Numerical solution of the Klein-Gordon equation in an unbounded domain

Gafari Abiodun Lukumon
217081936

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by

Gafari Abiodun Lukumon

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As the candidate's supervisors, we have approved this thesis for submission.

Signature: ________ Name: Dr. N. Parumasur Date: 19 /11/ 2018

Signature: ________ Name: Dr. S. Shindin Date: 19 /11/ 2018

Preface

The work described in this dissertation was carried out in the School of Mathematics, Statistics and Computer Science at University of KwaZulu-Natal, Durban,South Africa from January 2018 to November 2018, under the supervision of Dr N. Parumasur and Dr S. Shindin.

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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Gafari Abiodun Lukumon.

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I, Gafari Abiodun Lukumon, declare that

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Abstract

In this dissertation, we provide theoretical and numerical analyses of the Klein-Gordon equation (KGE) posed in the real line. In the first part of the work, using the weak compactness techniques, we show that the KGE equation is globally well-posed on the real line, moreover we show that the solutions are classical and compactly supported, provided the initial data is smooth and compactly supported. These properties form the theoretical foundation for the numerical analysis.

For numerical treatment, we use a Fourier-type pseudo-spectral scheme. In the second part of the dissertation, we provide its comprehensive stability and convergence analyses. Furthermore, we discuss technical issues connected with its efficient practical implementation, in particular, design of an appropriate time-stepping scheme that is able to preserve qualitative features of both the continuous and the space semi-discrete KGE models. The thesis is concluded with several computational examples.

Contents

Chapter 1

Introduction

In the field of numerical analysis, solutions of some evolution equations are difficult to obtain analytically and so we have to use a numerical approach. There are many types of numerical methods suitable for different problems, but when we refer to those set in regular domains, spectral methods are considered to be the most accurate and computationally efficient [Boy00, CQHZ06, HGG07, Kop09, STW11]. Spectral methods are collection of techniques that represent the solution of a differential equation as a finite linear combination of globally defined basis functions, where the coefficients in the sum are chosen to ensure the differential equation and perhaps some boundary conditions are satisfied as closely as possible [Boy00, CQHZ06, HGG07, Kop09, STW11].

In this dissertation, we provide theoretical and numerical analyses of a Fourier-type pseudo-spectral method in context of the nonlinear Klein-Gordon equation (KGE) posed on the real line. KGE has attracted significant attention in the area of applied sciences and engineering because of its important role in a wide variety of application [DEGM82]. Since it is one of the nonlinear partial differential equations (PDEs) examples, the exact solutions are not easy to compute and therefore, we resort to finding them numerically.

The outline of this thesis is as follows. Chapter 1 reviews some existing results from the literature. In Chapter 2, we present as preliminaries, some results from functional analysis. We provide a detailed account on the Fourier-type approximations in Chapter 3.

In Chapter 4, we demonstrate the well-posedness of the nonlinear KGE model in periodic settings and then extend the analysis to the real line. Account on a Fourier-type pseudo-spectral scheme for the nonlinear KGE equation with emphasis on its stability, consistency and convergence is presented in Chapter 5. In Chapter 6, we report the efficiency of our scheme by applying it to a special case of KGE known as Sine-Gordon equation (SGE). Finally, some conclusions, contributions to knowledge and possible future research based on our findings and numerical results are drawn in Chapter 7.

1.1 The Klein-Gordon equation

KGE, also known as Klein-Fock-Gordon equation or Klein-Gordon-Fock equation is a relativistic form of Schröndinger equation which define scalar spinless particle. It has root coming from the study of theoretical physics with importance in quantum mechanics, nonlinear optics, solid state physics, applied sciences and engineering [DEGM82]. The nonlinear KGE has the general form:

$$u_{tt} = a^2 \Delta u - \mathcal{V}'(u), \quad x \in \Omega, \quad t > 0, \tag{1.1.1a}$$

$$u(x,0) = u_0, \quad u_t(x,0) = v_0, \tag{1.1.1b}$$

where the nonlinearity $\mathcal{V}(u)$ represents the potential energy of the system modeled by (1.1.1). The concrete choice of the potential $\mathcal{V}(u)$ depends on the physical phenomenon under consideration. For example SGE, obtained when $\mathcal{V}(u) = 1 - \cos(u)$ is widely used in the modeling of shallow waves. A complete account on the various KGE forms can be found in [GI92].

Many authors have worked on KGE, including both its numerical and analytical aspect. We shall present a review of these in the coming sections.

1.2 Contemporary studies on well-posedness for the nonlinear KGE

For a given evolution system like KGE to be well-posed, one must ensure that solutions exist, are uniquely determined by input data (that normally involves a number of initial and boundary conditions) and depend on the data continuously. Mathematical studies that are pertinent to well-posedness of the nonlinear KGE have attracted a substantial number of authors [BW81, GV85, FT78, HW87, IMM06, KWY18, LYA$^+$18, Ma17, NO01, NMPZ84, Wed78, XD13, XZ13].

The concrete details depend strongly on the type of the nonlinearity $\mathcal{V}(u)$, the dimensionality of the spatial domain and the input data. E.g., in the Sobolev space, $H^s(\mathbb{R}^n)$ with $s \geq \frac{n}{2}$, the well-posedness of the pure Cauchy problem for nonlinear KGE is established in [NO01]. Study of the global well-posedness and scattering for a nonlinear KGE system in one dimensional domains is done by [XZ13]. The local and global existence results and finite blow-up time solutions of KGE, equipped with general power-type nonlinearities, is carried out in [GV85, LYA$^+$18]. The existence and uniqueness of global solutions for a Cauchy problem associated to a semilinear KGE, with exponential potentials, is proven by [IMM06] in two-dimensions. The well-posedness of the nonlinear KGE, with high energy initial data is investigated using the potential well method by [PT14]. Recent paper [Ma17] deals with global solution of quasi-linear wave Klein-Gordon system in two dimensional space. He is able to prove global existence of small regular solutions for a class of hyperbolic systems containing a wave equation and a KGE model with null couplings.

More details about the analysis of the Cauchy problem and global classical solution to KGE can be found in [BW81, FT78, KWY18, NMPZ84, HW87, Wed78, XD13, XZ13].

1.3 Contemporary studies of numerics for the nonlinear KGE

In numerical analysis realm, a number of semi- and fully- discrete schemes were proposed in the literature. In particular, study of three finite-difference approximations of the nonlinear KGE that respect the symplectic structure of the equation is done in [Dun97]. M. Dehghan and A. Shokri in [DS09] employ radial basis functions. Their scheme appears to be very similar to a finite-difference method and was successfully applied to solve one-dimensional nonlinear KGE with quadratic and cubic nonlinearities. The numerical techniques for the solution of nonlinear KGE based on the finite-difference and collocation methods are presented by [LD10]. The validity of these techniques is demonstrated with examples. Further details on classical finite-difference methods for solving nonlinear KGE can be found in [BOJM10, EMVQDGM15, HZ09].

A fully discrete approach, based on finite elements for the damped nonlinear KGE in one-dimension is implemented in [WC05]. The numerical schemes that are pertinent to Chebyshev-type wavelet spectral methods for the approximate solutions of KGE and SGE are presented in [IA16]. On the other hand, development of schemes that are associated with Legendre-type wavelets is done in [YTSZ15]. Fast and accurate fourth-order time-stepping schemes coupled with the discrete Fourier transform are proposed in [MAS11]. A Legendre-type pseudo-spectral scheme for solving initial-boundary value problems of nonlinear KGE is developed in [LGV96]. The authors investigate the stability and convergence of numerical solutions. Their numerical method exhibits high accuracy and extends to multi-dimensional settings. A variant of pseudo-spectral method for the solution of nonlinear KGE is proposed in [GW14]. A pseudo-spectral Fourier-type method for finding localized spherical soliton solutions of $(3+1)-$dimension KGE is presented in [ES16], where the classical fourth-order Runge-Kutta method is employed to perform time integration.

The continuous flow generated by KGE is symplectic, hence design of suitable high order time-stepping (marching) schemes preserving this structure is an important issue.

In this direction, in [LIW18], a class of symmetric and arbitrary high-order marching schemes suitable for time integration of KGE is proposed. The construction makes use of the two-point Hermite interpolation polynomial, which is applied directly to the operator-variation-of-constants formula. The high accuracy of the resulting scheme is demonstrated in a number of practical simulations. The numerical comparison of implicit and exponential time-differencing methods in context of ϕ^4 KGE is performed in [EMM13], where it was established that the former techniques are more accurate than the latter. Similarly, B. Weizhu and D. Xuanchun in [WX12], compared finite-difference and Fourier-type pseudo-spectral schemes combined with a Gaustschi-type exponential integrators for solving KGE in the non-relativistic limit region.

Further discussion of spectral and finite-element methods in context of KGE can be found in [CLC17, DT12, DXZ14, BZ15, ABI$^+$15].

To conclude, we note that developing appropriate numerics for KGE is an important area of modern research. However, despite a large number of various numerical techniques proposed in the literature, their rigorous analysis is far from being complete. There are very few works containing exhaustive stability/convergence analyses, in particular, in the realm of spectral methods. One of the main aims of the present dissertation is to fill in this gap for the class of Fourier-type pseudo-spectral schemes, applied to KGE with smooth potentials.

Chapter 2

Preliminaries

This Chapter is introductory. Here, we list some basic results in functional analysis that are used throughout our work.

2.1 Banach spaces

The results quoted below are standard and can be found in particular in [Bre11, Erw78, Lax02, RF10].

Definition 2.1.1. *Let X be a vector space over $\mathbb{R}$. A function $\|\cdot\|$ satisfying:*

(i) $\|u\| \geq 0$ *(non-negativity),*

(ii) $\|u\| = 0$ *if and only if* $u = 0$,

(iii) $\|u + v\| \leq \|u\| + \|v\|$ *(the triangle inequality),*

(iv) $\|\alpha u\| = |\alpha|\|u\|$ *(absolute homogeneity);*

for any $u, v \in X$ and $\alpha \in \mathbb{R}$, is called a norm in X. A vector space X equipped with a norm $\|\cdot\|$ is called a normed vector space.

A norm defines topology in X, in particular we have:

Definition 2.1.2. *A sequence, $\{u_n | n = 0, 1, 2, \cdots\}$ of X is said to converge to an element $u \in X$, if the distance $\|u_n - u\|$ tends to 0 as n increases.*

In a usual way, the Cauchy sequences are defined.

Definition 2.1.3. *A sequence, $\{u_n | n = 0, 1, 2, \cdots\}$ of X is said to be a Cauchy in X if given $\epsilon > 0$, there exist $N = N(\epsilon) > 0$ such that $\|u_n - u_m\| < \epsilon$, whenever $n, m > N(\epsilon)$.*

A complete normed vector space (i.e. the space where all Cauchy sequence converge in the topology induced by the norm) is called a Banach space. We give two examples below:

(i) Let $1 \leq p \leq \infty$. The finite-dimensional vector space $\mathbb{R}^n$, equipped with the norm

$$\|u\|_p = \Big(\sum_{k=1}^{n} |u_k|^p\Big)^{1/p},$$

is a Banach space.

(ii) Suppose Ω is an open measurable subset of $\mathbb{R}^n$ and $1 \leq p \leq \infty$. We say that two measurable functions $u, v : \Omega \to \mathbb{R}$ are equal almost everywhere ($u = v$ a.e.), if the measure of the set $\{x \in \Omega | u(x) \neq v(x)\}$ is zero. The equality understood in the almost everywhere sense is an equivalence relation. The collection (denoted by $L^p(\Omega)$) of all equivalence classes of measurable functions for which

$$\|u\|_p = \Big(\int_\Omega |u|^p dx\Big)^{1/p} < \infty$$

is a Banach space. The quantity $\|\cdot\|_p : L^p(\Omega) \to \mathbb{R}$, defined above, is its norm.

Definition 2.1.4. *Let X and Y be Banach spaces. A linear map $F : X \to Y$[1] is said to be bounded if there exists a constant $C > 0$ such that, for all $u \in X$, $\|Fu\|_Y \leq C\|u\|_X$.*

Note that every bounded linear map acting between two Banach spaces is continuous. The collection of all bounded maps from X to Y is usually denoted by $L(X, Y)$. $L(X, Y)$ is again a Banach space with the induced norm defined by

$$\|F\|_{X\to Y} = \sup_{\|u\|_X = 1} \|Fu\|_Y.$$

[1] In the special case when $Y = \mathbb{R}$, F is called a linear functional.

Definition 2.1.5. *A linear continuous map $F : X \to Y$ is said to be compact if for each bounded sequence $\{u_n \in X | n = 0, 1, \cdots\}$, one can find a subsequence $\{u_{nk} | k = 0, 1, \cdots\}$ and an element $u \in X$ such that $\{Fu_{nk} | k = 0, 1, \cdots\} \subset Y$ converges to Fu in Y.*

Definition 2.1.6. *Let X and Y be two Banach spaces. A bounded injective linear map $J : X \to Y$ is called an embedding of X into Y. We say that embedding J is compact if J is a compact map.*

The fact that X is embedded in Y is often expressed as $X \hookrightarrow Y$. When X is a subspace of Y and J acts as an identity on the elements of X, we speak about canonical embeddings.

2.2 Strong and weak convergence

Apart from the strong topology, induced by a norm, one may define other forms of convergence. To begin, we give the following

Definition 2.2.1. *Let X be a Banach space. The space of all bounded linear functionals on X is denoted by X' and is called the topological dual of X.*

By the remark above, X' is a Banach space under the norm

$$\|f\|_{X'} = \sup_{\|u\|_{X=1}} |fu|.$$

Since X' is a Banach space, one can define the second dual X'' of X. Then any $u \in X$ can be identified with a linear functional u' in X'' acting on the elements $f \in X'$ according to the formula

$$u'(f) = f(u).$$

The construction above defines a natural embedding J from X to X''. In general, the map J is injective but not surjective, i.e. X'' is in some sense larger than X. In the case when J is surjective, we say that the space X is reflexive. The connection between $u' \in X''$, $u \in X$ and $f \in X'$ is often written in the form

$$u'(f) = \langle u, f \rangle,$$

the bilinear form $\langle \cdot, \cdot \rangle$ is known as the duality paring.

Using the notion of dual spaces, we have

Definition 2.2.2. *We say that a sequence $\{u_n \in X | n = 0, 1, \cdots\}$ converges weakly to $u \in X$, if for every $f \in X'$*

$$\lim_{n\to\infty} \langle f, u_n \rangle = \langle f, u \rangle.$$

Definition 2.2.3. *We say that a sequence $\{f_n \in X' | n = 0, 1, \cdots\}$ converges weakly star to $f \in X'$, if for every $u \in X$*

$$\lim_{n\to\infty} \langle f_n, u \rangle = \langle f, u \rangle.$$

It is easy to verify that strong convergence implies weak convergence while weak convergence implies weakly star convergence. When X is a reflexive Banach space, weak and weak star convergences are equivalent. Below, we list several standard results that are used in our analysis. In our presentation, we follow [Bre11, Erw78, Eva90, Lax02, RF10, Son04].

Lemma 2.2.1. *Any bounded set in a reflexive Banach space is weakly compact, i.e. any bounded sequence has a weakly converging subsequence.*

Lemma 2.2.2. *Let X' be a dual of a Banach space X. Then any bounded set in X' is weakly star compact, i.e. any bounded sequence in X' has a weakly star converging subsequence.*

In what follows, we make use of one more notion of convergence.

Definition 2.2.4. *Let Ω be a measurable open subset of $\mathbb{R}^n$ and $\{u_n\}_{n\geq 0}$ be a sequence of measurable functions defined on Ω. We say that the sequence $\{u_n\}_{n\geq 0}$ converges almost everywhere in Ω to a measurable function u, provided that*

$$\lim_{n\to\infty} \sup_{\varepsilon>0} \lambda(\{x \in \Omega | |u_n(x) - u(x)| > \varepsilon\}) = 0,$$

where λ denotes the standard Lebesgue measure in $\mathbb{R}^n$.

The connections between different types of convergences are listed below, see [Eva90, Son04].

Lemma 2.2.3. *Let Ω be a measurable open subset of $\mathbb{R}^n$ and $\{u_n\}_{n\geq 0}$ be a sequence that converges strongly to $u \in L^p(\Omega)$, $1 \leq p < \infty$. Then there exists a subsequence that converges a.e. to u in Ω. When $p = \infty$ then the sequence itself converges almost everywhere to u in Ω.*

Lemma 2.2.4. *Let Ω be a measurable open subset of $\mathbb{R}^n$ and $\{u_n\}_{n\geq 0}$ be a bounded sequence in $L^p(\Omega)$, $1 \leq p < \infty$, that converges a.e. to u in Ω. Then $u \in L^p(\Omega)$ and u_n converges weakly to u in $L^p(\Omega)$.*

Later on, we deal with initial value problems, whose solutions $u(t)$ are elements of Bochner-type spaces $L^p([0,T], X')$, $1 \leq p \leq \infty$. The following result allows one to study values of such solutions at the boundary $t = 0$.

Lemma 2.2.5. *Let X be a Banach space. Assume that $1 \leq p < \infty$ and*

$$\begin{aligned} &u_n \to u \quad \textit{weakly star in } L^p([0,T], X'), \\ &\partial_t u_n \to \partial_t u \quad \textit{weakly star in } L^p([0,T], X'). \end{aligned}$$

Then,

$$u_n(0) \to u(0) \quad \textit{weakly star in } X'.$$

2.3 Hilbert spaces

Both theoretical and numerical analyses of KGE model make use of the notion of Hilbert spaces. Below, we summarize several fundamental results that are used in the dissertation. Our exposition follows closely [Ber61, Bre11, Erw78, Lax02, RF10].

Definition 2.3.1. *A vector space H over $\mathbb{R}$, equipped with a symmetric, bilinear positive definite map $\langle \cdot, \cdot \rangle : H \times H \to \mathbb{R}$, is called an inner product or Euclidean space.*

In an inner product space H, we let

$$\|u\| = \sqrt{\langle u, u \rangle}.$$

Function $\|\cdot\|$ induced by the inner product satisfies all axioms of the norm. Hence, any Euclidean space H is normed. If in addition H is complete with respect to $\|\cdot\|$, we say that H is a Hilbert space. For example, $\mathbb{R}^n$ and $L^2(\Omega)$, equipped with

$$\langle u, v\rangle = \sum_{k=1}^{n} u_k v_k \quad \text{and} \quad \langle u, v\rangle = \int_\Omega uv dx,$$

respectively, are Hilbert spaces.

According to the Riesz representation theorem, any bounded linear functional $f : H \to \mathbb{R}$ in a Hilbert space H can be realized as $f = \langle f', \cdot\rangle$, for some $f' \in H$. Hence, the dual space H' can be naturally identified with H itself, i.e. any Hilbert space is reflexive. The above identification has many important consequences. In particular, we have [Son04]

Lemma 2.3.1. *Assume $\{u_n\}_{n\geq 0} \subset H$ converges weakly to $u \in H$ and, in addition, $\lim_{n\to\infty} \|u_n\| = \|u\|$. Then the convergence is strong, i.e. $\lim_{n\to\infty} \|u_n - u\| = 0$.*

The inner product induces usual Euclidean structure in H.

Definition 2.3.2. *Two elements $u, v \in H$ are said to be orthogonal if $\langle u, v\rangle = 0$ and orthonormal if $\langle u, u\rangle = \langle v, v\rangle = 1$. An element u is said to be orthogonal to a subset Y of H, if it is orthogonal to each element of Y.*

A subset Y of a Hilbert space H is called everywhere dense in H if its closure is the whole of H. A Hilbert space that contains a countable everywhere dense subset is called separable.

Definition 2.3.3. *Let $\{u_\alpha\}_{\alpha\in A} \subset H$ be a collection of mutually orthogonal vectors in H. We say that the collection $\{u_\alpha\}_{\alpha\in A}$ is a basis of H if the linear span of $\{u_\alpha\}_{\alpha\in A}$ is everywhere dense in H.*

Theorem 2.3.2. *Any separable Hilbert space H has a countable orthonormal basis.*

Theorem 2.3.2 has fundamental consequences. It follows that any separable Hilbert space H contains a discrete set $\{u_n\}_{n\geq 0} \subset H$ of mutually orthonormal vectors that span the whole of H. Hence, any $u \in H$ is represented by its Fourier series

$$u = \sum_{n \geq 0} \hat{u}_n u_n, \quad \hat{u}_n = \langle u_n, u \rangle, \quad n \geq 0,$$

where convergence is strongly in H. For any $u, v \in H$, we have the Parseval identities

$$\langle u, v \rangle = \sum_{n \geq 0} \hat{u}_n \hat{v}_n,$$
$$\|u\|^2 = \sum_{n \geq 0} |\hat{u}_n|^2.$$

Further, if $H_k = \text{span}\{u_n\}_{n=0}^{k}$ and

$$S_k(u) = \sum_{n=0}^{k} \hat{u}_n u_n, \quad k \geq 0,$$

then for any $u \in H$,

$$\inf_{v \in H_k} \|u - v\| = \|u - S_k(u)\|.$$

In plain words, the partial Fourier sum $S_k(u)$ delivers the best approximation of u in the finite dimensional space H_k, $k \geq 0$. The extremal property lays the foundation for the large class of practical computational algorithms known as spectral methods.

2.4 Sobolev spaces

Let Ω be an open measurable subset of $\mathbb{R}^m$. Let $1 \leq p \leq \infty$ and $n \geq \mathbb{N}$. Sobolev space $W^{n,p}(\Omega)$ of order n is defined to be the linear subspace of functions (equivalence classes of functions) from $L^p(\Omega)$ whose distributional derivatives up to order n are also in $L^p(\Omega)$, see [AF03, Son04] and references therein. $W^{n,p}(\Omega)$, equipped with the norm

$$\|u\|_{W^{n,p}(\Omega)} = \sum_{|\alpha| \leq n} \|D^\alpha u\|_{L^p(\Omega)}^p,$$

where $\alpha \in \mathbb{N}^m$ is the multi-index, $|\alpha| = \sum_{i=1}^{m} \alpha_i$ and $D^\alpha u = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \cdots \partial x_n^{\alpha_m}}$, is a Banach space. When $p = 2$, $W^{n,2}(\Omega)$ is commonly denoted by $H^n(\Omega)$. The latter is a Hilbert space, endowed with inner product

$$\langle u, v\rangle_n = \langle u, v\rangle + \sum_{|\alpha|=n} \langle D^\alpha u, D^\alpha v\rangle.$$

In the literature, the definition of $W^{n,p}(\Omega)$ can be extended to any real $n \geq 0$, using the theory of interpolation [AF03]. Further, the negative order Sobolev spaces are defined via duality as $W^{-n,p}(\Omega) = (W^{n,p'}(\Omega))'$, where $p' = \frac{p}{p-1}$ is the exponent conjugate with $1 \leq p \leq \infty$.

Below, we make use of the following fundamental result, known as the Sobolev embedding theorem, see [Son04].

Theorem 2.4.1. *Let Ω be an open measurable subset of $\mathbb{R}^m$.*

(i) If $np < m$ and $q^* = \frac{mp}{m-np}$, then

$$W^{n,p}(\Omega) \hookrightarrow L^q(\Omega), \quad p \leq q \leq q^*. \tag{2.4.1a}$$

(ii) If $np = m$, then

$$W^{n,p}(\Omega) \hookrightarrow L^q(\Omega), \quad p \leq q < \infty. \tag{2.4.1b}$$

(iii) If $np > m > (n-1)p$, then

$$W^{n,p}(\Omega) \hookrightarrow C^{0,\alpha}(\overline{\Omega}), \quad 0 < \alpha \leq n - \tfrac{m}{p}, \tag{2.4.1c}$$

while if $m = (n-1)p$, (2.4.1c) *holds for all $0 < \alpha < 1$. In formula* (2.4.1c),

$$C^{0,\alpha}(\overline{\Omega}) = \left\{ f \in C(\overline{\Omega}) \middle| \sup_{x \neq y \in \overline{\Omega}} \tfrac{|f(x)-f(y)|}{|x-y|^\alpha} < \infty \right\}$$

denotes the space of Hölder continuous functions.

In the special case, when $\Omega \subset \mathbb{R}$ is bounded and has the cone property (which holds automatically for smooth domains, see [AF03]) all the embeddings (2.4.1) *are compact.*

In the dissertation, we deal with Banach spaces of vector valued functions. The following result, combined with the Sobolev embedding theorem, is essential.

Theorem 2.4.2 (see [Son04])**.** *Let X_0, X and X_1 be three Banach spaces and X_0, X_1 be reflexive. Assume that $X_0 \hookrightarrow X \hookrightarrow X_1$ and the embedding $X_0 \hookrightarrow X$ is compact. For any $1 < p, q < \infty$, let*

$$W = \{u | u \in L^p([0,T], X_0),\ u_t \in L^q((0,T), X_1)\}.$$

Then the embedding $W \hookrightarrow L^p([0,T], X)$ is compact.

Chapter 3

Fourier-type spectral methods

Spectral methods were endowed with first mathematical foundations in [GO77]. The general idea of the technique consists in expressing solutions of differential equations as a finite linear combination of specific globally defined smooth ”orthogonal basis functions”, where the coefficients in the sum are chosen so that the differential equation is satisfied as close as possible. Many important partial differential equations (PDEs), ordinary differential equations (ODEs) and eigenvalue problems are successfully solved using spectral methods.

There are three general ways spectral schemes are implemented, namely Galerkin, Tau and collocation methods [Boy00, CQHZ06, HGG07, Kop09, STW11]. All three techniques yield extremely accurate and efficient computational algorithms when applied to smooth problems posed on regular domains. However, they become less effective and accurate if complex geometries and/or discontinuous coefficients are involved.

To implement the Galerkin method, trial function and a weak formulation of a differential equation under consideration is required. The unknown coefficients are chosen so that the defect vanish on the subspace of trial functions [Boy00, CQHZ06, HGG07, Kop09, STW11]. Collocation schemes, also known as pseudo-spectral methods, make use of the strong formulation of a problem. The unknown coefficients, representing the numerical solution are chosen so that the problem is satisfied exactly at a given finite set of points known as collocation points. The Tau methods are used for problems with complicated boundary conditions, where the collocation techniques are extremely tedious and the Galerkin approach is not possible.

The computational properties of any spectral scheme depends on the properties of the orthogonal basis chosen to approximate solutions. In the case of compact regular domains, the common approach is to use trigonometric functions, Jacobi polynomials (in particular, Chebyshev and Legendre polynomials), tensor-product bases made up of these functions, spherical harmonics, e.t.c. The choice becomes less obvious when the spatial domain is unbounded. Here, several scenarios are possible: one can map the unbounded domain into a compact one and employ one of the bases listed above; depending on the geometry of the domain and the properties of solutions, one may use the Hermite or the Laguerre functions or specially designed rational bases; finally, when the asymptotic nature of solutions is known, one can artificially truncate the spatial domain. See [Boy00, CQHZ06, HGG07, Kop09, STW11] for general discussion.

In this dissertation, we deal with KGE equation that describes propagation of nonlinear waves. In the next Chapter, we show that the nonlinear flow, associated with KGE, maps compactly supported initial data back into compactly supported data. As a consequence, for compactly supported initial data, the dynamics of the model is completely confined to compact subdomains of $\mathbb{R}^2$. In view of this, we loose no information when restricting the spatial domain of the model to compact subintervals of $\mathbb{R}$. Doing so, we are forced to add some artificial boundary conditions. There are several options here, one can use e.g. homogeneous Dirichlet/Neumann or periodic boundary conditions. Either case imposes some restrictions on the choice of a computational basis. For example, in context of Dirichlet/Neumann boundary conditions, one can employ either Chebyshev or Legendre basis.

In the dissertation, we make use of the periodic boundary conditions and the classical trigonometric Fourier basis. With this approach, all differential operators are diagonal in the Fourier space and, as a result, associated spectral schemes allow very efficient practical implementation. In the sequel of this Chapter, we provide a detailed discussion of key properties of classical trigonometric Fourier basis.

3.1 The continuous Fourier expansion

Let $L_p^2(-\ell,\ell) := L^2(-\ell,\ell)$[1] be the space of square integrable 2ℓ-periodic functions. For $u(x) \in L_p^2(-\ell,\ell)$, we denote the trigonometric Fourier series of u by

$$\mathcal{F}[u] = \hat{a}_0 + \sum_{n=1}^{\infty} \hat{a}_n \cos(\tfrac{n\pi x}{\ell}) + \sum_{n=1}^{\infty} \hat{b}_n \sin(\tfrac{n\pi x}{\ell}). \tag{3.1.1}$$

The Fourier coefficients $\hat{a}_n$ and $\hat{b}_n$ are given respectively by

$$\hat{a}_n = \tfrac{1}{c_n \ell} \int_{-\ell}^{\ell} u(x) \cos(\tfrac{\pi n x}{\ell}) dx, \tag{3.1.2a}$$

$$\hat{b}_n = \tfrac{1}{\ell} \int_{-\ell}^{\ell} u(x) \sin(\tfrac{\pi n x}{\ell}) dx, \quad n > 0, \tag{3.1.2b}$$

where

$$c_n = \begin{cases} 2, & n = 0; \\ 1, & n > 1. \end{cases}$$

Alternatively, (3.1.1) can be rewritten in the complex form as

$$\mathcal{F}[u] = \tfrac{1}{2\ell} \sum_{|n| \le \infty} \hat{u}_n e^{i\frac{\pi n x}{\ell}}, \tag{3.1.3}$$

with the coefficients,

$$\hat{u}_n = \left\langle u, e^{i\frac{\pi n x}{\ell}} \right\rangle_{L_p^2} = \int_{-\ell}^{\ell} u(x) e^{-i\frac{\pi n x}{\ell}} dx = \tfrac{\ell}{2} \begin{cases} 2\hat{a}_0, & n = 0; \\ \hat{a}_n - i\hat{b}_n, & n > 0; \\ \hat{a}_{-n} + i\hat{b}_{-n}, & n < 0. \end{cases} \tag{3.1.4}$$

It is shown in classical texts on Fourier analysis (for example, see [Gra14, SS03, SW71]) that the collection of exponents $\left\{e^{-i\frac{\pi n}{\ell}x},\ n \in \mathbb{Z}\right\}$, provides a complete orthogonal basis in $L_p^2(-\ell,\ell)$. It follows from the standard theory of Hilbert space (see Section 2.3), that any function $u \in L_p^2(-\ell,\ell)$ can be represented by its Fourier series.

[1]Everywhere below, we add the subscript p to emphasize that we deal with spaces of periodic functions.

3.2 Trigonometric approximation of regular functions

Let $\mathcal{P}_N : L^2_p(-\ell,\ell) \to \bar{\mathbb{P}}_N$ be the orthogonal projector from $L^2_p(-\ell,\ell)$ onto $\bar{\mathbb{P}}_N$, where $\bar{\mathbb{P}}_N = \text{span}\{e^{i\frac{\pi n x}{\ell}}\}_{n=-N}^{N-1}$. We know from Section 2.3 that

$$\mathcal{P}_N[u](x) = \tfrac{1}{2\ell}\sum_{|n|\leq N} \hat{u} e^{i\frac{\pi n}{\ell}x} = \int_{-\ell}^{\ell} u(x-t)\frac{\sin\left(\frac{\pi(2N+1)t}{2\ell}\right)}{\sin\left(\frac{\pi t}{2\ell}\right)}dt$$

delivers the best approximation of u in $\bar{\mathbb{P}}_N$ and, according to Theorem 2.3.2, $\lim_{N\to\infty}\|(\mathcal{I}-\mathcal{P}_N)[u]\|_{L^2_p} = 0$. Hence, it is natural to approximate elements of $L^2_p(-\ell,\ell)$ by their truncated Fourier expansions. There is however a practical difficulty. For certain functions $u \in L^2_p(-\ell,\ell)$, the convergence speed of the spectral Fourier projections $\mathcal{P}_N[u]$ is extremely slow. Classical analysis, reproduced below (see [Boy00, CQHZ06, HGG07, Kop09, STW11]), indicates that we can control the convergence rate, provided functions are regular.

Theorem 3.2.1. *Assume $0 \leq \alpha < \beta$, then*

$$\|(\mathcal{I}-\mathcal{P}_N)[u]\|_{H^\alpha_p} \leq c\left(\tfrac{\ell}{\pi N}\right)^{\beta-\alpha}\|u\|_{H^\beta_p}, \tag{3.2.1}$$

where $c > 0$ is an absolute constant.

Proof. The proof is standard (see [HGG07]). We note that in terms of Fourier coefficients the Sobolev norm in $H^\alpha_p(-\ell,\ell) := H^\alpha(-\ell,\ell)$ can be written as

$$\|u\|^2_{H^\alpha_p} = \tfrac{1}{2\ell}\sum_{n\in\mathbb{Z}}\left(1+\left|\tfrac{\pi n}{\ell}\right|^{2\alpha}\right)|\hat{u}_n|^2.$$

Since the differentiation and projection commute, we have

$$\begin{aligned}
\|(\mathcal{I}-\mathcal{P}_N)[u]\|^2_{H^\alpha_p} &= \tfrac{1}{2\ell}\sum_{n>|N|}\left(1+\left|\tfrac{\pi n}{\ell}\right|^{2\alpha}\right)|\hat{u}_n|^2 \\
&= \tfrac{1}{2\ell}\sum_{n>|N|}\left(1+\left|\tfrac{\pi n}{\ell}\right|^{2\beta}\right)\frac{\left(1+\left|\frac{\pi n}{\ell}\right|^{2\alpha}\right)}{\left(1+\left|\frac{\pi n}{\ell}\right|^{2\beta}\right)}|\hat{u}_n|^2 \\
&\leq c^2\left(\tfrac{\ell}{\pi N}\right)^{2(\beta-\alpha)}\tfrac{1}{2\ell}\sum_{n>|N|}\left(1+\left|\tfrac{\pi n}{\ell}\right|^{2\beta}\right)|\hat{u}_n|^2,
\end{aligned}$$

and the claim is settled. ∎

The error bound (3.2.1) indicates that for functions of finite regularity (parameter β in Theorem 3.2.1), the convergence rate is at most algebraic in N. In the Sobolev scale $H_p^\beta(-\ell,\ell)$, the result is optimal [CQHZ06, HGG07, Kop09]. Faster convergence rates are obtained for analytic functions. The following result is classical, see [Boy00, CQHZ06, HGG07, Kop09, STW11] and reference therein.

Theorem 3.2.2. *Assume u is analytic in a bounded open region D with a rectifiable boundary ∂D, containing interval $[-\ell,\ell]$ in its interior. Then*

$$\|(\mathcal{I}-\mathcal{P}_N)[u]\|_{H_p^\alpha} \le c\tfrac{\gamma\sqrt{2\ell}}{2\pi}\left(\tfrac{\pi N}{\ell}\right)^{\alpha+1} e^{-\frac{\pi\delta}{\ell}N} \max_{z\in\partial D}|u(z)|, \tag{3.2.2}$$

where $c>0$ is an absolute constant, $\delta=\inf_{z\in\partial D, x\in[-\ell,\ell]}|z-x|>0$ is the distance from the interval $[-\ell,\ell]$ to the boundary ∂D and γ is the length of the boundary ∂D.

Proof. Under assumption of the Theorem, we have the following Cauchy estimate

$$|u^{(m)}(x)| \le \tfrac{m!}{2\pi}\oint_{\partial D}\frac{|u(z)|}{|z-x|^{m+1}}d|z| \le \tfrac{\gamma}{2\pi}\tfrac{m!}{\delta^{m+1}}\max_{z\in\partial D}|u(z)|,$$

which implies, in particular,

$$\|u\|_{H_p^m} \le c\tfrac{\gamma\sqrt{2\ell}}{2\pi}\tfrac{m!}{\delta^{m+1}}\max_{z\in\partial D}|u(z)|,$$

with an absolute constant $c>0$. In view of (3.2.1), we have

$$\|(\mathcal{I}-\mathcal{P}_N)[u]\|_{H_p^\alpha} \le c\tfrac{\gamma\sqrt{2\ell}}{2\pi}\left(\tfrac{\ell}{\pi N}\right)^{m-\alpha}\tfrac{m!}{\delta^{m+1}}\max_{z\in\partial D}|u(z)|,$$

for all $m\ge\alpha$. We have from Stirling's formula that $m!\le e^{1-m}m^{m+1}$, consequently, letting $m=\dfrac{\pi(N+1)\delta}{\ell}$ in the inequality above, we obtain (3.2.2). □

Theorem 3.2.2 indicates that for analytic functions, the approximation error decreases exponentially fast as the parameter N increases. In the texts on Numerical Analysis, the phenomenon is referred to as spectral convergence [Boy00, CQHZ06, HGG07, Kop09, STW11].

3.3 The discrete Fourier expansion

Unfortunately, the continuous Fourier approximation $\mathcal{P}_N[u]$ requires evaluation of (3.1.4). The integral that appears in the right-hand side of the equation may be impossible to compute analytically and, hence, one is forced to consider approximations by quadratures [Boy00, HGG07]. In the context of trigonometric Fourier expansions, it is a custom to use either the composite trapezoidal rule or the implicit mid-point with the nodes uniformly distributed in $[-\ell, \ell]$, [Boy00, HGG07]. The quadratures are given by the expressions

$$\int_{-\ell}^{\ell} f(x)dx \approx I^1_{2N+1}[f] := \tfrac{\ell}{N} \sum_{j=0}^{2N-1} f(x_j), \quad x_j = \frac{\ell(j-N)}{N}, \quad 0 \le j \le 2N, \tag{3.3.1a}$$

$$\int_{-\ell}^{\ell} f(x)dx \approx I^2_{2N+1}[f] := \tfrac{2\ell}{2N+1} \sum_{j=0}^{2N} f(x_j), \quad x_j = \frac{2\ell(j-N)}{2N+1}, \quad 0 \le j \le 2N, \tag{3.3.1b}$$

respectively. The key property of (3.3.1) is stated below, see [HGG07].

Lemma 3.3.1. *The quadrature formulas* (3.3.1a) *and* (3.3.1b) *are exact in* $\bar{\mathbb{P}}_{N-1}$ *and* $\bar{\mathbb{P}}_N$ *respectively, i.e.*

$$I^k_{2N+1}[u] = \int_{-\ell}^{\ell} u(x)dx, \quad k = 1, 2,$$

provided $k = 1$ *and* $u \in \bar{\mathbb{P}}_{N-1}$ *or* $k = 2$ *and* $u \in \bar{\mathbb{P}}_N$.

Proof. It is sufficient to verify the statement for the functions $\phi_n(x) = e^{i\frac{\pi n}{\ell}x}$, with $|n| \le 2N$. Substituting ϕ_n into (3.3.1) and taking into account definition of the quadratures nodes, we infer

$$I^1_{2N+1}[\phi_n] = \tfrac{\ell}{N} \sum_{|n|<2N} \frac{\sin(\pi n)}{\sin\left(\frac{\pi n}{2N}\right)} e^{-i\frac{\pi n}{2N}},$$

$$I^2_{2N+1}[\phi_n] = \tfrac{2\ell}{2N+1} \sum_{|n|\le 2N} \frac{\sin(\pi n)}{\sin\left(\frac{\pi n}{2N+1}\right)} e^{-i\frac{\pi n}{2N}},$$

where the last formulas are understood as limits when $n = 0$. Straightforward summation gives,

$$\int_{-\ell}^{\ell} \phi_n(x)dx = I^1_{2N+1}[\phi_n] = \delta_{n,0} 2\ell, \qquad |n| < 2N,$$

$$\int_{-\ell}^{\ell} \phi_n(x)dx = I^2_{2N+1}[\phi_n] = \delta_{n,0} 2\ell, \qquad |n| \le 2N,$$

and the claim is settled. $\square$

Using either of the quadratures, defined above, in practice one approximates the continuous Fourier coefficients by their discrete counterparts

$$\breve{u}_{1,n} = I^1_{2N+1}[u\overline{\phi_n}] =: \langle u, \phi_n \rangle_{1,2N+1}, \quad |n| \le N, \tag{3.3.2a}$$

$$\breve{u}_{2,n} = I^2_{2N+1}[u\overline{\phi_n}] =: \langle u, \phi_n \rangle_{2,2N+1}, \quad |n| \le N. \tag{3.3.2b}$$

The discrete Fourier coefficients give rise to the discrete expansions

$$\mathcal{I}^1_{2N+1}[u](x) = \tfrac{1}{2\ell} \sum_{|n|\le N} c_n \breve{u}_{1,n} e^{\frac{i\pi n}{\ell}x}, \quad c_{-N} = c_N = \tfrac{1}{2}, \quad c_n = 1, \quad |n| \le N-1, \tag{3.3.3a}$$

$$\mathcal{I}^2_{2N+1}[u](x) = \tfrac{1}{2\ell} \sum_{|n|\le N} \breve{u}_{2,n} e^{\frac{i\pi n}{\ell}x}, \tag{3.3.3b}$$

where the coefficients c_n in (3.3.3a) compensate inexactness of the composite trapezoidal rule for trigonometric polynomials of degree $2N$.

We observe that the discrete Fourier expansions $I^k_{2N+1}[u](x)$, $k = 1, 2$, are closely connected with the trigonometric interpolation [Boy00, HGG07]. Direct calculations show that

$$\mathcal{I}^1_{2N+1}[u](x) = \sum_{j=0}^{2N-1} u(x_j) \left[\frac{\cos\left(\frac{\pi}{2\ell}(x-x_j)\right)}{2N} \frac{\sin\left(\frac{\pi N}{\ell}(x-x_j)\right)}{\sin\left(\frac{\pi}{2\ell}(x-x_j)\right)} \right] = \sum_{j=0}^{2N-1} u(x_j) t^1_{2N+1,j}(x),$$

$$\mathcal{I}^2_{2N+1}[u](x) = \sum_{j=0}^{2N} u(x_j) \left[\frac{1}{2N+1} \frac{\sin\left(\frac{\pi(2N+1)}{2\ell}(x-x_j)\right)}{\sin\left(\frac{\pi}{2\ell}(x-x_j)\right)} \right] = \sum_{j=0}^{2N} u(x_j) t^2_{2N+1,j}(x).$$

Since $t^k_{2N,j}(x_m) = \delta_{j,m}$, it follows that both discrete operators $\mathcal{I}^k_{2N+1}[u](x)$, $k = 1, 2$, interpolate $u(x)$ at the quadrature nodes. Note that by Lemma 3.3.1, the interpolation operators $\mathcal{I}^1_{2N+1}[\cdot]$ and $\mathcal{I}^2_{2N+1}[\cdot]$ act as the identities in the respective finite dimensional spaces $\bar{\mathbb{P}}_{N-1}$ and $\bar{\mathbb{P}}_N$.

Formulas (3.3.2a), (3.3.3a), (3.3.2b) and (3.3.3b) provide a one-to-one linear correspondence between values of function u at the quadrature nodes and its discrete Fourier coefficients. For both quadrature formulas, the transformation matrix is Fourier [Boy00, CQHZ06, HGG07, Kop09, STW11], as a consequence, either of the four formulas can be computed at the cost of $\mathcal{O}(N\log_2 N)$ floating point operations using the classical divide-and-conquer strategy [Boy00, CQHZ06, HGG07, Kop09, STW11].

3.4 Trigonometric interpolation of regular functions

Unlike the projection operator $\mathcal{P}_N[\cdot]$ which is bounded as a map from $L^2_p(-\ell,\ell)$ to $\bar{\mathbb{P}}_N$, none of the interpolation operators of Section 3.3, is well defined on elements of $L^2_p(-\ell,\ell)$. The following result provides a partial substitute.

Lemma 3.4.1. *For any $\alpha > \frac{1}{2}$, the operators $\mathcal{I}^k_{2N+1} : H^\alpha_p(-\ell,\ell) \to L^2_p(-\ell,\ell)$, $k = 1,2$, satisfy*

$$\|\mathcal{I}^k_{2N+1}\|_{H^\alpha_p \to L^2_p} \le c_\alpha \sqrt{2N}, \quad k = 1,2, \tag{3.4.1}$$

where $c_\alpha > 0$ depends on the Sobolev embedding constant from $H^\alpha_p(-\ell,\ell)$ to $L^2_p(-\ell,\ell)$ only.

Proof. In view of (3.3.3a), the $L^2_p(-\ell,\ell)$ norm of $\mathcal{I}^1_{2N+1}[u]$ is given by $\|\mathcal{I}^1_{2N+1}[u]\|^2 = \frac{1}{2\ell}\sum_{|n|\le N} c_n^2 |\breve{u}_{1,n}|^2$. On the other hand, by virtue of (3.3.2a), we have

$$|\breve{u}_{1,n}| = \tfrac{\ell}{N}\sum_{j=0}^{2N-1} |u(x_j)| \le 2\ell \|u\|_{L^\infty}.$$

Combining the last two formulas together and taking into account that $\|u\|_{L^\infty} \le c_\alpha \|u\|_{H^\alpha_p}$. By the standard Sobolev embedding (see, (2.4.1)), we conclude that operator $\mathcal{I}^1_{2N+1}$ satisfies (3.4.1). The proof for $\mathcal{I}^2_{2N+1}$ is identical and omitted. $\square$

To proceed further, we observe that for $u \in \bar{\mathbb{P}}_N$, directly from the definition of $H^\alpha_p(-\ell,\ell)$ norm, we have

$$\|u\|_{H^\alpha_p} \le \big(\tfrac{\pi N}{\ell}\big)^{\max\{0,\alpha-\beta\}} \|u\|_{H^\beta_p}, \tag{3.4.2}$$

for any $\alpha,\beta \ge 0$. Using this fact, properties of the interpolation operators $\mathcal{I}^k_{2N+1}$ and Lemma 3.4.1, for functions of finite regularity, we obtain

Theorem 3.4.2. *Assume $\gamma > \frac{1}{2}$ and $\beta > \alpha + \gamma + \frac{1}{2}$. Then the interpolation error satisfies*

$$\|(\mathcal{I} - \mathcal{I}^k_{2N+1})[u]\|_{H^\alpha_p} \le c\big(\tfrac{\ell}{\pi N}\big)^{\beta-\alpha-\gamma-\frac{1}{2}} \|u\|_{H^\beta_p}, \quad k = 1,2, \tag{3.4.3}$$

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

Proof. We write

$$(\mathcal{I} - \mathcal{I}_{2N+1}^k)[u] = (\mathcal{I} - \mathcal{P}_{N-1})[u] - \mathcal{I}_{2N+1}^k(\mathcal{I} - \mathcal{P}_{N-1})[u].$$

The first term in the right-hand side of the last identity is bounded by Theorem 3.2.1, i.e.

$$\|(\mathcal{I} - \mathcal{P}_{N-1})[u]\|_{H_p^\alpha} \leq c\left(\tfrac{\ell}{\pi N}\right)^{\beta-\alpha}\|u\|_{H_p^\beta}.$$

Let $\gamma > \frac{1}{2}$, in view of (3.4.1) and (3.4.2), for the second term we obtain

$$\begin{aligned}\|\mathcal{I}_{2N+1}^k(\mathcal{I} - \mathcal{P}_{N-1})[u]\|_{H_p^\alpha} &\leq \left(\tfrac{\ell}{\pi N}\right)^{-\alpha}\|\mathcal{I}_{2N+1}^k(\mathcal{I} - \mathcal{P}_{N-1})[u]\|_{L_p^2} \\ &\leq c_\gamma\left(\tfrac{\ell}{\pi N}\right)^{-\alpha-\frac{1}{2}}\|(\mathcal{I} - \mathcal{P}_{N-1})[u]\|_{H_p^\gamma} \\ &\leq c\left(\tfrac{\ell}{\pi N}\right)^{\beta-\alpha-\gamma-\frac{1}{2}}\|u\|_{H_p^\beta}.\end{aligned}$$

Now the assertion follows directly from the last two estimates. □

Comparing Theorems 3.2.1 and 3.4.2, we see that accuracy of the discrete Fourier expansion drops by the factor $\mathcal{O}(N^{\gamma+\frac{1}{2}})$, as compared to the exact truncated Fourier series. This is the price we pay by replacing exact Fourier coefficients with their discrete counterparts.

For analytic functions, the interpolation error decays geometrically.

Theorem 3.4.3. *Assume u is analytic in a bounded open region D with a rectifiable boundary ∂D, containing the interval $[-\ell, \ell]$ in its interior. Then*

$$\|(\mathcal{I} - \mathcal{I}_{2N+1}^k)[u]\|_{H_p^\alpha} \leq c\tfrac{\gamma\sqrt{2\ell}}{2\pi}\left(\tfrac{\pi N}{\ell}\right)^{\alpha+1}e^{-\frac{\pi\delta}{\ell}N}\max_{z\in\partial D}|u(z)|, \quad k = 1, 2, \tag{3.4.4}$$

where $c > 0$ is an absolute constant, $\delta = \inf_{z\in\partial D, x\in[-\ell,\ell]}|z - x| > 0$ is the distance from the interval $[-\ell, \ell]$ to the boundary ∂D and γ is the length of the boundary ∂D.

Proof. Following similar steps as in Theorem 3.4.2 and using Theorem 3.2.2, we arrive at (3.4.4). □

Chapter 4

The Klein-Gordon equation in the real line

In this Chapter, we discuss the well-posedness of the KGE model posed in the real line. We start by checking the well-posedness in periodic settings. The result is then extended to the whole of real line.

4.1 The periodic Klein-Gordon equation

Let $\Omega = (-\ell, \ell)$, for some $\ell > 0$. We study the following equation

$$u_{tt} = a^2 \Delta u - \mathcal{V}'(u), \quad x \in \Omega, \quad t > 0, \tag{4.1.1a}$$

$$u(x, 0) = u_0, \quad u_t(x, 0) = v_0, \tag{4.1.1b}$$

where $\mathcal{V} \in C^2(\mathbb{R})$, $\mathcal{V} \geq 0$ in Ω and $\mathcal{V}(0) = 0$ and u is 2ℓ-periodic. The problem is Hamiltonian, i.e. introducing

$$U = \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} u \\ u_t \end{pmatrix}, \quad \mathcal{J} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

and

$$\mathcal{H}(U) = \frac{1}{2} \int_\Omega (v^2 + a^2 |\nabla u|^2 + 2\mathcal{V}(u)) dx,$$

it is easy to verify that (4.1.1) is equivalent to

$$U_t = \mathcal{J}\nabla\mathcal{H}(U) \quad x \in \Omega, \quad t > 0, \tag{4.1.2a}$$

$$U_0 = (u_0, v_0)^T. \tag{4.1.2b}$$

Also,

$$\frac{d}{dt}\mathcal{H}(u,v) = \frac{1}{2}\int_\Omega (2vv_t + 2a^2 u_{xt}u_x + 2u_t\mathcal{V}'(u))dx.$$

Using equation (4.1.1), integrating by parts and taking into account that v is 2ℓ-periodic, we infer that

$$\begin{aligned}\frac{d}{dt}\mathcal{H}(u,v) &= \int_\Omega (v[a^2u_{xx} - \mathcal{V}'(u)] + a^2v_xu_x + v\mathcal{V}'(u))dx \\ &= a^2\int_\Omega (-v_xu_x + v_xu_x)dx + (vu_x)|_{\partial\Omega} = 0.\end{aligned}$$

From the above, we conclude that the quantity $\mathcal{H}(U)$ is conserved along classical solutions of (4.1.1).

4.2 Well-posedness in the periodic settings

In what follows, we are interested in showing that (4.1.2) is well-posed in the Hilbert scale of spaces H_p^s of 2ℓ-periodic functions. For this, we replace equation (4.1.1) with its weak form. That is instead of (4.1.1), we consider the problem of finding $(u, v) \in C([0, T], H_p^1) \times C([0, T], L_p^2)$, with $(u_t, v_t) \in C([0, T], L_p^2) \times C([0, T], H_p^{-1})$, so that

$$\langle (u,v)_t, (\phi_1, \phi_2)\rangle = \langle v, \phi_1\rangle - a^2\langle \nabla u, \nabla\phi_2\rangle - \langle \mathcal{V}'(u), \phi_2\rangle, \tag{4.2.1a}$$

$$(u, v)_0 = (u_0, v_0), \tag{4.2.1b}$$

is satisfied for all $(\phi_1, \phi_2) \in L_p^2 \times H_p^1$.

We employ the Galerkin method. In the space of square integrable periodic functions L_p^2, we fix the standard orthonormal basis $\{\phi_n := \frac{1}{\sqrt{2\ell}}e^{-i\frac{\pi}{\ell}nx}\}_{n\in\mathbb{Z}}$ and denote $\mathbb{P}_N = \operatorname{span}\{\phi_n\}_{n=-N}^N$. With the orthonormal basis and the truncation index N, we associate the orthogonal projector $\mathcal{P}_N : L^2_p \to \mathbb{P}_N$. We note that the projection operator $\mathcal{P}_N$ commutes with the differentiation.

We approximate (u, v) by $(\hat{u}, \hat{v}) \in \mathbb{P}_N^2$, that satisfies

$$\langle (\hat{u}, \hat{v})_t, (\phi_1, \phi_2) \rangle = \langle \hat{v}, \phi_1 \rangle - a^2 \langle \nabla \hat{u}, \nabla \phi_2 \rangle - \langle \mathcal{V}'(\hat{u}), \phi_2 \rangle, \tag{4.2.2a}$$

$$\langle (u_0, v_0) - (\hat{u}_0, \hat{v}_0), (\phi_1, \phi_2) \rangle = 0, \tag{4.2.2b}$$

for all $(\phi_1, \phi_2) \in \mathbb{P}_N^2$.

The semi-discrete problem (4.2.2) is again Hamiltonian. Recalling that $\hat{u}_t = \hat{v}$ and replacing $(\hat{\phi}_1, \hat{\phi}_2)$ with $(\hat{u}, \hat{v})$, we infer that

$$\frac{d}{dt}\Big(\|\hat{u}\|^2_{L^2_p} + \|\hat{v}\|^2_{L^2_p} \Big) = \frac{d}{dt}\Big(\|\hat{u}\|^2_{L^2_p} - a^2 \|\nabla \hat{u}\|^2_{L^2_p} - 2\int_\Omega \mathcal{V}(\hat{u}) dx \Big),$$

which after rearranging of terms yields

$$2\frac{d}{dt}\mathcal{H}(\hat{u}, \hat{v}) = \frac{d}{dt}\Big(\|\hat{v}\|^2_{L^2_p} + a^2 \|\nabla \hat{u}\|^2_{L^2_p} + 2\int_\Omega \mathcal{V}(\hat{u}) dx \Big) = 0.$$

This shows that $\mathcal{H}(\hat{U})$ is conserved along Galerkin trajectories and the approximation satisfies

$$\hat{U}_t = \mathcal{J}\mathcal{P}_N \Big[\nabla \mathcal{H}(\hat{U}) \Big], \quad x \in \Omega, \quad t > 0, \tag{4.2.3a}$$

$$\hat{U}_0 = (\mathcal{P}_N[u_0], \mathcal{P}_N[v_0])^T. \tag{4.2.3b}$$

4.2.1 Global well-posedness of the Galerkin solutions

In this section, we study in detail the Galerkin solution, generated by (4.2.3). We begin with the following a priori estimates:

Lemma 4.2.1. *Assume* $(u_0, v_0) \in H^1_p \times L^2_p$. *Then a Galerkin solution* $(\hat{u}, \hat{v})$ *of* (4.2.3) *satisfies*

$$(\hat{u}, \hat{v}) \in C([0, T], H^1_p \times L^2_p),$$
$$(\hat{u}_t, \hat{v}_t) \in C((0, T), L^2_p \times H^{-1}_p).$$

The respective norms are uniformly bounded in N *and* ℓ.

Proof. (a) Equations (4.2.3) define a system of ordinary differential equation. If $\mathcal{V}(u) \in C^2(\mathbb{R})$, then the vector field of the system is one-time continuously differentiable, hence the standard theory of ODE's (see [AA14, MM07, Tes12]) implies existence of a local solution

$$(\hat{u}, \hat{v}) \in C^{(1)}((0,T), \mathbb{P}_N \times \mathbb{P}_N) \cap C([0,T], \mathbb{P}_N \times \mathbb{P}_N),$$

for some $T > 0$. Along the Galerkin trajectories $(\hat{u}, \hat{v})$, the Hamiltonian is preserved

$$\begin{aligned} 2\mathcal{H}(\hat{u}, \hat{v}) &= \|\hat{v}\|_{L_p^2}^2 + a^2 \|\nabla \hat{u}\|_{L_p^2}^2 + 2 \int_\Omega \mathcal{V}(\hat{u}) dx \\ &= \|\hat{v}_0\|_{L_p^2}^2 + a^2 \|\nabla \hat{u}_0\|_{L_p^2}^2 + 2 \int_\Omega \mathcal{V}(\hat{u}_0) dx = 2\mathcal{H}(\hat{u}_0, \hat{v}_0). \end{aligned}$$

It follows that $\|\hat{v}\|_{L_p^2}^2$, $\|\nabla \hat{u}\|_{L_p^2}^2$ and $\int_\Omega \mathcal{V}(\hat{u}) dx$ are uniformly bounded for any $t > 0$. In particular, for any $t > 0$

$$\|\hat{v}\|_{C([0,t], L_p^2)} \leq \mathcal{H}(\hat{u}_0, \hat{v}_0). \tag{4.2.4}$$

Furthermore, for any $b \neq 0$, $b \in \mathbb{R}$, we have

$$\hat{u}(x - bt, t) = \hat{u}_0(x) + \int_0^t \big(\hat{u}_t(x - b\tau, \tau) - b \nabla \hat{u}(x - b\tau, \tau) \big) d\tau.$$

Hence, if $t > 0$

$$\|\hat{u}\|_{L_p^2} \leq \|\hat{u}_0\|_{L_p^2} + t(1 + |b|) \mathcal{H}(\hat{u}_0, \hat{v}_0).$$

The calculations show that

$$\|\hat{u}\|_{C([0,t], H_p^1)} \leq \|\hat{u}_0\|_{L_p^2} + \big[\tfrac{1}{a^2} + (1 + |b|)t \big] \mathcal{H}(\hat{u}_0, \hat{v}_0). \tag{4.2.5}$$

Estimates (4.2.4) and (4.2.5) indicate that the solution $(\hat{u}, \hat{v})$ does not blow up in a finite time and hence is well defined in any finite time interval $[0,T]$.

(b) Directly from the equation, we have $\hat{u}_t = \hat{v}$, consequently

$$\|\hat{u}_t\|_{C((0,T), L_p^2)} \leq \mathcal{H}(\hat{u}_0, \hat{v}_0). \tag{4.2.6}$$

It remains to show that the quantity $\|\hat{v}_t\|_{C((0,T), H_p^{-1})}$ is bounded. In view of Theorem 2.4.1, $C([0,T], H_p^1) \hookrightarrow C([0,T], L^\infty)$, moreover,

$$\begin{aligned} \|\hat{u}\|_{C([0,T], L^\infty)} &\leq c_\ell \|\hat{u}\|_{C([0,T], L_p^2)}^{\frac{1}{2}} \cdot \|\hat{u}\|_{C([0,T], H_p^1)}^{\frac{1}{2}} \\ &\leq c_\ell \Big[\|\hat{u}_0\| + \big[\tfrac{1}{a^2} + (1 + |b|)T \big] \mathcal{H}(\hat{u}_0, \hat{v}_0) \Big], \end{aligned} \tag{4.2.7}$$

where the positive constant c_ℓ is uniformly bounded when $\ell \to \infty$. Further,

$$
\begin{aligned}
|\mathcal{V}'(\hat{u})| &\leq \int_0^{|\hat{u}|} |\mathcal{V}''(s)| ds \leq \max\{|\mathcal{V}''(s)| \mid , s \in [0, \|\hat{u}\|_{C([0,T],L^\infty)}]\} \cdot |\hat{u}| \\
&\leq C(\hat{u}_0, \hat{v}_0, T)|\hat{u}|, \qquad (4.2.8)
\end{aligned}
$$

where in view of (4.2.7), the positive constant $C(\hat{u}_0, \hat{v}_0, T)$ depends on the initial data $(\hat{u}_0, \hat{v}_0)$, terminal time T and the non-linearity $\mathcal{V}(u)$ only. Using (4.2.8), we infer that

$$
\begin{aligned}
\|\hat{v}_t\|_{H_p^{-1}} &\leq a^2 \|\nabla \hat{u}\|_{L_p^2} + \sup\{|\langle \mathcal{V}'(\hat{u}), \phi\rangle| \mid \|\phi\|_{H_p^1} = 1\} \\
&\leq \mathcal{H}(\hat{u}_0, \hat{v}_0) + \max\{|\mathcal{V}''(s)| \mid , s \in [0, \|\hat{u}\|_{C([0,T],L^\infty)}]\} \cdot \|\hat{u}\|_{C([0,T],L_p^2)} \\
&\leq \big[1 + C(\hat{u}_0, \hat{v}_0, T)T(1 + |b|)\big]\mathcal{H}(\hat{u}_0, \hat{v}_0) + C(\hat{u}_0, \hat{v}_0, T)\|\hat{u}_0\|_{L_p^2}.
\end{aligned}
$$

The last inequality shows that

$$
\|v_t\|_{C((0,T),H_p^{-1})} \leq M(\hat{u}_0, \hat{v}_0, T), \qquad (4.2.9)
$$

where the constant $M(\hat{u}_0, \hat{v}_0, T)$ depends on the initial data $(\hat{u}_0, \hat{v}_0)$, terminal time T and the non-linearity $\mathcal{V}(u)$ only.

(c) To conclude the proof, we note that the estimates (4.2.4), (4.2.5), (4.2.6) and (4.2.9) are uniform in N, provided the quantities $\mathcal{H}(\hat{u}_0, \hat{v}_0)$ and $\|\hat{u}_0\|_{L_p^2}$ are bounded independently of N. Since the projector $\mathcal{P}_N$ and differentiation commute, we have

$$
\|\hat{u}_0\|_{H_p^1} = \|\mathcal{P}_N u_0\|_{H_p^1} \leq \|u_0\|_{H_p^1}, \quad \|\hat{v}_0\|_{L_p^2} = \|\mathcal{P}_N v_0\|_{L_p^2} \leq \|v_0\|_{L_p^2}
$$

and then

$$
\|\hat{u}_0\|_{L_p^\infty} \leq c_\ell \|\hat{u}_0\|_{L_p^2}^{\frac{1}{2}} \cdot \|\hat{u}_0\|_{H_p^1}^{\frac{1}{2}} \leq c_\ell \|\hat{u}_0\|_{H_p^1} \leq c_\ell \|u_0\|_{H_p^1}.
$$

Using the last three inequalities, we infer as in (4.2.8)

$$
\begin{aligned}
\|\mathcal{V}(\hat{u}_0)\|_{L_p^1} &= \int_\Omega |\mathcal{V}(\hat{u}_0)| dx \leq \int_\Omega \int_0^{|\hat{u}_0|} \int_0^s |\mathcal{V}''(\tau)| d\tau ds dx \\
&\leq \int_\Omega \int_0^{|\hat{u}_0|} |\mathcal{V}''(\tau)| \cdot \big||\hat{u}_0| - \tau\big| d\tau dx \\
&\leq \max\{|\mathcal{V}''(\tau)| \mid \tau \in [0, \|\hat{u}_0\|_{L^\infty}]\} \cdot \|\hat{u}_0\|_{L_p^2}^2 \\
&= B(\|u_0\|_{H_p^1}) \cdot \|u_0\|_{L_p^2}^2,
\end{aligned}
$$

where $B(\|u_0\|_{H_p^1})$ depends on the initial data u_0 and the nonlinearity $\mathcal{V}(u)$ only. The calculations above show that

$$\mathcal{H}(\hat{u}_0, \hat{v}_0) \leq \frac{1}{2}\Big[\|v_0\|_{L_p^2} + a^2\|u_0\|^2_{H_p^1} + 2B(\|u_0\|_{H_p^1}).\|u_0\|^2_{L_p^2}\Big], \tag{4.2.10}$$

uniformly in N. The assertion of the Lemma follows directly from (4.2.4), (4.2.5), (4.2.6), (4.2.9) and (4.2.10). $\square$

In the case of regular initial data, we have the following extension of Lemma 4.2.1.

Lemma 4.2.2. *If* $(u_0, v_0) \in H_p^{s+1} \times H_p^s$ *and* $\mathcal{V} \in C^{s+2}(\mathbb{R})$, *with* $s \geq 0$, *then*

$$(\hat{u}, \hat{v}) \in C([0,T], H_p^{s+1} \times H_p^s),$$
$$(\hat{u}_t, \hat{v}_t) \in C((0,T), H_p^s \times H_p^{s-1}),$$

uniformly in N *and* ℓ.

Proof. (a) Since $(\hat{u}, \hat{v}) \in \mathbb{P}_N^2$, it follows that:

$$(\hat{u}, \hat{v}) \in C([0,T], H_p^{s+1} \times H_p^s), \tag{4.2.11a}$$
$$(\hat{u}_t, \hat{v}_t) \in C((0,T), H_p^s \times H_p^{s-1}), \tag{4.2.11b}$$

for all $s > 0$ as in the finite dimensional space $\mathbb{P}_N^2$, all norms are equivalent. We have to show that the respective norms are uniformly bounded in N and ℓ.

(b) In equation (4.2.2a), we let $\phi_1 = \partial_x^{2(s+1)}\hat{u}$ and $\phi_2 = \partial_x^{2s}\hat{v}$, where $s \geq 0$ is an integer. Integrating by parts and using the periodicity of $\phi_1, \phi_2, \hat{u}, \hat{v}$ we infer that

$$(-1)^{1+s}\frac{d}{dt}\Big[\|\partial_x^{1+s}\hat{u}\|^2_{L_p^2} + \|\partial_x^s\hat{v}\|^2_{L_p^2}\Big] = (-1)^{s+1}(1+a^2)\frac{d}{dt}\|\partial_x^{1+s}\hat{u}\|^2_{L_p^2} - 2\langle\mathcal{V}'(\hat{u}), \partial_x^{2s}\hat{v}\rangle,$$

which, after simplification, gives

$$\frac{d}{dt}\Big[a^2\|\partial_x^{1+s}\hat{u}\|^2_{L_p^2} + \|\partial_x^s\hat{v}\|^2_{L_p^2}\Big] = 2\langle\partial_x^s\mathcal{V}'(\hat{u}), \partial_x^s\hat{v}\rangle. \tag{4.2.12}$$

We estimate the inner product on the right-hand side of the last equation using the Faa di Bruno formula [Rom80]

$$\partial_x^s\mathcal{V}'(\hat{u}) = \sum_{k=1}^{s}\mathcal{V}^{(k+1)}(\hat{u})\sum_{|\pi|=k}\prod_{\pi_i\in\pi}\partial_x^{|\pi_i|}\hat{u},$$

where the second sum runs over all partitions $\pi = \{\pi_1, \dots, \pi_k\}$ of the set $\{1, \dots, s\}$ that contain exactly k nonempty and disjoint subsets $\pi_i \subset \{1, \dots, s\}$.

To begin, we observe that the same arguments as in Lemma 4.2.1, yield the bound

$$\begin{aligned}|\mathcal{V}^{(1+k)}(\hat{u})| &\le |\mathcal{V}^{(1+k)}(0)| + \int_0^{|\hat{u}|} |\mathcal{V}^{(2+k)}(s)| ds \\ &\le |\mathcal{V}^{(1+k)}(0)| + \max\{|\mathcal{V}^{(2+k)}(s)| \mid , s \in [0, \|\hat{u}\|_{L_p^\infty}]\} \cdot \|\hat{u}\|_{L_p^\infty} \\ &\le C_k(u_0, v_0, T), \quad k = 1, \dots, s, \end{aligned} \tag{4.2.13}$$

where each quantity $C_k(u_0, v_0, T)$ is controlled by the regularity of $\mathcal{V}(\cdot)$, the terminal time T and the initial data (u_0, v_0) only. Hence, using the Faa di Bruno formula [Rom80], the Cauchy-Schwartz and Young's inequalities and the fact that H_p^s are Banach algebras [AF03], when $s > \frac{1}{2}$, we infer that

$$\begin{aligned}2\big|\langle \mathcal{V}'(\hat{u}), \partial_x^{2s}\hat{v}\rangle\big| &\le C_1(u_0, v_0, T)\Big[\|\partial_x^s \hat{u}\|_{L_p^2}^2 + \|\partial_x^s \hat{v}\|_{L_p^2}^2\Big] \\ &\quad + \sum_{k=2}^{s} C_k(u_0, v_0, T) \sum_{|\pi|=k} \Big[\prod_{\pi_i \in \pi} \|\hat{u}\|_{H_p^{1+|\pi_i|}}^2 + \|\partial_x^s \hat{v}\|_{L_p^2}^2\Big] \\ &\le M_s(u_0, v_0, T)\|\partial_x^s \hat{v}\|_{L_p^2}^2 + F_s(\|\hat{u}\|_{H_p^s}),\end{aligned} \tag{4.2.14}$$

where $M_s(u_0, v_0, T)$ depends on the index s, the terminal time T and $\|u_0\|_{H_p^1}$ and $\|v_0\|_{L_p^2}$, while $F_s(\cdot)$ is a polynomial of degree $2s$, whose coefficients are controlled by the regularity of $\mathcal{V}$, the terminal time T and the initial data (u_0, v_0) only.

(c) Combining (4.2.12) and (4.2.14), we infer that

$$\frac{d}{dt}\Big[a^2\|\partial_x^{1+s}\hat{u}\|_{L_p^2}^2 + \|\partial_x^s \hat{v}\|_{L_p^2}^2\Big] \le M_s(u_0, v_0, T)\|\partial_x^s \hat{v}\|_{L_p^2}^2 + F_s(\|\hat{u}\|_{H_p^s}), \tag{4.2.15}$$

for any integer $s \ge 0$. The case $s = 0$ is established in Lemma 4.2.1. Assume $s = 1$, in view of Lemma 4.2.1, the quantity $F_1(\|\hat{u}\|_{C([0,T],H_p^1)})$ is uniformly bounded in N and ℓ. Hence we can apply Gronwall's inequality to obtain

$$\begin{aligned}&a^2\|\partial_x^2 \hat{u}\|_{L_p^2}^2 + \|\partial_x \hat{v}\|_{L_p^2}^2 \\ &\quad \le \exp\{T M_1(u_0, v_0, T)\}\Big[a^2\|\partial_x^2 \hat{u}_0\|_{L_p^2}^2 + \|\partial_x \hat{v}_0\|_{L_p^2}^2 + T F_1(\|\hat{u}\|_{C([0,T],H_p^1)})\Big].\end{aligned}$$

Since the projection $\mathcal{P}_N$ and differentiation commute, we have

$$a^2\|\partial_x^2\hat{u}_0\|_{L_p^2}^2 + \|\partial_x\hat{v}_0\|_{L_p^2}^2 \le a^2\|\partial_x^2 u_0\|_{L_p^2}^2 + \|\partial_x v_0\|_{L_p^2}^2.$$

Consequently,

$$(\hat{u}, \hat{v}) \in C([0,T], H_p^2 \times H_p^1),$$

with the respective norms bounded independently of N and/or ℓ.

The uniform bound on $\|\hat{v}_t\|_{C([0,T],L_p^2)}$, follows directly from equation (4.2.2). If we let $\phi_1 = 0$ and $\phi_2 = \hat{v}_t$ and use the already proven fact that the norm $\|\hat{u}\|_{C([0,T],H_p^2)}$ is uniformly bounded in terms of N and ℓ, this settles our claim for $s = 1$.

(d) With the aid of (4.2.15), the process described in part (c) of the proof, can be continued inductively for $s = 2, 3, \ldots$. We conclude that Lemma 4.2.2 holds for any $s \ge 0$, provided $(u_0, v_0) \in H_p^{s+1} \times H_p^s$ and $\mathcal{V} \in C^{s+2}(\mathbb{R})$. $\square$

4.2.2 Existence and uniqueness

Since the Galerkin solutions are globally defined and satisfy a priori estimates of Lemmas 4.2.1 and 4.2.2, we employ the weak compactness argument based on the results, presented in Section 2.2, to show that a solution to the periodic initial value problem (4.1.1) does exist and is unique.

Theorem 4.2.3. *Suppose that* $(u_0, v_0) \in H_p^1 \times L_p^2$. *Then problem* (4.1.1) *admits a weak solution*

$$(u, v) \in L^\infty([0,T], H_p^1 \times L_p^2),$$
$$(u_t, v_t) \in L^\infty([0,T], L_p^2 \times H_p^{-1}).$$

Proof. (a) In view of Lemma 4.2.1, the sequences $(\hat{u}, \hat{v})$ and $(\hat{u}_t, \hat{v}_t)$ are uniformly bounded in $C([0,T], H_p^1 \times L_p^2)$ and $C([0,T], L_p^2 \times H_p^{-1})$, respectively. Then, according to Lemma 2.2.2, there exists a subsequence $(\hat{u}, \hat{v})$, such that

$$\hat{u} \to u \quad \text{weakly star in} \quad L^\infty([0,T], H_p^1), \tag{4.2.16a}$$

$$\hat{v} \to v \quad \text{weakly star in} \quad L^\infty([0,T], L_p^2), \tag{4.2.16b}$$

$$\hat{v}_t \to v_t \quad \text{weakly star in} \quad L^\infty([0,T], H_p^{-1}). \tag{4.2.16c}$$

By Theorem 2.4.1, the embeddings $H_p^1 \hookrightarrow L_p^2 \hookrightarrow H_p^{-1}$ are compact, it follows from (4.2.16) and Theorem 2.4.2 that

$$\hat{u} \to u \quad \text{strongly in} \quad L^2([0,T], L_p^2), \tag{4.2.17a}$$

$$\hat{v} \to v \quad \text{strongly in} \quad L^2([0,T], H_p^{-1}). \tag{4.2.17b}$$

In view of (4.2.17) and Lemma 2.2.3, $\hat{u}$ converges to u almost everywhere in $[0,T] \times \Omega$, consequently, $\mathcal{V}'(\hat{u})$ converges a.e. to $\mathcal{V}'(u)$ in $[0,T] \times \Omega$. By virtue of (4.2.8), $\mathcal{V}'(\hat{u})$ is uniformly bounded in $L^\infty([0,T], L_p^2)$. With the aid of Lemma 2.2.4, we conclude that the quantities $\mathcal{V}'(\hat{u})$ converge weakly star to $\mathcal{V}'(u)$ in $L^\infty([0,T], L_p^2)$.

(b) Using (4.2.16a), (4.2.16b) and Lemma 2.2.5, we see that $(\hat{u}(0), \hat{v}(0))$ converges weakly to $(u(0), v(0))$ in $H_p^1 \times L_p^2$. On the other hand, by construction (see (4.2.2b)), $(\hat{u}(0), \hat{v}(0))$ converge strongly to (u_0, v_0) in $H_p^1 \times L_p^2$, hence $(u(0), v(0)) = (u_0, v_0)$.

(c) In view of parts (a) and (b) of the proof, we fix $N_0 > 0$, $(\phi_1, \phi_2) \in \mathbb{P}_{N_0}^2$ and pass to the limit in (4.2.2a), to obtain

$$\langle (u,v)_t, (\phi_1, \phi_2) \rangle = \langle v, \phi_1 \rangle - a^2 \langle \nabla u, \nabla \phi_2 \rangle - \langle \mathcal{V}'(u), \phi_2 \rangle, \tag{4.2.18a}$$

$$(u(0), v(0)) = (u_0, v_0), \tag{4.2.18b}$$

a.e. in $[0,T]$. Note that identity (4.2.18a) holds for any fixed $(\phi_1, \phi_2) \in \mathbb{P}_{N_0}^2$ and any fixed $N_0 > 0$. Since $\cup_{N>1} \mathbb{P}_N^2$ is everywhere dense in $L_p^2 \times H_p^1$, we conclude that (4.2.18) holds a.e. in $[0,T]$ for all $(\phi_1, \phi_2) \in L_p^2 \times H_p^1$, i.e (u,v) satisfies (4.1.1) in the weak sense. □

Remark 4.2.1. With an extra effort one can show that convergence of the subsequence $(\hat{u}, \hat{v})$, constructed in Theorem 4.2.3 is strong in $L^2([0,T], H_p^1 \times L_p^2)$.

Proof. By the choice of the subsequence, we have

$$\lim_{n\to\infty} \mathcal{H}(\hat{u}, \hat{u}) = \lim_{n\to\infty} \mathcal{H}(\hat{u}_0, \hat{u}_0) = \mathcal{H}(u_0, v_0). \tag{4.2.19}$$

Directly, from (4.2.18a), it follows that

$$\langle (v_t, a^2\nabla u), (\phi, \nabla\phi)\rangle = -\langle \mathcal{V}'(u), \phi\rangle,$$

for all $\phi \in H_p^1$ and a.e. in $[0, T]$. In the last formula, we let $\phi = \mathcal{P}_N v$ and integrate over interval $[0, t]$, to obtain initially $\mathcal{H}(\mathcal{P}_N u, \mathcal{P}_N v) = \mathcal{H}(\mathcal{P}_N u_0, \mathcal{P}_N v_0)$, and then $\mathcal{H}(u, v) = \mathcal{H}(u_0, v_0)$. Further, for almost all $t \in [0, T]$, we have

$$\left| \int_\Omega [\mathcal{V}(\hat{u}) - \mathcal{V}(u)]dx \right| \le M \int_\Omega |\hat{u} - u| dx \le M|\Omega|^{\frac{1}{2}} \|\hat{u} - u\|_{L_p^2}$$

and (4.2.17) implies that $\int_\Omega \mathcal{V}(\hat{u})dx$ converges to $\int_\Omega \mathcal{V}(u)dx$ a.e. in $[0, T]$. It follows that a.e. in $[0, T]$ the following holds

$$\lim_{n\to\infty} \left[\|\hat{v}\|_{L_p^2}^2 + a^2 \|\nabla \hat{u}\|_{L_p^2}^2 \right] = \|v\|_{L_p^2}^2 + a^2 \|\nabla u\|_{L_p^2}^2.$$

We conclude that

$$\lim_{n\to\infty} \|\hat{v}\|_{L_p^2}^2 = \|v\|_{L_p^2}, \quad \lim_{n\to\infty} \|\nabla \hat{u}\|_{L_p^2}^2 = \|\nabla u\|_{L_p^2}$$

and hence, by Lemma 2.3.1, $(\hat{u}, \hat{v})$ converges strongly to (u, v) in $H_p^1 \times L_p^2$ for almost all $t \in [0, T]$ and in $L^2([0, T], H_p^1 \times L_p^2)$. $\square$

Remark 4.2.2. Assuming, as in Lemma 4.2.2 that $(u_0, v_0) \in H^{s+1} \times H_p^s$ and $\mathcal{V} \in C^{s+2}(\mathbb{R})$, with $s \ge 0$, and repeating the proof of Theorem 4.2.3, one can show that the weak solutions satisfy

$$(u, v) \in L^\infty([0, T], H_p^{s+1} \times H_p^s),$$
$$(u_t, v_t) \in L^\infty((0, T), H_p^s \times H_p^{s-1}).$$

In particular, if $s \ge 1$, the solutions are classical.

Theorem 4.2.4. *The weak solution $(u, v) \in L^\infty([0, T], H_p^1 \times L_p^2)$ obtained in Theorem 4.2.3 is unique.*

Proof. Assume there exists another solution $(\overline{u},\overline{v}) \in L^\infty([0,T], H_p^1 \times L_p^2)$ that satisfies (4.2.18). We let $(e_1, e_2) = (u-\overline{u}, v-\overline{v}) \in H_p^1(\Omega \times L_p^2)$. Then the error satisfies

$$\langle (e_1,e_2)_t, (\phi_1,\phi_2)\rangle = \langle e_2, \phi_1\rangle - a^2\langle \nabla e_1, \nabla\phi_2\rangle - \langle \mathcal{V}'(u) - \mathcal{V}'(\overline{u}), \phi_2\rangle, \tag{4.2.20a}$$

$$(e_1, e_2) = 0, \tag{4.2.20b}$$

for all $(\phi_1,\phi_2) \in L_p^2 \times H_p^1$. As in Remark 4.2.1, we infer that

$$\begin{aligned}
\|e_1\|_{L_p^2}^2 &\le \int_0^t \big(\|e_1\|_{L_p^2}^2 + \|e_2\|_{L_p^2}^2\big) d\tau,\\
\|e_2\|_{L_p^2}^2 + a^2\|\nabla e_1\|_{L_p^2}^2 &\le 2\int_0^t |\langle \mathcal{V}'(u) - \mathcal{V}'(\overline{u}), e_2\rangle| d\tau\\
&\le 2M\int_0^t \langle |e_1|, |e_2|\rangle d\tau \le M\int_0^t \big(\|e_1\|_{L_p^2}^2 + \|e_2\|_{L_p^2}^2\big) d\tau.
\end{aligned}$$

Adding the inequalities together, we have

$$\|e_1\|_{L_p^2}^2 + a^2\|\nabla e_1\|_{L_p^2}^2 + \|e_2\|_{L_p^2}^2 \le (1+M)\int_0^t \big(\|e_1\|_{L_p^2}^2 + a^2\|\nabla e_1\|_{L_p^2}^2 + \|e_2\|_{L_p^2}^2\big) d\tau.$$

Gronwall's inequality indicates that $\|e_1\|_{H_p^1} = \|e_2\|_{L_p^2} = 0$ for all $t \in [0,T]$ and we conclude that $(\overline{u},\overline{v}) = (u,v)$ in $L^\infty([0,T], H_p^1 \times L_p^2)$. $\square$

4.2.3 Propagation of the initial data

The formulation (4.1.2) can be written in the form of the semilinear abstract Cauchy problem

$$U_t = \mathcal{A}U + \mathcal{F}(U), \quad U(0) = U_0, \tag{4.2.21}$$

where $\mathcal{A} = \operatorname{diag}\{1, -a^2\Delta\}\mathcal{J}$ generates a strongly continuous group $\{e^{\mathcal{A}t}\}_{t\in\mathbb{R}}$ of unitary operators in each of the spaces H_p^s.

Applying the variation of constants formula to (4.2.21), for classical solutions we have

$$U(t) = e^{\mathcal{A}t}U_0 + \int_0^t e^{\mathcal{A}(t-\tau)}\mathcal{F}(U(\tau))d\tau, \quad t \in \mathbb{R}. \tag{4.2.22}$$

Assume now the initial data U_0 is supported compactly in the interior of Ω, i.e. $\operatorname{supp} U_0 \subset (x_0-\varepsilon, x_0+\varepsilon) \subsetneq \Omega$, $x_0 \in \Omega$, $\varepsilon > 0$ and t is small. By virtue of D'Alembert formula, we have

$$e^{\mathcal{A}t}U_0 = \frac{1}{2}\begin{bmatrix} u_0(x+at)+u_0(x-at)+\frac{1}{a}\int_{x-at}^{x+at} v_0(s)ds \\ (1+a)v_0(x+at)+(1-a)v_0(x-at) \end{bmatrix}, \quad x \in \Omega.$$

The identity above indicates that the initial data propagates with finite speed a and $\operatorname{supp} e^{\mathcal{A}t}U_0 \subset [x_0-\varepsilon-at, x_0+\varepsilon+at] \subsetneq \Omega$, provided $t < \frac{1}{a}\min\{\ell - x_0 - \varepsilon, \ell + x_0 - \varepsilon\}$. Let $\chi_{x_0,T,\varepsilon}$ be the characteristic function of the set $\Omega \setminus [x_0-\varepsilon-aT, x_0+\varepsilon+aT]$, with $T < \frac{1}{a}\min\{\ell - x_0 - \varepsilon, \ell + x_0 - \varepsilon\}$. Then for $t \in [0,T]$, the solution $U(t)$ emanating from the initial data $\operatorname{supp} U_0 \in [x_0-\varepsilon, x_0+\varepsilon]$ satisfies

$$\begin{aligned} \|\chi_{x_0,T,\varepsilon}U(t)\|_{L^2_p} &= \left\| \int_0^t \chi_{x_0,T,\varepsilon} e^{\mathcal{A}(t-\tau)}\left[\chi_{x_0,\tau,\epsilon}\mathcal{F}(U(\tau)) + (1-\chi_{x_0,\tau,\varepsilon})\mathcal{F}(U(\tau))\right] d\tau \right\|_{L^2_p} \\ &\le \int_0^t \|\chi_{x_0,\tau,\varepsilon}\mathcal{F}(U(\tau))\|_{L^2_p} d\tau, \end{aligned}$$

where we employed the identities $\|e^{\mathcal{A}t}\|_{L^2_p} = 1$ and $\chi_{x_0,T,\varepsilon}e^{\mathcal{A}(t-\tau)}(1-\chi_{x_0,\tau,\varepsilon})\mathcal{F}(U(\tau)) = 0$, $\tau \in [0,t]$, that follow directly from the unitarity of the group $\{e^{\mathcal{A}t}\}_{t\in\mathbb{R}}$ and the D'Alembert formula.

By definition of the map $\mathcal{F}(\cdot)$, we have $\mathcal{F}(0) = 0$, furthermore, the nonlinearity is locally Lipschitz continuous (i.e. $\|\mathcal{F}(U) - \mathcal{F}(V)\|_{L^2_p} \le L(U,V)\|U-V\|_{L^2_p}$). Hence,

$$\|\chi_{x_0,T,\varepsilon}U(t)\|_{L^2_p} \le \int_0^t L(U(\tau),0)\|\chi_{x_0,T,\varepsilon}U(\tau)\|_{L^2_p} d\tau.$$

Applying the Gronwall lemma to the last inequality, we conclude that for small values of T, $\|\chi_{x_0,T,\varepsilon}U(t)\|_{L^2_p} = 0$, $t \in [0,T]$.

In calculations above, the size of $T > 0$ is controlled by the support of the initial data and by the Lipschitz constant $L = \sup_{t\in[0,T]} L(U(\tau),0)$. Using the standard continuation technique, it is not difficult to verify that for globally defined classical solutions, the latter restriction can be suppressed. Hence, we conclude that classical solutions of nonlinear problem (4.1.1) propagate with finite speed a. That is, if $\operatorname{supp} U_0 \subset [x_0-\varepsilon, x_0+\varepsilon]$ then $\operatorname{supp} U(t) \subset [x_0-\varepsilon-at, x_0+\varepsilon+at] \subsetneq \Omega$, provided $t < \frac{1}{a}\min\{\ell - x_0 - \varepsilon, \ell + x_0 - \varepsilon\}$.

4.3 Well-posedness in the real line

The discussion presented in Subsection 4.2.3 allow us to extend the well-posedness analysis from the periodic settings to the whole of real line.

Theorem 4.3.1. *Suppose* $(u_0, v_0) \in H^{s+1}(\mathbb{R}) \times H^s(\mathbb{R}), s \geq 0$*, then the Klein-Gordon equation*

$$u_{tt} = a^2 \Delta u - \mathcal{V}'(u), \quad x \in \mathbb{R}, \quad t > 0, \tag{4.3.1a}$$

$$u(x,0) = u_0, \quad u_t(x,0) = v_0, \tag{4.3.1b}$$

admits a unique global weak solution in the real line $\mathbb{R}$*. The solution is classical when* $s \geq 1$*.*

Proof. (a) From the analysis presented in Section 4.2 it follows that for any compactly supported initial data $(u_0, v_0) \in H^{s+1}(\mathbb{R}) \times H^s(\mathbb{R})$, $s \geq 0$, and any finite time-interval $[0, T]$, there exist a unique weak solution:

$$(u, v) \in L^\infty([0,T], H_p^{s+1}(\mathbb{R}) \times H_p^s(\mathbb{R})),$$
$$(u_t, v_t) \in L^\infty([0,T], H_p^s(\mathbb{R}) \times H_p^{s-1}(\mathbb{R})).$$

Indeed, such initial data can be fitted into a very large finite interval $\Omega = (-\ell, \ell)$ so that solution to the periodic problem with the data $\mathrm{supp}(u_0, v_0) \subset (-\ell, \ell)$ is compactly supported in $[-\ell, \ell] \times [0, T]$. Therefore, the solution of the periodic problem, extended by zero in $(\mathbb{R} \setminus [-\ell, \ell]) \times [0, T]$, solves the Klein Gordon equation in the real line $\mathbb{R}$.

(b) The Schwartz class $\mathcal{D}(\mathbb{R})$ of $C^\infty(\mathbb{R})$ and compactly supported functions is dense in each of the spaces $H^s(\mathbb{R})$, $s \geq 0$ (see e.g. [AF03]). Hence, any initial data $(u_0, v_0) \in H^{s+1}(\mathbb{R}) \times H^s(\mathbb{R}), s \geq 0$ can be approximated by a sequence $(u_{0n}, v_{0n})_{n \geq 0}$ of compactly supported and smooth functions. Each tuple $(u_{0n}, v_{0n})_{n \geq 0}$ gives rise to a weak solution $(u_n(t), v_n(t))$ of the Klein-Gordon equation in the real line.

Using the same approach as in Theorem 4.2.4, it is not difficult to verify that the sequence $\{(u_n(t), v_n(t))\}_{n\geq 0}$ converges strongly to a weak solution

$$(u, v) \in L^\infty([0,T], H_p^{s+1}(\mathbb{R}) \times H_p^s(\mathbb{R})),$$
$$(u_t, v_t) \in L^\infty([0,T], H_p^s(\mathbb{R}) \times H_p^{s-1}(\mathbb{R})),$$

of (4.3.1). Finally, uniqueness of weak solutions in context of the real line follows as in the proof of Theorem 4.2.4. $\square$

Chapter 5

The Fourier-type pseudo-spectral scheme for the nonlinear KGE

In this Chapter, we present a Fourier-type pseudo-spectral scheme for solving nonlinear KGE models with smooth nonlinearities. As it follows from the title of the Chapter, we approximate the exact solutions by the means of formula

$$(\overline{u}, \overline{v}) = \tfrac{1}{2\ell} \sum_{|n| \leq N} (\overline{u}, \overline{v})(t) \phi_n(x),$$

where the unknown discrete Fourier coefficients are chosen so that

$$\langle (\overline{u}, \overline{v})_t, (\phi_1, \phi_2) \rangle = \langle \overline{v}, \phi_1 \rangle - a^2 \langle \nabla \overline{u}, \nabla \phi_2 \rangle - \langle \mathcal{I}^2_{2N+1}[\mathcal{V}'(\overline{u})], \phi_2 \rangle, \tag{5.0.1a}$$

$$\langle (u_0, v_0)(x_j) = (\overline{u}_0, \overline{v}_0)(x_j) \rangle, \quad j = 0, 1, \ldots, 2N, \tag{5.0.1b}$$

for all $(\phi_1, \phi_2) \in \bar{\mathbb{P}}_N$. As in Section 4.2, we observe that the finite dimensional ODE (5.0.1) is Hamiltonian, i.e. (5.0.1) is equivalent to

$$\overline{U}_t = \mathcal{J} \nabla \overline{\mathcal{H}}(\overline{U}), \quad t > 0, \tag{5.0.2a}$$

$$\overline{U}_0 = (\mathcal{I}^2_{2N+1}[u_0], \mathcal{I}^2_{2N+1}[v_0])^T = (\bar{u}_0, \bar{v}_0)^T, \tag{5.0.2b}$$

where $\bar{U} = (\bar{u}, \bar{v})^T \in \bar{\mathbb{P}}^2_N$ and the discrete Hamiltonian is given by

$$\overline{\mathcal{H}}(\overline{u}, \overline{v}) = \frac{1}{2} \int_\Omega (\overline{v}^2 + a^2 |\nabla \overline{u}|^2 + 2\mathcal{I}^2_{2N+1}[\mathcal{V}(\overline{u})]) dx. \tag{5.0.2c}$$

5.1 Stability analysis

As in Lemma 4.2.1, the hamiltonicity of the pseudo-spectral semi-discretization (5.0.1) guarantees the numerical solutions remain uniformly bounded.

Lemma 5.1.1. *For any $t > 0$, the numerical solution $(\bar{u}, \bar{v})$ of (5.0.1) satisfies*

$$\|\nabla \bar{u}\|_{(C[0,T],L^2_p)} \leq \bar{\mathcal{H}}(\bar{u}_0, \bar{v}_0), \tag{5.1.1a}$$

$$\|\bar{v}\|_{(C[0,T],L^2_p)} \leq \bar{\mathcal{H}}(\bar{u}_0, \bar{v}_0), \tag{5.1.1b}$$

$$\|\bar{u}\|_{(C[0,T],L^2_p)} \leq \|\bar{u}_0\|_{L^2_p} + ct\bar{\mathcal{H}}(\bar{u}_0, \bar{v}_0), \tag{5.1.1c}$$

$$\|\bar{u}\|_{(C[0,T],L^\infty)} \leq \|\bar{u}_0\|_{L^2_p} + ct^{\frac{1}{2}}\bar{\mathcal{H}}(\bar{u}_0, \bar{v}_0), \tag{5.1.1d}$$

where the generic constant $c > 0$ is independent on $(\bar{u}, \bar{v})$ and/or $N > 0$. In addition, if $u_0 \in H^\alpha_p(-\ell, \ell)$ and $v_0 \in H^\beta_p(-\ell, \ell)$, with $\alpha > 2$ and $\beta > 1$, then

$$\bar{\mathcal{H}}(\bar{u}_0, \bar{v}_0) \leq C(\|u_0\|_{H^\alpha_p}, \|v_0\|_{H^\beta_p}), \tag{5.1.2a}$$

$$\|\bar{u}_0\|_{L^2_p} \leq \|u_0\|_{H^\alpha_p} + c\|u_0\|_{H^\alpha_p}, \tag{5.1.2b}$$

where function $C(\cdot,\cdot) > 0$ and generic constant $c > 0$ are independent on the initial data (u_0, v_0) and/or $N > 0$.

Proof. (a) The proof of (5.1.1) is identical to the proof of part (a) in Lemma 4.2.1 and is omitted.

(b) To show that (5.1.2) holds, we employ Theorem 3.4.2. For some $\gamma > \frac{1}{2}$ this gives the bound

$$\begin{aligned}
\|\bar{u}_0\|_{L^2_p} &\leq \|u_0\|_{L^2_p} + \|(\mathcal{I} - \mathcal{I}^2_{2N+1})[u_0]\|_{L^2_p} \\
&\leq \|u_0\|_{L^2_p} + c\left(\tfrac{\ell}{\pi N}\right)^{\alpha-\gamma-\frac{1}{2}}\|u_0\|_{H^\alpha_p} \leq \|u_0\|_{L^2_p} + c\|u_0\|_{H^\alpha_p},
\end{aligned}$$

which holds uniformly for all $N > 0$, provided $\alpha > 1$. When $\alpha > 2$ and $\beta > 1$, the same procedure yields also

$$\begin{aligned}
&\|\bar{v}_0\|_{L^2_p} \leq \|v_0\|_{L^2_p} + c\|v_0\|_{H^\beta_p}, \\
&\|\nabla \bar{u}_0\|_{L^2_p} \leq \|\bar{u}_0\|_{H^1_p} \leq \|u_0\|_{H^1_p} + c\|u_0\|_{H^\alpha_p}.
\end{aligned}$$

Finally, taking into account accuracy of the discrete quadrature (see Lemma 3.3.1) and the Sobolev Embedding Theorem 2.4.1, for smooth potentials $\mathcal{V}(u)$ we have

$$\int_\Omega \mathcal{I}^2_{2N+1}[\mathcal{V}(\bar{u}_0)]dx = \tfrac{2\ell}{2N+1}\sum_{j=0}^{2N}\left|\int_0^{u_0(x_j)}\mathcal{V}'(s)ds\right|$$
$$\leq 2\ell \sup\{|\mathcal{V}'(s)|\,|\,0 \leq s \leq \|u_0\|_{L^\infty}\}\|u_0\|_{L^\infty} \leq c\|u_0\|_{H^1_p}.$$

Combining our estimates and the definition of $\bar{\mathcal{H}}(\bar{u},\bar{v})$ (see formula (5.0.2c)), we arrive at (5.1.2). □

Next, we show that our numerical scheme (5.0.1) depends continuously on the input data, i.e. it is stable.

Lemma 5.1.2. *Let* $(\bar{u}^i,\bar{v}^i)$, $i=1,2$ *be two solutions of the following perturbed problems:*

$$\begin{cases} \langle(\bar{u}^i,\bar{v}^i)_t,(\phi_1,\phi_2)\rangle = \langle\bar{v}^i,\phi_1\rangle - a^2\langle\nabla\bar{u}^i,\nabla\phi_2\rangle - \langle\mathcal{I}^2_{2N+1}[\mathcal{V}(\bar{u}^i)],\phi_2\rangle + \langle f^i,\phi_2\rangle, \\ (\hat{u}^i(0),\hat{v}^i(0)) = (\hat{u}^i_0,\hat{v}^i_0), \quad \textit{for all} \quad (\phi_1,\phi_2)\in\bar{\mathbb{P}}_N, \end{cases} \tag{5.1.3}$$

that satisfy the estimates (5.1.1) *and* (5.1.2) *of Lemma 5.1.1. If* $(e_1,e_2) = (\bar{u}^2,\bar{v}^2)-(\bar{u}^1,\bar{v}^1)$, *then in any finite time interval* $[0,T]$, *the following is true:*

$$\|e_1\|_{(C([0,T]),H^1_p)} + \|e_2\|_{(C([0,T]),L^2_p)} \leq c\Big[\|e_{10}\|_{H^1_p} + \|e_{20}\|_{L^2_p} + \|f^1-f^2\|_{L^2([0,T]\times(-\ell,\ell))}\Big], \tag{5.1.4}$$

where the constant $c>0$ *does not depend on* $N>0$.

Proof. Subtracting equations with $i=1$ and $i=2$ from each other, we obtain

$$\begin{cases} \langle(e_1,e_2)_t,(\phi_1,\phi_2)\rangle &= \langle e_2,\phi_1\rangle - a^2\langle\nabla e_1,\nabla\phi_2\rangle \\ &\quad -\langle\mathcal{I}^2_{2N+1}[\mathcal{V}(\bar{u}^1)-\mathcal{V}(\bar{u}^2)],\phi_2\rangle + \langle(f^2-f^1),\phi_2\rangle, \\ (e_1(0),e_2(0)) &= (e_{10},e_{20}), \quad \text{for all} \quad (\phi_1,\phi_2)\in\bar{\mathbb{P}}_N. \end{cases} \tag{5.1.5}$$

Letting $(\phi_1,\phi_2)=(e_1,e_2)$ and taking into account that $e_{1t}=e_2$, we have

$$\frac{1}{2}\frac{d}{dt}\Big[\|e_2\|^2_{L^2_p} + a^2\|\nabla e_1\|^2_{L^2_p}\Big] = \langle(f^2-f^1),e_2\rangle - \langle\mathcal{I}^2_{2N+1}[\mathcal{V}(\bar{u}^1)-\mathcal{V}(\bar{u}^2)],e_2\rangle. \tag{5.1.6}$$

By Lemma 3.3.1 the quadrature is exact in $\bar{\mathbb{P}}_N$. Therefore, with the aid of the Cauchy-Schwartz and Young's inequalities, we infer

$$\begin{aligned}\left|\langle \mathcal{I}^k_{2N+1}[\mathcal{V}(\bar{u}^1) - \mathcal{V}(\bar{u}^2)], e_2\rangle\right| &\leq \frac{2\ell}{2N+1}\sum_{j=0}^{2N}|e_2(x_j)|\left|\int_{\bar{u}^1(x_j)}^{\bar{u}^2(x_j)}\mathcal{V}''(s)ds\right| \\ &\leq c\frac{2\ell}{2N+1}\sum_{j=0}^{2N}|e_2(x_j)||e_1(x_j)| \\ &\leq c\|e_1\|_{L^2_p}\|e_2\|_{L^2_p} \leq \frac{c}{2}\Big[\|e_1\|^2_{L^2_p} + \|e_2\|^2_{L^2_p}\Big],\end{aligned}$$

where

$$\begin{aligned}c &= \max\Big\{\mathcal{V}''(s)\,\Big|\,|s| \leq \max\{\|\bar{u}^1\|_{C([0,T],L^\infty)}, \|\bar{u}^2\|_{C([0,T],L^\infty)}\}\Big\} \\ &\leq \max\Big\{\mathcal{V}''(s)\,\Big|\,|s| \leq \|u_0\|_{H^1_p} + c\|u_0\|_{H^\alpha_p}\Big\}\end{aligned}$$

is independent of $N > 0$, by virtue of (5.1.2b).

The last estimate, combined with (5.1.6), yields the bound

$$\frac{d}{dt}\Big[\|e_2\|^2_{L^2_p} + a^2\|\nabla e_1\|^2_{L^2_p}\Big] \leq c\Big[\|e_1\|^2_{L^2_p} + \|e_2\|^2_{L^2_p}\Big] + \|f^1 - f^2\|^2_{L^2_p}, \tag{5.1.7}$$

where as before the generic constant $c > 0$ is independent of $N > 0$. Similarly, letting $(\phi_1, \phi_2) = (e_1, 0)$ in (5.1.5) and using Young's inequality, we have:

$$\tfrac{d}{dt}\|e_1\|^2_{L^2_p} \leq \|e_1\|^2_{L^2_p} + \|e_2\|^2_{L^2_p} \tag{5.1.8}$$

To end the proof, we add (5.1.7) and (5.1.8) together and apply Gronwall's inequality to obtain (5.1.4) and the claim is settled. □

5.2 Consistency and convergence

Let u be the exact weak solution of (4.1.1). For $N > 0$, and we denote $(\hat{u}, \hat{v}) = (\mathcal{P}_N[u], \mathcal{P}_N[v])$ and $(\hat{u}(0), \hat{v}(0)) = (\mathcal{P}_N[u]_0, \mathcal{P}_N[v]_0)$. It is not difficult to show that the spectral projection $(\hat{u}, \hat{v})$ satisfies:

$$\begin{cases}\langle(\hat{u}, \hat{v})_t, (\phi_1, \phi_2)\rangle = \langle\hat{v}, \phi_1\rangle - a^2\langle\nabla\hat{u}, \nabla\phi_2\rangle - \langle\mathcal{I}^2_{2N+1}[\mathcal{V}'(\hat{u})], \phi_2\rangle + \langle\mathcal{D}_N(u), \phi_2\rangle, \\ (\hat{u}(0), \hat{v}(0)) = (\mathcal{P}_N[u_0], \mathcal{P}_N[v_0]), \quad \text{for all} \quad (\phi_1, \phi_2) \in \bar{\mathbb{P}}^2_N,\end{cases} \tag{5.2.1}$$

where the quantity $\mathcal{D}_N(u) = \mathcal{I}^2_{2N+1}[\mathcal{V}'(\hat{u})] - \mathcal{P}_N[\mathcal{V}'(u)]$ is known as the defect. In what follows, we show that defect $\mathcal{D}_N(u)$ is small, provided the exact solution is sufficiently regular.

Lemma 5.2.1. *Let $s > \frac{3}{2}$, then*

$$\|\mathcal{D}_N(u)\|_{L^2_p} \leq c\big(\tfrac{\ell}{\pi N}\big)^{s-\frac{3}{2}}\Big(\|u\|_{H^s_p} + F_s(\|u\|_{H^s_p})\Big), \tag{5.2.2}$$

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

Proof. We recall that $\mathcal{I}^2_{2N+1}$ is identity in $\bar{\mathbb{P}}_N$, therefore

$$\begin{aligned}\|\mathcal{D}_N(u)\|_{L^2_p} &= \|\mathcal{I}^2_{2N+1}[\mathcal{V}'(\hat{u})] - \mathcal{P}_N[\mathcal{V}'(u)]\|_{L^2_p}\\ &= \|\mathcal{I}^2_{2N+1}\big[\mathcal{V}'(\hat{u}) - \mathcal{P}_N[\mathcal{V}'(u)]\big]\|_{L^2_p}.\end{aligned}$$

We infer from Lemma 3.4.1

$$\begin{aligned}\|\mathcal{D}_N(u)\|_{L^2_p} &\leq c_\alpha\sqrt{2N}\|[\mathcal{V}'(\hat{u})] - \mathcal{P}_N[\mathcal{V}'(u)]\|_{H^\alpha_p}\\ &\leq c_\alpha\sqrt{2N}\Big[\|\mathcal{V}'(\hat{u}) - \mathcal{V}'(u)\|_{H^\alpha_p} + \|(\mathcal{I} - \mathcal{P}_N)[\mathcal{V}'(u)]\|_{H^\alpha_p}\Big]\\ &=: c_\alpha\sqrt{2N}\Big[\|E_1\|_{H^\alpha_p} + \|E_2\|_{H^\alpha_p}\Big],\end{aligned}$$

with some $\frac{1}{2} < \alpha \leq 1$. To bound $\|E_1\|_{H^\alpha_p}$, we proceed as in the estimate (4.2.8) to obtain initially

$$\|E_1\|_{L^2_p} \leq c_0\|(\mathcal{I} - \mathcal{P}_N)[u]\|_{L^2_p}, \tag{5.2.3}$$

where $c_0 = \max\{|\mathcal{V}''(s)|\,|\,|s| \leq \|u\|_{L^\infty([0,T]\times(-\ell,\ell))}\}$. We also note that

$$\|\nabla E_1\|^2_{L^2_p} \leq \int_\Omega |\mathcal{V}''(\hat{u})\nabla\hat{u} - \mathcal{V}''(u)\nabla u|^2 dx.$$

Taking into account the regularity of $\mathcal{V}(\cdot)$ and in the same way as in (4.2.8), we have

$$\begin{aligned}\|\nabla E_1\|_{L^2_p} &\leq \|\mathcal{V}''(\hat{u})\nabla(\mathcal{I} - \mathcal{P}_N)[u]\|_{L^2_p} + \|[\mathcal{V}''(\hat{u}) - \mathcal{V}''(u)]\nabla u\|_{L^2_p}\\ &\leq \big(c_0 + c_1\|\nabla u\|_{L^\infty_p}\big)\|(\mathcal{I} - \mathcal{P}_N)[u]\|_{H^1_p},\end{aligned}$$

where $c_1 = \max\{|\mathcal{V}'''(s)|\,|\,|s| \leq \|u\|_{L^\infty([0,T]\times(-\ell,\ell))}\}$. With the aid of Theorem 3.2.1, we have that

$$\|E_1\|_{H^1_p} \leq \big(2c_0 + c_1\|\nabla u\|_{L^\infty_p}\big)\big(\tfrac{\ell}{\pi N}\big)^{s-1}\|u\|_{H^s_p}. \tag{5.2.4}$$

Next, we bound $\|E_2\|_{H_p^\alpha}$, again by Theorem 3.2.1, we have

$$\|E_2\|_{H_p^\alpha} \le c_2\big(\tfrac{\ell}{\pi N}\big)^{s-\alpha}\|\mathcal{V}'(u)\|_{H_p^s}.$$

Also, if $\mathcal{V} \in C^{s+2}$, then the Faa di Bruno formula and the fact that H_p^s is a Banach algebra yields as in (4.2.14) that

$$\|E_2\|_{H_p^\alpha} \le c_2\big(\tfrac{\ell}{\pi N}\big)^{s-\alpha}F_s(\|u\|_{H_p^s})^{\frac{1}{2}}. \tag{5.2.5}$$

Where $F_s(\cdot)$ is a polynomial of degree $2s$, whose coefficients are controlled by the regularity of $\mathcal{V}$. Formulas (5.2.4) and (5.2.5), combined together, imply (5.2.2). $\square$

Remark 5.2.1. In fact, results of Chapter 3 imply that the defect $\mathcal{D}_N(u)$ is exponentially small provided u and $\mathcal{V}$ are analytic. Indeed, when u and $\mathcal{V}(u)$ are analytic in the strip $S_\delta = \{|\mathrm{Im}\, z| < \delta\} \subset \mathbb{C}$ and continuous on its boundary ∂S_δ, from Theorem 3.4.3 we infer

$$\|\mathcal{D}(u)\|_{L_p^2} \le c\left(\tfrac{\pi N}{\ell}\right)^{\frac{5}{2}} e^{-\frac{\pi\delta}{\ell}N}\Big[\|u\|_{L^\infty(\partial S_\delta)} + \|\mathcal{V}'(u)\|_{L^\infty(\partial S_\delta)}\Big], \tag{5.2.6}$$

where the generic constant $c > 0$ does not depend on u, $\mathcal{V}'(u)$ and $N > 0$.

With the aid of Lemma 5.1.2 and 5.2.1, we obtain the main result of this section.

Theorem 5.2.2. *Assume $\gamma > \frac{1}{2}$ and $s > \frac{3}{2} + \gamma$. Then*

$$\begin{aligned}\|\bar{u} - u\|_{C([0,T],H_p^1)} &+ \|\bar{v} - v\|_{C([0,T],L_p^2)} \\ &\le c\big(\tfrac{\ell}{\pi N}\big)^{s-\frac{3}{2}-\gamma}\Big[\|u_0\|_{H_p^s} + \|v_0\|_{H_p^{s-1}} + G_s(\|u\|_{C([0,T],H_p^s)})\Big],\end{aligned} \tag{5.2.7}$$

where $G_s(\cdot) = \cdot + F_s(\cdot)$, function $F_s(\cdot)$ is defined in Lemma 5.2.1 and the generic constant $c > 0$ does not depend on u and $N > 0$ but depends on $T > 0$.

Proof. We apply stability Lemma 5.1.2 to the couple of problems (5.0.1) and (5.2.1). In view of Lemma 5.2.1 and Theorem 3.4.2, this gives

$$\begin{aligned}\|\bar{u} - \hat{u}\|_{H_p^1} + \|\bar{v} - \hat{v}\|_{L_p^2} &\le c\Big[\|(\mathcal{I}_{2N+1}^k - \mathcal{P}_N)[u_0]\|_{H_p^1} + \|(\mathcal{I}_{2N+1}^k - \mathcal{P}_N)[v_0]\|_{L_p^2} \\ &\quad + \|\mathcal{D}_N(u)\|_{L^2([0,T])\times(-\ell,\ell)}\Big] \\ &\le c\big(\tfrac{\ell}{\pi N}\big)^{s-\frac{3}{2}-\gamma}\Big[\|u_0\|_{H_p^s} + \|v_0\|_{H_p^{s-1}} + G_s(\|u\|_{C([0,T],H_p^s)})\Big],\end{aligned}$$

where $c > 0$ does not depend on u and $N > 0$ but depends on $T > 0$. Since $\|(\bar{u}, \bar{v}) - (u, v)\|_{L^2_p} \leq \|(\bar{u}, \bar{v}) - (\hat{u}, \hat{v})\|_{L^2_p} + \|(\mathcal{I} - \mathcal{P}_N)[(u, v)]\|_{L^2_p}$, straightforward application of Theorem 3.2.1 completes the proof. □

Theorem 5.2.2 shows that the numerical scheme (5.0.1) converges algebraically, provided that the exact solution is sufficiently smooth.

Remark 5.2.2. In view of Theorems 3.2.2, 3.4.2 and Remark 5.2.1, the discretization error decays geometrically if the exact solution (u, v) and potential $\mathcal{V}$ are analytic in the strip S_δ. In this case, we have

$$\begin{aligned} &\|\bar{u} - u\|_{C([0,T],H^1_p)} + \|\bar{v} - v\|_{C([0,T],L^2_p)} \\ &\qquad \leq c \left(\tfrac{\pi N}{\ell}\right)^{\frac{5}{2}} e^{-\frac{\pi\delta}{\ell}N} \Big[\|v_0\|_{L^\infty(S_\delta)} + \|u\|_{C([0,T],L^\infty(S_\delta))} + \|\mathcal{V}'(u)\|_{C([0,T],L^\infty(S_\delta))}\Big], \end{aligned} \tag{5.2.8}$$

where the generic constant $c > 0$ does not depend on (u, v), $\mathcal{V}'(u)$ and $N > 0$ but depends on $T > 0$.

The results of Subsection 4.2.3 imply, that in finite time intervals, the numerical scheme (5.0.1) is applicable to KGE models on the real line, provided the initial data is compactly supported. Since any (square integrable on $\mathbb{R}$) initial data can be approximated with arbitrary accuracy by compactly supported functions, we conclude that (5.0.1) yields spectrally accurate numerical solutions in $\mathbb{R}$, provided the truncation parameter $\ell > 0$ is sufficiently large.

Chapter 6

Implementation and simulations

In this Chapter, we present a brief discussion of several practical issues arising in connection with our scheme (5.0.1) and demonstrate its numerical accuracy and performance in a series of practical simulations.

6.1 Implementation

The numerical scheme (5.0.1) can be written in the form of the semi-linear Cauchy problem

$$U_t = \mathcal{A}U + \mathcal{F}(U), \quad U(0) = U_0. \tag{6.1.1}$$

Since exact solutions to the ODE (6.1.1) are not known, we shall integrate the system of ODE using an appropriate time-stepping algorithm. Two practical issues in connection with the time-stepping are discussed below.

6.1.1 Efficient evaluation of the semi-discrete vector field

Any time-stepping algorithm evaluates the right-hand side of (6.1.1) several times per time integration step. Hence, minimizing the computational cost of this procedure is critical for the overall efficiency of the numerical code. In context of (5.0.1), the computational cost is minimized when the linear part $\mathcal{A}U$ is evaluated in Fourier space[1], while the nonlinearity

[1]Note that in this case $\mathcal{A}U$ reduces to the matrix vector multiplication with a diagonal matrix.

$\mathcal{F}(U)$ is best computed directly in the physical space. Implemented this way, both operations require $\mathcal{O}(N)$ floating point operations. It follows from the above that irrespective of the concrete choice of the computational space (Fourier or physical), the procedure involves use of direct and inverse discrete Fourier transforms (3.3.2) and (3.3.3). As noted in Section 3.3, both operations can be accomplished in $\mathcal{O}(N \log_2 N)$ flops. Hence, the minimal computational cost of evaluating the semi-discrete KGE vector field is $\mathcal{O}(N \log_2 N)$.

6.1.2 Time-stepping

For large values of N, ODE (6.1.1) is stiff and integrating using standard Runge-Kutta explicit ODE solvers will be difficult. Also, the problem is Hamiltonian with symplectic flow. In order to handle the stiffness and preserve the flow associated with the symplectic structure of (6.1.1), we resort to a Strang-type symmetric splitting technique (see [HLW06] and references therein). That is, we rewrite the numerical Hamiltonian as

$$\mathcal{H}(\bar{u}, \bar{v}) = \tfrac{1}{2}\Big(\langle \bar{v}, \bar{v}\rangle + a^2 \langle \nabla \bar{u}, \nabla \bar{u}\rangle\Big) + \int_\Omega \mathcal{I}^2_{2N+1}[\mathcal{V}(\bar{u})] =: \mathcal{H}_1(\bar{u}, \bar{v}) + \mathcal{H}_2(\bar{u}) \tag{6.1.2a}$$

and consider couple of problems

$$(\bar{u}, \bar{v})_t = \mathcal{J} \nabla \mathcal{H}_1(\bar{u}, \bar{v}), \tag{6.1.2b}$$

$$(\bar{u}, \bar{v})_t = \mathcal{J} \nabla \mathcal{H}_2(\bar{u}), \tag{6.1.2c}$$

whose exact flows are given by Ψ^1_t and Ψ^2_t, respectively. With this notation, a one step of length τ of our Strang-type time-stepping splitting scheme can be written as

$$(\bar{u}, \bar{v})(t + \tau) = \big[\Psi^1_{\tau/2} \circ \Psi^2_\tau \circ \Psi^1_{\tau/2}\big](\bar{u}, \bar{v})(t) =: \Phi_\tau(\bar{u}, \bar{v})(t). \tag{6.1.3}$$

Since each of the flows Ψ^1_t and Ψ^2_t is symmetric, symplectic and can be computed exactly, (6.1.3) gives an A-stable, explicit, symmetric and symplectic Strang-type numerical scheme of classical order $p = 2$. In order to increase the convergence rate, we employ the symmetric composition approach described in [HLW06], i.e. instead of Φ_τ, we use

$$\Phi^s_\tau = \Phi_{\gamma_1 \tau} \circ \cdots \circ \Phi_{\gamma_s \tau}, \tag{6.1.4}$$

with $s = 17$ and

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

The procedure described above yields A-stable, explicit, symplectic and symmetric time-stepping scheme of classical order $p = 8$. In view of Subsection 6.1.1, the overall computational complexity of one time-integration step described above is $\mathcal{O}(N \log_2 N)$.

6.2 Numerical simulations

In this section, we present several numerical simulations demonstrating the numerical performance of our scheme. As a reference problem, we take the Sine-Gordon equation (SGE),

$$u_{tt} = \Delta u - \sin(u), \quad x \in \mathbb{R}, \quad t > 0, \tag{6.2.1a}$$

$$u(0) = u_0, \quad u_t(0) = v_0, \tag{6.2.1b}$$

which is a particular type of KGE, with $\mathcal{V}(u) = 1 - \cos u$. Problem (6.2.1) is known to be completely integrable via inverse scattering method (see [NMPZ84] and references therein). In our simulations, we make use of a subclass of exact solutions that describe propagation of n nonlinear traveling waves, known as n-solitons. These are given explicitly by the formulas [NMPZ84]

$$V = (v_{kj})_{k,j=1}^{n}, \quad v_{kj} = \tfrac{c_j}{\lambda_k + \lambda_j} \exp\!\left(2i\lambda_j x - \tfrac{it}{2\lambda_j}\right), \tag{6.2.2a}$$

$$u = -4 \arg \det(I + V), \tag{6.2.2b}$$

where parameters c_j and λ_j control the phase shift and the velocity of the associated traveling wave, respectively.

Using (6.2.2) one can verify that n-soliton solutions are analytic in a strip containing the real axis and are square integrable there, whenever n is even, $\lambda_{2i-1} = -\overline{\lambda_{2i}}$ and parameters $c_{2i-1} = c_{2i}$ are real. Hence, in this settings, the convergence theory developed in Chapter 5 applies.

6.2.1 A single breather

In our first example, we simulate the dynamics of a coupled pair of a soliton and an anti-soliton (known as a breather). We let $n = 2$,

$$\lambda_1 = \tfrac{2+2i}{\sqrt{8}}, \quad \lambda_2 = \tfrac{-2+2i}{\sqrt{8}}$$

and $c_i = 1$, $i = 1, 2$. With this settings, the breather components travel with the same constant speed of $v = \frac{4|\lambda_i|^2 - 1}{4|\lambda_i|^2 + 1} = \frac{3}{5}$ in the positive direction of x-axis. The results of simulations in time interval $[0, 10]$ are shown in Fig. 6.1.

The numerical solution, the pointwise and L^2-errors are plotted in the left- and the right-top diagrams and in the left-middle diagram of Fig. 6.1, respectively. The figures indicate that reasonable choice of the truncation parameter ℓ yields very accurate numerical results already for moderate values of N ($N = 2^6$ and $\ell = 5 \log_2 N$ in our simulation). In fact, 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 Remark 5.2.2, we expect geometric convergence. As illustrated by the left-bottom diagram of Fig. 6.1, this is indeed the case. Both $L^2(\mathbb{R})$ and $L^\infty(\mathbb{R})$ errors (blue and teal lines, respectively), obtained with $2^3 \le N \le 2^8$ and $\ell = 5 \log_2 N$, decrease geometrically as N increases.

The middle-right diagram ($N = 2^6$) and the red line in the bottom-left diagram illustrate the conservation properties of the semi-discretization (5.0.1), coupled with the composite time-stepping scheme (6.1.4). Since the space discretization preserves the hamiltonicity of the continuous model and the time discretization preserves symplecticity of the flow, the deviation in the semi-discrete Hamiltonian $\bar{\mathcal{H}}(\bar{u}, \bar{v})$ remains small (near 10^{-14}) independently of N. Finally, the work-precision diagram (the bottom-right panel of Fig. 6.1) demonstrates the overall efficiency of our scheme.

6.2.2 Two breathers interaction (A)

In our second example, we simulate an interaction of a stationary and a moving breather. To construct the exact solution, we employ (6.2.2) with $n = 4$,

$$\lambda_1 = \tfrac{1+i}{\sqrt{8}}, \quad \lambda_2 = \tfrac{-1+i}{\sqrt{8}}, \quad \lambda_3 = \tfrac{2+2i}{\sqrt{8}}, \quad \lambda_4 = \tfrac{-2+2i}{\sqrt{8}}$$

and $c_i = 1$, $i = 1, \ldots, 4$. We take the same values for parameters ℓ and N as in Example 6.2.1 and integrate the initial value problem (6.2.1) in the time interval $[0, 10]$. The results of numerical simulations, plotted in Fig. 6.2, demonstrate the same qualitative features as in Example 6.2.1. Again due to the analyticity of the exact solution, the L^2- and L^∞-errors (blue and teal lines in the left-bottom diagram, respectively) decrease geometrically as N increases and the scheme preserves the semi-discrete first integral $\bar{\mathcal{H}}(\bar{u}, \bar{v})$ almost exactly.

6.2.3 Two breathers interaction (B)

To provide further illustration, we slightly modify the settings of Example 6.2.2, i.e. we let

$$\lambda_3 = \tfrac{3+2i}{\sqrt{8}}, \quad \lambda_4 = \tfrac{-3+2i}{\sqrt{8}},$$

leave the remaining parameters unchanged and repeat the calculations of Example 6.2.2. As shown in Fig. 6.3, the results of simulations are almost identical to those obtained in Example 6.2.2.

6.2.4 Three breathers interaction

In our last example, we take $n = 6$,

$$\lambda_1 = \tfrac{1+i}{\sqrt{8}}, \quad \lambda_2 = \tfrac{-1+i}{\sqrt{8}}, \quad \lambda_3 = \tfrac{2+2i}{\sqrt{8}}, \quad \lambda_4 = \tfrac{-2+2i}{\sqrt{8}}, \quad \lambda_5 = \tfrac{3+3i}{\sqrt{8}}, \quad \lambda_6 = \tfrac{-3+3i}{\sqrt{8}},$$

$c_i = 1$, $i = 1, \ldots, 6$. This yields a three moving soliton/anti-soliton pairs. The simulations, with $2^3 \leq N \leq 2^8$ and $\ell = 5 \log_2 N$ are displayed in Fig. 6.4. We see that the qualitative behavior of both $L^2(\mathbb{R})$ and $L^\infty(\mathbb{R})$ errors (blue and teal lines, respectively) is the same as those observed in all our previous simulations. The errors decay geometrically as predicted by Theorem 5.2.2 and the time-stepping scheme preserves the semi-discrete first integral almost exactly.

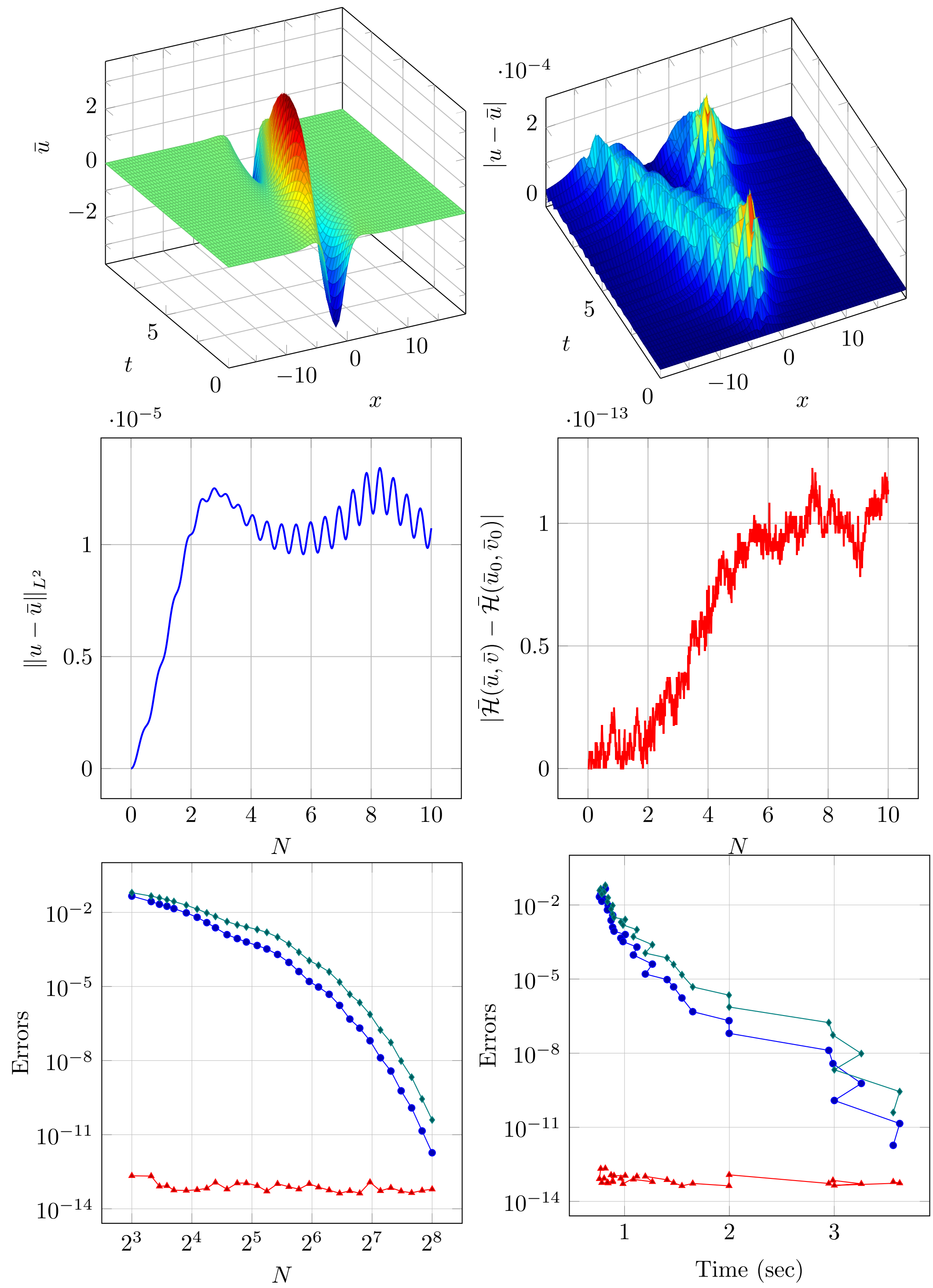

Figure 6.1: The numerical solution of (6.2.1) (left to right and top to bottom): $\bar{u}$, $|u - \bar{u}|$, $\|u - \bar{u}\|_{L^2}$, $|\mathcal{H}(\bar{u}, \bar{v}) - \mathcal{H}(\bar{u}_0, \bar{v}_0)|$, with $N = 2^6$; $\|u - \bar{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u - \bar{u}\|_{L^\infty(\mathbb{R})}$ (teal), and $|\mathcal{H}(\bar{u}, \bar{v}) - \mathcal{H}(\bar{u}_0, \bar{v}_0)|$ (red), work-precision diagram.

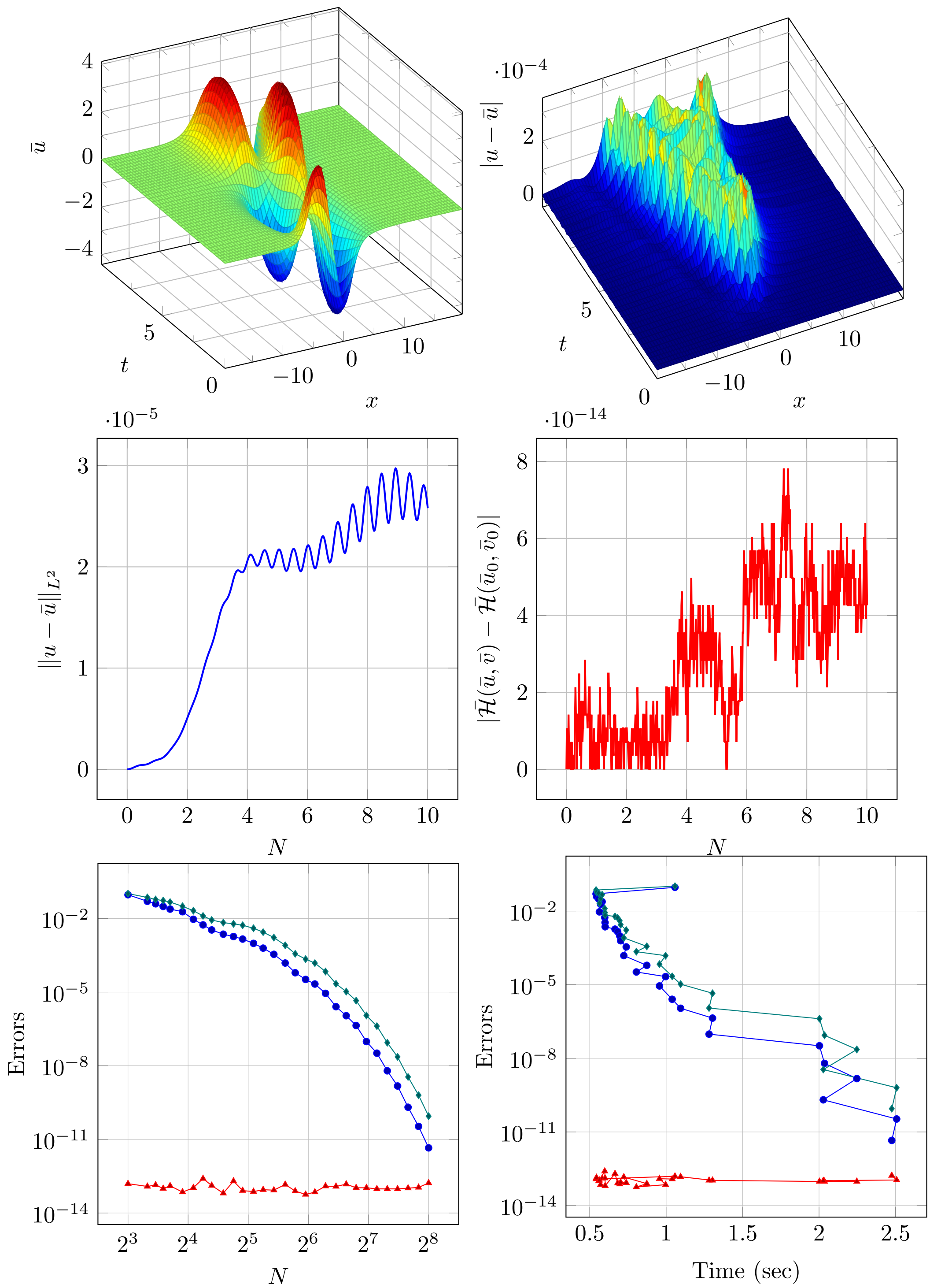

Figure 6.2: The numerical solution of (6.2.1) (left to right and top to bottom): $\bar{u}$, $|u-\bar{u}|$, $\|u-\bar{u}\|_{L^2}$, $|\mathcal{H}(\bar{u},\bar{v})-\mathcal{H}(\bar{u}_0,\bar{v}_0)|$, with $N=2^6$; $\|u-\bar{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u-\bar{u}\|_{L^\infty(\mathbb{R})}$ (teal), and $|\mathcal{H}(\bar{u},\bar{v})-\mathcal{H}(\bar{u}_0,\bar{v}_0)|$ (red), work-precision diagram.

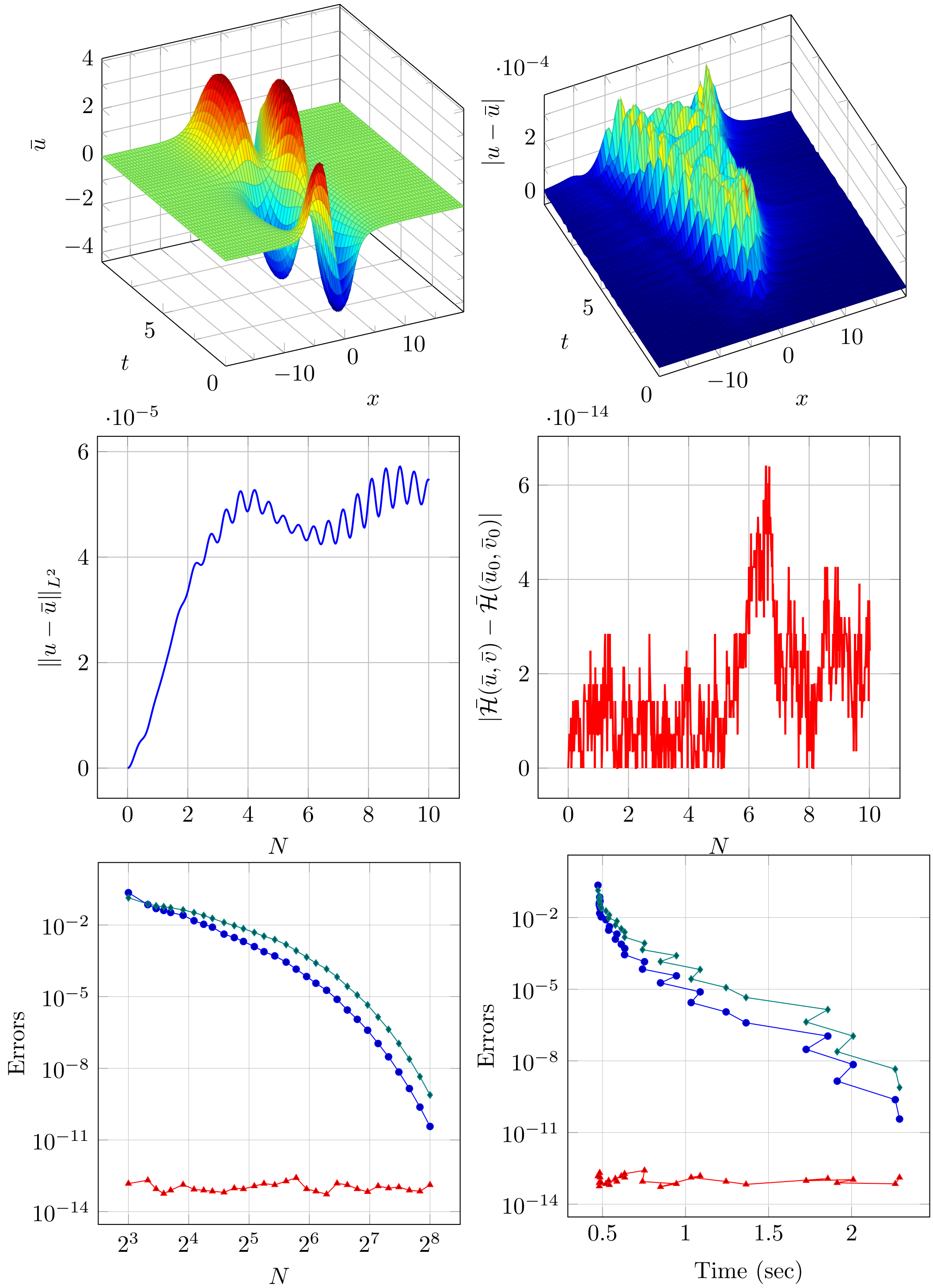

Figure 6.3: The numerical solution of (6.2.1) (left to right and top to bottom): $\bar{u}$, $|u-\bar{u}|$, $\|u-\bar{u}\|_{L^2}$, $|\mathcal{H}(\bar{u},\bar{v})-\mathcal{H}(\bar{u}_0,\bar{v}_0)|$, with $N=2^6$; $\|u-\bar{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u-\bar{u}\|_{L^\infty(\mathbb{R})}$ (teal), and $|\mathcal{H}(\bar{u},\bar{v})-\mathcal{H}(\bar{u}_0,\bar{v}_0)|$ (red), work-precision diagram.

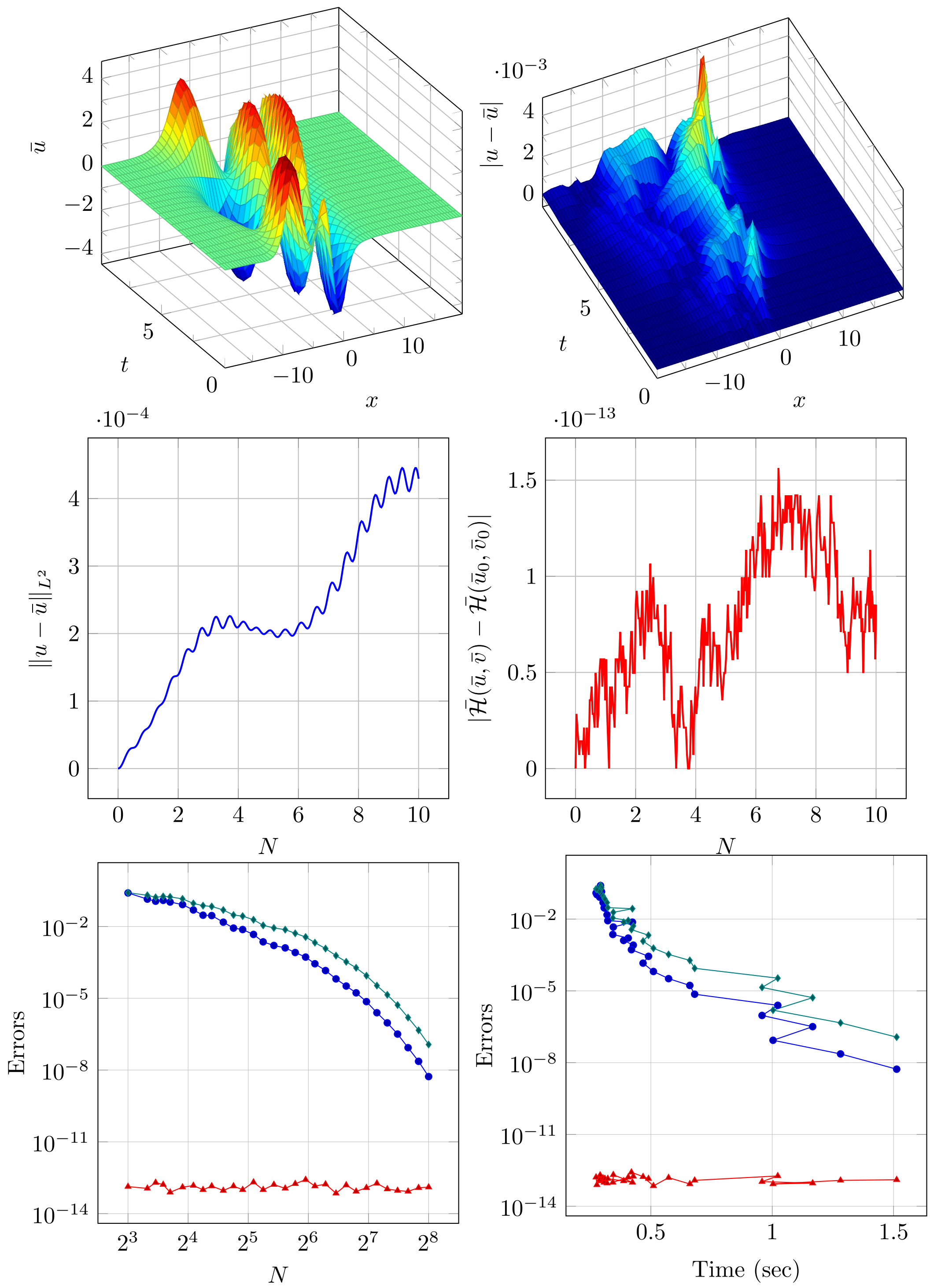

Figure 6.4: The numerical solution of (6.2.1) (left to right and top to bottom): $\bar{u}$, $|u-\bar{u}|$, $\|u-\bar{u}\|_{L^2}$, $|\mathcal{H}(\bar{u},\bar{v})-\mathcal{H}(\bar{u}_0,\bar{v}_0)|$, with $N=2^6$; $\|u-\bar{u}\|_{L^2(\mathbb{R})}$ (blue), $\|u-\bar{u}\|_{L^\infty(\mathbb{R})}$ (teal), and $|\mathcal{H}(\bar{u},\bar{v})-\mathcal{H}(\bar{u}_0,\bar{v}_0)|$ (red), work-precision diagram.

Chapter 7

Conclusion

In this dissertation, we provided theoretical and numerical analysis of the KGE model with smooth potentials $\mathcal{V}(u)$ in the periodic settings and in the real line. In Chapter 4, we did demonstrate that in the presence of smooth potentials the KGE model is globally well-posed in the periodic settings. In particular, we did show that the regularity of weak solutions is completely controlled by the input data and, hence, the solutions are classical, provided the initial data is sufficiently regular. Furthermore, using the propagation properties of the nonlinear KGE group, we managed to extend the well-posedness result from the periodic settings to the whole of real line.

In Chapter 5, we proposed a Fourier-type pseudo-spectral spatial semi-discrete scheme and provided its comprehensive stability and convergence analyses. The concrete implementation details are discussed in Chapter 6. In particular, we described an efficient way for computing the semi-discrete vector field and proposed an efficient, explicit, symmetric and symplectic high order time-stepping scheme. We concluded our work by running several concrete simulations. Numerical results, presented in Section 6.2 completely confirm theoretical investigations of Chapters 4 and 5 and demonstrate excellent accuracy and computational efficiency of our scheme.

Contribution to knowledge. Numerical solution of differential equations posed in unbounded domains is an important topic of modern research. Two approaches are commonly used, the first one treats the problem under consideration directly in the whole spatial domain, the second is based on the domain-truncation coupled with use of artificial boundary conditions. In the project, we did demonstrate that in context of KGE-type models (i.e. models whose flow groups preserve compactness of initial data) the second approach is nearly optimal. Part of the results obtained in this work shall be submitted for possible publication in a reputable journal.

Future research. Theoretical results and method used in this work can be extended to a range of nonlinear wave equation. Also, our scheme can be extended to problems posed in $\mathbb{R}^n$.

Bibliography

[AA14] S. Ahmad and A. Ambrosetti, *A textbook on ordinary differential equations*, Springer, 2014.

[ABI$^+$15] S. Aseeri, O. Batrasev, M. Icardi, B. Leu, A. Liu, N. Li, B.K. Muite, E. Müller, B. Palen, M. Quell, H. Servat, P. Sheth, R. Speck, M. Van-Moer, and J. Vienne, *Solving the Klein-Gordon equation using Fourier spectral methods: A benchmark test for computer performance*, CoRR, abs/1501.04552, (2015) 182–191.

[Ada70] R.A Adams, *Equivalent norms for Sobolev spaces*, American Mathematical Society **24 (1)** (1970), 63-66.

[AF03] R.A. Adams and J.J.F Fournier, *Sobolev spaces*, 2nd ed., Elsevier, New York, 2003.

[Ber61] S. Berberian, *Introduction to Hilbert space*, New York: Oxford University Press, 1961.

[BOJM10] G. Berikelashvili, S. Kharibegashvili O. Jokhadze, and B. Midodashvili, *Finite difference solution of a nonlinear Klein-Gordon equation with an external source*, Mathematics of Computation **80(274)** (2010), 847–862.

[Boy00] J.P. Boyd, *Chebyshev and Fourier spectral methods*, Dover Publications, Inc., New York, 2000.

[Bre11] H. Brezis, *Functional analysis, Sobolev spaces and partial differential equations*, Springer, New-York, Dordrecht, Heidelberg, London, 2011.

[BW81] P. Brenner and W. Wahl, *Global classical solutions of nonlinear wave equations*, International Journal of Computer Mathematics **176(1)** (1981), 87–121.

[BZ15] W. Bao and X. Zhao, *A uniformly accurate multiscale time integrator spectral method for the Klein-Gordon-Zakarov system in the high-plasma-frequency limit regime*, Journal of Computational Physics **327** (2015), 270–293.

[CLC17] H. Chen, S. Lu, and W. Chen, *A fully discrete spectral method for the nonlinear time fractional Klein-Gordon equation*, Taiwanese Journal of Mathematics **21(1)** (2017), 231–251.

[CQHZ06] C. Canuto, A. Quarteroni, M.Y. Hussani, and T.A. Zang, *Spectral methods: Fundamental in single domains*, Springer-verlag. Berlin, Heidelberg, 2006.

[DEGM82] R.K. Dodd, I.C. Eibeck, J.D. Gibbon, and H.C. Morris, *Solitons and nonlinear wave equations*, Academic London, 1982.

[DS09] M. Dehghan and A. Shokri, *Numerical solution of Klein-Gordon equations using radial basis functions*, Journal of Computational and Applied Mathematics **230** (2009), 400–410.

[DT12] M. Dehghan and A. Taleei, *Numerical solution of the yukawa-coupled Klein-Gordon-Schrödinger equations via a Chebyshev pseudospectral multidomain method.*, Applied Mathematical Modelling **36(6)** (2012), 2340–2349.

[Dun97] D. B. Duncan, *Sympletic finite difference approximations of the nonlinear Klein-Gordon equation*, SIAM Journal on Numerical Analysis **34(5)** (1997), 1742–1760.

[DXZ14] X. Dong, Z. Xu, and X. Zhao, *On time-splitting pseudospectral discretization for nonlinear Klein-Gordon equation in nonrelativistic limit regime*, Communications in Computational Physics **16(2)** (2014), 440–466.

[EMM13] F. H. Easif, S. A. Manaa, and D. Mekaeel, *The finite difference method for ϕ^4 - nonlinear Klein-Gordon equation*, IOSR Journal of Engineering (IOSRJEN) **3(11)** (2013), 01–05.

[EMVQDGM15] A.H. Encinasa, J. Martín-Vaqueroa, A. Queiruga-Diosa, and V. Gayoso-Martínezb, *Efficient high-order finite difference methods for nonlinear Klein-Gordon equations*, Nonlinear Analysis: Modelling and Control **20(2)** (2015), 274–290.

[Erw78] K. Erwin, *Introductory functional analysis with applications*, New York: Wiley, 1978.

[ES16] E. G. Ekomasov and R. K. Salimov, *Pseudo-spectral fourier method as applied to finding localized spherical soliton solutions of* $(3+1)$*-dimensional Klein-Gordon equations*, Journal of Computational Mathematics and Mathematical Physics **56(9)** (2016), 1604–1610.

[Eva90] L.C Evans, *Weak convergence methods for nonlinear partial differential equations*, 74th ed., CBMS Regional Conference Series in Mathematics, AMS, Providence, RI., 1990.

[FT78] I. Fukuda and M. Tsutsumi, *On coupled Klein-Gordon-Schrodinger equations, II*, Journal of mathematical Analysis and Applications **66(2)** (1978), 358–378.

[GI92] A.M. Grundland and E. Infeld, *A family of nonlinear Klein-Gordon equations and their solutions*, Journal of Mathematical Physics **33 (7)** (1992).

[GO77] D. Gottlieb and S.A. Orzag, *Numerical analysis of spectral methods: Theory and applications*, SIAM, 1977.

[Gra14] L. Grafakos, *Classical Fourier analysis*, 3rd ed., Springer, 2014.

[GV85] J. Ginibre and G. Velo, *The global Cauchy problem for the nonlinear Klein- Gordon equation.*, Math. Z. **189** (1985), 487–505.

[GW14] B. Guo and Z.Q Wang, *A collocation method for generalized nonlinear Klein-Gordon equation*, Advances in Computational Mathematics **40(2)** (2014), 377–398.

[HGG07] J. Hesthaven, S. Gottlieb, and D. Gottlieb, *Spectral method for time-dependent problems*, Cambridge University Press, Cambridge, UK, 2007.

[HLW06] E. Hairer, C. Lubich, and G. Wanner, *Geometric numerical integration*, Springer, 2006.

[HW87] N. Hayashi and W. Wahl, *On the global strong solutions of coupled Klein-Gordon-Schrödinger equations*, J. Math. Soc. Jpn., **39** (1987), 489–497.

[HZ09] H. Han and Z. Zhang, *An analysis of the finite-difference method for one-dimensional Klein-Gordon equation on unbounded domain*, Applied Numerical Mathematics **59(7)** (2009), 1568–1583.

[IA16] Javid Iqbal and Rustam Abass, *Numerical solution of Klein/ Sine-Gordon equations by spectral method coupled with Chebyshev wavelets*, Applied Mathematics **7(17)** (2016), 2097–2109.

[IMM06] S. Ibrahim, M. Majdoub, and M. Masmoudi, *Global solutions for a semilinear, two dimensional Klein-Gordon equation with exponential-type nonlinearity.*, Commun. Pure Appl. Math. **59** (2006), 1639–1658.

[Kop09] D.A. Kopriva, *Implementing spectral methods for partial differential equations: Algorithms for scientists and engineers*, Springer, 2009.

[KWY18] S. Klainerman, Q. Wang, and S. Yang, *Global solution for massive Maxwell-Klein-Gordon equations.*

[Lax02] P.D. Lax, *Functional analysis*, New York: Wiley, 2002.

[LD10] M. Lakestani and M. Dehghan, *Collocation and finite difference-collocation methods for the solution of nonlinear Klein-Gordon equation*, Computer Physics Communications **181(8)** (2010), 1392–1401.

[LGV96] X. Li, B. Y. Guo, and L. Vazquez, *A Legendre spectral method for solving the nonlinear Klein-Gordon equation*, Mathematics Applied and Computation **15** (1996), 19–36.

[LIW18] C. Liu, A. Iserles, and X. Wu, *Symmetric and arbitrarily high-order Birkhoff-Hermite time integrators and their long-time behaviour for solving nonlinear Klein-Gordon equations*, Journal of Computational Physics **356** (2018), 1–30.

[LYA+18] Y. Luo, Y. Yang, M. S. Ahmed, T. Yu, M. Zhang, L. Wang, and H. Xu, *Global existence and blow up of the solution for nonlinear Klein-Gordon equation with general power type nonlinearities at three initial energy levels*, Applied Numerical Mathematics **https://doi.org/10.1016/j.apnum.2018.05.018** (2018).

[Ma17] Y. Ma, *Global solutions of quasilinear wave Klein-Gordon system in two-space dimension: Technical tools*, Journal of Hyperbolic Differential Equations **14(4)** (2017), 591–625.

[MAS11] A. Mohebbia, Z. Asgarib, and A. Shahrezaee, *Fast and high accuracy numerical methods for the solution of nonlinear Klein-Gordon equations*, Verlag der Zeitschrift für Naturforschung Tubingen - Mainz **66a** (2011), 735–744.

[MM07] F.J. Murray and K.S. Miller, *Existence theorems for ordinary differential equations*, Dover Publications, 2007.

[NMPZ84] S. Novikov, S.V. Manakov, L.P. Pitaevskii, and V.E. Zakharov, *Theory of solitons, the inverse scaterring method*, Springer Science and Business Media, 1984.

[NO01] M. Nakamura and T. Ozawa, *The cauchy problem for nonlinear Klein-Gordon equations in the Sobolev spaces*, Publ. RMS, Kyoto Univ. **37** (2001).

[PT14] N. Polat and H. Taskesen, *On the existence of global solutions for a nonlinear Klein-Gordon equation*, Faculty of Sciences and Mathematics, University of Nis, Serbia **28(5)** (2014), 1073–1079.

[RF10] H. L. Royden and P. M. Fitzpatrick, *Real analysis*, 4th ed., Pearson Education Asia Limited and China Machine Press., 2010.

[Rom80] S. Roman, *The formula of Faa di Bruno*, Amer. Math. Monthly **87** (1980), 805–809.

[Son04] Z. Songmu, *Nonlinear evolution equations*, Boca Raton, Fla: Chapman and Hall/CRC Press, 2004.

[SS03] E.M. Stein and R. Shakarchi, *Fourier analysis, an introduction*, Princeton University Press, 2003.

[STW11] J. Shen, T. Tang, and L. Wang, *Spectral method: Algorithms, analysis and applications*, Springer-verlag. Berlin, Heidelberg, 2011.

[SW71] E.M. Stein and G. Weiss, *Introduction to Fourier analysis on euclidean spaces*, Princeton University Press, 1971.

[Tes12] G. Teschl, *Ordinary differential equations and dynamical systems*, American Mathematical Society, 2012.

[WC05] Q. F. Wang and D. Cheng, *Numerical solution of damped nonlinear Klein-Gordon equations using variational method and finite element approach*, Journal of Applied Mathematics and Computation **162** (2005), 381–401.

[Wed78] R.A. Weder, *Scattering theory for the Klein-Gordon equation*, J. Functional Analysis **27** (1978), 100–117.

[WX12] B. Weizhu and D. Xuanchun, *Analysis and comparison of numerical methods for the Klein-Gordon equation in the nonrelativistic limit regime*, Numerische Mathematik **120(2)** (2012), 189–229.

[XD13] R. Xu and Y. Ding, *Global solutions and finite time blow up for damped Klein-Gordon equation*, Acta Mathematica Scientia **33(3)** (2013), 634–652.

[XZ13] S. Xia and J. Zhang, *Global well-posedness and scattering for a nonlinear Klein-Gordon equation in low dimensions*, American Institute of Phyics **92** (2013).

[YTSZ15] F. Yin, T. Tian, J. Song, and M. Zhu, *Spectral methods using Legendre wavelets for nonlinear Klein/Sine-Gordon equations*, Journal of Computational and Applied Mathematics **275** (2015), 321–334.