Geometric numerical integration of nonlinear Schrödinger and nonlinear wave equations

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Contents

Preface

The present cumulative habilitation thesis (Habilitationsschrift) is about geometric numerical integration of Hamiltonian partial differential equations such as nonlinear Schrödinger equations and nonlinear wave equations. Besides a short introduction and summary of results, its main content are the following articles which have been written in the past years in collaboration with E. Faou (Rennes), E. Hairer (Genève), Ch. Lubich (Tübingen) and D. Weiss (Karlsruhe):

L. Gauckler (2016), Numerical long-time energy conservation for the nonlinear Schrödinger equation, *IMA J. Numer. Anal.* (2016), doi:10.1093/imanum/drw057 (online first).
(Appendix A)

E. Faou, L. Gauckler, C. Lubich (2013), Sobolev stability of plane wave solutions to the cubic nonlinear Schrödinger equation on a torus, *Comm. Partial Differential Equations* **38**, 1123–1140.
(Appendix B)

E. Faou, L. Gauckler, C. Lubich (2014), Plane wave stability of the split-step Fourier method for the nonlinear Schrödinger equation, *Forum Math. Sigma* **2**, e5, 45 pp.
(Appendix C)

L. Gauckler, E. Hairer, C. Lubich, D. Weiss (2012), Metastable energy strata in weakly nonlinear wave equations, *Comm. Partial Differential Equations* **37**, 1391–1413.
(Appendix D)

L. Gauckler, D. Weiss (2016), Metastable energy strata in numerical discretizations of weakly nonlinear wave equations, preprint, arXiv:1606.00647v2.
(Appendix E)

L. Gauckler (2015), Error analysis of trigonometric integrators for semilinear wave equations, *SIAM J. Numer. Anal.* **53**, 1082–1106.
(Appendix F)

L. Gauckler (2016), On a splitting method for the Zakharov system, preprint, arXiv:1607.07556v1.
(Appendix G)

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Berlin, January 2017 Ludwig Gauckler

Chapter 1

Introduction

Geometric numerical integration is concerned with the structure-preserving discretization of differential equations. The structure to be preserved by a numerical discretization is often of geometric nature, and hence the name.

An exemplary and important situation, which is considered in this thesis, is the discretization of *Hamiltonian differential equations*. These equations are characterized by the geometric property that their flow is a symplectic map. A typical geometric numerical integrator for a Hamiltonian differential equation aims for preserving this characteristic property in the sense that the numerical flow is again a symplectic map. Such methods are called *symplectic methods*. Many of them are in use today and have become standard methods for Hamiltonian differential equations.

But what is the benefit of a structure-preserving discretization? As a general rule of thumb, there is hope that a structure-preserving discretization is able to reproduce qualitative properties of the exact solution that are related to the structure that is preserved by the discretization.

To make this vague statement more precise, let us consider again the case of Hamiltonian differential equations and their discretization by symplectic methods. Solutions to such equations have remarkable qualitative properties on long time intervals. For example, they have conserved quantities such as the energy, and they behave stable under certain perturbations on long time intervals, which is the topic of the classical field of Hamiltonian perturbation theory. As symplectic methods preserve the characteristic structure of Hamiltonian differential equations, there is thus hope that they can reproduce such qualitative properties of solutions on *long time intervals*. And, in fact, symplectic methods do behave very well on long time intervals, which are much longer than those covered by a standard numerical analysis. Historically, this good long-time behaviour was actually the reason why they became so popular, long before this began to be analyzed mathematically.

In the case of (non-oscillatory) Hamiltonian *ordinary* differential equations, a good and mathematically rigorous understanding of the long-time behaviour of symplectic methods has been achieved meanwhile. This is well-documented in the monographs by Sanz-Serna & Calvo (1994), Leimkuhler & Reich (2004), Hairer, Lubich & Wanner (2006), Feng & Qin (2010) and Blanes & Casas (2016). For example, one of the remarkable properties of symplectic methods applied to non-oscillatory Hamiltonian ordinary differential equations is the near-conservation of the energy on long time intervals, which has been rigorously proven by Benettin & Giorgilli (1994).

The situation is different in the case of Hamiltonian *partial* differential equations. For these equations, the mathematical understanding of the long-time behaviour of symplectic methods lags

significantly behind the developments for Hamiltonian ordinary differential equations. One reason is of course the diversity of effects that can appear in different Hamiltonian partial differential equations. But even if one restricts to certain model classes of Hamiltonian partial differential equations and specific symplectic methods, there are significant difficulties that bedevil a sound mathematical understanding of the long-time behaviour in such special situations. One difficulty comes from the *oscillations* that are introduced in the dynamics by unbounded operators in the partial differential equation such as the Laplacian or more complicated differential operators. After a discretization in space, the largest frequency in the system will typically scale polynomially in the inverse of the spatial mesh width. The oscillations thus get higher and higher when the spatial discretization is refined. The presence of such high oscillations, however, is known (see, e.g., Hairer, Lubich & Wanner (2006) and Hairer (2009)) to be an obstacle to (directly) use those techniques (such as a backward error analysis) that have been developed over the years to analyze symplectic methods applied to (non-oscillatory) Hamiltonian ordinary differential equations, and that produced spectacular results on their long-time behaviour. A second difficulty comes from the fact that a Hamiltonian partial differential equation is an *infinite-dimensional* Hamiltonian system. After a discretization in space, the system is finite, but its size gets larger and larger when the spatial discretization is refined. The wish to have estimates that are uniform in the spatial mesh width thus requires to analyze the system independently of its size, using an appropriate functional analytic framework that accounts for the underlying infinite-dimensional problem.

In recent years, there is ongoing effort to shed some light on the long-time behaviour of symplectic methods applied to Hamiltonian *partial* differential equations. Rigorous results have been obtained using new techniques like modulated Fourier expansions or Birkhoff normal forms of numerical methods and careful adaptions of more classical tools like backward error analysis.

In the present thesis, some recent results in this context are collected. The focus is on nonlinear Schrödinger equations (Chapter 2) and nonlinear wave equations (Chapter 3). These equations are rather universal physical models to describe the propagation of nonlinear waves, see, e.g., Whitham (1974). The considered geometric numerical integrators for them are splitting integrators and trigonometric integrators, which are standard numerical methods for these equations.

To study whether symplectic methods can reproduce qualitative properties of the exact solution on long time intervals, a thorough understanding of the long-time behaviour of the exact solution itself is required. Therefore, also some results on the mathematical analysis of nonlinear Schrödinger and nonlinear wave equations are included in this thesis, always with the aim of understanding the corresponding long-time properties also after a numerical discretization.

Finally, some results on finite-time error bounds for the considered numerical methods are included as well.

Chapter 2

Geometric numerical integration of nonlinear Schrödinger equations

In this chapter, some results on the geometric numerical integration of nonlinear Schrödinger equations are described.

Nonlinear Schrödinger equations appear as a reduced model in a variety of physical applications, ranging from nonlinear optics to Bose–Einstein condensation. We refer to the monograph by Agrawal (2013) for their use in nonlinear optics and to Section 1.16 of Tao (2010) and the monographs by Kevrekidis, Frantzeskakis & Carretero-González (2008, 2015) for their use in Bose–Einstein condensation and a heuristic derivation. Triggered by the universality of the equations as a physical model and, at the same time, by their rich mathematical structure, there are also a lot of mathematical activities around these equations, see, e.g., the monographs by Sulem & Sulem (1999), Bourgain (1999), Zhidkov (2001), Cazenave (2003), Tao (2006), Carles (2008), Grébert & Kappeler (2014), Koch, Tataru & Vişan (2014), Linares & Ponce (2015) and Kevrekidis, Frantzeskakis & Carretero-González (2015). Of particular importance for us is the fact that nonlinear Schrödinger equations are classical examples of Hamiltonian partial differential equations. A standard numerical method for nonlinear Schrödinger equations is the split-step Fourier method. It is a symplectic method for these Hamiltonian differential equations, and hence a geometric numerical integrator.

This chapter on the geometric numerical integration of nonlinear Schrödinger equations is organized as follows. In Section 2.1, the considered cubic nonlinear Schrödinger equation is introduced. The split-step Fourier method is described in Section 2.2. The remaining sections are then concerned with the long-time behaviour of this symplectic method and also of the exact solution. In these Sections 2.3, 2.4 and 2.5, the results of the articles Gauckler (2016a), Faou, Gauckler & Lubich (2013) and Faou, Gauckler & Lubich (2014) are described, which are included in this thesis as Appendices A, B and C, respectively.

Throughout this chapter, the Euclidean norm on $\mathbb{R}^d$ (and also $\mathbb{C}^d$) is denoted by $|\cdot|$, and the corresponding scalar product on $\mathbb{R}^d$ is denoted by a dot ($x \cdot y = x^T y$ for $x, y \in \mathbb{R}^d$)

2.1 The nonlinear Schrödinger equation

The cubic nonlinear Schrödinger equation (NLS) is the time-dependent partial differential equation

$$\mathrm{i}\partial_t \psi = -\Delta\psi + \lambda|\psi|^2\psi, \qquad \psi = \psi(x,t), \tag{2.1}$$

where $t \geq 0$ denotes time and $x = (x_1, \dots, x_d) \in \mathbb{R}^d$ denotes space. The right-hand side of the equation consists of a linear part given by the Laplacian

$$-\Delta = -\partial_{x_1}^2 - \cdots - \partial_{x_d}^2$$

and a nonlinear part given by the cubic nonlinearity $\lambda|\psi|^2\psi$ with a given real-valued prefactor $\lambda \neq 0$. The sign of the factor λ in front of the nonlinearity makes the nonlinearity focusing if it is negative, and defocusing if it is positive. We assume in the following that this factor is normalized to

$$\lambda = \pm 1,$$

which can be achieved by rescaling $\psi \mapsto \sqrt{|\lambda|}\psi$.

Boundary conditions. Typical solutions to (2.1) decay in space to zero as $|x|$ goes to infinity. For a numerical discretization, the infinite spatial domain $\mathbb{R}^d$ of equation (2.1) is therefore usually truncated to a large but finite box, on which periodic boundary conditions are imposed. In the following, we therefore consider (2.1) on such a box. For simplicity, we assume that its side length is normalized to 2π, that is, we impose 2π-periodic boundary conditions in space. The spatial variable x thus belongs to the d-dimensional torus

$$\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d).$$

Hamiltonian structure. The nonlinear Schrödinger equation (2.1) is a Hamiltonian partial differential equation with Hamiltonian function (total energy) given by

$$H(\psi) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \Big(|\nabla\psi|^2 + \tfrac{1}{2}\lambda|\psi|^4 \Big) \,\mathrm{d}x. \tag{2.2}$$

We consider this Hamiltonian function for functions $\psi = \psi(x)$ in a Sobolev space $H^s(\mathbb{T}^d, \mathbb{C})$ of complex-valued functions on the torus $\mathbb{T}^d$, and we require $s \geq 1$ and $s > \frac{d}{2}$. In this situation, the Hamiltonian function is well-defined by the continuous Sobolev embedding of $H^s(\mathbb{T}^d, \mathbb{C})$ into $L^\infty(\mathbb{T}^d, \mathbb{C})$. In addition, the considered Sobolev space then forms an algebra.

To see that the function H is in fact a Hamiltonian function for the nonlinear Schrödinger equation (2.1), we write

$$\psi = \frac{q + \mathrm{i}p}{\sqrt{2}}$$

with real-valued q and p. In these new variables $(q, p) \in H^s(\mathbb{T}^d, \mathbb{R}) \times H^s(\mathbb{T}^d, \mathbb{R})$, the Hamiltonian function becomes

$$H(q, p) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \Big(\tfrac{1}{2}|\nabla q|^2 + \tfrac{1}{2}|\nabla p|^2 + \tfrac{1}{8}\lambda\big(q^2 + p^2\big)^2 \Big) \,\mathrm{d}x,$$

and the nonlinear Schrödinger equation reads[1]

$$\begin{aligned} \partial_t q &= -\Delta p + \tfrac{1}{2}\lambda\big(q^2 + p^2\big)p = \nabla_p H(q, p), \\ \partial_t p &= \Delta q - \tfrac{1}{2}\lambda\big(q^2 + p^2\big)q = -\nabla_q H(p, q). \end{aligned}$$

[1] We denote by $\nabla_q H(q, p) \in H^{-s}(\mathbb{T}^d, \mathbb{R})$ the gradient with respect to q in (q, p) of the Hamiltonian function $H\colon H^s(\mathbb{T}^d, \mathbb{R}) \times H^s(\mathbb{T}^d, \mathbb{R}) \to \mathbb{R}$, which is defined via the Fréchet derivative $d_q H(q, p)\colon H^s(\mathbb{T}^d, \mathbb{R}) \to \mathbb{R}$ of H with respect to q in (q, p) by the relation

$$d_q H(q, p)u = \big\langle \nabla_q H(q, p), u \big\rangle_{L^2} \qquad \text{for all} \qquad u \in H^s(\mathbb{T}^d, \mathbb{R}),$$

where $\langle \cdot, \cdot \rangle_{L^2}$ is the scalar product on $L^2(\mathbb{T}^d, \mathbb{R})$. Similarly, we denote by $\nabla_p H(q, p)$ the gradient of H with respect to p.

This is the classical form of a Hamiltonian differential equation, but on the *infinite-dimensional* state space $H^s(\mathbb{T}^d,\mathbb{R}) \times H^s(\mathbb{T}^d,\mathbb{R})$. In this sense, the nonlinear Schrödinger equation (2.1) is an infinite-dimensional Hamiltonian system or a Hamiltonian partial differential equation.

Resonances. Resonances form a problem that is omnipresent in the long-time analysis of Hamiltonian partial differential equations such as the nonlinear Schrödinger equation (2.1). More precisely, the problem are resonances among the eigenvalues (frequencies) of the linear part of the equation. Integer linear combinations of these frequencies are introduced into the dynamics by the nonlinearity in the equation, and resonances occur when these integer linear combinations equal a frequency. For the considered nonlinear Schrödinger equation (2.1), the linear part is $-\Delta$ on $\mathbb{T}^d$ with eigenvalues (frequencies) $|j|^2$, $j \in \mathbb{Z}^d$. They are resonant because some of their integer linear combinations vanish.

2.2 The split-step Fourier method

We describe the split-step Fourier method of Hardin & Tappert (1973) to discretize the nonlinear Schrödinger equation (2.1) in time and space. This method has become one of the standard numerical methods for this equation. It is a symplectic method, and hence a geometric numerical integrator for this Hamiltonian partial differential equation.

Discretization in space. We first discretize (2.1) in space by Fourier collocation. This Fourier pseudospectral method is based on the ansatz space

$$\mathcal{V}^K = \left\{ \sum_{j\in\mathcal{K}} \widehat{v}_j \mathrm{e}^{\mathrm{i}(j\cdot x)} : \widehat{v}_j \in \mathbb{C} \right\}, \qquad \mathcal{K} = \big\{-K,\dots,K-1\big\}^d,$$

of trigonometric polynomials of degree K. Recall that such a trigonometric polynomial is uniquely determined by its values in the discrete points

$$x_k = \frac{k\pi}{K}, \qquad k \in \mathcal{K}. \tag{2.3}$$

The idea is to replace, at each time t, the infinite spatial Fourier series of the solution $\psi(x,t)$ of (2.1) by a trigonometric polynomial $\psi^K(x,t)$ from the ansatz space $\mathcal{V}^K$:

$$\psi(x,t) \approx \psi^K(x,t) = \sum_{j\in\mathcal{K}} \widehat{\psi}_j^K(t) \mathrm{e}^{\mathrm{i}(j\cdot x)}.$$

Inserting this ansatz ψ^K into the nonlinear Schrödinger equation (2.1) obviously does not give a closed equation for ψ^K because the cubic nonlinearity leads to a trigonometric polynomial of higher degree than K. Instead of projecting the nonlinearity in an L^2-orthogonal way back to the ansatz space $\mathcal{V}^K$ (Galerkin method), we proceed here differently and use a *collocation* based on the discrete points x_k of (2.3), which turns out to be computationally efficient thanks to the fast Fourier transform. More precisely, we (only) require that the ansatz ψ^K satisfies (2.1) in the discrete points x_k of (2.3). This yields the spatially discrete and finite system of equations

$$\mathrm{i}\partial_t \psi^K(x_k,t) = \big(-\Delta\psi^K\big)(x_k,t) + \lambda\big|\psi^K(x_k,t)\big|^2\psi^K(x_k,t), \qquad k \in \mathcal{K}.$$

This spatially discrete system is the semi-discretization in space that we consider henceforth. It uniquely determines the trigonometric polynomial ψ^K because a trigonometric polynomial from the space $\mathcal{V}^K$ is uniquely determined by its values in the discrete points x_k of (2.3). Denoting by

$\mathcal{I}^K$ the corresponding trigonometric interpolation of degree K, that is, the operator that assigns a (sufficiently regular) 2π-periodic function the uniquely determined trigonometric polynomial from $\mathcal{V}^K$ that takes the same values in the discrete points x_k of (2.3), we can rewrite the spatially discrete system as an equation for the time-dependent trigonometric polynomial $\psi^K = \psi^K(x,t)$:

$$\mathrm{i}\partial_t \psi^K = -\Delta\psi^K + \lambda\,\mathcal{I}^K\big(|\psi^K|^2\psi^K\big). \tag{2.4}$$

Initial values at time $t_0 = 0$ are computed by

$$\psi^K(\cdot,0) = \mathcal{I}^K\big(\psi(\cdot,0)\big).$$

The spatial semi-discretization in this form is now discretized in time.

Discretization in time. The discretization in time is based on a splitting integrator. For a general introduction to these integrators, we refer to McLachlan & Quispel (2002) and Chapters II and III of Hairer, Lubich & Wanner (2006). In our concrete situation, we split the spatial semi-discretization (2.4) into its linear and its nonlinear part,

$$\mathrm{i}\partial_t \psi^K = -\Delta\psi^K \qquad \text{and} \qquad \mathrm{i}\partial_t \psi^K = \lambda\,\mathcal{I}^K\big(|\psi^K|^2\psi^K\big). \tag{2.5}$$

The main observation is that these split equations are easy to solve: The linear equation of (2.5) is easy to solve in Fourier space, where the jth Fourier coefficient $\widehat{\psi}_j^K(t)$ of the solution $\psi^K(x,t) = \sum_{j\in\mathcal{K}} \widehat{\psi}_j^K(t)\mathrm{e}^{\mathrm{i}(j\cdot x)}$ is given by

$$\widehat{\psi}_j^K(t) = \mathrm{e}^{-\mathrm{i}|j|^2 t}\widehat{\psi}_j^K(0), \qquad j \in \mathcal{K}. \tag{2.6}$$

The nonlinear equation of (2.5) is easy to solve pointwise in physical space, where we have in the discrete points x_k of (2.3)

$$\psi^K(x_k,t) = \mathrm{e}^{-\mathrm{i}\lambda|\psi^K(x_k,0)|^2 t}\psi^K(x_k,0), \qquad k \in \mathcal{K}, \tag{2.7}$$

from which the solution can be computed by trigonometric interpolation. In contrast to the flow of the nonlinear Schrödinger equation (2.1), the flows ϕ^t_{linear} and $\phi^t_{\text{nonlinear}}$ of the linear and the nonlinear equation in (2.5) are thus easy to compute. The idea of a splitting integrator is to use these easily computable flows to approximate the solution to the original equation at discrete times.

More precisely, denoting by τ a time step-size, the considered splitting integrator computes time-discrete approximations

$$\psi_n^K \approx \psi^K(\cdot,t_n), \qquad t_n = n\tau, \qquad n = 0,1,2,\ldots,$$

by the following composition of the flows of the split equations:

$$\psi_{n+1}^K = \phi^\tau_{\text{linear}} \circ \phi^\tau_{\text{nonlinear}}\big(\psi_n^K\big), \qquad \psi_0^K = \mathcal{I}^K\big(\psi(\cdot,0)\big). \tag{2.8}$$

Recall that the flows $\phi^\tau_{\text{linear}}$ and $\phi^\tau_{\text{nonlinear}}$ appearing in the method (2.8) can be computed from (2.6) and (2.7), respectively.

The method (2.8) is a (formally) first-order splitting integrator known as *Lie–Trotter splitting*. Its symmetric and (formally) second-order variant, the *Strang splitting*, reads

$$\psi_{n+1}^K = \phi^{\tau/2}_{\text{linear}} \circ \phi^\tau_{\text{nonlinear}} \circ \phi^{\tau/2}_{\text{linear}}\big(\psi_n^K\big), \qquad \psi_0^K = \mathcal{I}^K\big(\psi(\cdot,0)\big).$$

All results that are described in the following for the Lie–Trotter splitting (2.8) extend to this method. The methods are known as split-step Fourier methods.

Computational cost. One time step of the method (2.8) consists of computing the flows $\phi^\tau_{\text{linear}}$ and $\phi^\tau_{\text{nonlinear}}$ of the linear and the nonlinear equation in (2.5). As we have seen above, the flow $\phi^\tau_{\text{linear}}$ can be computed via (2.6) in Fourier space with a computational cost of order K^d, and the flow $\phi^\tau_{\text{nonlinear}}$ can be computed via (2.7) in the discrete points (2.3) with the same computational cost. The main computational cost comes from the need to switch between Fourier coefficients and function values in discrete points and vice versa. For such a discrete Fourier transform, the fast Fourier transform provides an efficient tool with computational cost of order $K^d \log K^d$.

Discretization error. An error analysis on finite time intervals of the split-step Fourier method has been given by Lubich (2008), Thalhammer (2012), Eilinghoff, Schnaubelt & Schratz (2016) and, in the case of small initial values, Chartier, Méhats, Thalhammer & Zhang (2016). See also Gauckler (2011), Shen & Wang (2013) and Hofstätter, Koch & Thalhammer (2014), where the Strang splitting in time is analyzed when combined with spectral collocation methods on the full space $\mathbb{R}^d$, and Koch & Lubich (2011) and Koch, Neuhauser & Thalhammer (2013), where splitting integrators for other nonlinear Schrödinger equations are analyzed.

Symplecticity. As we have seen in Section 2.1, the nonlinear Schrödinger equation (2.1) is a Hamiltonian partial differential equation with Hamiltonian function H given by (2.2). The spatial semi-discretization (2.4) inherits this Hamiltonian structure. In fact, with the same argument as in Section 2.1, the spatial semi-discretization (2.4) can be seen to be a Hamiltonian differential equation with Hamiltonian function

$$H^K(\psi^K) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \Big(\big|\nabla \psi^K\big|^2 + \tfrac{1}{2}\lambda \mathcal{I}^K\big(\big|\psi^K\big|^4\big) \Big)\, \mathrm{d}x$$

on the space $\mathcal{V}^K$ of trigonometric polynomials of degree K.

Similarly, the two split equations of (2.5) can be seen to be Hamiltonian differential equations corresponding to the Hamiltonian functions containing only the quadratic part

$$H^K_{\text{quadratic}}(\psi^K) = \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \big|\nabla \psi^K\big|^2\, \mathrm{d}x$$

and only the quartic part

$$H^K_{\text{quartic}}(\psi^K) = \frac{\lambda}{2(2\pi)^d} \int_{\mathbb{T}^d} \mathcal{I}^K\big(\big|\psi^K\big|^4\big)\, \mathrm{d}x$$

of H^K. The split-step Fourier method (2.8) is thus a composition of flows of Hamiltonian differential equations. As the flows of Hamiltonian differential equations are symplectic maps, and as the composition of symplectic maps is again a symplectic map, the split-step Fourier method is a symplectic numerical method.

Outline. In the remainder of this chapter, we are interested in the long-time behaviour of the split-step Fourier method (2.8). Does the symplecticity of the method yield a good long-time behaviour, in a similar way as it is known for symplectic methods applied to Hamiltonian ordinary differential equations, in spite of the high oscillations introduced by the Laplacian with eigenvalues (frequencies) $|j|^2$, $j \in \mathcal{K}$, and the size of the system?

In Section 2.3, the ability of the method to reproduce the conservation of energy on long time intervals is studied. Sections 2.4 and 2.5 are concerned with the stability of special solutions to the nonlinear Schrödinger equation, first for the exact solution (Section 2.4) and then for the numerical solution by the split-step Fourier method (Section 2.5).

2.3 Long-time energy conservation for the split-step Fourier method

One of the most fundamental long-time properties of Hamiltonian differential equations such as the nonlinear Schrödinger equation (2.1) is the exact conservation of the energy H (the Hamiltonian function, see (2.2)) along solutions $\psi = \psi(x,t)$ to (2.1):

$$H\big(\psi(\cdot,t)\big) = H\big(\psi(\cdot,0)\big) \qquad \text{for all times } t \geq 0.$$

The ability of the split-step Fourier method of Section 2.2 to nearly conserve the energy on long time intervals is investigated in the article Gauckler (2016a), which is included in this thesis as Appendix A.

The main result of Gauckler (2016a) (see also Gauckler (2016c)) is the following theorem which states long-time near-conservation of the energy under the following assumptions.

- The spatial dimension d is 1.
- The initial value is small in the Sobolev space $H^1 = H^1(\mathbb{T},\mathbb{C})$,

$$\big\|\psi_0^K\big\|_{H^1} \leq \varepsilon \ll 1. \tag{2.9}$$

- The time step-size τ (and the spatial discretization parameter K) satisfy, for some $0 \leq \mu \leq \frac{1}{2}$ and $0 < \nu \leq 1$ and with ε as in (2.9), the *non-resonance condition*

$$\frac{|1 - \mathrm{e}^{\mathrm{i}(k-j^2)\tau}|}{\tau} \geq c\varepsilon^{2\mu} \max\left(\frac{|k|+1}{|j|^2+1}, 1\right)^{\nu} \tag{2.10}$$

  for all $j \in \mathcal{K}$ and all integers $k \neq j^2$ with $|k| \leq NK^2$. This excludes *resonant or near-resonant time step-sizes* τ for which certain integer multiples are identical to or close to integer multiples of 2π. The behaviour of the method for resonant time step-sizes is illustrated in Section 3 of Gauckler (2016a), see Appendix A.

- The discretization parameters τ and K satisfy the condition

$$\varepsilon^2 \tau K^{6\nu} \leq c \tag{2.11}$$

  with ε as in (2.9) and ν as in (2.10).

Theorem (Theorem 3.1 and Corollary 3.2 of Gauckler (2016a), see Appendix A)**.** *Let $N \geq 3$, and assume that the initial value ψ_0^K, the time step-size τ and the spatial discretization parameter K satisfy the above assumptions. Then, for sufficiently small $\varepsilon \leq \varepsilon_0$ in (2.9), the numerical solution (2.8) nearly preserves the energy on a long time interval:*

$$\big|H\big(\psi_n^K\big) - H\big(\psi_0^K\big)\big| \leq C\varepsilon^{3-\mu} \qquad \text{for} \qquad 0 \leq t_n = nh \leq \varepsilon^{-2-(N-3)(1-\mu)}.$$

The constants C and ε_0 depend on N, c, μ and ν from the above assumptions, but they are independent of the size ε of the initial value, the time step-size τ and the spatial discretization parameter K.

We emphasize that the constants in the theorem are uniform in the discretization parameters and in the frequencies $|j|^2$, $j \in \mathcal{K}$.

Note that, in the considered situation of initial values of size ε, the energy H of (2.2) is of size ε^2, at least initially. The above theorem states that the accordingly rescaled energy $\varepsilon^{-2}H$ is still conserved up to $\mathcal{O}(\varepsilon^{1-\mu})$ on a long time interval. The length of this long time interval scales polynomially in ε^{-1}. The non-resonance condition (2.10) becomes stronger the larger the degree of this polynomial is.

Related results and techniques of proof. The near-conservation of energy on long time intervals by symplectic numerical methods applied to the nonlinear Schrödinger equation is one of the few problems in geometric numerical integration of Hamiltonian partial differential equations, where several results have already been obtained in the past years.

The first results by Gauckler & Lubich (2010b) and by Faou, Grébert & Paturel (2010a,b) date back to 2010. In these articles, long-time near-conservation of energy is proven for the split-step Fourier method applied to a *modified* nonlinear Schrödinger equation

$$\mathrm{i}\partial_t\psi = -\Delta\psi + V * \psi + \lambda|\psi|^2\psi.$$

In fact, long-time near-conservation of energy is obtained there as a corollary to a much stronger statement on long-time regularity of numerical solutions. The considered modified nonlinear Schrödinger equation has an additional convolution-type potential that removes resonances in the equation in the sense that the eigenvalues (frequencies) of the modified linear part $-\Delta + V*$ of the equation are not anymore resonant. Besides a control of resonances and also near-resonances in the equation itself, the results of Gauckler & Lubich (2010b) and Faou, Grébert & Paturel (2010a,b) require a numerical non-resonance condition on the time step-size τ, which is similar to the one used in the above theorem. In addition, they require that the initial values are not only small in H^1, but in a high-order Sobolev space H^s with $s \gg 1$. In contrast to the above theorem, however, they are not restricted to the one-dimensional case. They have been extended to a class of exponential integrators by Cohen & Gauckler (2012).

These first results have been obtained with Birkhoff normal form techniques (in Faou, Grébert & Paturel (2010a,b)) and with the technique of modulated Fourier expansions (in Gauckler & Lubich (2010b) and Cohen & Gauckler (2012)). The latter technique is also used to prove the above theorem of Gauckler (2016a), but now in a situation where the eigenvalues (frequencies) of the linear part of the equation are completely resonant, which requires a new completely resonant modulated Fourier expansion (see also Gauckler, Hairer & Lubich (2016)).

Further results on long-time near-conservation of energy by the split-step Fourier method for the nonlinear Schrödinger equation have been obtained by Faou & Grébert (2011) and by Faou (2012). They develop for that purpose a careful adaption of the backward error analysis familiar from the finite-dimensional case of Hamiltonian ordinary differential equations. In their results, near-conservation of energy on a time interval of length $\tau^{-(N-1)/2}$ is obtained for small initial values in H^1 under a CFL-type restriction on the discretization parameters of the form $(N+1)\tau K^2 < 4\pi$. Instead of assuming small initial values, these results also hold under the assumption that the numerical solution stays sufficiently regular, which is not clear a priori. Such a regularity assumption on the numerical solution is also needed in Wulff & Oliver (2016) to obtain long-time near-conservation of energy for symplectic Runge–Kutta methods from the backward error analysis described there.

In contrast to these previous results on long-time near-conservation of energy by the split-step Fourier method (or other methods), the above theorem of Gauckler (2016a) neither assumes an additional convolution-type potential in the equation, nor assumes very regular initial values, nor assumes any regularity of the numerical solution, nor assumes a CFL-type restriction of

the form $(N+1)\tau K^2 = \mathcal{O}(1)$ on the discretization parameters. Instead, the usual nonlinear Schrödinger equation (2.1) is considered with completely resonant frequencies stemming from $-\Delta$ on $\mathbb{T}$, with small initial values in H^1 as in Faou & Grébert (2011) and Faou (2012), with a very weak restriction (2.11) on the discretization parameters and with a non-resonance condition on the time step-size that is automatically fulfilled under the CFL-type step-size restriction of Faou & Grébert (2011) and Faou (2012), see Section 4 of Gauckler (2016a). It will be interesting to see whether the remaining restrictions on the spatial dimension and on the size of the initial value can be removed in future work.

2.4 Stability of plane wave solutions

In this section, the article Faou, Gauckler & Lubich (2013) is described, which is included in this thesis as Appendix B. In this article, a long-time property of the exact solution of the nonlinear Schrödinger equation (2.1) is proven. The correct reproduction of this property by the split-step Fourier method of Section 2.2 is then investigated in the following section.

Plane wave solutions. The nonlinear Schrödinger equation (2.1) has special solutions in the form of plane waves: for $\rho \in \mathbb{C}$ and $m \in \mathbb{Z}^d$, the plane wave

$$\psi(x,t) = \rho \mathrm{e}^{\mathrm{i}(m\cdot x)} \mathrm{e}^{-\mathrm{i}\omega t}$$

is a solution to (2.1) for

$$\omega = |m|^2 + \lambda|\rho|^2.$$

Recall that $|\cdot|$ denotes the Euclidean norm and $\cdot$ the Euclidean scalar product.

The long-time stability of these plane wave solutions under small perturbations of the initial value is the topic of the article Faou, Gauckler & Lubich (2013). The question as to whether special solutions such as plane wave solutions are stable under perturbations is a standard question from a mathematical point of view. But the very question about the stability of plane wave solutions in the nonlinear Schrödinger equation also arises in applications from nonlinear optics, see Section 5.1 of Agrawal (2013).

Linear stability. A first step in a stability analysis of plane wave solutions is the study of the linearization of the nonlinear Schrödinger equation (2.1) around a plane wave solution. With the ansatz

$$\psi(x,t) = \big(1+\eta(x,t)\big)\rho \mathrm{e}^{\mathrm{i}(m\cdot x)} \mathrm{e}^{-\mathrm{i}\omega t}, \qquad |\eta| \ll 1, \tag{2.12}$$

we get from the nonlinear Schrödinger equation (2.1) and the definition of ω the equation

$$\mathrm{i}\partial_t \eta = -\Delta\eta - 2\mathrm{i}(\nabla\eta \cdot m) + \lambda|\rho|^2\big(|1+\eta|^2 - 1\big)(1+\eta)$$

for the perturbation η. We then linearize this equation. Writing the perturbation η as a spatial Fourier series $\eta(x,t) = \sum_{j\in\mathbb{Z}^d} \widehat{\eta}_j(t)\mathrm{e}^{\mathrm{i}(j\cdot x)}$, this yields the system

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\widehat{\eta}_j = \big(|j|^2 + 2(j\cdot m) + \lambda|\rho|^2\big)\widehat{\eta}_j + \lambda|\rho|^2\overline{\widehat{\eta}_{-j}}, \qquad j \in \mathbb{Z}^d,$$

for the Fourier coefficients $\widehat{\eta}_j(t)$. Taking the equation for $\widehat{\eta}_j$ together with the complex conjugate of the equation for $\widehat{\eta}_{-j}$ finally yields the closed systems

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix}\widehat{\eta}_j \\ \overline{\widehat{\eta}_{-j}}\end{pmatrix} = \begin{pmatrix}|j|^2 + 2(j\cdot m) + \lambda|\rho|^2 & \lambda|\rho|^2 \\ -\lambda|\rho|^2 & -|j|^2 + 2(j\cdot m) - \lambda|\rho|^2\end{pmatrix}\begin{pmatrix}\widehat{\eta}_j \\ \overline{\widehat{\eta}_{-j}}\end{pmatrix}, \qquad j \in \mathbb{Z}^d.$$

To study the stability of this linearization, we compute the eigenvalues of the matrices in these linear 2×2-systems. They are given by

$$2(j \cdot m) \pm |j| \sqrt{|j|^2 + 2\lambda|\rho|^2}, \qquad j \in \mathbb{Z}^d. \tag{2.13}$$

The linearization of the nonlinear Schrödinger equation around a plane wave is stable if and only if all these eigenvalues are real, which is equivalent to the condition

$$1 + 2\lambda|\rho|^2 \geq 0. \tag{2.14}$$

This linear stability analysis and the resulting criterion (2.14) for linear stability have been known for a long time, see Bespalov & Talanov (1966) and Benjamin & Feir (1967). The possible instability is known as Benjamin–Feir instability or modulational instability.

Long-time orbital stability. The presented classical linear stability analysis can, by its very nature, only give information on short time intervals. Stability on longer time intervals is the topic of the article Faou, Gauckler & Lubich (2013) of Appendix B.

On longer time intervals, solutions to perturbed initial values cannot be expected to stay close to the unperturbed plane wave solution itself. What is proven in Faou, Gauckler & Lubich (2013), however, is that solutions to perturbed initial values stay, on long time intervals, close to the *orbit*

$$\left\{ \rho \mathrm{e}^{\mathrm{i}(m\cdot x)} \mathrm{e}^{\mathrm{i}\varphi} : \varphi \in \mathbb{R} \right\}$$

of the unperturbed plane wave solution $\rho \mathrm{e}^{\mathrm{i}(m\cdot x)} \mathrm{e}^{-\mathrm{i}\omega t}$. This orbital stability of plane wave solutions is true on long time intervals that scale polynomially in the inverse of the size of the perturbation.

More precisely, the main result of Faou, Gauckler & Lubich (2013) is the following theorem. Here we assume, without loss of generality, that $1 + \eta(\cdot, 0)$ in (2.12) is of unit L^2-norm, and hence $\|\psi(\cdot,0)\|_{L^2} = |\rho|$. In addition, we denote here and in the following by $\|\cdot\|_{H^s}$ the Sobolev norm on the Sobolev space $H^s = H^s(\mathbb{T}^d, \mathbb{C})$ and by $\widehat{\psi}_j(t)$ the jth Fourier coefficient of the solution

$$\psi(x,t) = \sum_{j \in \mathbb{Z}^d} \widehat{\psi}_j(t) \mathrm{e}^{\mathrm{i}(j\cdot x)}$$

to the nonlinear Schrödinger equation (2.1).

Theorem (Theorem 1.1 and equation (1.3) of Faou, Gauckler & Lubich (2013), see Appendix B)**.** *Let $\rho_0 > 0$ be such that $1 + 2\lambda\rho_0^2 > 0$, and let $N > 1$ be fixed arbitrarily. There exist $s_0 > 0$, $C \geq 1$ and a set $\mathcal{P}$ of full measure in the interval $(0, \rho_0]$ such that for every $s \geq s_0$ and every $|\rho| \in \mathcal{P}$, there exists $\varepsilon_0 > 0$ such that for every $m \in \mathbb{Z}^d$ the following holds: if the initial data $\psi(\cdot, 0)$ are such that*

$$\|\psi(\cdot,0)\|_{L^2} = |\rho| \qquad \text{and} \qquad \left\| \mathrm{e}^{-\mathrm{i}(m\cdot\bullet)} \psi(\cdot,0) - \widehat{\psi}_m(0) \right\|_{H^s} = \varepsilon \leq \varepsilon_0,$$

then the solution of (2.1) with these initial data satisfies

$$\left\| \mathrm{e}^{-\mathrm{i}(m\cdot\bullet)} \psi(\cdot,t) - \widehat{\psi}_m(t) \right\|_{H^s} \leq C\varepsilon \qquad \text{for} \qquad 0 \leq t \leq \varepsilon^{-N}$$

and

$$\inf_{\varphi \in \mathbb{R}} \left\| \mathrm{e}^{-\mathrm{i}(m\cdot\bullet)} \psi(\cdot,t) - \rho \mathrm{e}^{\mathrm{i}\varphi} \right\|_{H^s} \leq C\varepsilon \qquad \text{for} \qquad 0 \leq t \leq \varepsilon^{-N}.$$

Related results and techniques of proof. There are several other articles where stability of plane wave solutions to the nonlinear Schrödinger equation is investigated. Besides the classical

results on linear stability mentioned above, it is known that the above orbital stability holds for all times in the Sobolev space H^1, see Zhidkov (2001) and Gallay & Hărăguş (2007a,b), where also other periodic waves are considered. For perturbations in lower order spaces H^s, $s < 1$, some kind of instability of plane waves under certain perturbations has been established by Hani (2011, 2014).

In contrast to these previous results, the result from Faou, Gauckler & Lubich (2013) described above deals with perturbations in high-order Sobolev spaces H^s with large s and studies the behaviour of the corresponding high-order Sobolev norms along solutions. The behaviour of high-order Sobolev norms along solutions has recently attracted a lot of interest. This interest comes from the fact that a growth of higher Sobolev norms is related to a transfer of energy to smaller and smaller scales along solutions (weak turbulence). In particular, Bourgain asked in Bourgain (2000) whether higher Sobolev norms grow along solutions and tend to infinity as time goes to infinity. Recently, there are several articles that study this problem and establish a certain growth for certain initial values, see Colliander, Keel, Staffilani, Takaoka & Tao (2010), Guardia (2014), Guardia & Kaloshin (2015), Haus & Procesi (2015). In this direction, the theorem of Faou, Gauckler & Lubich (2013) described above shows that there is essentially no growth of higher Sobolev norms on long time intervals for initial values close to plane waves. It has been extended recently by Wilson (2015) to nonlinear Schrödinger equations with polynomial nonlinearities of the form $\lambda|\psi|^{2p}\psi$ with integers $p \geq 2$.

From a technical point of view, the article Faou, Gauckler & Lubich (2013) is related to a series of results on nonlinear perturbations of linear Hamiltonian partial differential equations with non-resonant frequencies, see Bambusi (2003), Bambusi & Grébert (2006), Grébert (2007), Cohen, Hairer & Lubich (2008b), Gauckler & Lubich (2010a) and Gauckler (2010). At first glance, this is a different situation, because the linear part $-\Delta$ of the nonlinear Schrödinger equation (2.1) has completely resonant eigenvalues (frequencies) $|j|^2$, $j \in \mathbb{Z}$, and, near plane waves, the nonlinearity cannot be considered as a small perturbation. A crucial step in the proof of the above theorem is then to show that it is possible to write the nonlinear Schrödinger equation (2.1) near plane waves as a Hamiltonian perturbation of a linear Hamiltonian system with frequencies that are non-resonant (in a certain sense). After this transformation, the tools and results of Bambusi (2003), Bambusi & Grébert (2006) and Grébert (2007) obtained with the technique of Birkhoff normal forms or, alternatively, the tools and results of Cohen, Hairer & Lubich (2008b), Gauckler & Lubich (2010a) and Gauckler (2010) obtained with the technique of modulated Fourier expansions can be applied to obtain the statement of the above theorem.

On the assumptions of the theorem. Recall that the linearization around a plane wave solution is stable if and only if $1 + 2\lambda|\rho|^2 \geq 0$, see (2.14). The condition $1 + 2\lambda\rho_0^2 > 0$ in the above theorem is thus essentially the requirement that this linearization is stable.

To go beyond this linear stability analysis and to cover longer intervals, further assumptions are needed in the above theorem. It is assumed there that the order s of the considered Sobolev space is large and that some values of $|\rho| = \|\psi(\cdot, 0)\|_{L^2}$ are excluded. These conditions are related to the control of certain resonances that might become relevant on longer time intervals. More precisely, these conditions allow us to control and to exclude to some extent resonances among the eigenvalues (frequencies) (2.13) that show up in the linearization around a pane wave. For a precise formulation of the required non-resonance condition, we refer to Lemma 2.2 of Faou, Gauckler & Lubich (2013), see Appendix B. The above theorem can thus be summarized as

$$\text{linear stability \& control of resonances} \implies \text{long-time orbital stability.}$$

2.5 Stability of plane wave solutions in the split-step Fourier method

In the article Faou, Gauckler & Lubich (2014), which is included in this thesis as Appendix C, the question is studied whether the split-step Fourier method of Section 2.2 is able to reproduce the stable behaviour of the exact solution near plane waves as described in the previous Section 2.4.

The question is in particular, whether the stability on *long* time intervals can be reproduced by this symplectic method in a qualitatively correct way. Stability on short times by means of a linear stability analysis following the procedure outlined in Section 2.4 (but now on a discrete level for the numerical method) has been investigated for the split-step Fourier method and also other methods already by Weideman & Herbst (1986) and more recently by Dahlby & Owren (2009), Khanamiryan, Nevanlinna & Vesanen (2012), Lakoba (2013) and Cano & González-Pachón (2016).

The main result of Faou, Gauckler & Lubich (2014) states that the split-step Fourier method is in fact able to reproduce the orbital stability of plane wave solutions even on long time intervals. Instead of reproducing here this main result in all details, we refer to Section 2.2 of the original article Faou, Gauckler & Lubich (2014) included in Appendix C and only state it vaguely as

$$\text{linear stability \& control of resonances} \implies \text{long-time orbital stability.}$$

This is, in fact, the same kind of result as for the exact solution, see the discussion of Section 2.4. However, "linear stability" now means that the linearization of the numerical method (and not the equation itself) has to be stable. Accordingly, the "control of resonances" requires a control of resonances among the frequencies that show up in the linearization of the numerical method (and not of the equation itself). A sufficient, though not necessary, condition under which these assumptions are fulfilled is stated in Theorem 3 of Faou, Gauckler & Lubich (2014) in Appendix C. In addition to the assumptions needed for orbital stability of the exact solution (see Section 2.4), its main ingredient is a CFL-type step-size restriction of the form

$$(N+1)d\tau K^2 = \mathcal{O}(1),$$

if the considered long time interval is supposed to be $\max(\varepsilon^{1/2}, \tau)^N$. Here, ε is again the size of the perturbation, τ the time step-size and K the spatial discretization parameter. Under these assumptions, the split-step Fourier method (2.8) reproduces the orbital stability of plane waves in the nonlinear Schrödinger equation (2.1) even on long time intervals. A related result on orbital stability of ground states of the nonlinear Schrödinger equation on $\mathbb{R}$ after a numerical discretization has been proven by Bambusi, Faou & Grébert (2013) on the basis of the backward error analysis of Faou & Grébert (2011) and Faou (2012).

Chapter 3

Geometric numerical integration of nonlinear wave equations

In this chapter, some results on the geometric numerical integration of nonlinear wave equations are described.

Wave equations are fundamental equations for the description of the propagation of waves. The propagation of nonlinear waves, for which, in particular, the superposition principle does not hold, is described by nonlinear equations. There are many different equations for such nonlinear wave phenomena, see, e.g., the monograph by Whitham (1974). The nonlinear Schrödinger equation of the previous chapter is actually one of them. In this chapter, we focus on a particular nonlinear wave equation that is a direct nonlinear extension of the linear wave equation $\partial_t^2 u = \partial_x^2 u$ or the linear Klein–Gordon equation $\partial_t^2 u = \partial_x^2 u - \rho u$ with $\rho > 0$. For some physical background on the considered equation, we refer to Section 14.1 of Whitham (1974). As the nonlinear Schrödinger equation of the previous chapter, the considered nonlinear wave equation is a Hamiltonian partial differential equation. Typical symplectic methods for the equation are trigonometric integrators.

This chapter is organized as follows. In Section 3.1, the considered nonlinear wave equation is introduced. In Section 3.2, trigonometric integrators for the discretization in time are described as well as their combination with a Fourier collocation method in space. The remaining sections are then concerned with the long-time behaviour of the exact solution and the long-time behaviour of these methods, and also with finite-time error bounds. In these Sections 3.3, 3.4, 3.5 and 3.6, the results of the articles Gauckler, Hairer, Lubich & Weiss (2012), Gauckler & Weiss (2016), Gauckler (2015) and Gauckler (2016b) are described, which are included in this thesis as Appendices D, E, F and G, respectively.

3.1 The nonlinear wave equation

We consider the one-dimensional nonlinear wave equation (NLW) with quadratic nonlinearity, which is the time-dependent partial differential equation

$$\partial_t^2 u = \partial_x^2 u - \rho u + u^2, \qquad u = u(x,t) \in \mathbb{R}, \tag{3.1}$$

where $t \geq 0$ denotes time and $x \in \mathbb{R}$ denotes space. We consider this equation with a positive parameter ρ. The equation is then also known as nonlinear Klein–Gordon equation. Throughout

this chapter, we write

$$v = \partial_t u$$

and consider the equation in first-order form

$$\begin{aligned} \partial_t u &= v, \\ \partial_t v &= \partial_x^2 u - \rho u + u^2. \end{aligned} \tag{3.2}$$

As the nonlinear Schrödinger equation of Chapter 2, this equation is an example of a Hamiltonian partial differential equation. On the one hand, sharing this property and others such as its semilinearity with the nonlinear Schrödinger equation of Chapter 2, makes both equations and the expected behaviour of solutions similar. On the other hand, there are considerable differences that often require a separate treatment. This latter case is the situation in many of the monographs on nonlinear Schrödinger equations mentioned in Chapter 2, where also nonlinear wave equations are considered with all their similarities and differences. We follow this style here in this separate chapter on the nonlinear wave equation (3.1).

Boundary conditions. As the nonlinear Schrödinger equation of Chapter 2, we consider the nonlinear wave equation (3.2) with 2π-periodic boundary conditions in space, that is, on the one-dimensional torus $\mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z})$.

Hamiltonian structure. The nonlinear wave equation (3.2) is a Hamiltonian partial differential equation with Hamiltonian function (total energy)

$$H(u,v) = \frac{1}{2\pi} \int_{\mathbb{T}} \Big(\tfrac{1}{2}|v|^2 + \tfrac{1}{2}|\partial_x u|^2 + \tfrac{1}{2}\rho|u|^2 - \tfrac{1}{3}u^3 \Big) \, \mathrm{d}x, \tag{3.3}$$

defined for functions u and v in the Sobolev space $H^1 = H^1(\mathbb{T}, \mathbb{R})$ of real-valued functions on the torus $\mathbb{T}$. In fact, with this Hamiltonian function and with the definition of the gradient of H from Section 2.1, we have

$$\begin{aligned} \partial_t u &= \nabla_v H(u,v), \\ \partial_t v &= -\nabla_u H(u,v) \end{aligned}$$

for the nonlinear wave equation in first-order form (3.2). As in the case of the nonlinear Schrödinger equation of Section 2.1, this is a Hamiltonian differential equation on an infinite-dimensional state space.

For later purposes, we consider the Hamiltonian function H also in Fourier space. We denote by $\widehat{u}_j$ and $\widehat{v}_j$, $j \in \mathbb{Z}$, the Fourier coefficients of $u(x) = \sum_{j\in\mathbb{Z}} \widehat{u}_j \mathrm{e}^{\mathrm{i}jx}$ and $v(x) = \sum_{j\in\mathbb{Z}} \widehat{v}_j \mathrm{e}^{\mathrm{i}jx}$. The Hamiltonian function H can then be written as

$$H(u,v) = \frac{1}{2} \sum_{j\in\mathbb{Z}} \Big(|\widehat{v}_j|^2 + \omega_j^2 |\widehat{u}_j|^2 \Big) - \frac{1}{6\pi} \int_{\mathbb{T}} u^3 \, \mathrm{d}x,$$

where

$$\omega_j = \sqrt{j^2 + \rho}, \qquad j \in \mathbb{Z}, \tag{3.4}$$

are the frequencies of the nonlinear wave equation (3.2). The individual summands of the quadratic part of H in this form are the energies associated to individual Fourier modes. These *mode energies*

$$E_j(u,v) = \tfrac{1}{2}|\widehat{v}_j|^2 + \tfrac{1}{2}\omega_j^2 |\widehat{u}_j|^2, \qquad j \in \mathbb{Z}, \tag{3.5}$$

will be studied in more detail below. Note that $E_j = E_{-j}$ as $\widehat{u}_j = \overline{\widehat{u}_{-j}}$ and $\widehat{v}_j = \overline{\widehat{v}_{-j}}$ for real-valued u and v.

3.2 Trigonometric integrators

Trigonometric integrators are exponential integrators for second-order differential equations, which appear in classical mechanics and molecular dynamics, but also as spatial semi-discretizations of nonlinear wave equations (3.1). Various instances of these methods have been introduced and analyzed, e.g., by García-Archilla, Sanz-Serna & Skeel (1999), Hochbruck & Lubich (1999), Hairer & Lubich (2000), Grimm (2005), Hairer, Lubich & Wanner (2006), Grimm & Hochbruck (2006) and Hochbruck & Ostermann (2010).

Discretization in space. For the discretization in space of (3.1), we use a Fourier collocation method as for the nonlinear Schrödinger equation in Section 2.2. We denote again by

$$\mathcal{V}^K = \left\{ \sum_{j\in\mathcal{K}} \widehat{v}_j \mathrm{e}^{\mathrm{i}jx} : \widehat{v}_j \in \mathbb{C} \right\}, \qquad \mathcal{K} = \{-K, \dots, K-1\},$$

the ansatz space of trigonometric polynomials of degree K, and we use again a collocation based on this ansatz space and the collocation points $x_k = k\pi/K$, $k \in \mathcal{K}$, of Section 2.2. This yields the spatially discrete and finite system of equations

$$\partial_t^2 u^K(x_k,t) = \big(\partial_x^2 u^K\big)(x_k,t) - \rho u^K(x_k,t) + \big(u^K(x_k,t)\big)^2, \qquad k \in \mathcal{K},$$

for the approximation

$$u^K(x,t) = \sum_{j\in\mathcal{K}} \widehat{u}_j^K(t)\mathrm{e}^{\mathrm{i}jx} \approx u(x,t)$$

from $\mathcal{V}^K$. With the trigonometric interpolation $\mathcal{I}^K$, we can rewrite this system as an equation for the time-dependent trigonometric polynomial $u^K = u^K(x,t)$:

$$\partial_t^2 u^K = \partial_x^2 u^K - \rho u^K + \mathcal{I}^K\big((u^K)^2\big). \tag{3.6}$$

In the following, we write

$$g\big(u^K\big) = \mathcal{I}^K\big((u^K)^2\big) \qquad \text{and} \qquad -\Omega^2 = \partial_x^2 - \rho,$$

i.e., Ω denotes the operator that multiplies the jth Fourier coefficient of its argument with the frequency $\omega_j = \sqrt{j^2+\rho}$ of (3.4). The spatial semi-discretization (3.6) in first-order form then takes the form

$$\begin{aligned} \partial_t u^K &= v^K, \\ \partial_t v^K &= -\Omega^2 u^K + g\big(u^K\big). \end{aligned} \tag{3.7}$$

Discretization in time. Trigonometric integrators are exponential integrators and, as such, they are based on a discretization of the variation-of-constants formula

$$\begin{pmatrix} u^K(\cdot,t) \\ v^K(\cdot,t) \end{pmatrix} = R(t-t_0) \begin{pmatrix} u^K(\cdot,t_0) \\ v^K(\cdot,t_0) \end{pmatrix} + \int_{t_0}^t R(t-\sigma) \begin{pmatrix} 0 \\ g\big(u^K(\cdot,\sigma)\big) \end{pmatrix} \mathrm{d}\sigma$$

for the system (3.7), where

$$R(t) = \begin{pmatrix} \cos(t\Omega) & t\,\mathrm{sinc}(t\Omega) \\ -\Omega\sin(t\Omega) & \cos(t\Omega) \end{pmatrix}$$

denotes the flow of the linear problem $\partial_t u^K = v^K$, $\partial_t v^K = -\Omega^2 u^K$. Using the trapezoidal rule to discretize the integral in the variation-of-constants formula yields, with the time step-size τ, the basic trigonometric integrator

$$\begin{pmatrix} u_{n+1}^K \\ v_{n+1}^K \end{pmatrix} = R(\tau) \begin{pmatrix} u_n^K \\ v_n^K \end{pmatrix} + \frac{\tau}{2} \begin{pmatrix} \tau\,\mathrm{sinc}(\tau\Omega) g\big(u_n^K\big) \\ \cos(\tau\Omega) g\big(u_n^K\big) + g\big(u_{n+1}^K\big) \end{pmatrix}. \tag{3.8}$$

This basic trigonometric integrator computes approximations

$$u_n^K \approx u^K(\cdot, t_n) \qquad \text{and} \qquad v_n^K \approx v^K(\cdot, t_n) = \partial_t u^K(\cdot, t_n)$$

at discrete times $t_n = n\tau$, $n = 1, 2, \ldots$. Note that the method is explicit because u_{n+1}^K on the right-hand side only appears in the equation for v_{n+1}^K. The method was introduced by Deuflhard (1979) and by Grubmüller, Heller, Windemuth & Schulten (1991), Tuckerman, Berne & Martyna (1992). It is known as method of Deuflhard or impulse method. Initial values for (3.8) are computed by trigonometric interpolation,

$$u_0^K \approx \mathcal{I}^K\big(u^K(\cdot, 0)\big) \qquad \text{and} \qquad v_0^K \approx \mathcal{I}^K\big(v^K(\cdot, 0)\big).$$

Extensions of the above basic trigonometric integrator use filters in the nonlinearity to deal with certain resonant situations. The first such extension is due to García-Archilla, Sanz-Serna & Skeel (1999). The general class of trigonometric integrators considered in the literature takes the form

$$\begin{pmatrix} u_{n+1}^K \\ v_{n+1}^K \end{pmatrix} = R(\tau) \begin{pmatrix} u_n^K \\ v_n^K \end{pmatrix} + \frac{\tau}{2} \begin{pmatrix} \tau\Psi g\big(\Phi u_n^K\big) \\ \Psi_0 g\big(\Phi u_n^K\big) + \Psi_1 g\big(\Phi u_{n+1}^K\big) \end{pmatrix}, \tag{3.9}$$

where

$$\Psi = \psi(\tau\Omega), \qquad \Phi = \phi(\tau\Omega), \qquad \Psi_0 = \psi_0(\tau\Omega), \qquad \Psi_1 = \psi_1(\tau\Omega)$$

are filters computed from real-valued and even filter functions ψ, ϕ, ψ_0 and ψ_1. The filter functions ψ_0 and ψ_1 are typically chosen as

$$\psi_0 = \cos \cdot\, \psi_1 \qquad \text{and} \qquad \psi_1 = \mathrm{sinc}^{-1} \cdot\, \psi, \tag{3.10}$$

which is equivalent to the symmetry of the trigonometric integrator (3.9), see equation (2.9) in Chapter XIII of Hairer, Lubich & Wanner (2006). Popular choices for the remaining free filter functions ψ and ϕ are then

(a) $\psi = \mathrm{sinc}$ and $\phi = 1$, see Deuflhard (1979) and Grubmüller, Heller, Windemuth & Schulten (1991), Tuckerman, Berne & Martyna (1992) (this is the basic trigonometric integrator (3.8) above),

(b) $\psi = \mathrm{sinc}^2$ and $\phi = \mathrm{sinc}$, see García-Archilla, Sanz-Serna & Skeel (1999) (this method is known as mollified impulse method),

(c) $\psi = \mathrm{sinc}^2$ and $\phi = 1$, see Hairer & Lubich (2000),

(d) $\psi = \mathrm{sinc}^3$ and $\phi = \mathrm{sinc}$, see Grimm & Hochbruck (2006),

(e) $\psi = \mathrm{sinc}(\frac{1}{2}\cdot)$ and $\phi = 1$, see Gautschi (1961),

(f) $\psi = \mathrm{sinc}(\frac{1}{2}\cdot)$ and $\phi = \mathrm{sinc} \cdot \big(1 + \frac{1}{3}\sin(\frac{1}{2}\cdot)^2\big)$, see Hochbruck & Lubich (1999).

While trigonometric integrators (3.9) were originally derived for highly oscillatory second-order ordinary differential equations from classical mechanics and molecular dynamics, they are now also used extensively for nonlinear wave equations like (3.2), see, e.g., Grimm (2006), Cohen, Hairer & Lubich (2008a), Bao & Dong (2012), Cano (2013), Dong (2014) and Gauckler (2015). They have been extended to higher order by Cano & Moreta (2010, 2013) and to stochastic wave equations by Cohen, Larsson & Sigg (2013), Cohen & Quer-Sardanyons (2016) and Anton, Cohen, Larsson & Wang (2016).

Computational cost. As for the split-step Fourier method of Section 2.2, the main computational cost of a trigonometric integrator (3.9) is to switch between the Fourier coefficients (in which the multiplication with the filters and with R is computed) and the values in the collocation points (in which the nonlinearity is computed). The computational cost per time step is thus proportional to the cost of a discrete Fourier transform.

Symplecticity. In order to study the symplecticity of trigonometric integrators (3.9), we interpret them as splitting integrators applied to an averaged equation. This interpretation is at the basis of the derivation of the mollified impulse method of García-Archilla, Sanz-Serna & Skeel (1999) and has been used very recently by Buchholz, Gauckler, Grimm, Hochbruck & Jahnke (2016) to prove error bounds.

More precisely, we use filters $\Phi = \phi(\tau\Omega)$ and $\Psi_1 = \psi_1(\tau\Omega)$ and consider the averaged version

$$\begin{aligned} \partial_t u^K &= v^K, \\ \partial_t v^K &= -\Omega^2 u^K + \Psi_1 g\big(\Phi u^K\big) \end{aligned} \tag{3.11}$$

of the spatial semi-discretization (3.7). This averaged version is then split into

$$\begin{aligned} \partial_t u^K &= 0, \\ \partial_t v^K &= \Psi_1 g\big(\Phi u^K\big) \end{aligned} \qquad \text{and} \qquad \begin{aligned} \partial_t u^K &= v^K, \\ \partial_t v^K &= -\Omega^2 u^K. \end{aligned} \tag{3.12}$$

Both of these split equations are easy to solve, and the corresponding Strang splitting (solving first the first equation of (3.12) over a time interval $\frac{1}{2}\tau$, then the second one over a time interval τ and finally again the first one over a time interval $\frac{1}{2}\tau$) reads

$$\begin{aligned} v_{n,+}^K &= v_n^K + \tfrac{1}{2}\tau\Psi_1 g\big(\Phi u_n^K\big), \\ \begin{pmatrix} u_{n+1}^K \\ v_{n+1,-}^K \end{pmatrix} &= R(\tau) \begin{pmatrix} u_n^K \\ v_{n,+}^K \end{pmatrix}, \\ v_{n+1}^K &= v_{n+1,-}^K + \tfrac{1}{2}\tau\Psi_1 g\big(\Phi u_{n+1}^K\big). \end{aligned}$$

Eliminating the intermediate variables $v_{n,+}^K$ and $v_{n+1,-}^K$, this Strang splitting is seen to be equivalent to the trigonometric integrator (3.9) with filter functions satisfying the symmetry condition (3.10). In other words, symmetric trigonometric integrators are a Strang splitting applied to averaged versions of the equation. This interpretation is now used to study their symplecticity in a similar way as it has been done in Section 2.2 for the split-step Fourier method.

If the filter functions satisfy the symmetry condition (3.10) and in addition the condition

$$\psi = \operatorname{sinc} \cdot \phi, \tag{3.13}$$

then we have $\psi_1 = \phi$. The above averaged equation (3.11) is then a Hamiltonian differential equation with Hamiltonian function

$$H^K\big(u^K, v^K\big) = \frac{1}{2\pi} \int_{\mathbb{T}} \Big(\tfrac{1}{2}\big|v^K\big|^2 + \tfrac{1}{2}\big|\partial_x u^K\big|^2 + \tfrac{1}{2}\rho\big|u^K\big|^2 - \tfrac{1}{3}\mathcal{I}^K\big((\Phi u^K)^3\big) \Big)\, \mathrm{d}x$$

on the space $\mathcal{V}^K$ of trigonometric polynomials of degree K. Similarly, the split equations of (3.12) are in this case Hamiltonian differential equations with Hamiltonian functions

$$H^K_{\text{cubic}}(u^K, v^K) = -\frac{1}{6\pi}\int_{\mathbb{T}} \mathcal{I}^K\big((\Phi u^K)^3\big)\,\mathrm{d}x$$

and

$$H^K_{\text{quadratic}}(u^K, v^K) = \frac{1}{2\pi}\int_{\mathbb{T}} \Big(\tfrac{1}{2}\big|v^K\big|^2 + \tfrac{1}{2}\big|\partial_x u^K\big|^2 + \tfrac{1}{2}\rho\big|u^K\big|^2\Big)\,\mathrm{d}x.$$

Under the conditions (3.10) and (3.13), the trigonometric integrator (3.9) is thus a composition of flows of Hamiltonian differential equations, and hence a symplectic method.

Outline. In the remainder of this chapter, we are interested in the long-time behaviour of solutions to the nonlinear wave equation (3.2) and of trigonometric integrators (3.9), but also in finite-time error bounds for such methods.

In Section 3.3, a long-time property of exact solutions to the nonlinear wave equation (3.2) is described. Its correct reproduction by symplectic trigonometric integrators is then discussed in Section 3.4. The final Sections 3.5 and 3.6 are concerned with finite-time error bounds for trigonometric integrators (3.9) applied to (3.2) and for a related class of methods applied to the Zakharov system, a wave equation that is nonlinearly coupled to a Schrödinger equation.

3.3 Metastable energy strata

In this section, the article Gauckler, Hairer, Lubich & Weiss (2012) is described, which is included in this thesis as Appendix D. The topic of this article is a long-time property of the exact solution of the nonlinear wave equation (3.2).

Energy strata on a short time interval. In analogy to the plane wave solutions of the nonlinear Schrödinger equation discussed in Sections 2.4 and 2.5, we consider for the nonlinear wave equation (3.2) initial values that are located in a single Fourier mode. As we consider real-valued solutions, this means that $u(x,0) = a\mathrm{e}^{\mathrm{i}mx} + \overline{a}\mathrm{e}^{-\mathrm{i}mx}$ and $v(x,0) = b\mathrm{e}^{\mathrm{i}mx} + \overline{b}\mathrm{e}^{-\mathrm{i}mx}$ for some $m \in \mathbb{Z}$ and $a, b \in \mathbb{C}$. For simplicity, we restrict in the following to the case $m = 1$, i.e.,

$$u(x,0) = a\mathrm{e}^{\mathrm{i}x} + \overline{a}\mathrm{e}^{-\mathrm{i}x} \qquad \text{and} \qquad v(x,0) = b\mathrm{e}^{\mathrm{i}x} + \overline{b}\mathrm{e}^{-\mathrm{i}x}, \tag{3.14a}$$

but all results can be extended to general $m \in \mathbb{Z}$.

For such initial values, the solution to the *linear* wave equation $\partial_t^2 u = \partial_x^2 u - \rho u$ remains in the first Fourier mode for all times, that is, it remains a linear combination of $\mathrm{e}^{\mathrm{i}x}$ and $\mathrm{e}^{-\mathrm{i}x}$ for all times. This, however, is no longer true in the presence of a nonlinear coupling term, as for example the quadratic nonlinearity u^2 considered in (3.2). In fact, the right-hand side of the nonlinear wave equation (3.2) evaluated at the initial value is then

$$\partial_x^2 u(x,0) - \rho u(x,0) + \big(u(x,0)\big)^2 = 2|a|^2 - (1+\rho)\big(a\mathrm{e}^{\mathrm{i}x} + \overline{a}\mathrm{e}^{-\mathrm{i}x}\big) + \big(a^2\mathrm{e}^{2\mathrm{i}x} + \overline{a}^2\mathrm{e}^{-2\mathrm{i}x}\big),$$

which shows that the solution does not remain a linear combination of $\mathrm{e}^{\mathrm{i}x}$ and $\mathrm{e}^{-\mathrm{i}x}$. In a weakly nonlinear regime, in which the initial values (3.14a) are small, i.e.,

$$|a| \le \varepsilon \ll 1, \qquad |b| \le \varepsilon \ll 1, \tag{3.14b}$$

this calculation suggests at the same time that the zeroth and second Fourier modes are significantly smaller than the first one. In fact, the zeroth and the second Fourier modes of the solution are

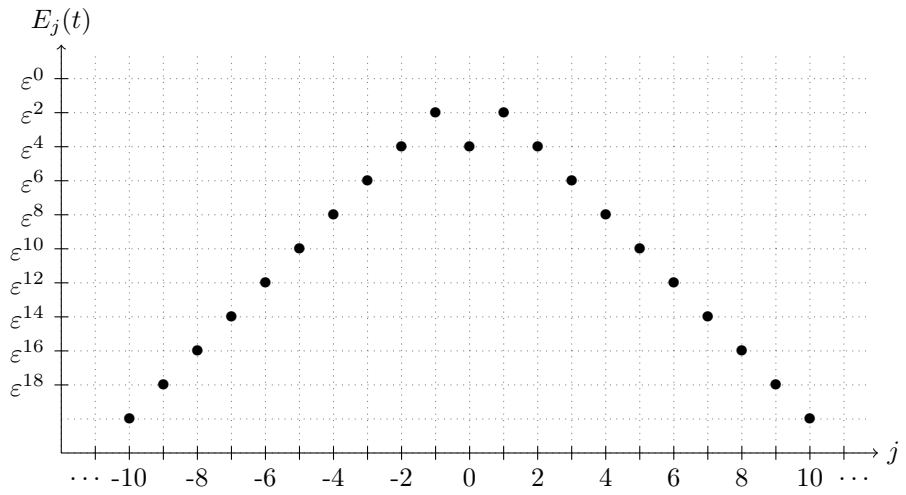

Figure 3.1: Expected upper bounds for the mode energies $E_j(t)$ on a short time interval.

expected to be of order ε^2, at least on short time intervals, whereas the first mode is of order ε. Iterating the above computation of the right-hand side of the nonlinear wave equation (3.2) further suggests that the jth Fourier mode with $|j| \geq 3$ is of order $\varepsilon^{|j|}$, again at least on short time intervals.

For initial values of the form (3.14), we thus expect that the mode energies (3.5) of the nonlinear wave equation behave like

$$E_0(t) = \mathcal{O}\big(\varepsilon^4\big), \qquad E_j(t) = E_{-j}(t) = \mathcal{O}\big(\varepsilon^{2|j|}\big), \qquad |j| \geq 1,$$

on a short time interval. A schematic description of these *energy strata* is given in Figure 3.1.

Metastable energy strata on a long time interval. The main result of Gauckler, Hairer, Lubich & Weiss (2012) states that the described energy strata are in fact stable on a *long* time interval. More precisely, it is shown for fixed but arbitrary $N \geq 2$ and $0 < \theta \leq 1$ that the mode energies decay as

$$E_j(t) = E_{-j}(t) = \mathcal{O}\big(\varepsilon^{2e(j)}\big), \qquad j \in \mathbb{Z},$$

with the energy profile

$$e(j) = \begin{cases} 2, & j = 0, \\ |j|, & 0 < |j| \leq N, \\ |j|(1-\theta) + N\theta, & |j| > N, \end{cases}$$

on a long time interval

$$0 \leq t \leq c\varepsilon^{-\theta N}.$$

This situation is depicted in Figure 3.2 for $N = 5$ and $\theta = \frac{1}{2}$. For a finite number of modes, the expected decay of the mode energies is thus observed indeed on a long time interval. This time interval is much longer than the interval on which a standard perturbation analysis is possible. For the remaining modes, we get a decay that is close to the decay that is expected on a short time interval.

More precisely, the main result of Gauckler, Hairer, Lubich & Weiss (2012) is the following theorem.

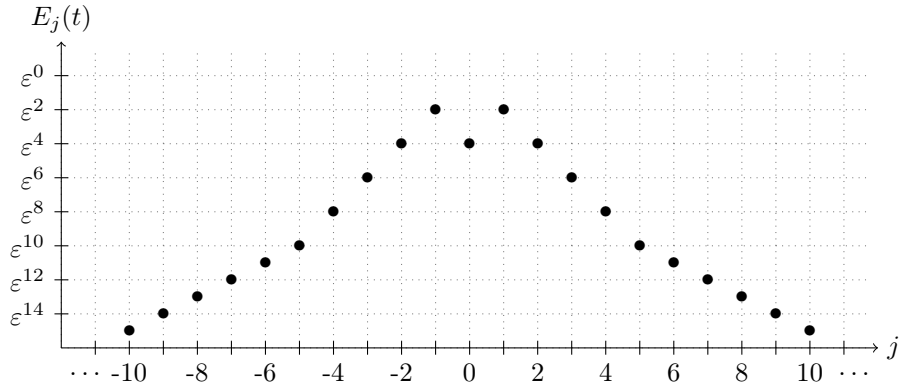

Figure 3.2: Upper bounds for the mode energies $E_j(t)$ on a long time interval (for $N = 5$ and $\theta = \frac{1}{2}$).

Theorem (Theorem 1 of Gauckler, Hairer, Lubich & Weiss (2012), see Appendix D)**.** *Fix an integer $N \geq 2$ and real numbers $s > \frac{1}{2}$ and $\rho_0 > 0$. For all except finitely many $0 < \rho < \rho_0$ the following holds: There exist $\delta_0 > 0$ and positive c and C such that for $0 < \theta \leq 1$ the mode energies of solutions to the nonlinear wave equation (3.2) for initial data (3.14) with $0 < \varepsilon^\theta \leq \delta_0$ satisfy, over long times*

$$0 \leq t \leq c\varepsilon^{-\theta N},$$

the bound

$$\sum_{j=-\infty}^{\infty} \varepsilon^{-2e(j)} \big(1 + |j|^2\big)^s E_j(t) \leq C.$$

On the assumption of the theorem. In the above theorem, some values of the parameter ρ in the nonlinear wave equation (3.2) have to be excluded. These are those values of ρ, for which the frequencies $\omega_j = \sqrt{j^2 + \rho}$ of (3.4) are in resonance or almost-resonance. More precisely, the required non-resonance condition reads

$$\left| \sum_{\ell=0}^{\infty} k_\ell \omega_\ell \right| \geq \gamma > 0 \tag{3.15}$$

for all non-zero and finite integer sequences $(k_0, k_1, k_2, \dots)$ of a special form. The types of sequences $(k_0, k_1, k_2, \dots)$ that have to be considered are determined by the interactions of Fourier modes introduced by the nonlinearity into the dynamics (see Section 3.2 of Gauckler, Hairer, Lubich & Weiss (2012) in Appendix D for more details). This non-resonance condition can be shown to be satisfied for all except finitely many values of the parameter ρ in a given interval, see Theorem 2 of Gauckler, Hairer, Lubich & Weiss (2012).

3.4 Metastable energy strata in trigonometric integrators

The topic of this section is the article Gauckler & Weiss (2016), which is included in this thesis as Appendix E. In that article, the metastability of energy strata in the nonlinear wave equation (3.2) from the previous section is studied from a numerical point of view. More precisely, the ability of some symplectic methods to reproduce these metastable energy strata on a long time interval is

studied. The considered numerical methods are the trigonometric integrators (3.9) of Section 3.2. These integrators applied to nonlinear wave equations are known to behave well with respect to conserved quantities on long time intervals, see Cohen, Hairer & Lubich (2008a), Faou, Grébert & Paturel (2010a,b), Gauckler (2010), Faou & Grébert (2011) and Cano (2013).

The main result of the article Gauckler & Weiss (2016) states that symplectic trigonometric integrators indeed reproduce the metastable energy strata of the exact solution on a long time interval in a qualitatively correct way, uniformly in the discretization parameters. This result holds under a non-resonance condition. In contrast to the non-resonance condition (3.15) for the exact solution, this non-resonance condition does not only involve the frequencies $\omega_j = \sqrt{j^2+\rho}$ of (3.4), but also the time step-size τ of the numerical method (3.9): Instead of bounding certain integer linear combinations of the frequencies away from zero, this non-resonance condition requires to bound these integer linear combinations away from integer multiples of $2\pi/\tau$ with the time step-size τ. There are thus also numerical resonances that have to be excluded. The bad behaviour of a trigonometric integrator in such a numerically resonant situation is illustrated in Section 2.4 of Gauckler & Weiss (2016), see Appendix E.

3.5 Error analysis of trigonometric integrators

In the article Gauckler (2015), which is included in this thesis as Appendix F, an error analysis of the trigonometric integrators (3.9) applied to the spatial semi-discretization (3.7) of the nonlinear wave equation (3.2) is given. The analysis relies on a regularity assumption on the exact solution of (3.7) and an assumption on the filter functions ϕ, ψ, ψ_0 and ψ_1 of the trigonometric integrator (3.9).

Regularity assumption. We fix $s \geq 0$, $M \geq 1$ and $T > 0$, and we assume that the exact solution $(u^K(\cdot,t), v^K(\cdot,t))$ of the spatial semi-discretization (3.7) of the nonlinear wave equation (3.2) satisfies

$$\left\|u^K(\cdot,t)\right\|_{H^{s+1}} + \left\|v^K(\cdot,t)\right\|_{H^s} \leq M \tag{3.16}$$

for $0 \leq t - t_0 \leq T$, uniformly in the spatial discretization parameter K. Here, we denote again by $\|\cdot\|_{H^s}$ the Sobolev norm on the Sobolev space $H^s = H^s(\mathbb{T},\mathbb{R})$.

This assumption can be shown to hold locally in time if it is satisfied at the initial value. It can also be shown to hold if it satisfied for the exact solution of the nonlinear wave equation (3.2) itself.

In the important case $s = 0$, the above regularity assumption just requires boundedness of (u^K, v^K) in $H^1 \times H^0$, which is closely related to a bounded energy (3.3). Previous error bounds for trigonometric integrators as given, e.g., by García-Archilla, Sanz-Serna & Skeel (1999), Hochbruck & Lubich (1999), Grimm (2005), Hairer, Lubich & Wanner (2006), Grimm & Hochbruck (2006), Grimm (2006) or Buchholz, Gauckler, Grimm, Hochbruck & Jahnke (2016) all require this property of the exact solution.

Assumptions on the filter functions. For the filter functions ϕ, ψ, ψ_0 and ψ_1 of the trigonometric integrator (3.9), the analysis of Gauckler (2015) requires, for all $\xi \geq 0$, the bounds

$$\begin{aligned} &|\chi(\xi)| \leq c, \qquad |1-\chi(\xi)| \leq c\,\xi^2 \qquad \text{for} \qquad \chi = \phi, \psi_0, \psi_1, \\ &|\psi(\xi)| \leq c, \qquad |\psi(\xi)| \leq c\,\xi^{-1}, \qquad |1-\psi(\xi)| \leq c\,\xi. \end{aligned} \tag{3.17}$$

These assumptions are in particular fulfilled for the impulse method/method of Deuflhard, the mollified impulse method of García-Archilla, Sanz-Serna & Skeel (1999) and the methods of Hairer

& Lubich (2000) and Grimm & Hochbruck (2006) (methods (a)–(d) of Section 3.2).

Under these assumptions on the exact solution and the filter functions, the main result of Gauckler (2015) is the following error bound for the time discretization with the trigonometric integrators (3.9).

Theorem (Theorem 2.1 of Gauckler (2015), see Appendix F)**.** *Let $s \geq 0$, $M \geq 1$ and $T > 0$, and assume that the exact solution $(u^K(\cdot,t), v^K(\cdot,t))$ of the spatial semi-discretization (3.7) of the nonlinear wave equation (3.2) satisfies (3.16) for $0 \leq t - t_0 \leq T$. Assume further that the filter functions ϕ, ψ, ψ_0 and ψ_1 of the trigonometric integrator (3.9) satisfy the bounds (3.17) for all $\xi \geq 0$ with a constant c.*

Then, there exists $\tau_0 > 0$ such that for all time step-sizes $\tau \leq \tau_0$ the following global error bound holds for the numerical solution (u_n^K, v_n^K) computed with the trigonometric integrator (3.9):

$$\left\|u^K(\cdot,t_n) - u_n^K\right\|_{H^{s+1-\alpha}} + \left\|v^K(\cdot,t_n) - v_n^K\right\|_{H^{s-\alpha}} \leq C\tau^{1+\alpha}$$

for $0 \leq t_n - t_0 = nh \leq T$ and $-1 \leq \alpha \leq 1$. The constants C and τ_0 depend only on M and s from the regularity assumption (3.16), on the final time T and on the constant c from the filter bounds (3.17).

We emphasize that the constants in the above theorem are uniform in the spatial discretization parameter K. In particular, the theorem yields

- second-order convergence in the time step-size τ in the space $H^0 \times H^{-1}$ uniformly in K,
- first-order convergence in the time step-size τ in the space $H^1 \times H^0$ uniformly in K,

if the exact solution is bounded in $H^1 \times H^0$.

Related results. Error bounds for various trigonometric integrators (3.9) are available in the literature, see García-Archilla, Sanz-Serna & Skeel (1999), Hochbruck & Lubich (1999), Grimm (2005), Section XIII.4 of Hairer, Lubich & Wanner (2006), Grimm & Hochbruck (2006), Grimm (2006) and Buchholz, Gauckler, Grimm, Hochbruck & Jahnke (2016). However, all these results cannot be applied directly to semilinear wave equations because they would require for example (with $s = 0$ in the language of our wave equation (3.2)) that the nonlinearity u^2 is bounded in L^2 for functions $u \in L^2$, which is not true.

In addition, the model problems considered in the literature and the analysis presented there require significantly stronger assumptions on the filter functions than (3.17) to obtain second-order error bounds under a finite-energy assumption on the exact solution. In particular, they require that the filter functions should vanish at integer multiples of 2π, which is, for example, not the case for the filters of the impulse method/method of Deuflhard. The analysis of Gauckler (2015) shows that such strong assumptions on the filter functions are not necessary in the case of semilinear wave equations. In particular, the impulse method/method of Deuflhard works well for semilinear wave equations, contrary to what was believed before.

3.6 A splitting integrator for the Zakharov system

The *Zakharov system*

$$\begin{aligned} \mathrm{i}\partial_t \psi &= -\Delta\psi + u\psi, \\ \partial_t^2 u &= \Delta u + \Delta|\psi|^2 \end{aligned} \tag{3.18}$$

combines the nonlinear Schrödinger equation as considered in Chapter 2 and the nonlinear wave equation as considered in this chapter. In fact, it is a Schrödinger equation for the complex-valued function

$$\psi = \psi(x,t) \in \mathbb{C}$$

that is nonlinearly coupled to a wave equation for the real-valued function

$$u = u(x,t) \in \mathbb{R}.$$

It is a model from plasma physics which has been introduced by Zakharov (1972) to describe the propagation of Langmuir waves. As in the previous sections and chapters, we consider this equation here with 2π-periodic boundary conditions on $\mathbb{R}^d$, i.e., $x \in \mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$. In addition, we write again

$$v = \partial_t u.$$

In the article Gauckler (2016b), which is included in this thesis as Appendix G, an error analysis is given for one of the standard numerical methods for this equation. The method, introduced by Jin, Markowich & Zheng (2004) and Jin & Zheng (2006), is a (structure-preserving) Lie–Trotter splitting integrator in time combined with a Fourier collocation in space similar to the split-step Fourier method of Section 2.2 and the trigonometric integrators of Section 3.2. We do not give a precise definition of the method here, but refer to the original articles by Jin, Markowich & Zheng (2004) and Jin & Zheng (2006) and to Section 2.2 of Gauckler (2016b) in Appendix G. We denote by ψ_n^K, u_n^K and v_n^K the trigonometric polynomials of degree K as computed by the method, which are supposed to approximate the exact solution $\psi(\cdot,t_n)$, $u(\cdot,t_n)$ and $v(\cdot,t_n) = \partial_t u(\cdot,t_n)$, respectively, at time $t_n = n\tau$ with the time step-size τ.

As in the case of the nonlinear wave equation of the previous section, we require regularity of the exact solution to prove error bounds. In addition, we now require a CFL-type coupling of the time step-size τ and the spatial discretization parameter K.

Regularity assumption. We fix $s > \frac{d}{2}$, $\sigma \geq 2$, $M \geq 1$ and $T > 0$, and we assume that the exact solution to the Zakharov system (3.18) satisfies

$$\|\psi(\cdot,t)\|_{H^{s+2+\sigma}} + \|u(\cdot,t)\|_{H^{s+1+\sigma}} + \|v(\cdot,t)\|_{H^{s+\sigma}} \leq M \tag{3.19}$$

for $0 \leq t - t_0 \leq T$. As before, we denote here again by $\|\cdot\|_{H^s}$ the Sobolev norm on the Sobolev spaces $H^s = H^s(\mathbb{T}^d,\mathbb{C})$ or $H^s = H^s(\mathbb{T}^d,\mathbb{R})$. This regularity assumption on the exact solution can be expected to hold locally in time by the well-posedness theory for the Zakharov system, see Kishimoto (2013) and references therein.

CFL condition. We assume that the time step-size τ and the spatial discretization parameter K are coupled as

$$d\tau K^2 \leq c < 2\pi, \tag{3.20}$$

where d is the spatial dimension.

Under these assumptions, the following error bound for the method of Jin, Markowich & Zheng (2004) and Jin & Zheng (2006) is proven in Gauckler (2016b).

Theorem (Theorem 2.3 of Gauckler (2016b), see Appendix G)**.** *Let $s > \frac{d}{2}$, $\sigma \geq 2$, $M \geq 1$ and $T > 0$, and assume that the exact solution to the Zakharov system (3.18) satisfies (3.19) for $0 \leq t - t_0 \leq T$. Assume further that the time step-size τ and the spatial discretization parameter K satisfy the CFL-type step-size restriction (3.20) with constant c.*

Then, the global error of the Lie–Trotter splitting of Jin, Markowich & Zheng (2004) and Jin & Zheng (2006) with time step-size $\tau \leq \tau_0$ and spatial discretization parameter $K \geq K_0$ is bounded by

$$\big\|\psi(\cdot,t_n) - \psi_n^K\big\|_{H^{s+2}} + \big\|u(\cdot,t_n) - u_n^K\big\|_{H^{s+1}} + \big\|v(\cdot,t_n) - v_n^K\big\|_{H^s} \leq C\big(\tau + K^{-\sigma}\big)$$

for $0 \leq t_n - t_0 = n\tau \leq T$. The constants C, K_0 and τ_0 depend on the dimension d, on M, s and σ from the regularity assumption (3.19), on the final time T and on the constant c from the CFL condition (3.20).

The numerical examples of Section 6 of Gauckler (2016b) show that CFL condition (3.20) of the theorem is necessary. We note, however, that this CFL condition is a natural restriction in view of the proven spatial and temporal error bound, which suggests to choose $\tau = \mathcal{O}(K^{-\sigma}) = \mathcal{O}(K^{-2})$.

Related results and technique of proof. In view of the available error analysis for the split-step Fourier method for the Schrödinger equation, see Lubich (2008) and Thalhammer (2012), and for trigonometric integrators for wave equations, see Gauckler (2015) and Section 3.5, the proof of this theorem might seem to be an easy combination of these results and their proofs. This, however, is not the case. The reason is the term $\Delta|\psi|^2$ in the wave equation of (3.18), which leads to a loss of spatial derivatives when applying the arguments of the mentioned articles on Schrödinger and wave equations in a direct way. By a loss of spatial derivatives we mean that a control of a certain number of spatial derivatives of the numerical solution requires a control of *more* spatial derivatives at a previous time step. Such properties, of course, make this approach to analyze the method failing.

In Gauckler (2016b), a new technique is developed to analyze the splitting method for the Zakharov system (3.18). It is based on a transformation of the numerical solution to new variables, in which a loss of spatial derivatives can be excluded and which finally leads to the error bound of the above theorem. This transformation is a fully discrete analogon of a transformation that has been introduced by Ozawa & Tsutsumi (1992) to analyze the Zakharov system itself.

The only other methods for the Zakharov system, for which rigorous error bounds have been proven so far, are, to the best of the author's knowledge, the methods derived by Herr & Schratz (2016). They are based on a discretization of the Zakharov system *after* applying the mentioned transformation of Ozawa & Tsutsumi (1992), and they don't require the CFL condition (3.20). In contrast, the transformation of Ozawa & Tsutsumi (1992) is translated in Gauckler (2016b) to the discrete level of a numerical method, and it is shown how this can be used to analyze an existing and well-established numerical method. It is expected that this approach is also useful to analyze other numerical methods for a wider class of equations where it is difficult to exclude a loss of spatial derivatives, for example for derivative nonlinear Schrödinger equations.

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Appendix A

Numerical long-time energy conservation for the nonlinear Schrödinger equation

This appendix consists of a copy of the article

> L. Gauckler (2016), Numerical long-time energy conservation for the nonlinear Schrödinger equation, *IMA J. Numer. Anal.* (2016), doi:10.1093/imanum/drw057 (online first).

In the online version, this article is not included. It is available online at

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Appendix B

Sobolev stability of plane wave solutions to the cubic nonlinear Schrödinger equation on a torus

This appendix consists of a copy of the article

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Appendix C

Plane wave stability of the split-step Fourier method for the nonlinear Schrödinger equation

This appendix consists of a copy of the article

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Appendix D

Metastable energy strata in weakly nonlinear wave equations

This appendix consists of a copy of the article

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Appendix E

Metastable energy strata in numerical discretizations of weakly nonlinear wave equations

This appendix consists of a copy of the article

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Appendix F

Error analysis of trigonometric integrators for semilinear wave equations

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Appendix G

On a splitting method for the Zakharov system

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