi_x\rangle + 2\nu\langle i\mathcal{I}_N[|\hat{u}^j|^2\hat{u}^j], \phi\rangle + \langle f^j, \phi\rangle, \quad \textit{for all} \quad \phi \in \mathbb{P}_N, \\ \hat{u}^j(0) = \hat{u}^j_0. \end{cases} \tag{4.2.4}$$

Assume that each solution $\hat{u}^j$, $j = 0, 1$, satisfies a priori estimates (4.2.1). Then, the error $e = \hat{u}^0 - \hat{u}^1$ satisfies

$$\|e\|_{L^\infty([0,T],L^2(\mathbb{R}))} \leq c\big(\|e_0\|_{L^2(\mathbb{R})} + \|f^0 - f^1\|_{L^2([0,T],L^2(\mathbb{R}))}\big). \tag{4.2.5}$$

The constant $c > 0$ depends on T and the initial data $\hat{u}^j_0$, $j = 0, 1$, but is independent on the discretization parameter $N > 0$.

Proof. Subtracting equations with $j = 0$ and $j = 1$ from each other, we see that the error satisfies:

$$\begin{cases} \langle e_t, \phi\rangle = -\langle ie_x, \phi_x\rangle + 2\nu\langle i\mathcal{I}_N[|\hat{u}^0|^2\hat{u}^0 - |\hat{u}^1|^2\hat{u}^1], \phi\rangle \\ \qquad\qquad + \langle f^0 - f^1, \phi\rangle, \quad \text{for all} \quad \phi \in \mathbb{P}_N, \\ e(0) = e_0 = \hat{u}^0_0 - \hat{u}^1_0. \end{cases}$$

In the last equation, we set $\phi = e$ and then employ Cauchy-Schwartz and Young inequalities:

$$\begin{aligned}
\frac{d}{dt}\|e\|^2_{L^2(\mathbb{R})} &= 2\nu\langle i\mathcal{I}_N[|\hat{u}^0|^2\hat{u}^0 - |\hat{u}^1|^2\hat{u}^1], e\rangle + \langle f_0 - f_1, e\rangle \\
&= 2\nu\langle i\mathcal{I}_N[(|\hat{u}^0|^2 + |\hat{u}^1|^2)e + \hat{u}^0\hat{u}^1\bar{e}], e\rangle + \langle f_0 - f_1, e\rangle \\
&\le \left(\frac{1}{2} + 2|\nu|\big(\|\hat{u}^0\|_{L^\infty(\mathbb{R})} + \|\hat{u}^1\|_{L^\infty(\mathbb{R})}\big)^2\right)\|e\|^2_{L^2(\mathbb{R})} + \frac{1}{2}\|f_0 - f_1\|^2_{L^2(\mathbb{R})} \\
&\le \kappa(\hat{u}^0, \hat{u}^1)\|e\|^2_{L^2(\mathbb{R})} + \frac{1}{2}\|f_0 - f_1\|^2_{L^2(\mathbb{R})}.
\end{aligned}$$

The last formula, together with Gronwall's inequality, yields

$$\|e\|_{L^2(\mathbb{R})} \le e^{t\kappa(\hat{u}^0,\hat{u}^1)}\Big(\|e_0\|_{L^2(\mathbb{R})} + \int_0^t \|f^0 - f^1\|^2_{L^2(\mathbb{R})}d\tau\Big).$$

By our assumption, $\hat{u}^j$ satisfies a priori estimates (4.2.1). Hence, by virtue of (4.2.2), the positive constant $\kappa(\hat{u}^0, \hat{u}^1)$ is completely controlled by the initial data $\|\hat{u}^j_0\|_{L^2(\mathbb{R})}$ and $\|\hat{u}^j_{0x}\|_{L^2(\mathbb{R})}$, $j = 0, 1$. Hence, in the finite time interval $[0, T]$, (4.2.5) holds with $c = e^{T\kappa(\hat{u}^0,\hat{u}^1)}$. □

4.3 Consistency and convergence

Let u be the exact weak solution to (4.1.2) and let $N > 0$ be fixed. We denote $\tilde{u} = \mathbb{P}_N[u]$. It is not difficult to verify that the spectral projection $\tilde{u}$ satisfies

$$\begin{cases}
\langle \tilde{u}_t, \phi\rangle = -\langle i\tilde{u}_x, \phi_x\rangle + 2\nu\langle i\mathcal{I}_N[|\tilde{u}|^2\tilde{u}], \phi\rangle + \langle f, \phi\rangle, \quad \text{for all} \quad \phi \in \mathbb{P}_N, \\
\tilde{u}(0) = \tilde{u}_0 = \mathcal{P}_N[u_0],
\end{cases} \tag{4.3.1a}$$

where

$$\begin{aligned}
f &= i\frac{d^2}{dx^2}(\mathcal{P}_{N+4} - \mathcal{P}_N)[u] + i2\nu(\mathcal{I} - \mathcal{I}_N)\big[|u|^2u\big] + i2\nu\mathcal{I}_N\big[|u|^2u - |\tilde{u}|^2\tilde{u}\big] \\
&= f_1 + f_2 + f_3.
\end{aligned} \tag{4.3.1b}$$

The following result shows that the defect f is small, provided that the exact solution is sufficiently regular.

Lemma 4.3.1. *Let $1 < 2\gamma < \beta$. Then*

$$\|f\|_{L^2([0,T],L^2(\mathbb{R}))} \leq c\ell^{-2\gamma}(\ell N)^{1+2\gamma-\beta}\|u\|^3_{L^6([0,T],H^{2,\beta}_{2\beta})}, \tag{4.3.2}$$

where $c > 0$ does not depend on $N > 0$ or u.

Proof. We estimate each part of the defect separately. To estimate f_1, we employ Theorem 3.1.2:

$$\begin{aligned}\|f_1\|_{L^2(\mathbb{R})} &\leq \|(\mathcal{P}_{N+4} - \mathcal{P}_N)[u]\|_{H^{2,2}} \leq \|(\mathcal{I} - \mathcal{P}_{N+4})[u]\|_{H^{2,2}} + \|(\mathcal{I} - \mathcal{P}_N)[u]\|_{H^{2,2}} \\ &\leq c(\ell N)^{2-\beta}\|u\|_{H^{2,\beta}_{2\beta}}.\end{aligned}$$

Next, we apply Corollary 3.2.2 and (1.3.9) to obtain

$$\|f_2\|_{L^2(\mathbb{R})} \leq c(\ell N)^{1+\gamma-\beta}\||u|^2u\|_{H^{2,\beta}_{2\beta}} \leq c(\ell N)^{1+\gamma-\beta}\|u\|^3_{H^{2,\beta}_{2\beta}}.$$

Finally, Lemma 3.2.2, inequality (1.3.9) and Theorem 3.1.2 yield the basic bound

$$\begin{aligned}\|f_3\|_{L^2(\mathbb{R})} &\leq c(\ell N)\||u|^2u - |\tilde{u}|^2\tilde{u}\|_{H^{2,\gamma}} \\ &\leq c(\ell N)\big(\||u|^2(\mathcal{I} - \mathcal{P}_N)[u]\|_{H^{2,\gamma}} + \|\tilde{u}\bar{u}(\mathcal{I} - \mathcal{P}_N)[u]\|_{H^{2,\gamma}} + \|\tilde{u}^2(\mathcal{I} - \mathcal{P}_N)[u]\|_{H^{2,\gamma}}\big) \\ &\leq c(\ell N)\big(\|u\|_{H^{2,\gamma}} + \|\tilde{u}\|_{H^{2,\gamma}}\big)^2\|(\mathcal{I} - \mathcal{P}_N)u\|_{H^{2,\gamma}} \\ &\leq c(\ell N)^{1+\gamma-\beta}\big(\|u\|_{H^{2,\gamma}} + \|\tilde{u}\|_{H^{2,\gamma}}\big)^2\|u\|_{H^{2,\beta}_{2\beta}}.\end{aligned}$$

By virtue of inverse inequality (3.2.6),

$$\|\tilde{u}\|_{H^{2,\gamma}} \leq c\Big(\frac{N}{\ell}\Big)^{\gamma}\|u\|_{L^2(\mathbb{R})}.$$

Therefore trivial embedding $H^{2,\beta}_{\beta} \subset H^{2,\gamma}$, implies

$$\|f_3\|_{L^2(\mathbb{R})} \leq c\ell^{-2\gamma}(\ell N)^{1+2\gamma-\beta}\|u\|^3_{H^{2,\beta}_{2\beta}}.$$

To complete the proof, we combine all our estimates together and integrate with respect to t over $[0,T]$, to obtain (4.3.2). □

With the aid of Lemmas 4.2.2 and 4.3.1, we obtain the main result of this section:

Theorem 4.3.2. *Let* $1 < 2\gamma < \beta$. *Then*

$$\|u - \hat{u}\|_{L^\infty([0,T],L^2(\mathbb{R}))} \le c\ell^{-2\gamma}(\ell N)^{1+2\gamma-\beta}\|u\|^3_{L^\infty([0,T],H^{2,\beta}_{2\beta})}, \tag{4.3.3}$$

uniformly in N*, provided that the norm in the right-hand side of the inequality is finite.*

Proof. (a) It is easy to verify that the exact solution u satisfies (4.2.1). We turn now to its spectral projection. First of all,

$$\|\tilde{u}\|_{L^2(\mathbb{R})} \le \|u\|_{L^2(\mathbb{R})} = \|u_0\|_{L^2(\mathbb{R})}.$$

Second, using the triangle inequality, we obtain

$$\|\tilde{u}_x\|_{L^2(\mathbb{R})} \le \|(\mathcal{I} - \mathcal{P}_N)[u]\|_{H^{2,1}} + c\big(\|u_0\|_{L^2(\mathbb{R})}, \|u_{0x}\|_{L^2(\mathbb{R})}\big),$$

where $c(x, y)$ is the bounded function from Lemma 4.2.1. By virtue of Theorem 3.1.2,

$$\|(\mathcal{I} - \mathcal{P}_N)[u]\|_{H^{2,1}} \le c(\ell N)^{1-\beta}\|u\|_{H^{2,\beta}_{2\beta}},$$

for each $t \in [0, T]$. This allows us to conclude that $\|u_x\|_{L^2(\mathbb{R})}$ is uniformly bounded with respect to N.

(b) Now we can apply the stability Lemma 4.2.2 to the couple of problems (4.1.4) and (4.3.1) to obtain

$$\|\hat{u} - \tilde{u}\|_{L^\infty([0,T],L^2(\mathbb{R}))} \le c\Big(\|(\mathcal{I}_N - \mathcal{P}_N)[u_0]\|_{L^2(\mathbb{R})} + \|f\|_{L^2([0,T],L^2(\mathbb{R}))}\Big),$$

with constant $c > 0$ that depends on the exact solution u and terminal time T but is independent of $N > 0$. In view of Theorem 3.1.1, Corollary 3.2.2 and Lemma 4.3.1, we have

$$\|\hat{u} - \tilde{u}\|_{L^\infty([0,T],L^2(\mathbb{R}))} \le c\ell^{-2\gamma}(\ell N)^{1+2\gamma-\beta}\Big(\|u_0\|_{H^{2,\beta}_{2\beta}} + \|u\|^3_{L^6([0,T],H^{2,\beta}_{2\beta})}\Big).$$

Since

$$\|\hat{u}-u\|_{L^\infty([0,T],L^2(\mathbb{R}))} \leq \|\hat{u}-\tilde{u}\|_{L^\infty([0,T],L^2(\mathbb{R}))} + \|(\mathcal{I}-\mathcal{P}_N)[u]\|_{L^\infty([0,T],L^2(\mathbb{R}))},$$

Theorem 3.1.1 and obvious embedding $L^\infty([0,T],H^{2,\beta}_{2\beta}) \subset L^6([0,T],H^{2,\beta}_{2\beta})$ completes the proof. $\square$

Theorem 4.3.2 shows that the numerical scheme (4.1.4) converges algebraically, provided that the exact solution is regular and decays to zero sufficiently fast at infinity.

4.4 Implementation

The numerical scheme (4.1.2) leads to the semi-linear system of ordinary differential equations of the form

$$\dot{Y} = iDY + ig(Y), \tag{4.4.1}$$

where $D \in \mathbb{R}^{(N+1)\times(N+1)}$ is the differentiation matrix, $g(Y)$ is nonlinearity and the neutral symbol Y represents either vector of pseudo-spectral coefficients

$$F(t) = (f_n(t), 0 \leq n \leq N),$$

or vector

$$U(t) = (\hat{u}(x_{k,N},t), 0 \leq k \leq N),$$

containing values of $\hat{u}$ at Gauss-Chebyshev nodes. Particular forms of D and g differ when (4.1.2) is formulated in Fourier or physical space. For instance, the differentiation matrix D is dense in physical space and is five-diagonal (according to formula (3.2.5)) in Fourier space. Similarly, the nonlinearity is given explicitly by

$$g(Y) = 2\nu(|\hat{u}(x_{k,N})|^2\hat{u}(x_{k,N},t), 0 \leq k \leq N), \tag{4.4.2}$$

in physical space, while its exact representation in Fourier space is not so straightforward.

Note that the exact solutions to ODE (4.4.1) are not known. In practice, it shall be integrated using an appropriate time-stepping algorithm. There are two important practical issues that arise in this connection. First of all, computing the vector field $iDY + ig(Y)$ requires transformations of physical data $U(t)$ into its Fourier counterpart $F(t)$ and vice versa. Straightforward implementation of both transforms, written in a matrix-vector form, would require $\mathcal{O}(N^2)$ operations and hence is not numerically feasible for large values of N. Second, the problem (4.4.1) is stiff and symplectic, i.e. the exact flow φ_t of (4.4.1) preserves the quadratic form

$$\Big(\overline{\frac{\partial\varphi_t}{\partial Y_0}}\Big)^T\Big(\frac{\partial\varphi_t}{\partial Y_0}\Big)$$

A reasonable time-stepping algorithm must be able to cope with stiffness and at the same time be reasonably cheap and preserve the symplectic structure of the exact flow. Both issues are briefly discussed below.

4.4.1 Fast direct and inverse Chebyshev-Fourier transforms

First, we discuss fast direct and inverse Chebyshev-Fourier transforms. As was observed by many authors (see [CQHZ06] and references therein) both can be computed in $\mathcal{O}(N\log N)$ flops with the aid of fast discrete direct and inverse Fourier transforms (FFT). Indeed, components of F and U are connected by the identities (see formulas (3.2.1) and (3.2.2)):

$$f_n = \frac{\pi}{\ell(N+1)}\sum_{k=0}^{N}[\ell^2 + x_{k,n}^2]TB_n(x_{k,N})u_k, \quad 0 \le n \le N; \tag{4.4.3a}$$

$$u_k = \sum_{n=0}^{N} \frac{f_n}{\kappa_n} TB_n(x_{k,N}), \quad 0 \le k \le N. \tag{4.4.3b}$$

To evaluate (4.4.3a), we define

$$w_k = \frac{\pi\sqrt{\ell}}{\sin\left(\pi\frac{4k+1}{2(N+1)}\right)} \begin{cases} u_{2k}, & 0 \le k \le \lfloor\frac{N}{2}\rfloor; \\ -u_{2(N+1-k)-1}, & \lfloor\frac{N}{2}\rfloor \le k \le N, \end{cases} \tag{4.4.4a}$$

$$\hat{w}_n = \frac{1}{N+1} \sum_{k=0}^{N} w_k e^{-2\pi i \frac{kn}{N+1}}, \quad 0 \le n \le N, \quad \hat{w}_{N+1} = \hat{w}_0. \tag{4.4.4b}$$

Then, the pseudo-spectral coefficients are given explicitly by

$$f_n = \frac{1}{2}\left[\hat{w}_n e^{\pi i \frac{n}{N+1}} + \hat{w}_{N+1-n} e^{-\pi i \frac{n}{N+1}}\right], \quad 0 \le n \le N. \tag{4.4.4c}$$

We note that formulas (4.4.4a) and (4.4.4c) each require $\mathcal{O}(N)$ arithmetic operations, while (4.4.4b) can be accomplished in $\mathcal{O}(N \log N)$ flops using standard discrete inverse FFT. Hence, the overall complexity of the algorithm is $\mathcal{O}(N \log N)$.

The inverse fast Chebyshev-Fourier transform is obtained by inverting formulas (4.4.4). In particular, inversion of (4.4.4b) involves standard discrete direct FFT, so that the computational complexity of the resulting algorithm is again $\mathcal{O}(N \log N)$.

4.4.2 Time-stepping

Now, we turn to practical time-stepping. As mentioned earlier on, when N is large, the problem (4.4.1) is stiff and cannot be integrated using explicit ODE solvers. Furthermore, the problem is Hamiltonian and its flow is symplectic. To cope with the stiffness and at the same time, to preserve the symplectic structure of the flow, we apply the Strang-type symmetric splitting technique, see [HLW06] and references therein. That is, we rewrite the numerical Hamiltonian as:

$$\hat{\mathcal{H}}(\hat{u}) = -\frac{1}{2}\langle \hat{u}_x, \hat{u}_x\rangle + \frac{\nu}{2}\langle \mathcal{I}_N[|\hat{u}|^2\hat{u}], \hat{u}\rangle =: \hat{\mathcal{H}}_1(\hat{u}) + \hat{\mathcal{H}}_2(\hat{u}),$$

and introduce two sub-problems:

Find $\hat{u}^1$, $\hat{u}^2$ so that:

$$\langle \hat{u}_t^1, \phi\rangle = \langle i\nabla\hat{\mathcal{H}}_1(\hat{u}^1), \phi\rangle, \quad \text{for all} \quad \phi \in \mathbb{P}_N, \tag{4.4.5a}$$

$$\langle \hat{u}_t^2, \phi\rangle = \langle i\nabla\hat{\mathcal{H}}_2(\hat{u}^2), \phi\rangle, \quad \text{for all} \quad \phi \in \mathbb{P}_N. \tag{4.4.5b}$$

If Φ_t^1, Φ_t^2 denote the flows of problems (4.4.5a) and (4.4.5b), respectively, then the exact solution of (4.4.1) is given by:

$$\hat{u}(h) = \Phi^1_{\frac{h}{2}} \circ \Phi^2_h \circ \Phi^1_{\frac{h}{2}}(\hat{u}(0)) + \mathcal{O}(h^3), \tag{4.4.6}$$

when time-step h is small.

We observe that calculating the exact flow $\Phi^1_{\frac{h}{2}}$ requires evaluation of a matrix exponent times a vector. This can be done using Krylov type algorithm as described in [HL97]. To simplify matters, we solve (4.4.5a) numerically, using the implicit midpoint rule

$$\hat{u}^1(h) = \Phi^1_h(\hat{u}^1(0)) = \Psi^1_h(\hat{u}^1(0)) + \mathcal{O}(h^3) = \Big[2\Big(I - i\frac{h}{2}D\Big)^{-1} - I\Big]\hat{u}^1(0) + \mathcal{O}(h^3). \tag{4.4.7}$$

The above procedure involves the solution of a system of linear equations with five diagonal matrix and can be accomplished in $\mathcal{O}(\mathcal{N})$ operations per time integration step. The second flow Φ_h^2 can be computed exactly. Elementary calculations yield the formula:

$$\Phi^2_h(\hat{u}^2(x,0)) = \exp\big\{i2\nu h|u_0^2(x,0)|^2\big\}\hat{u}^2(x,0), \quad x \in \mathbb{R}. \tag{4.4.8}$$

Combining (4.4.6), (4.4.7) and (4.4.8), we advance the numerical solution by one time step, using the following one-step splitting scheme:

$$\hat{u}(t_{n+1}) = \Psi^1_{\frac{h}{2}} \circ \Phi^2_h \circ \Psi^1_{\frac{h}{2}}(\hat{u}(t_n)) = \Psi_h(\hat{u}(t_n)), \quad h = t_{n+1} - t_n. \tag{4.4.9}$$

By construction, time-stepping scheme (4.4.9) is symmetric, symplectic and has classical order of convergence $p = 2$. To lift its order, we employ the composition

$$\hat{\Psi}_h = \Psi_{\gamma_1 h} \circ \cdots \circ \Psi_{\gamma_m h}, \tag{4.4.10}$$

as described in [HLW06]. In particular, taking the composition coefficients (see [HLW06])

$$\begin{aligned}
\gamma_1 =& \gamma_{17} = 0.13020248308889008087881763, \\
\gamma_2 =& \gamma_{16} = 0.56116298177510838456196441, \\
\gamma_3 =& \gamma_{15} = -0.38947496264484728640807860, \\
\gamma_4 =& \gamma_{14} = 0.15884190655515560089621075, \\
\gamma_5 =& \gamma_{13} = -0.39590389413323757733623154, \\
\gamma_6 =& \gamma_{12} = 0.18453964097831570709183254, \\
\gamma_7 =& \gamma_{11} = 0.25837438768632204729397911, \\
\gamma_8 =& \gamma_{10} = 0.29501172360931029887096624, \\
& \gamma_9 = -0.60550853383003451169892108,
\end{aligned}$$

we obtain a symplectic and symmetric time stepping method of order $p = 8$. Note that the overall computational complexity of one time integration step described above is $\mathcal{O}(N \log N)$.

4.5 Numerical simulations

In this section, we demonstrate the performance of numerical scheme (4.1.2). In our simulations, we solve the nonlinear Schrödinger equation (4.1.1) with $\nu = 1$ only. We note that the stability and convergence theory presented in Sections 4.2 and 4.3 applies to all nonzero values of ν. However, it is impossible to obtain closed reference solutions when $\nu < 0$ (so called defocusing mode). The opposite case $\nu > 0$ (the focusing mode) is easier to deal with. Here, the discrete spectrum of Lax operator $i\frac{\partial^2}{\partial x^2} + \mathcal{I}$ is nonempty and yields traveling wave (J-soliton) solutions, [APT04]. Every J-soliton solution is controlled by a number of real parameters, such as amplitudes — a_j, velocities — v_j, centers — ξ_j and phases — ϕ_j, $1 \leq j \leq J$, and can be easily reconstructed using the explicit formula (see [APT04] for derivations):

$$u(x,t) = 2i\frac{\det G^c}{\det G}, \tag{4.5.1}$$

where

$$\begin{aligned}
&k = \left(\frac{v_j + ia_j}{2}, 0 \leq j \leq J\right), \quad K = \left(\frac{1}{k_i - k_j^*}, 0 \leq i,j \leq J\right), \\
&y = i\left(a_j e^{a_j\xi_j + i(\phi_j + 2xk_j - 4tk_j^2)}\, 0 \leq j \leq J\right), \\
&G = I + K\operatorname{diag}(y^*)K^*\operatorname{diag}(y), \quad G^c = \begin{pmatrix} 0 & y^T \\ \mathbb{1} & G \end{pmatrix}.
\end{aligned}$$

4.5.1 Example 1.

In our first example, we integrate (4.1.2) in the time interval $[0, 2\pi]$, with $\nu = 1$ and initial condition obtained from (4.5.1), with $J = 1$ and $a_1 = 1$, $v_1 = \xi_1 = \phi_1 = 0$. In these settings, the exact solution is a single stationary soliton centered at the origin. Furthermore, the exact solution is analytic in a strip containing the real axis and decays to zero exponentially at $\pm\infty$. The situation is ideal and, in view of Theorem 4.3.2, we expect rapid convergence.

The results of simulations, with $2^4 \leq N \leq 2^7$ and $\ell = 4$, (see Figure 4.1) show that this is indeed the case. Both, $L^2(\mathbb{R})$ and $L^\infty(\mathbb{R})$ (blue and teal lines, respectively) errors decrease geometrically as N increases. For large values of N, both errors stabilize near 10^{-11}. This phenomenon is the consequence of round-off errors accumulation. These errors (approximately 10^{-16} in IEEE arithmetics) are amplified by the quantity $\|D\| \sim \mathcal{O}(N^2)$ when solving linear systems in (4.4.7).

According to Lemma 4.2.1, the quantities $\|\hat{u}(t)\|_{L^2(\mathbb{R})}$ and $\hat{\mathcal{H}}(\hat{u}(t))$ are conserved along exact trajectories of (4.1.4). This is confirmed by our simulations, and both first integrals remain almost constantly (within the machine precision) independent on the discretization parameter N.

4.5.2 Example 2.

Here, we integrate (4.1.2) in the time interval $[0, 2\pi]$, with $\nu = 1$ and initial condition obtained from (4.5.1), with $J = 1$ and $a_1 = 1$, $v_1 = \frac{1}{2}$, $\xi_1 = -1$, $\phi_1 = 0$. In these settings, the exact solution is a single traveling wave. As in Example 1, the exact solution is analytic in a strip containing the real axis and decays to zero exponentially at $\pm\infty$.

The results of simulations, with $2^4 \leq N \leq 2^8$ and $\ell = 4$ are presented in Figure 4.2. As in Example 1, we see that both, $L^2(\mathbb{R})$ and $L^\infty(\mathbb{R})$ (blue and teal lines, respectively) errors decrease geometrically and the scheme preserves both first integrals to remain almost exactly. However, this time the wave is moving from the region with a large number of spatial grid points to the region with relatively few grid points. For this reason, resolving the wave with higher accuracy requires more grid points than in our previous example. Compare, for instance, upper right diagrams in Figures 4.1 and 4.2.

4.5.3 Example 3.

In this example, we set $\nu = 1$, $J = 2$ and $a_1 = 2$, $a_2 = 1$, $v_1 = v_2 = 0$, $\xi_1 = -\frac{1}{2}$, $\xi_2 = \frac{1}{2}$, $\phi_1 = 0$, $\phi_2 = \frac{\pi}{3}$. This yields a stationary 2-soliton solution. The results of simulations (we use $2^4 \leq N \leq 2^8$ and $\ell = 4$) are qualitatively

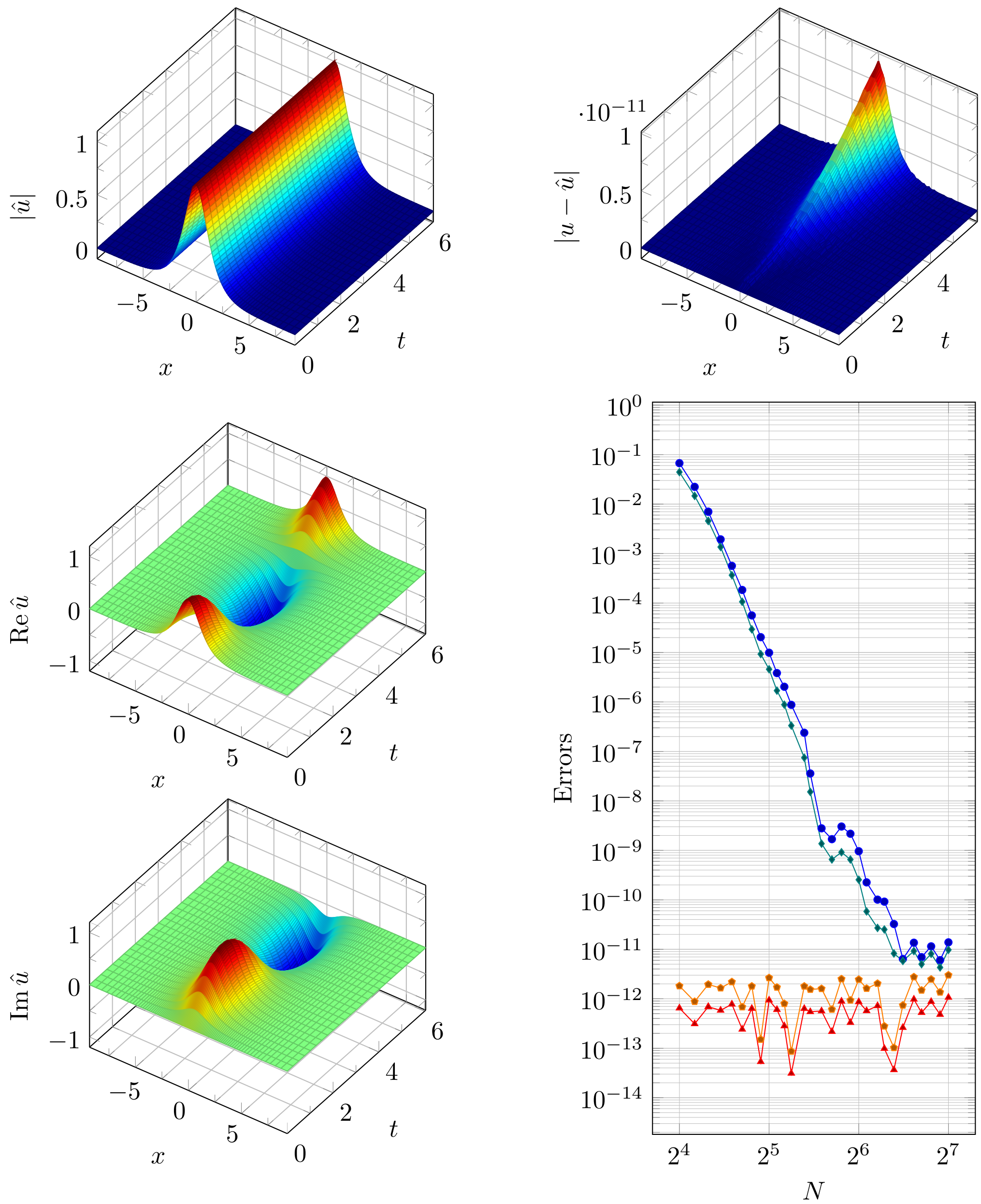

Figure 4.1: The numerical solution of (4.1.2) (top to bottom and left to right): $|\hat{u}|$, $\operatorname{Re}\hat{u}$, $\operatorname{Im}\hat{u}$, $|u-\hat{u}|$, with $N = 2^7$. The bottom right diagram: $\|u-\hat{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u-\hat{u}\|_{L^\infty(\mathbb{R})}$ (teal), $\max_t\big|\|\hat{u}(t)\|_{L^2(\mathbb{R})} - \|\hat{u}_0\|_{L^2(\mathbb{R})}\big|$ (red) and $\max_t\big|\hat{\mathcal{H}}(\hat{u}(t)) - \hat{\mathcal{H}}(\hat{u}_0)\big|$ (orange).

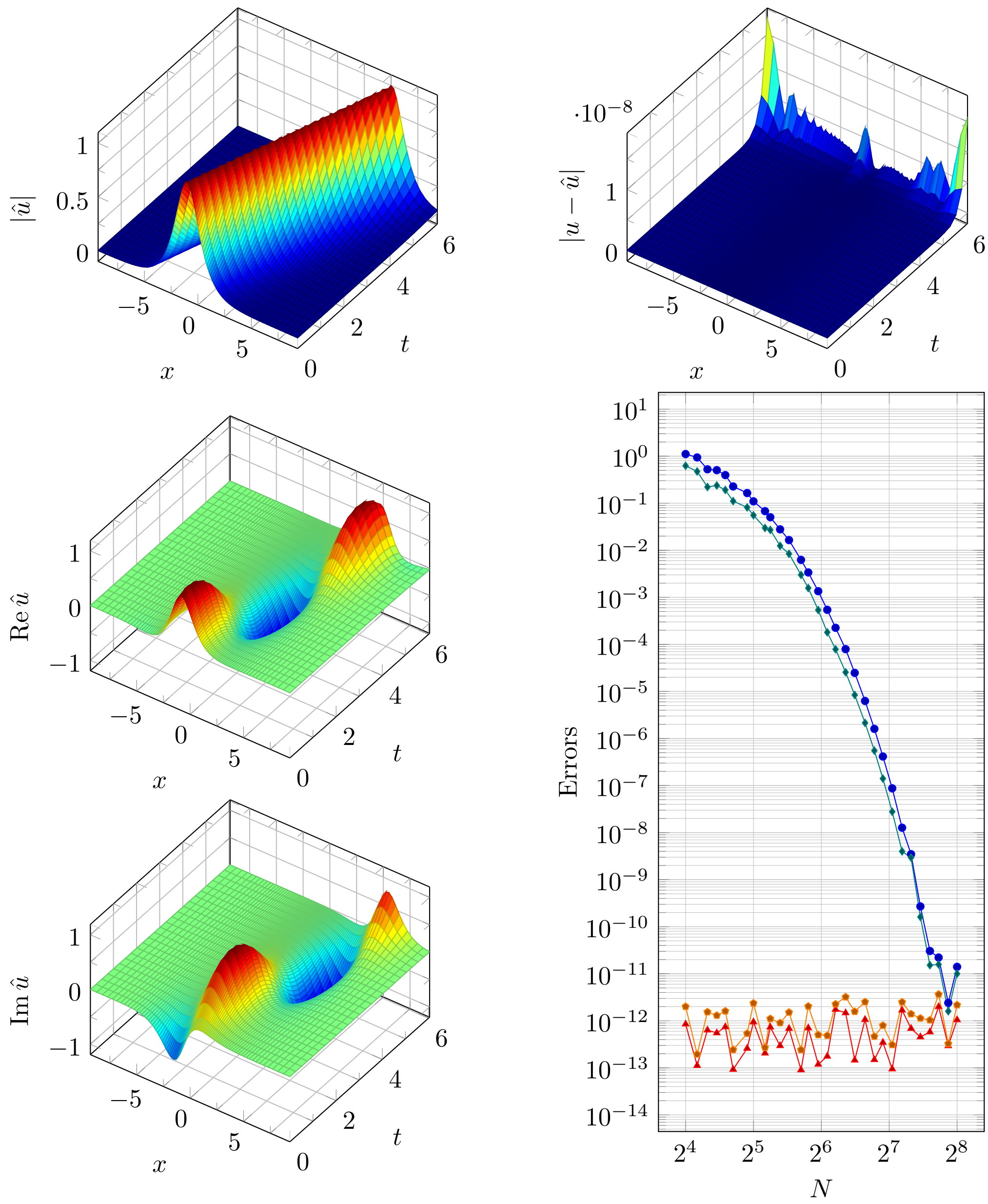

Figure 4.2: The numerical solution of (4.1.2) (top to bottom and left to right): $|\hat{u}|$, $\mathrm{Re}\,\hat{u}$, $\mathrm{Im}\,\hat{u}$, $|u - \hat{u}|$, with $N = 2^7$. The bottom right diagram: $\|u - \hat{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u - \hat{u}\|_{L^\infty(\mathbb{R})}$ (teal), $\max_t \big| \|\hat{u}(t)\|_{L^2(\mathbb{R})} - \|\hat{u}_0\|_{L^2(\mathbb{R})} \big|$ (red) and $\max_t \big| \hat{\mathcal{H}}(\hat{u}(t)) - \hat{\mathcal{H}}(\hat{u}_0) \big|$ (orange).

the same as in Example 2. The errors decay geometrically as predicted by Theorem 4.3.2, see Figure 4.3.

4.5.4 Example 4.

As another example, we take $\nu = 1$, $J = 2$ and $a_1 = 2$, $a_2 = 1$, $v_1 = -\frac{1}{2}$, $v_2 = \frac{1}{2}$, $\xi_1 = 2$, $\xi_2 = -\frac{1}{2}$, $\phi_1 = \phi_2 = 0$. The resulting 2-soliton solution represents two colliding traveling waves.

The results of simulations, with $2^4 \leq N \leq 2^8$ and $\ell = 4$ are presented in Figure 4.4. We see that the qualitative behavior of both $L^2(\mathbb{R})$ and $L^\infty(\mathbb{R})$ (blue and teal lines, respectively) errors is the same as those observed in all our previous simulations. The convergence is geometric (the error curves are concave). However, the absolute accuracy drops. The reason is — as the time increases, the waves enter a region with relatively few grid points, where solutions cannot be resolved accurately. The situation can be improved by taking larger values for N.

4.5.5 Example 5.

In our last example, we simulate a 3-soliton colliding scenario. Here, we set $\nu = 1$, $J = 3$ and $a_1 = 2$, $a_2 = 3$, $a_3 = 1$, $v_1 = \frac{1}{2}$, $v_2 = 0$, $v_3 = -\frac{1}{2}$, $\xi_1 = 0$, $\xi_2 = 2$, $\xi_3 = 5$, $\phi_1 = \phi_2 = \phi_3 = 0$. The results of simulations (we use $2^4 \leq N \leq 2^8$ and $\ell = 4$) are almost identical to those obtained in Example 4, see Figure 4.5.

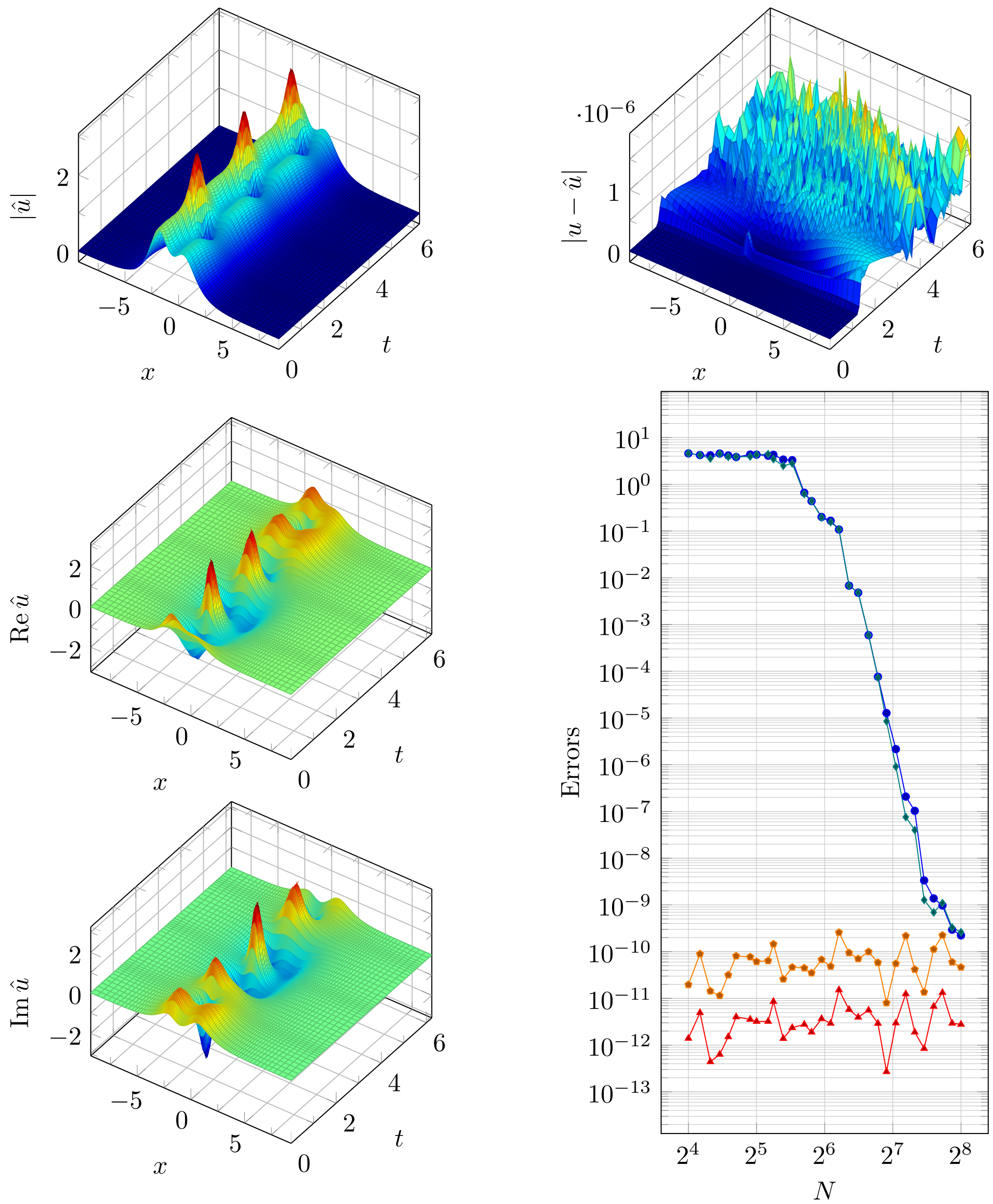

Figure 4.3: The numerical solution of (4.1.2) (top to bottom and left to right): $|\hat{u}|$, $\mathrm{Re}\,\hat{u}$, $\mathrm{Im}\,\hat{u}$, $|u-\hat{u}|$, with $N = 2^7$. The bottom right diagram: $\|u-\hat{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u-\hat{u}\|_{L^\infty(\mathbb{R})}$ (teal), $\max_t\big|\|\hat{u}(t)\|_{L^2(\mathbb{R})} - \|\hat{u}_0\|_{L^2(\mathbb{R})}\big|$ (red) and $\max_t\big|\hat{\mathcal{H}}(\hat{u}(t)) - \hat{\mathcal{H}}(\hat{u}_0)\big|$ (orange).

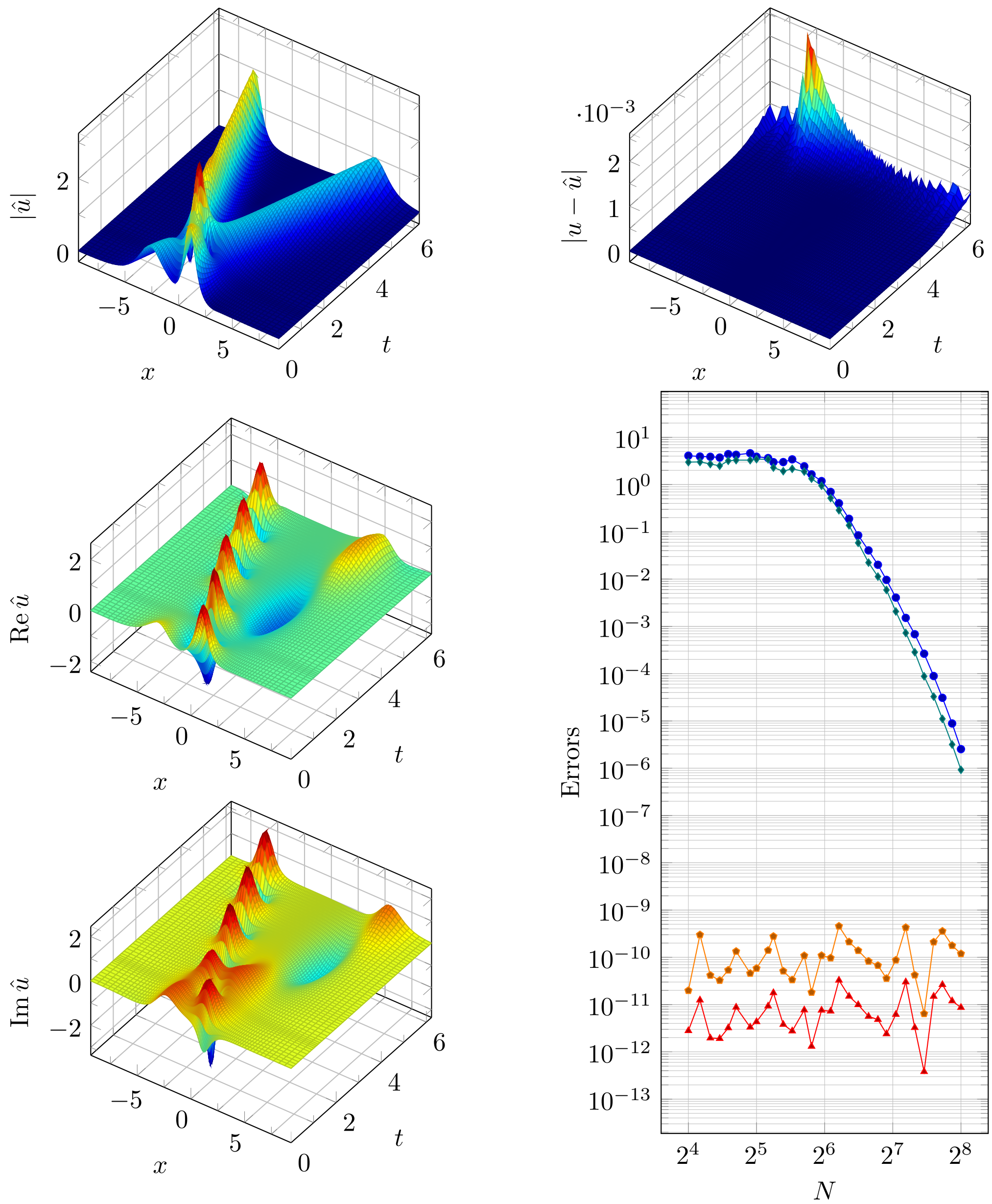

Figure 4.4: The numerical solution of (4.1.2) (top to bottom and left to right): $|\hat{u}|$, $\operatorname{Re} \hat{u}$, $\operatorname{Im} \hat{u}$, $|u - \hat{u}|$, with $N = 2^7$. The bottom right diagram: $\|u - \hat{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u - \hat{u}\|_{L^\infty(\mathbb{R})}$ (teal), $\max_t \big| \|\hat{u}(t)\|_{L^2(\mathbb{R})} - \|\hat{u}_0\|_{L^2(\mathbb{R})} \big|$ (red) and $\max_t \big| \hat{\mathcal{H}}(\hat{u}(t)) - \hat{\mathcal{H}}(\hat{u}_0) \big|$ (orange).

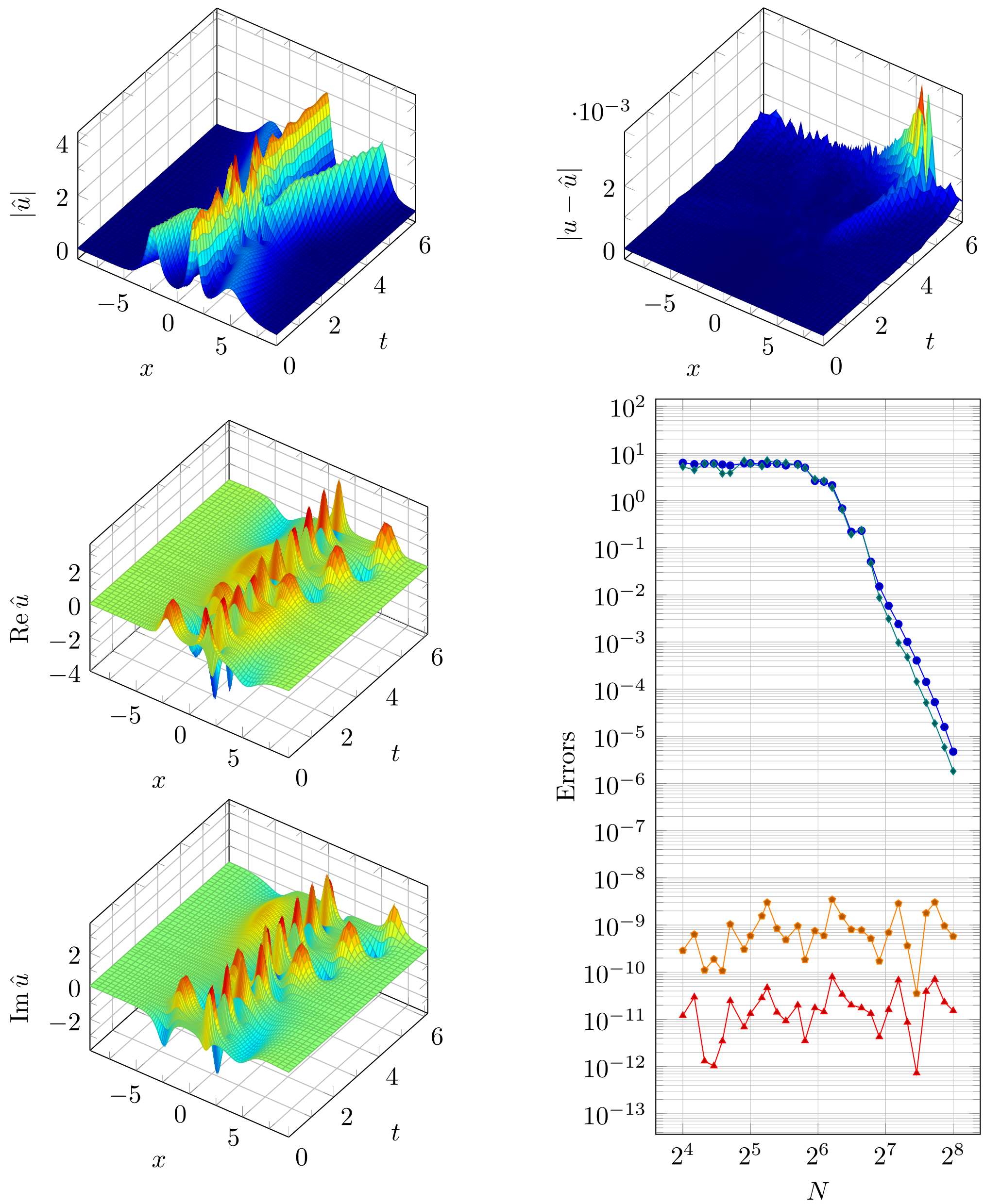

Figure 4.5: The numerical solution of (4.1.2) (top to bottom and left to right): $|\hat{u}|$, $\operatorname{Re}\hat{u}$, $\operatorname{Im}\hat{u}$, $|u-\hat{u}|$, with $N = 2^7$. The bottom right diagram: $\|u-\hat{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u-\hat{u}\|_{L^\infty(\mathbb{R})}$ (teal), $\max_t\big|\|\hat{u}(t)\|_{L^2(\mathbb{R})} - \|\hat{u}_0\|_{L^2(\mathbb{R})}\big|$ (red) and $\max_t\big|\hat{\mathcal{H}}(\hat{u}(t)) - \hat{\mathcal{H}}(\hat{u}_0)\big|$ (orange).

Conclusion

In the project, we dealt with Chebyshev-type spectral and pseudo-spectral methods in unbounded domains. Such methods are widely used in simulations as they have a number of important computational advantages. In particular, they admit very efficient practical implementation, see [Fun92, Boy00, Tre00, CQHZ06, HGG07, STW11] and references therein. However, the stability and convergence analysis of these methods require deep understanding of approximation properties of the underlying functional basis.

This was the core part of our research. Using the connection between algebraically mapped Chebyshev basis and Laguerre functions, established in Chapter 2, we obtained sharp approximation and interpolation estimates in $L^2(\mathbb{R})$ and $H^{2,\alpha}(\mathbb{R})$ settings. These results provided the complete description of numerical errors in terms of regularity of functions being approximated. Once the behavior of stationary errors were fully understood, we turned to applications.

In the thesis, we applied Chebyshev-type pseudo-spectral method to the classical nonlinear Schrödinger equation. We explained how to construct an appropriate numerical scheme that preserves symplecticity of the exact flow. Next, we provided a rigorous and comprehensive stability and convergence analysis. Exactly at this point, our approximation and interpolation estimates played a pivotal role and yielded the precise description of the discretization errors.

With these results at hand, we switched to practical simulations. Following [CQHZ06], we observed that Chebyshev-type bases allow very efficient numerical implementation. In particular, the direct and inverse discrete Chebyshev-Fourier transforms can be computed using standard direct and inverse discrete FFT. This significantly reduces the computational cost of the algorithm and makes it suitable for large scale simulations. Though the thesis dealt with space discretization only, we provided a brief account on practical time-stepping. In context of Schrödinger's equation, whose flow is a nonlinear one-parameter group, we proposed the use of a simple composite Strang-type splitting scheme. Finally, we presented several simulations that were done using the computer. We observed that the numerical data agreed well with our theoretical investigations.

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