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Long-Time Analysis of Hamiltonian Partial Differential Equations and Their Discretizations

Dissertation

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Zusammenfassung in deutscher Sprache

I ventured to write this thesis in English
because it will be more easily read
in poor English than in good German
by many of my intended readers.

frei nach [49]

Hamiltonsche partielle Differentialgleichungen sind partielle Differentialgleichungen, die in Form eines Hamiltonsystems geschrieben werden können, wie beispielsweise die Bewegungsgleichungen der klassischen Mechanik, allerdings auf einem *unendlichdimensionalen* Phasenraum. Wichtige Beispiele sind Schrödinger- und Wellengleichungen, die sowohl wegen ihrer mathematischen Struktur als auch wegen ihrer Anwendungen in der Physik, zum Beispiel der Quantenmechanik, viel untersucht werden.

Erhaltungsgrößen oder *Invarianten* spielen in der Theorie Hamiltonscher partieller Differentialgleichungen eine wichtige Rolle. Hierbei handelt es sich um Größen, die entlang einer jeden Lösung einer solchen Gleichung erhalten werden. Sie stehen für wichtige physikalische Eigenschaften wie beispielsweise Energieerhaltung sind aber auch bei einer mathematischen Analyse der Gleichungen von entscheidender Bedeutung, um zum Beispiel Wohlgestelltheit zu beweisen. Aus Sicht der numerischen Mathematik stellt sich nun zwangsläufig die folgende Frage:

> Wie verhalten sich Erhaltungsgrößen einer Hamiltonschen partiellen Differentialgleichung entlang einer numerischen Lösung dieser Gleichung?

Hierbei handelt es sich um ein grundlegendes Problem der *geometrischen numerischen Integration*, die sich mit der Konstruktion und Analyse strukturerhaltender Algorithmen für Differentialgleichungen beschäftigt. Wie sich herausstellt, ist diese Frage eng verwandt mit einer Frage aus der *Störungstheorie*.

> Wie ändert eine kleine (nichtlineare) Störung die Dynamik einer linearen Hamiltonschen partiellen Differentialgleichung?

Die vorliegende Dissertation trägt zur Beantwortung beider Fragen bei. Es wird gezeigt, dass exakte Erhaltungsgrößen einer linearen Hamiltonschen partiellen Differentialgleichung entlang von Lösungen einer nichtlinear gestörten Variante der Gleichung zumindest annähernd erhalten werden, und zwar auf einem unerwartet *langen Zeitintervall*. Dieses Ergebnis wird mit Hilfe einer *modulierten Fourierentwicklung* der Lösung erzielt. Diese Methode erlaubt auch eine Beantwortung der ersten Frage nach dem Verhalten von Erhaltungsgrößen entlang einer geeigneten numerischen Lösung der Gleichung. Es werden weit verbreitete numerische Vefahren untersucht mit dem Ergebnis, dass Erhaltungsgrößen der exakten Lösung entlang einer numerischen Lösung wenigstens näherungsweise erhalten werden, und zwar wieder auf bemerkenswert langen Zeitintervallen.

Danke. Mein herzlicher Dank gilt Prof. Dr. Christian Lubich für die exzellente Betreuung. Durch sein enormes Wissen und seine ständige Bereitschaft zur Diskussion war er mir eine große Hilfe.

Allen Kolleginnen und Kollegen, die ich "daheim" im Arbeitsbereich *Numerische Mathematik* und auf den Dienstreisen kennenlernen durfte, und besonders meiner Familie danke ich für die Unterstützung.

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Introduction

Hamiltonian partial differential equations are partial differential equations, that can be written in the form of a Hamiltonian system as for instance the equations of motion in classical mechanics but on an *infinite* dimensional phase space. Important examples are Schrödinger equations and wave equations which attract much interest because of both, their beautiful mathematical structure but also their applications in physics, for instance in quantum mechanics.

In the theory of (finite or infinite dimensional) Hamiltonian systems *invariants* or *conserved quantities* play a dominant role. These quantities are conserved along a solution of such equations and represent important physical properties such as energy conservation, but they are also fundamental in a mathematical analysis of the equations, for instance to show well-posedness. From the point of view of numerical analysis the following question is then inevitable.

> What is the behaviour of invariants of Hamiltonian partial differential equations along a numerical solution of such equations?

This is a fundamental problem in the field of *geometric numerical integration* which is concerned with the construction and the analysis of structure-preserving algorithms for differential equations. This question turns out to be closely related to a question in *perturbation theory* concerning the exact solution of Hamiltonian partial differential equations.

> How does a small (nonlinear) perturbation change the dynamics of a linear Hamiltonian partial differential equation?

The present thesis contributes to the answers of both questions. We show that exact invariants of a linear Hamiltonian partial differential equation are approximately conserved along solutions of a nonlinearly perturbed version of the equation on remarkably *long time intervals*. This is done with the help of a *modulated Fourier expansion* of the solution. It turns out that this technique also allows to study rigorously the first question, namely to study conserved quantities of the exact solution of such Hamiltonian partial differential equations along a numerical solution. We consider widely used numerical discretizations with the result that invariants of the exact solution of weakly nonlinear Hamiltonian partial differential equations are at least approximately conserved along suitable numerical solutions, again on remarkably long time intervals.

Let us give a more detailed introduction to the above questions from perturbation theory and geometric numerical integration.

Perturbation Theory for Hamiltonian Ordinary Differential Equations. Hamiltonian perturbation theory aims for an understanding of Hamiltonian differential equations that are perturbations of simple (completely integrable) equations with explicitly known solution. The interest in this problem arose in the 18th and 19th century when many ordinary differential equations of classical mechanics were noticed to be such perturbations but resisted their global and explicit integration. In order to understand the global behaviour of the solution one began to study the influence of the perturbation, developing a rich theory of such perturbed Hamiltonian ordinary differential equations, culminating in the developments of Lindstedt–Poincaré series in the late 19th century and Kolmogorov–Arnold–Moser theory (KAM theory) in the middle of the 20th century, see [2], [5], and [36, Chapter X].

A main result states that solutions of the perturbed equation stay close to the torus on which solutions of the underlying completely integrable equation evolve. This seems not surprising at first glance since one expects the influence of a perturbation of size ε to be small on an appropriate time interval, namely on a time interval of length ε^{-1}. Remarkably, however, the result is valid on a *long* time interval of length ε^{-N} or even exponentially long in a negative power of ε [36, Chapters X.2 and X.4]. In this thesis we are interested in this kind of result. Let us mention that the famous KAM result states that some tori of the underlying completely integrable equations persist under a small perturbation for all times [36, Chapter X.5], see also the original articles [37], [44], and [1].

Perturbation Theory for Hamiltonian Partial Differential Equations. All the above results have been established for Hamiltonian *ordinary* differential equations. Their extension to Hamiltonian *partial* differential equations, which are *infinite* dimensional Hamiltonian systems, has just begun to attract interest. KAM-type results for Hamiltonian partial differential equations are due to Kuksin, see his monograph [38]. These results, however, affect only finite dimensional tori. Concerning tori of infinite dimension, long-time results have been obtained by Bourgain in [8] and [10] and by Bambusi and/or Grébert in [3], [4], and [31]. Cohen, Hairer, and Lubich [17] and Lubich together with the author of the present thesis [29] obtain similar results using a completely different technique of proof, the so called modulated Fourier expansions.

Let us comment more on the results on Hamiltonian partial differential equations taking as an example the *cubic nonlinear Schrödinger equation*

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + \varepsilon|\psi(x,t)|^2\psi(x,t) \tag{NLS}$$

with periodic boundary conditions in one dimension, $x \in \mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z})$. Here and in the following, Δ denotes the Laplacian operator acting on the spatial variable x. This equation considered with a small parameter ε is *weakly nonlinear*. It is a perturbation of the *linear Schrödinger equation* ($\varepsilon = 0$)

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t). \tag{LS}$$

Along solutions of this underlying unperturbed equation (LS), the *actions*

$$I_j(\psi) = |\psi_j|^2 \quad \text{for } j \in \mathbb{Z}$$

are exactly conserved, where ψ_j denotes the jth Fourier coefficient of $\psi(x) = \sum_{j\in\mathbb{Z}} \psi_j e^{ijx}$. In fact, the linear Schrödinger equation (LS) reads in terms of the Fourier coefficients $i\frac{d}{dt}\psi_j(t) = j^2\psi_j(t)$, i.e., $\psi_j(t) = e^{-ij^2(t-t_0)}\psi_j(t_0)$ is its solution. In other words, solutions of the linear Schrödinger equation (LS) evolve on tori

$$\mathbb{T}_\eta = \{\, \psi : I_j(\psi) = \eta_j \,\}$$

for $\eta = (\eta_j)_{j\in\mathbb{Z}}$. If only finitely many η_j are nonzero, the torus is of finite dimension as studied in the KAM-type results by Kuksin. Concerning infinite dimensional tori, results of the following type are proven in all the works mentioned above.

> The actions I_j are *nearly conserved* along solutions of the nonlinear equation (NLS) over *long times* ε^{-N}, i.e., solutions starting on an invariant torus of the linear equation (LS) stay close to this torus over long times.

In order to prove such a result the *frequencies*, the eigenvalues of the operator $-\Delta$ describing the linear part, have to satisfy a *non-resonance condition* as in the finite dimensional context (but now involving infinitely many frequencies). The frequencies of the nonlinear Schrödinger equation (NLS) are j^2, $j \in \mathbb{Z}$, which are obviously resonant, $3^2 + 4^2 = 5^2$. For this reason one has to consider modifications of the nonlinear Schrödinger equation (NLS) with non-resonant frequencies.

Geometric Numerical Integration of Hamiltonian Ordinary Differential Equations. Geometric numerical integration is concerned with a structure-preserving numerical integration of differential equations. An outstanding (and characteristic) structure of Hamiltonian differential equations is the *symplecticity* of their flow, and much effort has been put in a *symplectic numerical integration* of such equations that preserves the symplecticity, see the monographs [36], [47], and [39]. Often, a symplectic numerical integration is achieved by splitting the Hamiltonian function into two or more Hamiltonian functions whose equations of motion are easy to solve and then composed, yielding a symplectic scheme. Such schemes are called *splitting integrators* or *split-step methods*.

A major benefit of a symplectic numerical integration is that the preservation of the symplectic structure leads to an advantageous behaviour concerning other structures of the equation, namely *invariants* such as *energy*. Indeed, one can show in the case of Hamiltonian ordinary differential equations that symplectic integrators nearly conserve energy over long times, see [36, Chapter IX]. The tool to prove such a result is a *backward error analysis* where the numerical scheme is interpreted as a solution of a modified differential equation which turns out to be again Hamiltonian if the method is symplectic.

Geometric Numerical Integration of Hamiltonian Partial Differential Equations. Concerning Hamiltonian partial differential equations, backward error analysis seems not to be an appropriate tool to explain the long-time behaviour of symplectic schemes. The reason for this failure is that backward error analysis requires the product of the time step-size and the highest frequency of the system to be small, and due to the unbounded frequencies in partial differential equations this would lead to an undesirable, severe, and unrealistic step-size restriction for the results to be valid. Indeed, the frequencies for instance in the nonlinear Schrödinger equation are j^2, and a backward error analysis would require the time step-size to be significantly smaller than $1/j^2$ where j^2 is the largest frequency appearing in the spatial semi-discretization of the equation.

Clearly, the same problem occurs in the numerical integration of highly oscillatory Hamiltonian ordinary differential equations. In [33] the technique of modulated Fourier expansion was developed by Hairer and Lubich to explain the good long-time behaviour of some trigonometric methods applied to these highly oscillatory equations, see also [36, Chapter XIII]. Just recently, this was adapted in [16] by Cohen, Hairer, and Lubich and in [30] by Lubich and the author of the present thesis to the situation of infinitely many high frequencies in partial differential equations such as the nonlinear wave and the nonlinear Schrödinger equation. These were the first results explaining the favourable long-time behaviour of symplectic methods applied to Hamiltonian partial differential equations. It is shown for perturbations of linear equations such as (NLS) that the conserved quantities energy and momentum are nearly conserved along suitable symplectic numerical solutions over long times ε^{-N}. The key for such results is the proof of the long-time near-conservation of actions along the numerical solutions as observed along the exact solution.

Discretizations for a general class of Hamiltonian partial differential equations have been studied recently and independently by Faou, Grébert, and Paturel [25] and [26] adapting the technique of proof used by Bambusi and/or Grébert [3], [4], and [31] for the analysis of the exact solution. Let us finally mention the long-time results concerning discretizations of *linear* Schrödinger equations due to Dujardin and Faou [22], Castella and Dujardin [11], and Debussche and Faou [20].

The above problems and results all affect the numerical discretization in time. Concerning the (semi-)discretization in space, there are also interesting problems and solutions. A structure-preserving semi-discretization in space of a Hamiltonian partial differential equation leads to a Hamiltonian ordinary differential equation whose long-time behaviour can, in principle, be understood by applying the classical results to this ordinary differential equation. This, however, yields different constants for different resolutions of the spatial domain, i.e., for different spatial discretization parameters, which is unsatisfactory from a numerical point of view. In order to understand the influence of the spatial discretization parameter on long-time results it seems to be inevitable to take the underlying infinite dimensional structure into account. First long-time results for spatial semi-discretizations of Hamiltonian partial differential equations with constants independent of the spatial discretization parameter have been obtained by Hairer and Lubich in [34] for nonlinear wave equations and in [29] for nonlinear Schrödinger equations.

Modulated Fourier Expansions. The proofs of the main results in this thesis rely on a modulated Fourier expansion of the solution of a Hamiltonian partial differential equation or of its discretization. Modulated Fourier expansions are particularly appealing because they allow to transfer the results for the exact solution and in particular their proofs in an easy way to numerical discretizations.

A modulated Fourier expansion is an expansion of the exact or of the numerical solution of a differential equation such as (NLS) in terms of products of solutions of the underlying simple equation such as (LS). This turns out to be a two-scale expansion since the coefficients of these products evolve on a slow time scale εt.

In the context of a long-time analysis, modulated Fourier expansions were introduced by Hairer and Lubich in [33] in order to study numerical methods for highly oscillatory differential equations with one high frequency over long times. In [14], together with Cohen, they used modulated Fourier expansions to analyse exact solutions of these highly oscillatory differential equations over long times, and in [15] this trio extended [33] to the case of multiple high frequencies, see also the thesis of Cohen [12]. Another class of highly oscillatory ordinary differential equations was considered by Cohen in [13]. Many of these results can be found in the monograph [36, Chapter XIII]. The case of a time-dependent high frequency was considered by Sigg [48].

In [17], Cohen, Hairer, and Lubich extended the technique of modulated Fourier expansions to weakly nonlinear wave equations and in [16] to their discretizations by trigonometric integrators. Modulated Fourier expansions were also used by Hairer and Lubich to study spectral semi-discretizations of such nonlinear wave equations over long times in [34]. In [29] and [30] modulated Fourier expansions are used to analyse exact and numerical solutions of nonlinear Schrödinger equations.

Reviews of long-time results obtained with modulated Fourier expansions are given in [35] and [32]. Yet, modulated Fourier expansions are not only used as a tool to analyse differential equations and numerical methods but also as a numerical scheme for highly oscillatory ordinary differential equations, see Miranker and van Veldhuizen [43], Cohen [12], Sigg [48], and the recent contribution [18] by Condon, Deaño, and Iserles. Moreover, modulated Fourier expansions can be used to analyse the convergence of numerical methods, see Hairer, Lubich, and Wanner [36, Chapter XIII.4] and Sanz-Serna [46].

How does the present thesis contribute to the above fields? In this thesis we show how modulated Fourier expansions can be used to study the long-time behaviour of a *general class* of Hamiltonian partial differential equations and their discretizations. This class consists of weakly nonlinear Hamiltonian partial differential equations which are perturbations of linear Hamiltonian partial differential equations. In particular, this generalises and unifies the theory of modulated Fourier expansions developed in [17], [34], and [16] for nonlinear wave equations and in [29] and [30] for nonlinear Schrödinger equations. The thesis mainly builds up on the joint work [29] and [30] of the author with Lubich.

As a main result for the *exact solution* of a Hamiltonian partial differential equation belonging to the general class mentioned above we prove the *long-time near-conservation of actions* along its solution over long times. There is a similar result for a general class

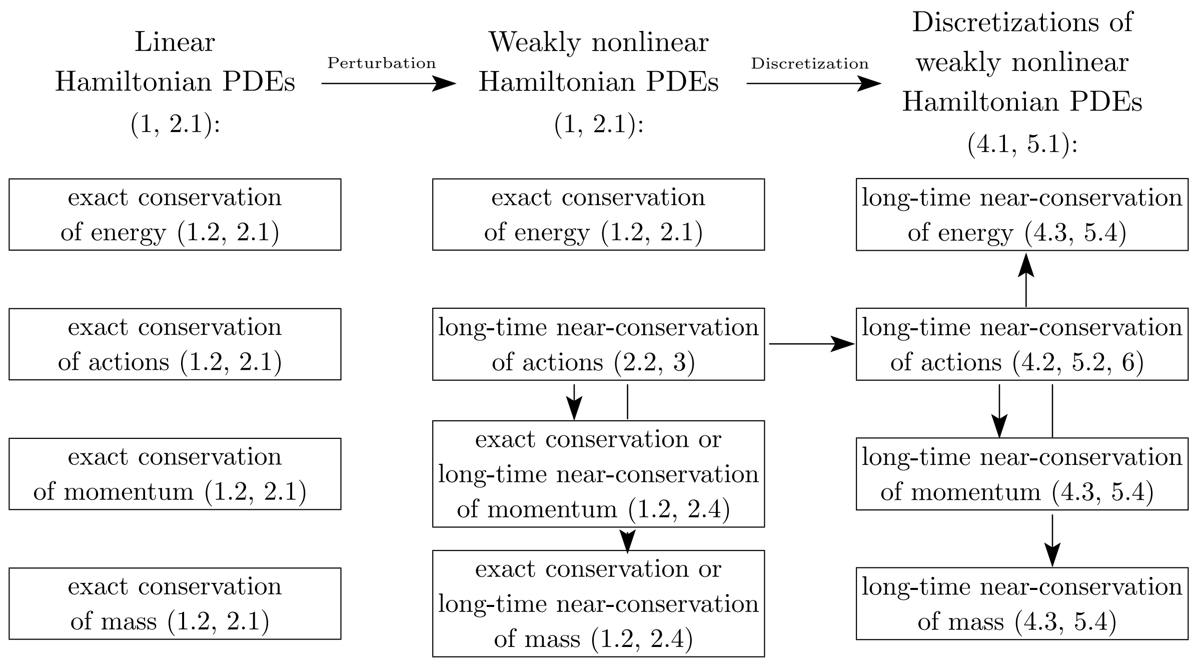

Figure 1: Outline

of equations by Bambusi and Grébert [4] obtained by Birkhoff normal form techniques. The result in the present thesis is obtained with a completely different technique of proof. It is slightly stronger than their result though we are working under less restrictive assumptions.

The understanding of the actions is the starting point to study other invariants of the linear equation that are not necessarily invariants of the nonlinear equation such as mass and momentum. We can prove that both are at least nearly conserved over long times along solutions of the nonlinear equations, see Figure 1. We apply our general results to nonlinear Schrödinger and nonlinear wave equations.

Moreover, we use a refinement of the result to study the problem of *energy distribution* in Hamiltonian partial differential equations. There, one studies initial values with only finitely many nonzero Fourier coefficients, i.e., all the energy is located in a finite number of modes, and tries to understand how this energy is distributed among the other modes. We are able to show that the expected energy distribution is nearly conserved on an again remarkably long time interval.

The results for the exact solution of Hamiltonian partial differential equations are formulated in such a way that they are directly applicable also to suitable *spatial semi-discretizations* of these equations. We show that invariants and near-invariants of the exact solution are nearly conserved along solutions of the semi-discretization over long times, see Figure 1. These results are independent of the spatial discretization parameter. The examples include spectral semi-discretizations for nonlinear Schrödinger equations and nonlinear wave equations.

Finally, we study *full discretizations* of Hamiltonian partial differential equations that are based on a splitting of the semi-discretization in space in its linear and its nonlinear part. Trigonometric integrators for nonlinear wave equations as studied in [16] and splitting integrators for nonlinear Schrödinger equations as studied in [30] can be interpreted as such symplectic numerical schemes. They are standard integrators for these equations. As for the spatial semi-discretization we show that invariants and near-invariants of the exact solution are nearly conserved along solutions of the full discretization over long times, see again Figure 1. Moreover, we show that the results on energy distribution along exact solutions are also true along these numerical solutions.

The present thesis is organised as follows. In the first chapter we introduce Hamiltonian partial differential equations in an abstract framework and derive their (possibly) conserved quantities actions, energy, mass, and momentum. In the following Chapter 2 we formulate the main results on the exact solution of Hamiltonian partial differential equations in a weakly nonlinear setting — long-time near-conservation of actions (Theorems 2.5, 2.7, and 2.12), long-time regularity (Corollary 2.9), long-time near-conservation of mass and momentum (Corollaries 2.10 and 2.11), and long-time energy distribution (Corollaries 2.13 and 2.14). We exemplify the results using nonlinear Schrödinger and nonlinear wave equations. Chapter 3 is solely devoted to the proof of the main results of Chapter 2. This proof is based on modulated Fourier expansions.

In Chapter 4 we study spatial semi-discretizations for which the results of Chapter 2 are also valid, see Theorems 4.2 and 4.3 and Corollaries 4.4, 4.5, and 4.6. Full discretizations of Hamiltonian partial differential equations are considered in Chapter 5. Again, our main results state long-time near-conservation of actions (Theorems 5.4, 5.6, and 5.12), long-time regularity (Corollary 5.9), long-time near-conservation of energy, mass, and momentum (Corollaries 5.10 and 5.11), and long-time energy distribution (Corollaries 5.13 and 5.14). These results are proven in the final Chapter 6 adapting the proof for the exact solution of Chapter 3 to the fully discrete setting. Once again, the main tool is a modulated Fourier expansion.

1 Hamiltonian Partial Differential Equations

In this chapter we give a short and self-contained introduction to Hamiltonian partial differential equations with an emphasis on conserved quantities and examples. For more information we refer the reader to the monograph [38].

1.1 Hamiltonian Functions and Hamiltonian Equations of Motion

We introduce Hamiltonian partial differential equations as infinite dimensional Hamiltonian systems extending the well-known finite dimensional Hamiltonian formalism. Following [4] and [31] we work on complex phase spaces.

Functional Analytic Setting. By $\mathcal{N} \subseteq \mathbb{Z}^d$ we denote a set of indices, and we write for an index $j \in \mathcal{N}$

$$|j| = \max\Bigl(1, \sqrt{j_1^2 + \cdots + j_d^2}\Bigr).$$

For any $s \in \mathbb{R}$ we consider the Hilbert space

$$l_s^2 = l_s^2(\mathbb{C}^{\mathcal{N}}) = \{\, \xi \in \mathbb{C}^{\mathcal{N}} : \|\xi\|_s < \infty \,\}$$

of sequences $\xi = (\xi_j)_{j\in\mathcal{N}} \in \mathbb{C}^{\mathcal{N}}$ of complex numbers equipped with the norm

$$\|\xi\|_s = \Bigl(\sum_{j\in\mathcal{N}} |j|^{2s} |\xi_j|^2\Bigr)^{\frac{1}{2}},$$

which is induced by the scalar product $(\xi, \eta)_s = \sum_{j\in\mathcal{N}} |j|^{2s} \overline{\xi_j} \eta_j$ for $\xi = (\xi_j)_{j\in\mathcal{N}} \in l_s^2$ and $\eta = (\eta_j)_{j\in\mathcal{N}} \in l_s^2$. Note that $\|\xi\|_s = \|\overline{\xi}\|_s$ where $\overline{\xi}$ denotes the entrywise complex conjugate of ξ.

Differentiability. Let $\mathcal{U}$ be an open subset of l_s^2. A map $F : \mathcal{U} \to \mathbb{C}$ is called *Fréchet differentiable* in $\xi \in \mathcal{U}$ if there exists a bounded linear operator $DF(\xi) : l_s^2 \to \mathbb{C}$, such that

$$\lim_{\kappa\to 0} \frac{|F(\xi+\kappa) - F(\xi) - DF(\xi)\kappa|}{\|\kappa\|_s} = 0.$$

The *gradient* of F in ξ is then the sequence $\nabla F(\xi) = (\frac{\partial F}{\partial \xi_j}(\xi))_{j\in\mathcal{N}} \in l_{-s}^2$ with

$$DF(\xi)\kappa = (\overline{\nabla F(\xi)}, \kappa)_0 \quad \text{for any } \kappa \in l_s^2,$$

which exists by the Riesz representation theorem.

Hamiltonian Systems. Let $H : \mathcal{U}\times\mathcal{U} \to \mathbb{C}$ be Fréchet differentiable in both components and write

$$X_H(\xi,\eta) = -i\begin{pmatrix} \nabla_\eta H(\xi,\eta) \\ -\nabla_\xi H(\xi,\eta)\end{pmatrix} = -i\begin{pmatrix} \left(\frac{\partial H}{\partial \eta_j}(\xi,\eta)\right)_{j\in\mathcal{N}} \\ -\left(\frac{\partial H}{\partial \xi_j}(\xi,\eta)\right)_{j\in\mathcal{N}}\end{pmatrix} \in l^2_{-s}\times l^2_{-s}.$$

X_H is called the *Hamiltonian vector field* of the *Hamiltonian function* H on the *phase space* $\mathcal{U}\times\mathcal{U}$. The *Hamiltonian equations of motion* are

$$\frac{d}{dt}\begin{pmatrix}\xi(t)\\ \eta(t)\end{pmatrix} = X_H(\xi(t),\eta(t))$$

or

$$\begin{aligned} i\frac{d}{dt}\xi_j(t) &= \frac{\partial H}{\partial \eta_j}(\xi(t),\eta(t)), \quad j\in\mathcal{N}, \\ -i\frac{d}{dt}\eta_j(t) &= \frac{\partial H}{\partial \xi_j}(\xi(t),\eta(t)), \quad j\in\mathcal{N}. \end{aligned}$$

We further assume for Hamiltonian functions H that

$$\overline{H(\xi,\eta)} = H(\overline{\eta},\overline{\xi})$$

in an open neighbourhood of $\{(\xi,\overline{\xi}) : \xi\in\mathcal{U}\}$, implying $\nabla_\xi H(\xi,\overline{\xi}) = \overline{\nabla_\eta H(\xi,\overline{\xi})}$ for all $\xi\in\mathcal{U}$. Then, for initial values satisfying $\eta(t_0)=\overline{\xi(t_0)}$, the Hamiltonian equations of motion imply $\eta(t)=\overline{\xi(t)}$ for all t where the solution exists, and the Hamiltonian equations of motion reduce to

$$i\frac{d}{dt}\xi_j(t) = \frac{\partial H}{\partial \eta_j}(\xi(t),\overline{\xi(t)}), \quad j\in\mathcal{N}. \tag{1.1}$$

A partial differential equation of the form (1.1) is called a *Hamiltonian partial differential equation*, and we will always consider Hamiltonian functions leading to such equations.

Real Hamiltonian Systems. We consider again the equation (1.1). Introducing the real variables

$$p_j = \sqrt{2}\,\mathrm{Re}(\xi_j) \quad \text{and} \quad q_j = \sqrt{2}\,\mathrm{Im}(\xi_j)$$

and the real Hamiltonian function $\widetilde{H}(q,p) = H(\xi,\overline{\xi})$, an easy calculation shows that $\sqrt{2}\nabla_p\widetilde{H}(q,p) = \nabla_\xi H(\xi,\overline{\xi}) + \nabla_\eta H(\xi,\overline{\xi})$ and $-i\sqrt{2}\nabla_q\widetilde{H}(q,p) = \nabla_\xi H(\xi,\overline{\xi}) - \nabla_\eta H(\xi,\overline{\xi})$. Hence, the Hamiltonian equations of motion (1.1) become

$$\begin{aligned} \frac{d}{dt}q_j(t) &= \frac{\partial \widetilde{H}}{\partial p_j}(q(t),p(t)), \quad j\in\mathcal{N}, \\ \frac{d}{dt}p_j(t) &= -\frac{\partial \widetilde{H}}{\partial q_j}(q(t),p(t)), \quad j\in\mathcal{N}. \end{aligned}$$

(In fact, the above change of variables is a symplectic transformation preserving the Hamiltonian structure of the system.) For finite sets $\mathcal{N}$ we recover the well-known finite dimensional Hamiltonian formalism, see for example [36, Chapter VI].

Various partial differential equations fit into the abstract framework presented here. Some of them are discussed in Sections 1.3, 1.4, and 1.5.

1.2 Conserved Quantities

A very important topic in the theory of Hamiltonian partial or ordinary differential equations are quantities which are conserved along any solution of the Hamiltonian equations of motion (1.1). These *conserved quantities* (or *invariants*) represent important physical properties such as energy conservation and are also very useful in a mathematical analysis of the equations, see for example [50]. We assume throughout this section that the Hamiltonian function $H(\xi,\eta)$ is defined on a phase space $\mathcal{U}\times\mathcal{U}\subseteq l_s^2\times l_s^2$ with $s\geq 0$.

Energy. The *energy* is defined as the Hamiltonian function $H(\xi,\eta)$. It is conserved along any solution of the Hamiltonian equations of motion (1.1).

Proposition 1.1 (Conservation of Energy)**.** *Let $\xi(t)$ be a solution of the Hamiltonian equations of motion* (1.1)*. Then the energy H is conserved along $\xi(t)$,*

$$\frac{d}{dt}H(\xi(t),\overline{\xi(t)})=0.$$

Proof. We compute

$$\frac{d}{dt}H(\xi(t),\overline{\xi(t)})=\Big(\overline{\nabla_\xi H(\xi(t),\overline{\xi(t)})},\frac{d}{dt}\xi(t)\Big)_0+\Big(\overline{\nabla_\eta H(\xi(t),\overline{\xi(t)})},\frac{d}{dt}\overline{\xi(t)}\Big)_0.$$

The Hamiltonian equations of motion (1.1) imply

$$\frac{d}{dt}H(\xi(t),\overline{\xi(t)})=\Big(i\frac{d}{dt}\xi(t),\frac{d}{dt}\xi(t)\Big)_0+\Big(\overline{i\frac{d}{dt}\xi(t)},\frac{d}{dt}\overline{\xi(t)}\Big)_0=0.$$ □

In addition to the energy, symmetries in the Hamiltonian function induce other conserved quantities along solutions of the Hamiltonian equations of motion (1.1) such as the "classical" invariants mass, momentum, and actions. This is made precise in the following proposition closely related to Noether's Theorem [36, Chapter VI, Theorem 6.5], see also [2].

Proposition 1.2 (Noether's Theorem)**.** *For $\theta\in\mathbb{R}$ let $g_\theta:\mathcal{U}\to\mathcal{U}$ be such that $g_0=\mathrm{id}$ and $\frac{d}{d\theta}|_{\theta=0}g_\theta(\xi)=iA\xi$ with a self-adjoint and bounded linear operator $A:l_s^2\to l_0^2$. If the Hamiltonian function $H(\xi,\overline{\xi})$ is invariant under the transformation $\xi\mapsto g_\theta(\xi)$ for all $\theta\in\mathbb{R}$, then*

$$(\xi,A\xi)_0$$

is conserved along any solution $\xi(t)$ of the Hamiltonian equations of motion (1.1)*,*

$$\frac{d}{dt}(\xi(t),A\xi(t))_0=0.$$

Conversely, if the Hamiltonian function $H(\xi,\overline{\xi})$ is not invariant under the transformation g_θ as above for $\theta\to 0$ (i.e., there exists ξ and a sequence $\theta_n\to 0$ such that $H(\xi,\overline{\xi})$ is not invariant under $g_{\theta_n}(\xi)$), then $(\xi,A\xi)_0$ is not conserved along every solution of (1.1)*.*

Proof. Since $H(g_\theta(\xi), \overline{g_\theta(\xi)}) = H(\xi, \overline{\xi})$ for all $\xi \in \mathcal{U}$ and $\theta \in \mathbb{R}$, we have for a solution $\xi(t)$ of (1.1)

$$0 = \frac{d}{d\theta}\Big|_{\theta=0} H(g_\theta(\xi(t)), \overline{g_\theta(\xi(t))}) = \Big(\overline{\nabla_\xi H(\xi(t), \overline{\xi(t)})}, iA\xi(t)\Big)_0 + \Big(\overline{\nabla_\eta H(\xi(t), \overline{\xi(t)})}, \overline{iA\xi(t)}\Big)_0.$$

The Hamiltonian equations of motion (1.1) and the self-adjointness of A imply

$$0 = \Big(i\frac{d}{dt}\xi(t), iA\xi(t)\Big)_0 + \Big(\overline{i\frac{d}{dt}\xi(t)}, \overline{iA\xi(t)}\Big)_0 = \Big(\frac{d}{dt}\xi(t), A\xi(t)\Big)_0 + \Big(\xi(t), A\frac{d}{dt}\xi(t)\Big)_0.$$

The result follows. □

Mass. We define the *mass*

$$m(\xi, \eta) = (\xi, \overline{\eta})_0 = \sum_{j\in\mathcal{N}} \overline{\xi_j \eta_j}.$$

If $H(\xi, \overline{\xi})$ is invariant under the transformation $g_\theta(\xi) = e^{i\theta}\xi$, $\theta \in \mathbb{R}$, then the mass $m(\xi, \overline{\xi})$ is conserved by Proposition 1.2. Indeed, we have $\frac{d}{d\theta}|_{\theta=0} g_\theta(\xi) = i\xi$ ($A = \mathrm{id}$).

Proposition 1.3 (Conservation of Mass)**.** *Let $\xi(t)$ be a solution of the Hamiltonian equations of motion* (1.1) *and assume that $H(\xi, \overline{\xi})$ is invariant under the transformation $\xi \mapsto e^{i\theta}\xi$, $\theta \in \mathbb{R}$. Then the mass m is conserved along $\xi(t)$,*

$$\frac{d}{dt} m(\xi(t), \overline{\xi(t)}) = 0.$$ □

Momentum. The *momentum* is defined as

$$K(\xi, \eta) = \sum_{j\in\mathcal{N}} j\xi_j\eta_j.$$

The conservation of the lth component of the momentum ($l = 1, \ldots, d$) along solutions of the Hamiltonian equations of motion (1.1) is a direct consequence of Proposition 1.2 provided that the Hamiltonian function $H(\xi, \overline{\xi})$ is invariant under the transformation $g_\theta(\xi)_j = e^{i\theta j_l}\xi_j$, $\theta \in \mathbb{R}$ and $j \in \mathcal{N}$ (in this situation $(A\xi)_j = j_l\xi_j$ and A maps to l_0^2 for $s \geq 1$).

Proposition 1.4 (Conservation of Momentum)**.** *Let $s \geq 1$, let $\xi(t)$ be a solution of the Hamiltonian equations of motion* (1.1)*, and assume that $H(\xi, \overline{\xi})$ is invariant under the transformation $\xi_j \mapsto e^{i\theta j_l}\xi_j$, $\theta \in \mathbb{R}$, for an $l = 1, \ldots, d$. Then the lth component K_l of the momentum is conserved along $\xi(t)$,*

$$\frac{d}{dt} K_l(\xi(t), \overline{\xi(t)}) = 0.$$ □

Actions. By Proposition 1.2, invariance of $H(\xi, \overline{\xi})$ under the transformation $g_\theta(\xi)_j = e^{i\theta}\xi_j$ for fixed $j \in \mathcal{N}$ and $g_\theta(\xi)_l = 1$ for all $j \neq l \in \mathcal{N}$ implies the conservation of the jth *action*

$$I_j(\xi, \overline{\xi}) = |\xi_j|^2$$

along solutions of the Hamiltonian equations of motion (1.1).

Proposition 1.5 (Conservation of Actions). *Let $\xi(t)$ be a solution of the Hamiltonian equations of motion* (1.1) *and assume that $H(\xi,\overline{\xi})$ is invariant under the transformation $g_\theta(\xi)_j = e^{i\theta}\xi_j$, $\theta \in \mathbb{R}$ and fixed $j \in \mathcal{N}$, and $g_\theta(\xi)_l = 1$ for all $j \neq l \in \mathcal{N}$. Then the jth action I_j is conserved along $\xi(t)$,*

$$\frac{d}{dt} I_j(\xi(t), \overline{\xi(t)}) = 0. \qquad \square$$

In particular, if $H(\xi,\overline{\xi})$ depends only on the actions $(|\xi_j|^2)_{j\in\mathcal{N}}$, then all the actions are conserved along any solution of (1.1).

Examples of Hamiltonian partial differential equations with and without conserved quantities are given in the following Sections 1.3, 1.4, and 1.5.

1.3 Example — Linear Schrödinger Equations

Linear Schrödinger equations are fundamental in quantum mechanics. They are used to describe non-relativistic particles, see for example [40, Chapter I], [42], or [52]. For convenience we omit here all constants appearing in a physical context.

Free Schrödinger Equations. Consider the Hamiltonian function $H : l_1^2 \times l_1^2 \to \mathbb{C}$,

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j, \tag{1.2}$$

with $\mathcal{N} = \mathbb{Z}^d$ and the *frequencies* $\omega_j = j_1^2 + \cdots + j_d^2$. Then

$$X_H(\xi,\eta) = -i \begin{pmatrix} (\omega_j \xi_j)_{j\in\mathcal{N}} \\ -(\omega_j \eta_j)_{j\in\mathcal{N}} \end{pmatrix},$$

and the Hamiltonian equations of motion (1.1) are

$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t).$$

These are precisely the equations determining the Fourier coefficients $\xi_j(t)$ along a solution $\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t) e^{i(j\cdot x)}$, where $j\cdot x = j_1x_1 + \cdots + j_dx_d$, of the *free Schrödinger equation*

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) \tag{1.3}$$

with periodic boundary conditions on $[-\pi,\pi]^d$, that is $x \in \mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$.

Linear Schrödinger Equations with a Potential of Convolution Type. Considering the Hamiltonian function (1.2) with frequencies $\omega_j = j_1^2 + \cdots + j_d^2 + V_j$ for $j \in \mathcal{N} = \mathbb{Z}^d$ instead of $j_1^2 + \cdots + j_d^2$ as for the free Schrödinger equation, where V_j are the Fourier coefficients of a 2π-periodic potential $V(x) \in L^2(\mathbb{T}^d)$ with real Fourier coefficients, leads to the *linear Schrödinger equation*

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x) * \psi(x,t) \tag{1.4}$$

on $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$. The potential $V(x) = \sum_{j\in\mathcal{N}} V_j e^{i(j\cdot x)}$ acts by convolution on ψ, i.e., by multiplication in the frequency domain.

Comparing (1.4) with the free Schrödinger equation (1.3), we notice that the potential does not change the eigenfunctions $e^{i(j\cdot x)}$, $j \in \mathcal{N}$, of the operators on the right-hand sides of the equations ($-\Delta$ and $-\Delta + V(x)*$) with periodic boundary conditions but the corresponding eigenvalues ω_j. This will be important in our investigations since we can keep the comfortable eigenfunctions $e^{i(j\cdot x)}$ but obtain frequencies ω_j which can be expected to be not anymore *resonant* — for the frequencies ω_j of the free Schrödinger equation (1.3) in one dimension ($d = 1$) we have for instance the resonance $\omega_3 + \omega_4 = \omega_5$ whereas the potential V in the linear Schrödinger equation (1.4) can be used to exclude such resonances.

A more difficult situation than in (1.4), where the potential acts by multiplication instead of convolution on ψ, is presented now in the case of Dirichlet boundary conditions on $[0,\pi]$ (dimension $d = 1$).

Linear Schrödinger Equations with a Multiplicative Potential. Another *linear Schrödinger equation* is

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x)\psi(x,t) \tag{1.5}$$

with Dirichlet boundary conditions $\psi(x,t) = 0$ for x on the boundary of $[0,\pi]$. The real potential $V(x)$ satisfying Dirichlet boundary conditions acts here by multiplication on ψ.

As for the free Schrödinger equation (1.3) and the linear Schrödinger equation with a potential of convolution type (1.4) we aim for a decomposition of the solution $\psi(\cdot,t)$ in terms of the eigenfunctions of the operator $-\Delta + V(x)$ on the right-hand side of the linear Schrödinger equation (1.5). There is a rich theory on such eigenvalue problems

$$-\Delta\varphi(x) + V(x)\varphi(x) = \lambda\varphi(x)$$

with Dirichlet boundary conditions which are referred to as Sturm–Liouville problems, see for example [53, §27 and §28] and [45, Chapter 2]. In particular, there exists a complete $L^2([0,\pi])$-orthonormal set of eigenfunctions φ_j with corresponding eigenvalues ω_j, $j \in \mathcal{N} = \mathbb{N} \setminus \{0\}$, such that $\psi(\cdot,t)$ can be expanded in terms of these eigenfunctions,

$$\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t)\varphi_j(x).$$

The equations determining the coefficients $\xi_j(t)$ are the equations of motion corresponding to the Hamiltonian function (1.2) with the above eigenvalues ω_j as frequencies. Since these eigenvalues satisfy

$$c_2|j|^2 \le |\omega_j| \le C_2|j|^2 \quad \text{for all } j \in \mathcal{N} \tag{1.6}$$

with positive constants c_2 and C_2, the Hamiltonian function is again defined on $l_1^2 \times l_1^2$.

For $V = 0$ we have $\varphi_j(x) = \sin(jx) = \frac{1}{2i}(e^{i(jx)} - e^{-i(jx)})$ and $\omega_j = j^2$. A choice $V \neq 0$ changes the eigenvalues ω_j as well as the eigenfunctions φ_j. This is different to the situation of a potential of convolution type in (1.4) where the eigenfunctions do not change for different potentials (but the eigenvalues do).

Conservation of Energy. According to Proposition 1.1 the energy

$$H(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} \omega_j |\xi_j|^2$$

is conserved along any solution of linear Schrödinger equations (1.3), (1.4), and (1.5). In terms of the function $\psi = \psi(x)$ the energy becomes due to Parseval's equality

$$H(\xi,\overline{\xi}) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} \overline{\psi}(-\Delta\psi)\,dx = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} |\nabla\psi|^2\,dx$$

for the free Schrödinger equation (1.3),

$$H(\xi,\overline{\xi}) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} \Big(|\nabla\psi|^2 + \overline{\psi}(V * \psi)\Big)\,dx$$

for the linear Schrödinger equation with a potential of convolution type (1.4), and

$$H(\xi,\overline{\xi}) = \frac{1}{\pi}\int_{[0,\pi]} \Big(|\nabla\psi|^2 + V|\psi|^2\Big)\,dx$$

for the linear Schrödinger equation with a multiplicative potential (1.5).

Conservation of Mass. The invariance of the Hamiltonian function (1.2) under the transformation $\xi \mapsto e^{i\theta}\xi$ implies by Proposition 1.3 the conservation of mass

$$m(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} |\xi_j|^2$$

along solutions of linear Schrödinger equation (1.3), (1.4), and (1.5), which reads in terms of $\psi = \psi(x)$ by Parseval's equality for the linear Schrödinger equations (1.3) and (1.4)

$$m(\xi,\overline{\xi}) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} |\psi|^2\,dx = \|\psi\|^2_{L^2(\mathbb{T}^d)}$$

and

$$m(\xi,\overline{\xi}) = \frac{1}{\pi}\int_{[0,\pi]} |\psi|^2\,dx = \|\psi\|^2_{L^2([0,\pi])}$$

for the linear Schrödinger equation (1.5).

Conservation of Momentum. Since the Hamiltonian function (1.2) is also invariant under the transformations $\xi_j \mapsto e^{i\theta j_l}\xi_j$ for $l = 1, \dots, d$, we have conservation of momentum

$$K(\xi, \overline{\xi}) = \sum_{j\in\mathcal{N}} j|\xi_j|^2$$

along solutions of linear Schrödinger equations (1.3), (1.4), and (1.5) due to Proposition 1.4. Once again, we can rewrite this quantity in terms of the function $\psi = \psi(x)$ itself using Parseval's equality,

$$K(\xi, \overline{\xi}) = \mathrm{Im}\Big(\sum_{j\in\mathcal{N}} ij|\xi_j|^2\Big) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} \mathrm{Im}(\overline{\psi}\nabla\psi)\, dx$$

for the free Schrödinger equation (1.3) and the linear Schrödinger equation with a potential of convolution type (1.4).

Conservation of Actions. The Hamiltonian function (1.2) is also invariant under the transformations $\xi_j \mapsto e^{i\theta}\xi_j$ for fixed $j \in \mathcal{N}$ and $\xi_l \mapsto 1$ for all $j \neq l \in \mathcal{N}$. This implies the conservation of the actions

$$I_j(\xi, \overline{\xi}) = |\xi_j|^2$$

along solutions of linear Schrödinger equations (1.3), (1.4), and (1.5) by Proposition 1.5.

In fact, the conservation of actions can also be seen directly from the solution $\xi_j(t) = e^{-i\omega_j t}\xi_j(0)$ of linear Schrödinger equations. Since energy, mass, and momentum are all sums of the actions in the case of linear Schrödinger equations, the conservation of actions also implies conservation of energy, mass, and momentum.

1.4 Example — Nonlinear Schrödinger Equations

A linear Schrödinger equation describing non-relativistic particles is defined on a space whose dimension d equals three times the number of particles. In order to handle this high dimensional problem one usually studies reduced models which result in Schrödinger equations in lower dimensional spaces, see for example [40, Chapter II]. Often these equations are nonlinear of the types discussed below. Such nonlinear Schrödinger equations also appear in various other physical contexts, see for example [50].

Nonlinear Schrödinger Equations with a Potential of Convolution Type. Consider the *nonlinear Schrödinger equation*

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x) * \psi(x,t) + g(|\psi(x,t)|^2)\psi(x,t) \tag{1.7}$$

on $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$, which is a nonlinear version of (1.4). As for the linear Schrödinger equation with a potential of convolution type (1.4), $V(x)$ is in $L^2(\mathbb{T}^d)$ with real Fourier coefficients, and the function $g : \mathbb{R} \to \mathbb{R}$ is assumed to be real-valued and analytic in a neighbourhood of zero, $g(y) = \sum_{m=0}^{\infty} y^m g^{(m)}(0)/m!$. Such nonlinear Schrödinger equations can be seen as a first attempt to understand the (physically) interesting situation where the potential of convolution type is replaced by a multiplicative potential. They have been considered for example by Bambusi and Grébert [4], Bourgain [9], and Eliasson and Kuksin [23].

In terms of the Fourier coefficients $\xi_j(t)$, $j \in \mathcal{N} = \mathbb{Z}^d$, of $\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t) e^{i(j\cdot x)}$ this equation reads

$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{\substack{j^1+\cdots+j^{m+1}\\ -j^{m+2}-\cdots-j^{2m+1}=j}} \xi_{j^1}(t)\cdots\xi_{j^{m+1}}(t)\overline{\xi_{j^{m+2}}(t)\cdots\xi_{j^{2m+1}}(t)} \tag{1.8}$$

with the frequencies $\omega_j = j_1^2 + \cdots + j_d^2 + V_j$. Hence, the nonlinear Schrödinger equation (1.7) is a Hamiltonian partial differential equation with Hamiltonian function

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{\substack{j^1+\cdots+j^{m+1}\\ -j^{m+2}-\cdots-j^{2m+2}=0}} \xi_{j^1}\cdots\xi_{j^{m+1}}\eta_{j^{m+2}}\cdots\eta_{j^{2m+2}},$$

or in terms of $\psi = \psi(x) = \sum_{j\in\mathcal{N}} \xi_j e^{i(j\cdot x)}$

$$H(\xi,\overline{\xi}) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} \Big(\overline{\psi}\,(-\Delta\psi + V * \psi) + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} |\psi|^{2m+2} \Big)\, dx.$$

We now show that this Hamiltonian function is defined on a neighbourhood $\mathcal{U}\times\mathcal{U}$ of zero in $l_s^2 \times l_s^2$ for any $s > \frac{d}{2}$ and $s \geq 1$. We first note that $\sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j$ is defined on $l_1^2 \times l_1^2$. For the term resulting from the nonlinearity in (1.7) we have

$$\Big| \sum_{\substack{j^1+\cdots+j^{m+1}\\ -j^{m+2}-\cdots-j^{2m+2}=0}} \xi_{j^1}\cdots\xi_{j^{m+1}}\eta_{j^{m+2}}\cdots\eta_{j^{2m+2}} \Big| \leq \Big(\sum_j |\xi_j|\Big)^{m+1} \Big(\sum_j |\eta_j|\Big)^{m+1}$$

and

$$\sum_{j\in\mathcal{N}} |\xi_j| \leq \Big(\sum_{j\in\mathcal{N}} \frac{1}{|j|^{2s}}\Big)^{\frac12} \Big(\sum_{j\in\mathcal{N}} |j|^{2s}|\xi_j|^2\Big)^{\frac12} = \Big(\sum_{j\in\mathcal{N}} \frac{1}{|j|^{2s}}\Big)^{\frac12} \|\xi\|_s$$

by the Cauchy–Schwarz inequality. We finally show that

$$\sum_{j\in\mathcal{N}} \frac{1}{|j|^{2s}} \quad \text{converges for } s > \frac{d}{2}, \tag{1.9}$$

since this implies together with the analyticity of g that the second term of the Hamiltonian function H is defined for sufficiently small $\xi, \eta \in l_s^2$ with $s > \frac{d}{2}$. To show (1.9) we note that for given $0 \neq n \in \mathbb{N}$ a crude estimate of the number of $j \in \mathcal{N}$ with $|j| = n$ is $2(2n+1)^{d-1}$, and hence

$$\sum_{j\in\mathcal{N}} \frac{1}{|j|^{2s}} \leq 2\sum_{n=1}^{\infty} \frac{(2n+1)^{d-1}}{n^{2s}} \leq 2\cdot 3^{d-1} \sum_{n=1}^{\infty} n^{d-1-2s}.$$

The latter series is the well-known generalized harmonic series which converges for $s > \frac{d}{2}$. Note that this estimate is optimal with respect to the possible choice of s since we can show that $\sum_{j\in\mathcal{N}} \frac{1}{|j|^{2s}}$ diverges for $s \leq \frac{d}{2}$, see [29, Lemma 1] and references therein. Summarising, we have shown that the second term in the Hamiltonian function H can be estimated for $s > \frac{d}{2}$ by

$$\Big|\sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{\substack{j^1+\cdots+j^{m+1} \\ -j^{m+2}-\cdots-j^{2m+2}=0}} \xi_{j^1}\cdots\xi_{j^{m+1}}\eta_{j^{m+2}}\cdots\eta_{j^{2m+2}}\Big| \leq \sum_{m=0}^{\infty} \frac{|g^{(m)}(0)|}{m!(m+1)} C^{2m+2}\|\xi\|_s^{m+1}\|\eta\|_s^{m+1}, \tag{1.10}$$

and the latter series converges for sufficiently regular g and sufficiently small $\|\xi\|_s$ and $\|\eta\|_s$.

Schrödinger–Poisson Equations. We consider an equation of Schrödinger–Poisson type where $g(|\psi(x,t)|^2)$ in the nonlinear Schrödinger equation (1.7) is replaced by a potential $W(x,t)$ which is coupled to the solution $\psi(x,t)$ through a Poisson equation. In particular, we study the *Schrödinger–Poisson equation*

$$\begin{aligned} i\frac{\partial}{\partial t}\psi(x,t) &= -\Delta\psi(x,t) + V(x) * \psi(x,t) + W(x,t)\psi(x,t), \\ -\Delta W(x,t) &= |\psi(x,t)|^2 - \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} |\psi(x,t)|^2\,dx, \\ \int_{\mathbb{T}^d} W(x,t)\,dx &= 0 \end{aligned} \tag{1.11}$$

on $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$ with a potential $V(x)$ as in (1.4) and (1.7).

In the "standard" Schrödinger–Poisson equation defined on $\mathbb{R}^d$ with asymptotic boundary condition $\psi(x,t) \to 0$ as $|x| \to \infty$ instead of periodic boundary conditions, the potential $W(x,t)$ is defined by the Poisson equation

$$-\Delta W(x,t) = |\psi(x,t)|^2$$

with asymptotic boundary condition $W(x,t) \to 0$ as $|x| \to \infty$. Since we consider here periodic boundary conditions for ψ and W, we give this Poisson equation a meaning by requiring $\int_{\mathbb{T}^d} W(x,t)\,dx = 0$ (note that the zeroth Fourier coefficient of $W(x,t)$ is not defined by the Poisson equation with periodic boundary conditions) and by subtracting $\frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} |\psi(x,t)|^2\,dx$ on the right-hand side of the Poisson equation (note that the Poisson equation with periodic boundary conditions only has a solution if the zeroth Fourier coefficient on the right-hand side is zero).

Writing the Schrödinger–Poisson equation (1.11) in terms of the Fourier coefficients

$\xi_j(t)$ and $W_j(t)$, $j \in \mathcal{N} = \mathbb{Z}^d$, of $\psi(x,t)$ and $W(x,t)$, respectively, yields

$$\begin{aligned} i\frac{d}{dt}\xi_j(t) &= \omega_j \xi_j(t) + \sum_{j^1+j^2=j} \xi_{j^1}(t) W_{j^2}(t), \\ (j_1^2 + \cdots + j_d^2) W_j(t) &= \sum_{j^1-j^2=j} \xi_{j^1}(t)\overline{\xi_{j^2}(t)} \quad \text{for } j \neq 0, \\ W_j(t) &= 0 \quad \text{for } j = 0 \end{aligned}$$

with the frequencies $\omega_j = j_1^2 + \cdots + j_d^2 + V_j$, or

$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) + \sum_{\substack{j^1+j^2-j^3=j \\ j^2 \neq j^3}} \frac{1}{(j_1^2 - j_1^3)^2 + \cdots + (j_d^2 - j_d^3)^2} \xi_{j^1}(t)\xi_{j^2}(t)\overline{\xi_{j^3}(t)}. \tag{1.12}$$

Hence, the Schrödinger–Poisson equation (1.11) is a Hamiltonian partial differential equation with Hamiltonian function

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + \frac{1}{2} \sum_{\substack{j^1+j^2-j^3-j^4=0 \\ j^2 \neq j^3}} \frac{1}{(j_1^2 - j_1^3)^2 + \cdots + (j_d^2 - j_d^3)^2} \xi_{j^1}(t)\xi_{j^2}(t)\eta_{j^3}(t)\eta_{j^4}(t).$$

As for the nonlinear Schrödinger equation with a potential of convolution type (1.7) this Hamiltonian function is defined on a neighbourhood $\mathcal{U} \times \mathcal{U}$ of $l_s^2 \times l_s^2$ for $s > \frac{d}{2}$ and $s \geq 1$.

Nonlinear Schrödinger Equations with a Multiplicative Potential. We consider a nonlinear variant of (1.5) leading to the *nonlinear Schrödinger equation*

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x)\psi(x,t) + g(|\psi(x,t)|^2)\psi(x,t) \tag{1.13}$$

with Dirichlet boundary conditions $\psi(x,t) = 0$ for x on the boundary of $[0,\pi]$, where g is once again assumed to be real-valued and analytic in a neighbourhood of zero. Expressing $\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t)\varphi_j(x)$ as in the linear situation (1.5) in terms of the (real-valued) eigenfunctions $\varphi_j(x)$, $j \in \mathcal{N} = \mathbb{N}\setminus\{0\}$, of $-\Delta + V(x)$, the nonlinear Schrödinger equation (1.13) reduces to

$$\begin{aligned} i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{j^1,\ldots,j^{2m+1}} & P_{j,(j^1,\ldots,j^{m+1}),(j^{m+2},\ldots,j^{2m+1})} \\ & \xi_{j^1}(t)\cdots\xi_{j^{m+1}}(t)\overline{\xi_{j^{m+2}}(t)\cdots\xi_{j^{2m+1}}(t)}, \end{aligned}$$

where ω_j are the eigenvalues corresponding to the eigenfunctions φ_j and

$$P_{j,(j^1,\ldots,j^{m+1}),(j^{m+2},\ldots,j^{2m+1})} = \frac{1}{\pi}\int_{[0,\pi]} \varphi_j(x)\varphi_{j^1}(x)\cdots\varphi_{j^{2m+1}}(x)\,dx$$

by the orthonormality of the eigenfunctions φ_j. These are the Hamiltonian equations of motion corresponding to the Hamiltonian function

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{j^1,\dots,j^{2m+2}} P_{j^{2m+2},(j^1,\dots,j^{m+1}),(j^{m+2},\dots,j^{2m+1})} \xi_{j^1}\cdots\xi_{j^{m+1}}\eta_{j^{m+2}}\cdots\eta_{j^{2m+2}}$$

(note that $P_{j^{2m+2},(j^1,\dots,j^{m+1}),(j^{m+2},\dots,j^{2m+1})}$ is symmetric in the indices $j^1,\dots,j^{2m+2}$). We can show as for the nonlinear Schrödinger equation with a potential of convolution type (1.7) that this Hamiltonian function is defined on a neighbourhood $\mathcal{U}\times\mathcal{U}$ of zero in $l^2_s\times l^2_s$ for $s>\frac{d}{2}$ and $s\geq 1$.

Conservation of Energy. By Proposition 1.1 the energy $H(\xi,\overline{\xi})$ is conserved along any solution of the nonlinear Schrödinger equations (1.7), (1.11), and (1.13). We can write the energy in terms of the function $\psi=\psi(x)$ as

$$H(\xi,\overline{\xi}) = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}\Big(|\nabla\psi|^2 + \overline{\psi}(-\Delta\psi + V*\psi) + \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!(m+1)}|\psi|^{2m+2}\Big)\,dx$$

for the nonlinear Schrödinger equation with a potential of convolution type (1.7),

$$\begin{aligned} H(\xi,\overline{\xi}) &= \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}\Big(|\nabla\psi|^2 + V|\psi|^2 + W|\psi|^2\Big)\,dx,\\ -\Delta W &= |\psi|^2 - \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}|\psi|^2\,dx,\\ \int_{\mathbb{T}^d} W\,dx &= 0 \end{aligned}$$

for the Schrödinger–Poisson equation (1.11), and

$$H(\xi,\overline{\xi}) = \frac{1}{\pi}\int_{[0,\pi]}\Big(|\nabla\psi|^2 + V|\psi|^2 + \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!(m+1)}|\psi|^{2m+2}\Big)\,dx$$

for the nonlinear Schrödinger equation with a multiplicative potential (1.13).

Conservation of Mass. The Hamiltonian functions $H(\xi,\overline{\xi})$ of the nonlinear Schrödinger equations (1.7), (1.11), and (1.13) are all invariant under the transformation $\xi\mapsto e^{i\theta}\xi$, and hence Proposition 1.3 ensures the conservations of mass

$$m(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}}|\xi_j|^2 = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d}|\psi|^2\,dx = \|\psi\|^2_{L^2(\mathbb{T}^d)}$$

along any solution of (1.7) and (1.11), and

$$m(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}}|\xi_j|^2 = \frac{1}{\pi}\int_{[0,\pi]}|\psi|^2\,dx = \|\psi\|^2_{L^2([0,\pi])}$$

along any solution of (1.13).

Conservation or Non-Conservation of Momentum. For the nonlinear Schrödinger equation with a potential of convolution type (1.7) and for the Schrödinger–Poisson equation (1.11) the Hamiltonian functions $H(\xi,\overline{\xi})$ are invariant under the transformation $\xi_j \mapsto e^{i\theta j_l}\xi_j$ for $l = 1,\dots,d$, and hence the momentum

$$K(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} j|\xi_j|^2 = \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} \mathrm{Im}(\overline{\psi}\nabla\psi)\,dx$$

is conserved along any solution of these nonlinear Schrödinger equations.

However, the Hamiltonian function $H(\xi,\overline{\xi})$ of the nonlinear Schrödinger equation with a multiplicative potential (1.13) is not anymore invariant under the above transformation, and Propositions 1.2 and 1.4 do not ensure the conservation of momentum $K(\xi,\overline{\xi})$ along solutions of this nonlinear Schrödinger equation.

Non-Conservation of Actions. None of the Hamiltonian functions $H(\xi,\overline{\xi})$ for the nonlinear Schrödinger equations (1.7), (1.11), and (1.13) is in general invariant under the transformation $\xi_j \mapsto e^{i\theta}\xi_j$ for fixed $j \in \mathcal{N}$ and $\xi_l \mapsto 1$ for all $j \neq l \in \mathcal{N}$, and the actions

$$I_j(\xi,\overline{\xi}) = |\xi_j|^2$$

are in general not conserved along a solution of the nonlinear Schrödinger equations (1.7), (1.11), and (1.13), see Propositions 1.2 and 1.5. Note however that the actions are conserved quantities for the linear variants of these equations, see Section 1.3.

	linear	nonlinear		
	(equations (1.3), (1.4), and (1.5))	potential of convolution type (equation (1.7))	Schrödinger – Poisson (equation (1.11))	multiplicative potential (equation (1.13))
actions	exact conservation	non-conservation		
energy	exact conservation			
mass	exact conservation			
momentum	exact conservation			non-conservation

Table 1: Conservation properties of Schrödinger equations.

The different results on conservation properties of linear and nonlinear Schrödinger equations are summarised in Table 1. In Sections 2.6, 2.7, and 2.8 we will show that we have at least long-time near-conservation for all items which are non-conserved.

1.5 Example — Nonlinear Wave Equations

In this section we introduce nonlinear wave equations as Hamiltonian partial differential equations. We restrict our attention here to wave equations in one spatial dimension since the theory of the following sections is restricted in the case of wave equations to this situation. Moreover, we consider only real-valued initial values resulting in real-valued solutions.

Nonlinear Wave Equations with Periodic Boundary Conditions. Consider the *nonlinear wave equation*

$$\frac{\partial^2}{\partial t^2}u(x,t) = \Delta u(x,t) - \rho u(x,t) + g(u(x,t)) \tag{1.14}$$

with a nonnegative real number ρ and a real-valued and analytic function g. We consider this equation on $\mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z})$, i.e., with periodic boundary conditions. The *Sine–Gordon equation* $\frac{\partial^2}{\partial t^2}u(x,t) = \Delta u(x,t) - \rho \sin(u(x,t))$ is an example for this type of equation, where the nonlinearity is chosen as $g(u) = -\rho\sin(u) + \rho u$.

Introducing $v(x,t) = \frac{\partial}{\partial t}u(x,t)$, this equation can be written as a first order equation (in time), which reads in terms of the Fourier coefficients $u_j(t)$ and $v_j(t)$, $j \in \mathcal{N} = \mathbb{Z}$, of $u(x,t)$ and $v(x,t)$, respectively,

$$\begin{aligned} \frac{d}{dt}u_j(t) &= v_j(t), \\ \frac{d}{dt}v_j(t) &= -\omega_j^2 u_j(t) + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{j^1+\cdots+j^m=j} u_{j^1}(t)\cdots u_{j^m}(t) \end{aligned} \tag{1.15}$$

with $\omega_j = \sqrt{j^2+\rho}$. Assuming real-valued initial data $u(x,0)$ and $v(x,0)$, i.e., $u_j(0) = \overline{u_{-j}(0)}$ and $v_j(0) = \overline{v_{-j}(0)}$ for $j \in \mathcal{N}$, we also have real-valued solutions $u(x,t)$ and $v(x,t)$.

For $j \in \mathcal{N}$ we set

$$\xi_j = \frac{\omega_j^{\frac{1}{2}} u_j + i\omega_j^{-\frac{1}{2}} v_j}{\sqrt{2}}.$$

Then, $u_j = \overline{u_{-j}}$ ensures that $u_j = \frac{\xi_j + \overline{\xi_{-j}}}{\sqrt{2\omega_j}}$ and

$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) - \frac{1}{\sqrt{2\omega_j}} \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{j^1+\cdots+j^m=j} \frac{\xi_{j^1} + \overline{\xi_{-j^1}}}{\sqrt{2\omega_{j^1}}} \cdots \frac{\xi_{j^m} + \overline{\xi_{-j^m}}}{\sqrt{2\omega_{j^m}}}.$$

Hence, the nonlinear wave equation (1.14) is a Hamiltonian partial differential equation with Hamiltonian function

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j - \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{j^1+\cdots+j^{m+1}=0} \frac{\xi_{j^1} + \eta_{-j^1}}{\sqrt{2\omega_{j^1}}} \cdots \frac{\xi_{j^{m+1}} + \eta_{-j^{m+1}}}{\sqrt{2\omega_{j^{m+1}}}}. \tag{1.16}$$

Nonlinear Wave Equations with Dirichlet Boundary Conditions. Instead of periodic boundary conditions on $[-\pi,\pi]$ in (1.14) we can consider the same *nonlinear wave equation*

$$\frac{\partial^2}{\partial t^2}u(x,t) = \Delta u(x,t) - \rho u(x,t) + g(u(x,t)) \tag{1.17}$$

with Dirichlet boundary conditions $u(x,t) = v(x,t) = 0$ for x on the boundary of $[0,\pi]$. We assume in addition that the nonlinearity g is odd,

$$g(u) = -g(-u).$$

This implies that an odd continuation $u(-x,t) = -u(x,t)$ of a solution of (1.17) is a solution of the nonlinear wave equation with periodic boundary conditions (1.14). In particular, the nonlinear wave equation with Dirichlet boundary conditions (1.17) can be considered as a Hamiltonian partial differential equation with the same Hamiltonian function as the nonlinear wave equation with periodic boundary conditions (1.14).

We derive now another Hamiltonian function defined on a different phase space for (1.17). We study $u(x,t)$ and $v(x,t) = \frac{\partial}{\partial t}u(x,t)$ in terms of the eigenfunctions $\sin(jx)$, $j \in \widetilde{\mathcal{N}} = \mathbb{N} \setminus \{0\}$ of $-\Delta + \rho$ with Dirichlet boundary conditions and their corresponding eigenvalues $\omega_j^2 = j^2 + \rho$. By the theory of Sturm–Liouville problems, see [53, §27 and §28] and [45, Chapter 2], we can express $u(x,t) = \sum_{j\in\widetilde{\mathcal{N}}} \widetilde{u}_j(t)\sin(jx)$ and $v(x,t) = \sum_{j\in\widetilde{\mathcal{N}}} \widetilde{v}_j(t)\sin(jx)$ in terms of these eigenfunctions. Note that the equations (1.15) then take the form

$$\begin{aligned}
&\frac{d}{dt}\widetilde{u}_j(t) = \widetilde{v}_j(t),\\
&\frac{d}{dt}\widetilde{v}_j(t) = -\omega_j^2\widetilde{u}_j(t) + \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!}\sum_{j^1,\dots,j^m\in\widetilde{\mathcal{N}}} P_{j,(j^1,\dots,j^m)}\widetilde{u}_{j^1}(t)\cdots\widetilde{u}_{j^m}(t)
\end{aligned}$$

with

$$P_{j,(j^1,\dots,j^m)} = \frac{1}{\pi}\int_{[0,\pi]} \sin(jx)\sin(j^1x)\cdots\sin(j^mx)\,dx.$$

Since solutions of (1.17) are assumed to be real-valued, we have $\widetilde{u}_j(t) \in \mathbb{R}$ and $\widetilde{v}_j(t) \in \mathbb{R}$. Similar as for (1.14) we can introduce complex variables

$$\widetilde{\xi}_j = \frac{\omega_j^{\frac12}\widetilde{u}_j + i\omega_j^{-\frac12}\widetilde{v}_j}{\sqrt{2}} \quad\text{and}\quad \widetilde{\eta}_j = \overline{\widetilde{\xi}_j} = \frac{\omega_j^{\frac12}\widetilde{u}_j - i\omega_j^{-\frac12}\widetilde{v}_j}{\sqrt{2}}$$

to see that the same nonlinear wave equation with Dirichlet boundary conditions (1.17) is also a Hamiltonian partial differential equation with Hamiltonian function

$$\begin{aligned}
H(\widetilde{\xi},\widetilde{\eta}) = \sum_{j\in\widetilde{\mathcal{N}}}\omega_j\widetilde{\xi}_j\widetilde{\eta}_j - \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!(m+1)}&\\
\sum_{j^1,\dots,j^{m+1}\in\widetilde{\mathcal{N}}} P_{j^{m+1},(j^1,\dots,j^m)}\frac{\widetilde{\xi}_{j^1}+\widetilde{\eta}_{j^1}}{\sqrt{2\omega_{j^1}}}\cdots\frac{\widetilde{\xi}_{j^{m+1}}+\widetilde{\eta}_{j^{m+1}}}{\sqrt{2\omega_{j^{m+1}}}}&,
\end{aligned}\tag{1.18}$$

which is denoted again by H by a slight abuse of notation.

Conservation of Energy. We have conservation of energy $H(\xi,\overline{\xi})$ along solutions of the nonlinear wave equation with periodic boundary conditions (1.14) and Dirichlet boundary conditions (1.17) by Proposition 1.1. In terms of the functions $u = u(x,t)$ and $v = v(x,t)$ the energy reads by Parseval's equality

$$H(\xi,\overline{\xi}) = \frac{1}{2\pi}\int_{\mathbb{T}}\Big(|v|^2 + |\nabla u|^2 + \rho|u|^2 - \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!(m+1)}u^{m+1}\Big)\,dx$$

in the case of periodic boundary conditions (1.14) and two times the same expression with the integral only over $[0,\pi]$ in the case of Dirichlet boundary conditions (1.17) (this is true for both Hamiltonian formulations (1.16) and (1.18) of this equation presented above).

Non-Conservation of Mass. The Hamiltonian functions $H(\xi,\overline{\xi})$ for the nonlinear wave equation with periodic boundary conditions (1.14) and Dirichlet boundary conditions (1.17) are in general not invariant under the transformation $\xi \mapsto e^{i\theta}\xi$, and hence the mass $m(\xi,\overline{\xi})$ is in general not conserved along a solution of the nonlinear wave equations (1.14) and (1.17) by Propositions 1.2 and 1.3.

Conservation or Non-Conservation of Momentum. For the nonlinear wave equation with periodic boundary conditions (1.14) the Hamiltonian function $H(\xi,\overline{\xi})$ is invariant under the transformations $\xi \mapsto e^{i\theta j_l}\xi_j$ for $l = 1,\dots,d$. Hence, the momentum

$$\begin{aligned} K(\xi,\overline{\xi}) &= \sum_{j\in\mathcal{N}} j|\xi_j|^2 = \frac{1}{2}\sum_{j\in\mathcal{N}} j(\omega_j|u_j|^2 + \omega_j^{-1}|v_j|^2 + i\overline{u_j}v_j - iu_j\overline{v_j}) \\ &= \sum_{j\in\mathcal{N}} iju_{-j}v_j = -\frac{1}{2\pi}\int_{\mathbb{T}}\Big(\frac{\partial}{\partial x}u\Big)\Big(\frac{\partial}{\partial t}u\Big)\,dx \end{aligned}$$

is conserved along any solution of the nonlinear wave equations with periodic boundary conditions (1.14), see Proposition 1.4.

For the nonlinear wave equation with Dirichlet boundary conditions we have to distinguish the two Hamiltonian formulations derived in this section. For the first formulation (1.16), whose Hamiltonian function agrees with the one for periodic boundary conditions, we have again conservation of the momentum $K(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} j|\xi_j|^2$. However, since the solution satisfies Dirichlet boundary conditions, we have in this formulation that the coefficients u_j and v_j, $j \in \mathcal{N} = \mathbb{Z}$ are purely imaginary. This implies that $\xi_{-j} = -\xi_j$ and

$$K(\xi,\overline{\xi}) = 0.$$

For the second Hamiltonian formulation with Hamiltonian function (1.18) we do not have invariance under the transformations $\xi \mapsto e^{i\theta j_l}\xi_j$ for $l = 1,\dots,d$ anymore. Hence, we have for this formulation no conservation of momentum

$$K(\widetilde{\xi},\overline{\widetilde{\xi}}) = \sum_{j\in\widetilde{\mathcal{N}}} j|\widetilde{\xi}_j|^2 = \frac{1}{2}\sum_{j\in\widetilde{\mathcal{N}}} j(\omega_j|\widetilde{u}_j|^2 + \omega_j^{-1}|\widetilde{v}_j|^2).$$

This example shows that for different Hamiltonian formulations of Hamiltonian partial differential equations different notions of momentum (for instance) occur with even different conservation properties.

Non-Conservation of Actions. The Hamiltonian functions $H(\xi,\overline{\xi})$ for the nonlinear wave equations (1.14) and (1.17) are not invariant under the transformation $\xi_j \mapsto e^{i\theta}\xi_j$ for fixed $j \in \mathcal{N}$ and $\xi_l \mapsto 1$ for all $j \neq l \in \mathcal{N}$. By Propositions 1.2 and 1.5 the actions

$$I_j(\xi,\overline{\xi}) = |\xi_j|^2 = \frac{1}{2}(\omega_j|u_j|^2 + \omega_j^{-1}|v_j|^2 + i\overline{u_j}v_j - iu_j\overline{v_j})$$

for periodic boundary conditions (1.14) and

$$I_j(\xi,\overline{\xi}) = |\xi_j|^2 = \frac{1}{2}(\omega_j|u_j|^2 + \omega_j^{-1}|v_j|^2) = I_{-j}(\xi,\overline{\xi})$$

respectively

$$I_j(\widetilde{\xi},\overline{\widetilde{\xi}}) = |\widetilde{\xi}_j|^2 = \frac{1}{2}(\omega_j|\widetilde{u}_j|^2 + \omega_j^{-1}|\widetilde{v}_j|^2)$$

for Dirichlet boundary conditions (1.17) are not conserved along solutions of these nonlinear wave equations.

	linear	nonlinear		
		periodic boundary conditions (equation (1.14))	Dirichlet boundary conditions: formulation (1.16) (equation (1.17))	Dirichlet boundary conditions: formulation (1.18) (equation (1.17))
actions	exact conservation	non-conservation		
energy	exact conservation			
mass	exact conservation	non-conservation		
momentum	exact conservation			non-conservation

Table 2: Conservation properties of wave equations.

As in the case of Schrödinger equations we can also consider *linear wave equations*

$$\frac{\partial^2}{\partial t^2}u(x,t) = \Delta u(x,t)$$

which result in the same Hamiltonian system (1.2) as linear Schrödinger equations (1.3), (1.4), and (1.5) with the same conserved quantities actions, energy, mass, and momentum. All conservation results on wave equations are summarised in Table 2. The non-conserved quantities are nearly conserved over long times, as we will show in Sections 2.9 and 2.10.

2 Long-Time Analysis of Hamiltonian Partial Differential Equations

We study solutions of Hamiltonian partial differential equations in the general framework described in Chapter 1 on a long time interval (see the first two columns in Figure 1).

2.1 Weakly Nonlinear Hamiltonian Partial Differential Equations

We consider Hamiltonian functions of the form

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + P(\xi,\eta) \tag{2.1}$$

on an appropriate phase space $\mathcal{U}\times\mathcal{U} \subseteq l_s^2 \times l_s^2$ whose Hamiltonian equations of motion (1.1) become

$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) + \frac{\partial P}{\partial \eta_j}(\xi,\eta), \quad j\in\mathcal{N}\subseteq\mathbb{Z}^d. \tag{2.2}$$

P is a function with $\overline{P(\xi,\eta)} = P(\overline{\eta},\overline{\xi})$ having a zero of order (at least) three at the origin, and we will further specify it later on. The assumption $\overline{P(\xi,\eta)} = P(\overline{\eta},\overline{\xi})$ together with our general assumption $\overline{H(\xi,\eta)} = H(\overline{\eta},\overline{\xi})$ implies that the *frequencies* ω_j in the Hamiltonian function (2.1) have to be real. The examples of Schrödinger and wave equations discussed in Sections 1.3, 1.4, and 1.5 are of this form.

Linear Hamiltonian Partial Differential Equations. In the absence of the function P in (2.1), the Hamiltonian equations of motion (2.2) reduce to linear equations[1] with solution $\xi_j(t) = e^{-i\omega_j t}\xi_j(0)$. The linear Schrödinger equations discussed in Section 1.3 are of this form. By Proposition 1.1 the energy

$$H(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} \omega_j |\xi_j|^2$$

is conserved along any solution of (2.2). Moreover, since (for $P=0$) $H(\xi,\overline{\xi})$ is obviously invariant under the transformations $\xi\mapsto e^{i\theta}\xi$, $\xi_j\mapsto e^{i\theta j_l}\xi_j$, and $\xi_j\mapsto e^{i\theta}\xi_j$ for fixed $j\in\mathcal{N}$ and $\xi_l\mapsto 1$ for all $j\neq l\in\mathcal{N}$, also mass

$$m(\xi,\overline{\xi}) = (\xi,\xi)_0 = \sum_{j\in\mathcal{N}} |\xi_j|^2,$$

momentum

$$K(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} j|\xi_j|^2,$$

[1] For this reason we refer to P as the nonlinearity in (2.1).

and all actions

$$I_j(\xi,\overline{\xi}) = |\xi_j|^2, \quad j \in \mathcal{N},$$

are conserved by Propositions 1.3, 1.4, and 1.5 along any solution of (2.2) if $P = 0$. In fact, the conservation of actions can also be seen directly from the solution $\xi_j(t) = e^{-i\omega_j t}\xi_j(0)$ (since the frequencies ω_j are real) and implies the conservation of energy, mass, and momentum which all are sums of the actions. These are the properties mentioned in the first column of Figure 1.

Problem Setting. In the case $P \neq 0$, the equations of motion (2.2) are not necessarily linear anymore. The conservation of energy

$$H(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} \omega_j |\xi_j|^2 + P(\xi,\overline{\xi})$$

is still ensured by Proposition 1.1. However, in contrast to the linear situation, the behaviour of mass m, momentum K, and actions I_j along solutions of (2.2) is not clear anymore. For instance, along solutions of nonlinear Schrödinger equations, we have conservation of mass and sometimes also of momentum, whereas the actions are not conserved in general, see Section 1.4. For nonlinear wave equations mass, momentum, and actions are not conserved in general, see Section 1.5.

In other words, the presence of the nonlinearity P in the Hamiltonian function (2.1) can turn conserved quantities into non-conserved ones. Our aim is to study the influence of the nonlinearity P on these quantities when the nonlinear effects are small. Can we still expect mass, momentum, and actions to be at least approximately conserved? And if so, on which time interval is this true?

The nonlinear effects are small if the initial value $\xi(0)$ is small, of size ε say. This is the situation we study here. Then, after changing to new variables of size 1 by $\xi \mapsto \varepsilon^{-1}\xi$, the Hamiltonian equations of motion (2.2) take the form

$$i\frac{d}{dt}\xi_j(t) = \omega_j\xi_j(t) + \varepsilon^{-1}\frac{\partial P}{\partial \eta_j}(\varepsilon\xi(t), \varepsilon\overline{\xi(t)}), \quad j \in \mathcal{N}. \tag{2.3}$$

Since P is assumed to have a zero of order (at least) three at the origin, the nonlinearity in the equations of motion is expected to be of size ε. We refer to this situation as *weakly nonlinear*.

What We Can Expect. Since the nonlinearity in the equations of motion (2.3) is of size ε, we can expect the nonlinear effects to be small on a time interval of length ε^{-1}. This will be made rigorous in Section 3.4. In particular, we have at least *near-conservation* of mass, momentum, and actions on such time intervals. We show here that this is actually true on much longer time intervals of length ε^{-N} for any given number N.

Birkhoff Normal Form Techniques. In order to understand the problem just described in the finite dimensional context, Birkhoff [7], see also [31, Section 3], introduced in the early 20th century a sequence of changes of variables bringing the Hamiltonian function (2.1) to the form

$$H_0^{(n)}(|\xi^{(n)}|^2) + P^{(n)}(\xi^{(n)}, \eta^{(n)})$$

after n changes of variables. Here, $H_0^{(n)}$ depends only on the actions $(|\xi_j^{(n)}|^2)_{j\in\mathcal{N}}$, and $P^{(n)}$ has a zero of order (at least) $n+3$ at the origin. Without $P^{(n)}$ we have exact conservation of actions due to Proposition 1.5. As above, the nonlinear effects introduced by $P^{(n)}$ can be considered small on a time interval of length ε^{-n-1}, since the nonlinearity $P^{(n)}$ is assumed to have a zero of order at least $n+3$ at the origin. This implies near-conservation of actions on time intervals of length ε^{-n-1}. Since mass and momentum are sums of the actions, this is the key to understand also the behaviour of these quantities on long time intervals.

This Birkhoff normal form technique was just recently adapted to the infinite dimensional context by Bourgain [8], Bambusi [3], Bambusi and Grébert [4], and Grébert [31]. Here we follow a different approach based on modulated Fourier expansions, see Chapter 3. This approach has been so far applied to the examples of nonlinear wave equations by Cohen, Hairer, and Lubich [17] and nonlinear Schrödinger equations [29], and it is extended here to a general class of Hamiltonian partial differential equations.

2.2 Long-Time Near-Conservation of Actions

The key for understanding the long-time behaviour of weakly nonlinear Hamiltonian partial differential equations as introduced in the preceding section is the near-conservation of actions on a long time interval $0 \le t \le \varepsilon^{-N}$, where ε describes the smallness of the initial value.

We fix N. For our study of the influence of the nonlinearity P in (2.1) on the conservation of actions we will need the following assumptions on the nonlinearity P and on the frequencies ω_j.

Assumption 2.1 (Regularity Assumption on P)**.** We assume that there is an s_0 such that $\frac{\partial P}{\partial \eta_j}$ is analytic for any $j \in \mathcal{N}$ in a neighbourhood of zero in $l_s^2 \times l_s^2$ for all $s \ge s_0$ with an expansion

$$\frac{\partial P}{\partial \eta_j}(\xi,\eta) = \sum_{m,m'=0}^{\infty} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l}\,\xi_{k^1}\cdots\xi_{k^m}\eta_{l^1}\cdots\eta_{l^{m'}}, \tag{2.4}$$

and has a zero of order at least 2 at the origin,

$$P_{j,k,l} = 0 \quad \text{for } j \in \mathcal{N},\ k \in \mathcal{N}^m, \text{ and } l \in \mathcal{N}^{m'} \text{ with } m + m' < 2. \tag{2.5}$$

Writing moreover

$$|P|_j^{m,m'}(\xi^1,\dots,\xi^m,\eta^1,\dots,\eta^{m'}) = \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} |P_{j,k,l}|\,\xi^1_{k^1}\cdots\xi^m_{k^m}\eta^1_{l^1}\cdots\eta^{m'}_{l^{m'}}$$

for $\xi^1,\ldots,\xi^m,\eta^1,\ldots,\eta^{m'}\in l_s^2$ we assume that $|P|^{m,m'}=(|P|_j^{m,m'})_{j\in\mathcal{N}}\in l_s^2$ with

$$\||P|^{m,m'}(\xi^1,\ldots,\xi^m,\eta^1,\ldots,\eta^{m'})\|_s\le C_{m,m',s}\|\xi^1\|_s\cdots\|\xi^m\|_s\|\eta^1\|_s\cdots\|\eta^{m'}\|_s. \tag{2.6a}$$

$C_{m,m',s}$ are constants depending only on P, m, m', and s, such that

$$\sum_{m+m'=2}^{\infty} C_{m,m',s}|z|^{m+m'-2}\le C_s \quad \text{for all } |z|\le C_1 \tag{2.6b}$$

with a constant C_1 and a constant C_s depending only on P and s. For convenience we write $C_{L,s}=\max_{m+m'\le L} C_{m,m',s}$.

Taking the modulus of the coefficients $P_{j,k,l}$ in Assumption 2.1 is referred to as taking the modulus of a map in [4]. The regularity assumption implies in particular

$$\Big\|\frac{\partial P}{\partial \eta_j}(\xi,\bar\xi)\Big\|_s\le \sum_{m+m'=2}^{\infty} C_{m,m',s}\|\xi\|_s^{m+m'}\le C_s\|\xi\|_s^2 \tag{2.7}$$

for $\|\xi\|_s\le C_1$.

Assumption 2.2 (Condition of Small Dimension or Zero Momentum)**.** We assume that the frequencies ω_j grow like a power of $|j|$, i.e., there exist positive constants c_2, C_2, and σ such that

$$c_2|j|^\sigma\le|\omega_j|\le C_2|j|^\sigma \quad \text{for all } j\in\mathcal{N}. \tag{2.8}$$

Moreover, we assume that

$$s_0\le\sigma \quad \text{and} \quad s\ge N+3+3s_0 \tag{2.9a}$$

with s_0 and s from the regularity assumption 2.1. If (2.9a) is not fulfilled, we alternatively assume that

$$P_{j,k,l}\ne 0 \text{ implies } j=k^1+\cdots+k^m-l^1-\cdots-l^{m'} \tag{2.9b}$$

for $j\in\mathcal{N}$, $k\in\mathcal{N}^m$, and $l\in\mathcal{N}^{m'}$. In the latter assumption the addition $+$ of indices is not necessarily the addition in $\mathbb{Z}^d$. Any addition such that the triangle inequality for $|\cdot|$ is fulfilled can be considered.[2]

As we will see in the examples in Sections 2.6, 2.7, 2.8, and 2.9, we have $\sigma=2$ and $\sigma=1$ for d-dimensional Schrödinger and wave equations, respectively, and s_0 can be chosen as any number greater than $\frac{d}{2}$. Accordingly, the assumption (2.9a) can be interpreted as a condition of small dimension.

In [4], $k^1+\cdots+k^m-l^1-\cdots-l^{m'}-j$ is referred to as the *momentum* of (j,k,l). Accordingly, condition (2.9b) is a condition of zero momentum which is indeed fulfilled

[2] If we study for instance the equations of motion of a semi-discretization in space of a Hamiltonian partial differential equation, the addition of indices can be the addition modulo $2M$ for $M\in\mathbb{N}$, see Sections 4.5 and 4.6.

in many examples. We emphasize that only one of the conditions, either the condition of zero momentum (2.9b) or the condition of small dimension (2.9a), has to be satisfied.

We now turn to the formulation of a non-resonance condition on the frequencies ω_j, $j \in \mathcal{N}$. For a sequence $\mathbf{k} = (k_l)_{l\in\mathcal{N}} \in \mathbb{Z}^{\mathcal{N}}$ of integers k_l indexed by $\mathcal{N}$ and the sequence $\boldsymbol{\omega} = (\omega_l)_{l\in\mathcal{N}}$ of frequencies we write

$$\mathbf{k}\cdot\boldsymbol{\omega} = \sum_{l\in\mathcal{N}} k_l\omega_l, \quad \|\mathbf{k}\| = \sum_{l\in\mathcal{N}} |k_l|, \quad \mathbf{j}^{(s-s_0)|\mathbf{k}|} = \prod_{l\in\mathcal{N}} |l|^{(s-s_0)|k_l|}, \quad j(\mathbf{k}) = \sum_{l\in\mathcal{N}} k_l l,$$

where $j(\mathbf{k})$ is only defined (and also needed) if the condition of zero momentum (2.9b) in Assumption 2.2 is satisfied with the addition of indices used there. Since we have to divide by $\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j$ in our analysis, we impose the following non-resonance condition in order to control the effect of possibly small denominators.

Assumption 2.3 (Non-Resonance Condition)**.** Let $\varepsilon \le \varepsilon_0$ for fixed $\varepsilon_0 \le 1$. We define an *(ε-)near-resonant* index $(j, \mathbf{k})$ as an index with

$$\|\mathbf{k}\| \le 2N + 4 + 4s_0, \quad \mathbf{k} \ne \langle j\rangle, \quad \text{and} \quad |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| < \varepsilon^{\frac{1}{2}},$$

where $\langle j\rangle = (\delta_{jl})_{l\in\mathcal{N}}$ with Kronecker's delta. For given N and $s \ge s_0$ from the regularity assumption 2.1 we impose the non-resonance condition

$$\frac{|j|^{s-s_0}}{\mathbf{j}^{(s-s_0)|\mathbf{k}|}}\varepsilon^{\frac{1}{2}\|\mathbf{k}\|} \le C_0\varepsilon^{N+3+2s_0} \quad \text{for any } (\varepsilon\text{-})\text{near-resonant index } (j,\mathbf{k}) \tag{2.10}$$

and any $\varepsilon \le \varepsilon_0 \le 1$ on the frequencies ω_l, $l \in \mathcal{N}$, with a constant C_0 independent of ε and $(j, \mathbf{k})$. If the condition of zero momentum (2.9b) is satisfied in Assumption 2.2, only near-resonant indices of the form $(j(\mathbf{k}), \mathbf{k})$ have to be considered in (2.10).

This non-resonance condition 2.3 can be interpreted as follows. Whenever a sum of frequencies becomes small (in terms of $\varepsilon^{\frac{1}{2}}$), at least three of its frequencies have to be large (in terms of ε^{-1}).

The following additional non-resonance condition is not needed in our theorems and their proofs, but we can prove stronger estimates if it is fulfilled in combination with the condition of zero momentum (2.9b) in Assumption 2.2. It allows to avoid near-resonances among three frequencies.

Assumption 2.4 (Additional (Optional) Non-Resonance Condition)**.** There exists a positive constant C_3 such that

$$|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_{j(\mathbf{k})}| \ge C_3^{-1} \quad \text{for all } \mathbf{k} \ne \langle j\rangle \text{ with } \|\mathbf{k}\| \le 2, \tag{2.11}$$

and the condition of zero momentum (2.9b) is satisfied in Assumption 2.2.

Under these assumptions we have the following theorem.

Theorem 2.5 (Long-Time Near-Conservation of Actions). *Fix N and let the regularity assumption 2.1, the condition of small dimension or zero momentum 2.2, and the non-resonance condition 2.3 be satisfied. Then for any ε sufficiently small compared to C_1, C_{s_0}, C_s, and $s \geq 2s_0$ from 2.1, c_2, C_2, and σ from 2.2, C_0 and ε_0 from 2.3, and N and for small initial values*

$$\|\xi(0)\|_s \leq \varepsilon$$

we have near-conservation of actions

$$\sum_{l \in \mathcal{N}} |l|^{2s} \frac{|I_l(\xi(t), \overline{\xi(t)}) - I_l(\xi(0), \overline{\xi(0)})|}{\varepsilon^2} \leq C \varepsilon^{\frac{1}{2}} \tag{2.12}$$

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

along any solution $\xi(t)$ of the Hamiltonian equations of motion (2.2) *with a constant C depending only on C_1, C_{s_0}, C_s, s_0, s, c_2, C_2, σ, C_0, and N, but not on ε.*

The near-conservation of actions improves to $C\varepsilon$ with a constant C depending in addition on C_3 if in addition the non-resonance condition 2.4 is satisfied.

The following Chapter 3 is devoted to the proof of this theorem.

Invariant Tori of Linear Hamiltonian Partial Differential Equations. Solutions $\xi_j(t) = e^{-i\omega_j t}\xi_j(0)$ of linear Hamiltonian partial differential equations with $P = 0$ in the Hamiltonian function (2.1) evolve on the torus

$$\mathbb{T}_\eta = \{\, \xi : I_j(\xi, \overline{\xi}) = \eta_j \,\}$$

for $\eta = (\eta_j)_{j \in \mathcal{N}} = \xi(0)$. Theorem 2.5 implies that solutions $\xi(t)$ of the nonlinear partial differential equation (2.2) starting on the torus $\mathbb{T}_{\xi(0)}$ with $\|\xi(0)\|_s \leq \varepsilon$ stay close to this torus,

$$d_s(\xi(t), \mathbb{T}_{\xi(0)}) \leq C \varepsilon^{\frac{5}{4}}, \tag{2.13}$$

over long times. Here, d_s denotes the distance in l_s^2 defined by $d_s(\xi, \eta) = \|\xi - \eta\|_s$. In order to prove (2.13) we choose for $\xi = \xi(t)$ an $\eta \in \mathbb{T}_{\xi(0)}$ in such a way that $\|\xi - \eta\|_s = \||\xi(t)| - |\xi(0)|\|_s$ and use $||\xi_j(t)| - |\xi_j(0)||^2 \leq ||\xi_j(t)|^2 - |\xi_j(0)|^2|$.

In the remaining part of this chapter we formulate adaptations of this theorem to slightly more general situations, derive important implications, and apply it to various examples.

The Case of Partial Resonances. For the nonlinear wave equation with periodic boundary conditions as discussed in Section 1.5 the frequencies $\omega_j = \sqrt{j^2 + \rho}$ are *completely resonant* in the sense that a nontrivial linear combination of them can equal zero. This is caused by the fact that $\omega_j = \omega_{-j}$. However, if this is the only reason for complete resonances among the frequencies, we can adapt Theorem 2.5 on the long-time near-conservation of actions to a long-time near-conservation of certain sums of actions. This condition is now formulated precisely, replacing the non-resonance condition 2.3.

Assumption 2.6 (Non-Resonance Condition in the Presence of Completely Resonant Frequencies)**.** We denote the *resonance module* (see [6] or [15]) by

$$\mathcal{M} = \{\, \mathbf{k} \in \mathbb{Z}^{\mathcal{N}} : \mathbf{k} \cdot \boldsymbol{\omega} = 0 \,\}.$$

The non-resonance condition 2.3 is then relaxed to the condition that only near-resonant indices $(j, \mathbf{k})$ with $\mathbf{k} - \langle j \rangle \notin \mathcal{M}$ are assumed to satisfy the non-resonance condition (2.10). In order to control the complete resonances in $\mathcal{M}$ we assume that for any $m \in \mathbb{N}$

$$\text{if } \mathbf{k} \in \mathcal{M}, \text{ then } \sum_{j \in \mathcal{N}:|j|=m} k_j = \sum_{j \in \mathcal{N}:|j|=m} k_j \omega_j = 0. \tag{2.14}$$

Note that this non-resonance condition 2.6 does not control resonances which appear for example for $\rho = 0$ in the nonlinear wave equation. It is an open problem how to deal with such "hyper-resonant" Hamiltonian partial differential equations. For hyper-resonant nonlinear Schrödinger equations ((1.7) with $V = 0$) long-time regularity in spatial dimension one ($d = 1$) is shown for many initial values by Bourgain [10].

If the non-resonance condition 2.3 is replaced by the non-resonance condition 2.6, we cannot expect the actions to be approximately conserved anymore since exchanges among the modes ξ_l with constant $|l|$ are possible due to the resonances. However, we can control the sums of actions

$$\sum_{l \in \mathcal{N}:|l|=m} I_l(\xi, \overline{\xi})$$

for $m \in \mathbb{N}$ in which the possibly exchanging actions are collected.

Theorem 2.7 (Long-Time Near-Conservation of Sums of Actions)**.** *Under the assumptions of Theorem 2.5 but with the non-resonance condition 2.3 replaced by the non-resonance condition 2.6 we have near-conservation of sums of actions*

$$\sum_{m \in \mathbb{N}} m^{2s} \frac{\left|\sum_{l \in \mathcal{N}:|l|=m} I_l(\xi(t), \overline{\xi(t)}) - \sum_{l \in \mathcal{N}:|l|=m} I_l(\xi(0), \overline{\xi(0)})\right|}{\varepsilon^2} \le C \varepsilon^{\frac{1}{2}} \tag{2.15}$$

over long times

$$0 \le t \le \varepsilon^{-N}$$

with the constant C of Theorem 2.5.

As there, the estimate improves to $C\varepsilon$ if in addition the non-resonance condition 2.4 is satisfied.

The proof of this theorem is also given in Chapter 3.

Comparison with the Dynamic Consequences of Birkhoff Normal Form Results (Bambusi and Grébert [4], [31])**.** Similar results as in Theorems 2.5 and 2.7 have been obtained by Bambusi and Grébert [4, Corollary 2.16] and [31, Corollary 4.8]. Our result on the near-conservation of actions is slightly stronger since their result is an estimate of the individual summands in (2.12) and (2.15), whereas we estimate the total sum.

As in the present thesis they consider a general class of Hamiltonian partial differential equations. Our assumptions defining the considered class are weaker than the assumptions used by Bambusi and Grébert [4], [31]. In [4], a so called "tame estimate" replaces our assumption (2.6) on the regularity of the nonlinearity P in 2.1. In this tame estimate the product on the right-hand side of (2.6) is replaced by a sum of such products with only one factor in the l_s^2-norm and all the other factors in lower norms, see [4, Definition 2.2]. This is clearly a stronger assumption than our Assumption 2.1. Moreover, the proof of [31, Proposition 6.1] shows that the assumption used in [31] also implies a kind of tame estimate stronger than our Assumption 2.1. In the following section we will moreover show in Lemma 2.8 that the non-resonance condition used by Bambusi and Grébert implies our non-resonance condition 2.3. Concerning our Assumption 2.2, we mention that Bambusi and Grébert use a condition of zero momentum similar to (2.9b) if they consider partial differential equations in more than one spatial dimension (which do not satisfy the condition of small dimension (2.9a)).

2.3 On the Non-Resonance Condition

The non-resonance condition 2.3 (or 2.6 for partially resonant frequencies) turns out to be the most crucial assumption we made. It excludes in particular hyper-resonant Hamiltonian partial differential equations such as nonlinear Schrödinger equations (1.7) with $V = 0$ and nonlinear wave equations (1.14) and (1.17) with $\rho = 0$. However, we can show that the non-resonance condition is satisfied in many situations. We do this by reducing our non-resonance condition 2.3 to the one used by Bambusi and Grébert [3], [4], and [31] which has been shown to be valid in many situations. Their non-resonance condition reads as follows, see [4, Inequality (2.22)], [3, Inequality (3.3)], and [31, Definition 4.4].

Non-Resonance Condition by Bambusi and Grébert. For any $r' \in \mathbb{N}$ there exist $\gamma > 0$ and $\alpha \in \mathbb{R}$ such that for any $r \in \mathbb{N}$ and any $\widetilde{\mathbf{k}} \in \mathbb{Z}^{\mathcal{N}}$

$$|\widetilde{\mathbf{k}} \cdot \boldsymbol{\omega}| \geq \frac{\gamma}{r^\alpha} \quad \text{if} \quad 0 \neq \|\widetilde{\mathbf{k}}\| \leq r' + 2 \text{ and } \sum_{|l|>r} |\widetilde{k}_l| \leq 2. \tag{2.16}$$

Similar to our non-resonance condition 2.3, this condition can be interpreted as a condition requiring that a small sum of frequencies contains at least three large frequencies. However, the sizes are here measured in terms of $|j|$ for frequencies ω_j whereas they are measured in terms of ε in our non-resonance condition 2.3. Indeed, the non-resonance condition 2.3 is implied by the non-resonance condition (2.16) used by Bambusi and Grébert.

Lemma 2.8 ([17, Lemma 1]). *If the asymptotics of the frequencies* (2.8) *in Assumption 2.2 is valid and if* $\varepsilon \leq 1$*, then we have the following result.*

If the non-resonance condition (2.16) *is fulfilled for* $\widetilde{\mathbf{k}} = \mathbf{k} - \langle j \rangle$ *with a near-resonant index* $(j, \mathbf{k})$*, then this near-resonant index also satisfies the non-resonance condition* (2.10) *in Assumption 2.3 for* $s \geq 2\alpha(N+3+2s_0)+s_0$ *and a constant* C_0 *depending only on* α, γ, s_0, c_2, C_2, σ, *and* N, *where* α *and* γ *are chosen in* (2.16) *for* $r' = 2N+3+4s_0$.

In particular, the non-resonance condition (2.16) *implies the non-resonance condition 2.3.*

Proof. Let $(j, \mathbf{k})$ be near-resonant, i.e., $|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| < \varepsilon^{\frac{1}{2}}$, $\mathbf{k} \neq \langle j\rangle$, and $\|\mathbf{k}\| \leq 2N+4+4s_0$. We have to show that

$$\frac{|j|^{s-s_0}}{\mathbf{j}^{(s-s_0)|\mathbf{k}|}}\varepsilon^{\frac{1}{2}\|\mathbf{k}\|} \leq C_0 \varepsilon^{N+3+2s_0}$$

for a constant C_0.

The asymptotics of the frequencies (2.8) implies (without loss of generality we assume $C_2 \geq 1$)

$$|j| \leq \Big(\frac{|\omega_j|}{c_2}\Big)^{\frac{1}{\sigma}} \leq \Big(\frac{|\mathbf{k}\cdot\boldsymbol{\omega}| + \varepsilon^{\frac{1}{2}}}{c_2}\Big)^{\frac{1}{\sigma}} \leq \Big(\frac{2C_2\|\mathbf{k}\||\bar{l}|^{\sigma}}{c_2}\Big)^{\frac{1}{\sigma}}, \tag{2.17}$$

where $\bar{l} \in \mathcal{N}$ denotes the largest index (not necessarily unique) with respect to $|\cdot|$ with $k_{\bar{l}} \neq 0$. Now, let $r \in \mathbb{N}$ be minimal such that $\sum_{|l|>r}|k_l| \leq 1$. In particular, we have $r = |\bar{l}|$ and $|k_{\bar{l}}| \geq 2$, or there exists $\bar{l} \neq l \in \mathcal{N}$ with $r = |l| \leq |\bar{l}|$ and $k_l \neq 0$. In both cases $\mathbf{j}^{(s-s_0)|\mathbf{k}|} \geq |\bar{l}|^{s-s_0} r^{s-s_0}$, and in conjunction with (2.17) we get

$$\frac{|j|^{s-s_0}}{\mathbf{j}^{(s-s_0)|\mathbf{k}|}} \leq \Big(\frac{2C_2\|\mathbf{k}\|}{c_2}\Big)^{\frac{s-s_0}{\sigma}} \frac{1}{r^{s-s_0}}. \tag{2.18}$$

This means that we can control $\frac{|j|}{\mathbf{j}^{|\mathbf{k}|}}$ by $\frac{1}{r}$ where ω_l with $|l| = r$ is asymptotically the second largest frequency in $\mathbf{k}\cdot\boldsymbol{\omega}$.

We now use the non-resonance condition (2.16), where we choose $r' = 2N+3+4s_0$, which gives us a control on r. We write $\widetilde{\mathbf{k}} = \mathbf{k} - \langle j\rangle$ and note that $0 \neq \|\widetilde{\mathbf{k}}\| \leq r'+2$ and $\sum_{|l|>r}|\widetilde{k}_l| \leq 2$. Then by (2.16)

$$\frac{\gamma}{r^{\alpha}} \leq |\widetilde{\mathbf{k}}\cdot\boldsymbol{\omega}| = |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| < \varepsilon^{\frac{1}{2}},$$

and with (2.18)

$$\frac{|j|^{s-s_0}}{\mathbf{j}^{(s-s_0)|\mathbf{k}|}} \leq \Big(\frac{2C_2\|\mathbf{k}\|}{c_2}\Big)^{\frac{s-s_0}{\sigma}} \Big(\frac{\varepsilon^{\frac{1}{2}}}{\gamma}\Big)^{\frac{s-s_0}{\alpha}}.$$

In other words, $(j, \mathbf{k})$ satisfies (2.10) for s as specified in the lemma and

$$C_0 = \Big(\frac{2C_2\|\mathbf{k}\|}{c_2}\Big)^{\frac{s-s_0}{\sigma}} \gamma^{-\frac{s-s_0}{\alpha}}.$$

Since the condition (2.10) becomes weaker the larger s, we can indeed choose C_0 independently of s. □

2.4 Long-Time Regularity and Long-Time Analysis of Mass and Momentum

Theorems 2.5 and 2.7 on the long-time near-conservation of actions or sums of them along solutions of (2.2) have several important consequences. A first implication of these theorems is the long-time regularity of the solution of (2.2).

Corollary 2.9 (Long-Time Regularity). *Under the assumptions of Theorem 2.5 or Theorem 2.7 we have regularity*

$$\|\xi(t)\|_s \leq 2\varepsilon \tag{2.19}$$

over long times

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

Proof. This follows immediately from Theorem 2.5 since

$$\|\xi\|_s = \Big(\sum_{l\in\mathcal{N}} |l|^{2s} I_l(\xi,\overline{\xi})\Big)^{\frac{1}{2}} = \Big(\sum_{m\in\mathbb{N}} m^{2s} \sum_{l\in\mathcal{N}:|l|=m} I_l(\xi,\overline{\xi})\Big)^{\frac{1}{2}}$$

and $\|\xi(0)\|_s \leq \varepsilon$ (we choose ε sufficiently small compared to the constant of Theorem 2.5 which depends only on C_1, C_{s_0}, C_s, s_0, s, c_2, C_2, σ, C_0, and N). □

We now study mass

$$m(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} |\xi_j|^2$$

and momentum

$$K(\xi,\overline{\xi}) = \sum_{j\in\mathcal{N}} j|\xi_j|^2$$

along solutions of (2.2). Propositions 1.3 and 1.4 imply their exact conservation provided that the Hamiltonian function is invariant under some transformations. If this is not the case, Theorem 2.5 and for the mass also Theorem 2.7 still allow us to show their near-conservation over long times, since they both are sums of the actions $I_j(\xi,\overline{\xi}) = |\xi_j|^2$.

Corollary 2.10 (Long-Time Near-Conservation of Mass). *Under the assumptions of Theorem 2.5 or Theorem 2.7 we have near-conservation of mass*

$$\frac{|m(\xi(t),\overline{\xi(t)}) - m(\xi(0),\overline{\xi(0)})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{2.20}$$

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

with the constant C of Theorem 2.5.

As there, the estimate improves to $C\varepsilon$ if in addition the non-resonance condition 2.4 is satisfied.

Proof. We just note that

$$
\begin{aligned}
|m(\xi(t),\overline{\xi(t)}) - m(\xi(0),\overline{\xi(0)})| &\le \sum_{m\in\mathbb{N}} \Big| \sum_{l\in\mathcal{N}:|l|=m} I_l(\xi(t),\overline{\xi(t)}) - I_l(\xi(0),\overline{\xi(0)}) \Big| \\
&\le \sum_{l\in\mathcal{N}} |I_l(\xi(t),\overline{\xi(t)}) - I_l(\xi(0),\overline{\xi(0)})|.
\end{aligned}
$$

The result now follows from Theorem 2.5 or Theorem 2.7. □

Corollary 2.11 (Long-Time Near-Conservation of Momentum)**.** *Under the assumptions of Theorem 2.5 and for $s \ge \frac{1}{2}$ we have near-conservation of momentum*

$$
\frac{|K_l(\xi(t),\overline{\xi(t)}) - K_l(\xi(0),\overline{\xi(0)})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{2.21}
$$

for $l = 1,\dots,d$ over long times

$$
0 \le t \le \varepsilon^{-N}
$$

with the constant C of Theorem 2.5.

As there, the estimate improves to $C\varepsilon$ if in addition the non-resonance condition 2.4 is satisfied.

Proof. We have

$$
|K_l(\xi(t),\overline{\xi(t)}) - K_l(\xi(0),\overline{\xi(0)})| \le \sum_{j\in\mathcal{N}} |j_l||I_j(\xi(t),\overline{\xi(t)}) - I_j(\xi(0),\overline{\xi(0)})|,
$$

and since $|j_l| \le |j|$ the result once again follows from Theorem 2.5. □

The proof of Corollary 2.11 is not applicable in the case of partial resonances discussed in Theorem 2.7 (in contrast to the proof of Corollary 2.10). Long-time investigations of the momentum in this situation rely on the particular structure of the Hamiltonian function H, see for example Section 4.5.

2.5 Long-Time Energy Distribution

In this section we study again solutions of the Hamiltonian equations of motion (2.2) with small initial values

$$
\|\xi(0)\|_s \le \varepsilon.
$$

In addition we assume that there are only finitely many nonzero coefficients $\xi_j(0)$ in the initial value. We distinguish two different situations.

(a) All nonzero coefficients of the initial value are located in a finite band (of width $2B$, centered at zero),

$$
\xi_j(0) = 0 \quad \text{for } |j| > B, \tag{2.22a}
$$

see also Figure 2.

(b) There is a pair of nonzero coefficients $\xi_{\tilde{j}}(0)$ and $\xi_{-\tilde{j}}(0)$ with $\tilde{j} \neq 0$ in the initial value,

$$\xi_j(0) = 0 \quad \text{for all } \pm\tilde{j} \neq j \in \mathcal{N}, \tag{2.22b}$$

see also Figure 3.

In other words, all the energy is initially located in a finite number of modes (the energy in a mode ξ_j is defined as the action $I_j(\xi, \overline{\xi})$ multiplied with the frequency ω_j). In this section we examine how this energy is distributed among the other modes along a solution of (2.2).

What We Can Expect. First of all, Theorem 2.5 (or Theorem 2.7 in the case of partial resonances) ensures that the actions I_j (i.e., the energy in the jth mode) stay of size $\varepsilon^{\frac{5}{2}}$ (or even ε^3) in all modes which are zero initially on a long time interval of length ε^{-N}. We have

$$\sum_{j \notin \mathcal{B}} |j|^{2s} I_j(\xi(t), \overline{\xi(t)}) \leq C\varepsilon^{\frac{5}{2}} \quad (\text{or even } C\varepsilon^3),$$

where $\mathcal{B} = \{\, j \in \mathcal{N} : |j| \leq B \,\}$ in situation (2.22a) and $\mathcal{B} = \{\pm\tilde{j}\}$ in situation (2.22b), over long times

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

If we impose the condition of zero momentum (2.9b) in Assumption 2.2, we can expect more, at least on a short time interval. The Hamiltonian equations of motion (2.2) then take the form (see also (2.4))

$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) + \sum_{m+m'=2}^{\infty} \sum_{\substack{k^1+\cdots+k^m \\ -l^1-\cdots-l^{m'}=j}} P_{j,k,l}\, \xi_{k^1} \cdots \xi_{k^m} \overline{\xi_{l^1} \cdots \xi_{l^{m'}}} \tag{2.23}$$

with $k = (k^1, \ldots, k^m)$ and $l = (l^1, \ldots, l^{m'})$.

(a) Assuming an initial value as in (2.22a) with all the energy located in a finite band we notice that for $(m-1)B < |j| \leq mB$ the nonlinearity in (2.23) is of size ε^m since it contains at least m modes of the initially excited band $|j| \leq B$. Since $\xi_j(0) = 0$ for $|j| > B$, we can therefore expect the modes ξ_j with $(m-1)B < |j| \leq mB$ to be of size ε^m, at least on a short time interval, see Figure 2.

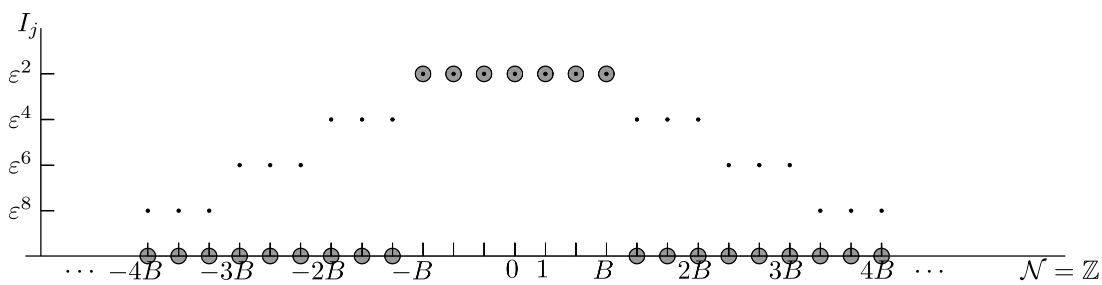

Figure 2: Initial (grey dots) and expected (black dots) energy distribution for (2.22a).

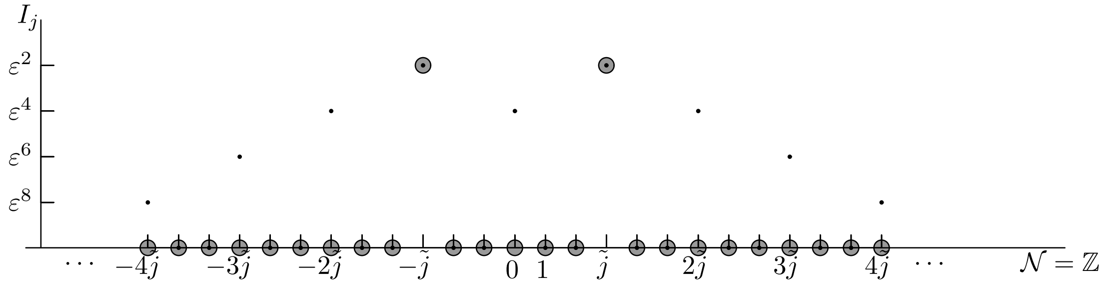

Figure 3: Initial (grey dots) and expected (black dots) energy distribution for (2.22b).

(b) For initial values with only an excited pair of modes $\xi_{\tilde{j}}$ and $\xi_{-\tilde{j}}$ as in (2.22b) we expect that — due to the condition of zero momentum — this mode distributes its energy only among the modes ξ_j with $j \in \{\, m\tilde{j} : m \in \mathbb{Z}\,\}$. Here and in the following, the addition used in the condition of zero momentum (2.9b) is used to compute $m\tilde{j}$. Moreover, we expect by an analysis of the nonlinearity in (2.23) that ξ_0 and $\xi_{\pm 2\tilde{j}}$ are of size ε^2, $\xi_{\pm 3\tilde{j}}$ are of size ε^3, and so on, see Figure 3.

As it turns out, we are able to study all these situations on a long time interval by the following generalisation of Theorem 2.5 (or Theorem 2.7) which enables us to treat scaled norms

$$\|\xi\|_{s,e} = \Big(\sum_{j\in\mathcal{N}} \varepsilon^{-2e(j)(1-\mu)} |j|^{2s} |\xi_j|^2\Big)^{\frac{1}{2}} = \|(\varepsilon^{-e(j)(1-\mu)}\xi_j)_{j\in\mathcal{N}}\|_s$$

and correspondingly scaled actions. As a scaling function we will later choose $e(j)$ such that $\varepsilon^{2e(j)}$ represents the expected energy distribution.

Theorem 2.12 (Long-Time Near-Conservation of Scaled Actions)**.** *Let $e : \mathcal{N} \to \mathbb{R}_+$ satisfy the triangle inequality and let $0 < \mu \le 1$. (If the nonlinearity $\frac{\partial P}{\partial \eta_j}$ is at least cubic for all $j \in \mathcal{N}$ and $P_{j,k,l} \neq 0$ only for $k \in \mathcal{N}^{m+1}$ and $l \in \mathcal{N}^m$, then the triangle inequality has to be satisfied only for sums of at least three indices.)*

Under the assumptions of Theorem 2.5 with the condition of zero momentum (2.9b) *satisfied in Assumption 2.2 and for small initial values*

$$\|\xi(0)\|_{s,e} \le \varepsilon^{\mu}$$

instead of $\|\xi(0)\|_s \le \varepsilon$ with ε^μ satisfying the smallness assumption of Theorem 2.5 we have near-conservation of scaled actions

$$\sum_{l\in\mathcal{N}} |l|^{2s} \frac{|I_l(\xi(t),\overline{\xi(t)}) - I_l(\xi(0),\overline{\xi(0)})|}{\varepsilon^{2e(l)(1-\mu)+2\mu}} \le C\varepsilon^{\frac{1}{2}\mu}$$

over long times

$$0 \le t \le \varepsilon^{-N\mu}$$

with the constant C of Theorem 2.5.

In the situation of partial resonances as in Theorem 2.7 we have near-conservation of sums of scaled actions

$$\sum_{m\in\mathbb{N}} m^{2s} \frac{\left|\sum_{l\in\mathcal{N}:|l|=m} I_l(\xi(t),\overline{\xi(t)}) - \sum_{l\in\mathcal{N}:|l|=m} I_l(\xi(0),\overline{\xi(0)})\right|}{\varepsilon^{2e(m)(1-\mu)+2\mu}} \leq C\varepsilon^{\frac{1}{2}\mu}$$

over long times $0 \leq t \leq \varepsilon^{-N\mu}$ if $e(l) = e(|l|)$ depends only on $|l|$.

The near-conservation of actions or sums of actions improves to $C\varepsilon^{\mu}$ with a constant C depending in addition on C_3 if in addition the non-resonance condition 2.4 is satisfied.

The proof of this theorem is given in Section 3.7 and consists of an easy modification of the proofs of Theorems 2.5 and 2.7 given in Chapter 3. For $\mu = 1$ Theorem 2.12 reduces to Theorems 2.5 and 2.7. In applying this theorem we focus first on the situation (2.22a) of a finite band initial value $\xi(0)$.

Corollary 2.13 (Long-Time Energy Distribution (a))**.** *Let $0 < \mu \leq 1$. Under the assumptions of Theorem 2.5 or Theorem 2.7 with the condition of zero momentum* (2.9b) *satisfied in Assumption 2.2 and for small initial values*

$$\|\xi(0)\|_s \leq \varepsilon \quad \textit{with } (2.22a)$$

we have for any ε, such that ε^{μ} satisfies the smallness assumption of Theorem 2.5 or 2.7, the energy distribution

$$\sum_{(m-1)B<|l|\leq mB} |l|^{2s} I_l(\xi(t),\overline{\xi(t)}) \leq C\varepsilon^{2m(1-\mu)+\frac{5}{2}\mu}$$

for $m \geq 2$ over long times

$$0 \leq t \leq \varepsilon^{-N\mu}$$

with the constant C of Theorem 2.5.

The estimate improves to $C\varepsilon^{2m(1-\mu)+3\mu}$ if in addition the non-resonance condition 2.4 is satisfied.

Proof. Motivated by Figure 2 we apply Theorem 2.12 with the scaling function

$$e(l) = \left\lceil \frac{|l|}{B} \right\rceil.$$

This scaling function satisfies the triangle inequality since

$$e(l+j) = \left\lceil \frac{|l+j|}{B} \right\rceil \leq \left\lceil \frac{|l|+|j|}{B} \right\rceil \leq \left\lceil \frac{|l|}{B} \right\rceil + \left\lceil \frac{|j|}{B} \right\rceil = e(l) + e(j),$$

and we have for the initial value

$$\|\xi(0)\|_{s,e} = \Big(\sum_{|j|\leq B} \varepsilon^{-2e(j)(1-\mu)} |j|^{2s} |\xi_j(0)|^2\Big)^{\frac{1}{2}} = \varepsilon^{-(1-\mu)} \|\xi(0)\|_s \leq \varepsilon^{\mu}.$$

The statement now follows from Theorem 2.12. □

Corollary 2.13 shows that the expected behaviour (see Figure 2) can be observed on long time intervals up to a factor $1-\mu$ in the exponent of ε. In the case of no partial resonances, Corollary 2.13 holds true if the (modified) Euclidean norm $|\cdot|$ in $(m-1)B<|l|\le mB$ is replaced by any other norm (or any other map satisfying the triangle inequality). In this way we are able to treat not only finite bands with the form of a circle, but also cubes, and so on.

Now we study the situation (b) where a pair of modes $\xi_{\tilde{j}}$ and $\xi_{-\tilde{j}}$ is excited initially. We denote for $l\in\{\,m\tilde{j}:m\in\mathbb{Z}\,\}\cap\mathcal{N}$ by $m(l)$ the minimal integer with respect to $|\cdot|$ such that $l=m(l)\tilde{j}$.[3] Again, we obtain the expected behaviour (see Figure 3) up to a factor $1-\mu$ on a long time interval.

Corollary 2.14 (Long-Time Energy Distribution (b))**.** *Let $0<\mu\le 1$. Under the assumptions of Theorem 2.5 with the condition of zero momentum* (2.9b) *satisfied in Assumption 2.2 and for small initial values*

$$\|\xi(0)\|_s\le\varepsilon\quad\textit{with }(2.22\text{b})$$

we have for any ε, such that ε^μ satisfies the smallness assumption of Theorem 2.5, the energy distribution

$$I_0(\xi(t),\overline{\xi(t)})\le C\varepsilon^{4(1-\mu)+\frac{5}{2}\mu},$$
$$|l|^{2s}I_l(\xi(t),\overline{\xi(t)})\le C\varepsilon^{2|m(l)|(1-\mu)+\frac{5}{2}\mu}$$

for $0,\pm\tilde{j}\ne l\in\{\,m\tilde{j}:m\in\mathbb{Z}\,\}\cap\mathcal{N}$ over long times

$$0\le t\le\varepsilon^{-N\mu}$$

with the constant C of Theorem 2.5. If $l\notin\{\,m\tilde{j}:m\in\mathbb{Z}\,\}$, then $\xi_l(t)=0$ for all times t.

The same result holds true in the situation of Theorem 2.7 in dimension one ($d=1$). The estimates improve by a factor $\varepsilon^{\frac{1}{2}\mu}$ if in addition the non-resonance condition 2.4 is satisfied.

Proof. We first show that

$$\xi_l(t)=0\quad\text{for all times } t \text{ if } l\ne m\tilde{j}\text{ for all } m\in\mathbb{Z}. \tag{2.24}$$

This is done by differentiating the Hamiltonian equations of motion (2.23) several times with respect to t and evaluating at $t=0$. Due to the condition of zero momentum the nonlinearity then cancels for all $l\ne m\tilde{j}$. We thus have $\frac{d^n}{dt^n}\xi_l(0)=0$ for all $n\ge 0$ and all $l\ne m\tilde{j}$. This proves (2.24).

[3] Recall that in order to compute $m\tilde{j}$ the addition of indices introduced in the condition of zero momentum (2.9b) is used. If this is the addition in $\mathbb{Z}^d$, then an integer m with $l=m\tilde{j}$ is unique. If the addition is, however, the addition modulo $2M$ for instance, an integer m with $l=m\tilde{j}$ is not necessarily unique.

We now apply Theorem 2.12 with the scaling function

$$e(l) = \begin{cases} |m(l)|, & \text{if } 0 \neq l = m\tilde{j} \text{ for an } m \in \mathbb{Z}, \\ 2, & \text{if } l = 0, \\ \infty, & \text{else} \end{cases}$$

and the convention $\varepsilon^{-\infty}0 = 0$. The latter convention is justified by (2.24). The function e satisfies the triangle inequality since we have for $0 \neq l + j = m(l+j)\tilde{j} = (m(l)+m(j))\tilde{j}$

$$e(l+j) = |m(l+j)| \leq |m(l)| + |m(j)| \leq e(l) + e(j)$$

by the minimal choice of $m(l)$. Moreover $e(l+j) = 2 \leq e(l) + e(j)$ if $0 = l + j$. If $e(l+j) = \infty$, then $e(l) = \infty$ or $e(j) = \infty$ and the triangle inequality is clear. For the initial value we have $\|\xi(0)\|_{s,e} \leq \varepsilon^{\mu}$ since $e(l) \geq 1$ for all $l \in \mathcal{N}$. The statement now follows from Theorem 2.12.

In dimension one ($d = 1$) and the situation of Theorem 2.7 the property (2.24) remains valid and $e(l) = \text{const}$ if $|l| = \text{const}$, and hence Theorem 2.12 can be applied also in the situation of Theorem 2.7. □

2.6 Example — Nonlinear Schrödinger Equations of Convolution Type

In this section, we apply Theorem 2.5 on the long-time near-conservation of actions and its Corollaries 2.9 on the long-time regularity and 2.13 and 2.14 on the long-time energy distribution to nonlinear Schrödinger equations with a potential of convolution type (1.7),

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x) * \psi(x,t) + g(|\psi(x,t)|^2)\psi(x,t), \tag{2.25}$$

as discussed in Section 1.4, i.e., on $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$. In particular, $V(x) \in L^2(\mathbb{T}^d)$ is assumed to have real Fourier coefficients, and g is assumed to be real-valued and analytic in a neighbourhood of zero. As explained there, this partial differential equation is Hamiltonian, and its Hamiltonian function $H(\xi,\eta)$ is of the form (2.1). Note that the Corollaries 2.10 on the long-time near-conservation of mass and 2.11 on the long-time near-conservation of momentum are not of interest for the nonlinear Schrödinger equation (2.25) since they are exact invariants of a solution, see Section 1.4. In order to apply Theorem 2.5 we verify its various assumptions.

Verification of the Regularity Assumption 2.1. *The regularity assumption 2.1 on the nonlinearity* $\frac{\partial P}{\partial \eta_j}(\xi,\eta)$ *of the nonlinear Schrödinger equation* (2.25) *is fulfilled for* $s \geq s_0 > \frac{d}{2}$ *and* $g(0) = 0$. *The constants* C_1, C_{s_0}, C_s, *and* $C_{L,s}$ *depend only on* g, d, s_0, *and* s *(and* L*).*

Since g is assumed to be analytic in a neighbourhood of zero, the nonlinearity in this equation allows an expansion of the form (2.4) with

$$P_{j,k,l} = \begin{cases} \frac{g^{(m')}(0)}{m'!}, & m = m'+1,\ k^1 + \cdots + k^m - l^1 - \cdots - l^{m'} = j, \\ 0, & \text{else} \end{cases} \tag{2.26}$$

for $j \in \mathcal{N}$, $k \in \mathcal{N}^m$, and $l \in \mathcal{N}^{m'}$, see (1.8). In order to satisfy (2.5) in Assumption 2.1 we require $g(0) = 0$, i.e., the nonlinearity in (2.25) is at least cubic.

We now turn to the main assumptions (2.6a) and (2.6b) of 2.1. Note that with the notation $|P|^{m,m'}$ as in Assumption 2.1 we have

$$\||P|^{m,m'}(\xi^1,\dots,\xi^m,\eta^1,\dots,\eta^{m'})\|_s = \frac{|g^{(m')}(0)|}{m'!} \Big\| \Big(\sum_{\substack{k^1+\cdots+k^m \\ -l^1-\cdots-l^{m'}=j}} \xi^1_{k^1} \cdots \xi^m_{k^m} \eta^1_{l^1} \cdots \eta^{m'}_{l^{m'}} \Big)_{j\in\mathcal{N}} \Big\|_s .$$

for $m = m'+1 \geq 2$ and $|P|^{m,m'} = 0$ else. Moreover, the Cauchy–Schwarz inequality yields

$$\begin{aligned} \Big\| \Big(\sum_{\substack{k^1+\cdots+k^m \\ -l^1-\cdots-l^{m'}=j}} \xi^1_{k^1} \cdots \xi^m_{k^m} \eta^1_{l^1} \cdots \eta^{m'}_{l^{m'}} \Big)_{j\in\mathcal{N}} \Big\|_s^2 &= \sum_{j\in\mathcal{N}} |j|^{2s} \Big| \sum_{\substack{k^1+\cdots+k^m \\ -l^1-\cdots-l^{m'}=j}} \xi^1_{k^1} \cdots \xi^m_{k^m} \eta^1_{l^1} \cdots \eta^{m'}_{l^{m'}} \Big|^2 \\ &\leq \sum_{j\in\mathcal{N}} \Big(\sum_{k^1+r=j} \frac{|j|^{2s}}{|k^1|^{2s}|r|^{2s}} \Big) \Big(\sum_{k^1+r=j} |k^1|^{2s} |\xi^1_{k^1}|^2 |r|^{2s} \Big| \sum_{\substack{k^2+\cdots+k^m \\ -l^1-\cdots-l^{m'}=r}} \xi^2_{k^2} \cdots \xi^m_{k^m} \eta^1_{l^1} \cdots \eta^{m'}_{l^{m'}} \Big|^2 \Big). \end{aligned}$$

The triangle inequality (which is valid for $|\cdot|$) yields $|k^1| \geq \frac{1}{2}|j|$ or $|r| \geq \frac{1}{2}|j|$ if $k^1 + r = j$, and hence

$$\sum_{k^1+r=j} \frac{|j|^{2s}}{|k^1|^{2s}|r|^{2s}} \leq 4 \sum_{r\in\mathcal{N}} \frac{1}{|r|^{2s}}.$$

The latter sum converges for $s > \frac{d}{2}$ by (1.9). Then we get inductively for $s > \frac{d}{2}$

$$\Big\| \Big(\sum_{\substack{k^1+\cdots+k^m \\ -l^1-\cdots-l^{m'}=j}} \xi^1_{k^1} \cdots \xi^m_{k^m} \eta^1_{l^1} \cdots \eta^{m'}_{l^{m'}} \Big)_{j\in\mathcal{N}} \Big\|_s \leq C^{m+m'} \|\xi^1\|_s \cdots \|\xi^m\|_s \|\eta^1\|_s \cdots \|\eta^{m'}\|_s,$$

i.e., (2.6a) is satisfied with $C_{m,m',s} = C^{m+m'} \frac{|g^{(m')}(0)|}{m'!}$ for $m = m'+1 \geq 2$ (and $C_{m,m',s} = 0$ for $m \neq m'+1$ or $m \leq 1$),

$$\||P|^{m,m'}(\xi^1,\dots,\xi^m,\eta^1,\dots,\eta^{m'})\|_s \leq C^{m+m'} \frac{|g^{(m')}(0)|}{m'!} \|\xi^1\|_s \cdots \|\xi^m\|_s \|\eta^1\|_s \cdots \|\eta^{m'}\|_s$$

with a constant C depending only on d and s. Thus we can choose in Assumption 2.1 $s \geq s_0 > \frac{d}{2}$ arbitrarily in order to satisfy (2.6a) with constants $C_{m,m',s}$ depending only on g, d, s, m, and m'.

We now turn to the last assumption (2.6b) in 2.1. Let ρ be the convergence radius of the Taylor series of g which is positive by the assumption on g. Then

$$\sum_{m+m'=2}^{\infty} C_{m,m',s}|z|^{m+m'-2} = |z|^{-2} \sum_{m'=1}^{\infty} \frac{|g^{(m')}(0)|}{m'!} C^{2m'+1}|z|^{2m'+1}$$

converges towards a constant C_s depending only on g, d, and s, provided that $0 \neq |z| \leq C^{-1}\rho^{\frac{1}{2}} = C_1$. This verifies assumption (2.6b) and concludes the verification of the regularity of the nonlinearity.

Verification of the Condition of Small Dimension or of Zero Momentum 2.2. *Assumption 2.2 is fulfilled with $\sigma = 2$ and constants c_2 and C_2 depending only on V. The condition of zero momentum* (2.9b) *in this assumption is fulfilled.*

For the nonlinear Schrödinger equation (2.25) the frequencies

$$\omega_j = j_1^2 + \cdots + j_d^2 + V_j$$

satisfy the growth condition (2.8) in Assumption 2.2 with $\sigma = 2$ and constants c_2 and C_2 depending only on the potential V.

As we learned from the verification of the regularity assumption, we can choose $s_0 > \frac{d}{2}$. Hence, the condition of small dimension (2.9a) can only be satisfied in dimensions one to three. However, the alternative condition of zero momentum (2.9b) is satisfied for the nonlinear Schrödinger equation in any dimension d, see (2.26) (we choose as an addition of indices the natural addition in $\mathcal{N} = \mathbb{Z}^d$). This concludes the verification of Assumption 2.2.

Verification of the Non-Resonance Condition 2.3. *For $m > \frac{d}{2}$ and $R > 0$ let*

$$\mathcal{V} = \Big\{ V(x) = \sum_{j \in \mathcal{N}} V_j e^{i(j\cdot x)} : |V_j||j|^m/R \leq \frac{1}{2} \Big\}$$

be a set of potentials endowed with the product probability measure. Then there exists a subset $\mathcal{S} \subseteq \mathcal{V}$ of full measure, such that the non-resonance condition 2.3 is fulfilled for any potential $V \in \mathcal{S}$ with a constant C_0 depending only on V, s_0, and N.

Let us first consider indices $(j, \mathbf{k}) = (j, \langle l \rangle)$ with $|j| = |l| \geq 2$ but $j \neq l$. Those indices are usually near-resonant since

$$|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| = |\omega_l - \omega_j| = |V_l - V_j| \to 0 \quad \text{for } |j| = |l| \to \infty. \tag{2.27}$$

However, they obviously do not satisfy the non-resonance condition (2.10). The same remark applies to indices of the form $(j, \langle j \rangle + \langle l \rangle - \langle \bar{l} \rangle)$ with $|l| = |\bar{l}|$ but $l \neq \bar{l}$.

But, since the condition of zero momentum is fulfilled for the nonlinear Schrödinger equation of convolution type (2.25), the non-resonance condition 2.3 only has to cover indices $(j, \mathbf{k})$ with $j = j(\mathbf{k})$. In particular, if $\mathbf{k} = \langle l \rangle$ as above, then $j = j(\mathbf{k}) = l$ and $(j, \mathbf{k}) = (j, \langle j \rangle)$ is not near-resonant. Similar, if $\mathbf{k} = \langle j \rangle + \langle l \rangle - \langle \bar{l} \rangle$, then $j = j(\mathbf{k}) = j + l - \bar{l}$

and also $(j, \mathbf{k}) = (j, \langle j \rangle)$ is not near-resonant. This means that the situation described above in (2.27) can be avoided.

The verification of the non-resonance condition 2.3 now mainly relies on Lemma 2.8 which allows us to reduce our non-resonance condition 2.3 to the one used by Bambusi and Grébert [4]. It is shown in [4, Theorem 3.22] that there exists a subset $\mathcal{S}$ of $\mathcal{V}$ of full measure, such that the non-resonance condition (2.16) is fulfilled for all $\widetilde{\mathbf{k}} \in \mathbb{Z}^{\mathcal{N}}$ with the properties in (2.16) and in addition

$$\widetilde{\mathbf{k}} \neq \langle l \rangle - \langle \bar{l} \rangle \quad \text{with} \quad |l| = |\bar{l}|,$$

see also [29, Proposition 1] and the comment following this proposition. By Lemma 2.8 any near-resonant index $(j, \mathbf{k})$ with $\mathbf{k} - \langle j \rangle \neq \langle l \rangle - \langle \bar{l} \rangle$ then satisfies also (2.10) in Assumption 2.3. As explained above, near-resonant indices with $\mathbf{k} - \langle j \rangle = \langle l \rangle - \langle \bar{l} \rangle$ need not to be considered in Assumption 2.3 due to the condition of zero momentum. In summary, our non-resonance condition 2.3 is fulfilled for any potential $V \in \mathcal{S}$.

Verification of the Additional Non-Resonance Condition 2.4. *The additional non-resonance condition 2.4 is fulfilled with a constant C_3 depending only on V in dimension one ($d = 1$).*

We have to control $|\mathbf{k} \cdot \boldsymbol{\omega} - \omega_{j(\mathbf{k})}|$ for $\mathbf{k} \neq \langle j \rangle$ and $\|\mathbf{k}\| \leq 2$. For $\|\mathbf{k}\| = 0$ we have $\mathbf{k} = \mathbf{0}$ and

$$|\mathbf{k} \cdot \boldsymbol{\omega} - \omega_{j(\mathbf{k})}| = |\omega_0| = |V_0|,$$

which clearly can be controlled from below by a positive constant depending only on the potential V, provided that the non-resonance condition 2.3 is satisfied.

For $\|\mathbf{k}\| = 1$ we have necessarily $\mathbf{k} = -\langle j \rangle$ with $j \in \mathcal{N}$, and

$$|\mathbf{k} \cdot \boldsymbol{\omega} - \omega_{j(\mathbf{k})}| = |-\omega_j - \omega_{-j}| = |2(j_1^2 + \cdots + j_d^2) + V_j + V_{-j}|$$

can be controlled from below by a positive constant depending only on V.

For $\|\mathbf{k}\| = 2$ we have $\mathbf{k} = \pm\langle j \rangle \pm \langle l \rangle$. In one dimension ($d = 1$) we can control $|\mathbf{k} \cdot \boldsymbol{\omega} - \omega_{j(\mathbf{k})}|$ from below by a positive constant depending only on V, whereas this is not possible in higher dimensions. For instance we have in dimension one for $\mathbf{k} = \langle j \rangle + \langle l \rangle$

$$|\mathbf{k} \cdot \boldsymbol{\omega} - \omega_{j(\mathbf{k})}| = |\omega_j + \omega_l - \omega_{j+l}| = |-2jl + V_j + V_l - V_{j+l}|$$

and for $\mathbf{k} = \langle j \rangle - \langle l \rangle$

$$|\mathbf{k} \cdot \boldsymbol{\omega} - \omega_{j(\mathbf{k})}| = |\omega_j - \omega_l - \omega_{j-l}| = |2l(j - l) + V_j + V_l - V_{j-l}|.$$

Hence the additional non-resonance condition 2.4 is fulfilled in one dimension with a constant C_3 depending only on V, but it is not satisfied in higher dimensions.

Summarising our results we get as corollary of Theorem 2.5 and Corollary 2.9.

Corollary 2.15 (Long-Time Analysis of Nonlinear Schrödinger Equations (2.25))**.** *Fix N, $s \geq 2s_0 > d$, and assume $g(0) = 0$ and $V \in \mathcal{S}$. Then for any ε sufficiently small compared to the nonlinearity g, the dimension d, the potential V, s_0, s, and N and for small initial values*

$$\|\psi(\cdot, 0)\|_s = \|\xi(0)\|_s = \Big(\sum_{j\in\mathcal{N}} |j|^{2s} |\xi_j(0)|^2\Big)^{\frac{1}{2}} \leq \varepsilon$$

we have

- *near-conservation of actions* (2.12),
- *exact conservation of energy, mass, and momentum,*
- *and regularity* (2.19)

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

along any solution $\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t) e^{i(j\cdot x)}$ of the nonlinear Schrödinger equation with a potential of convolution type (2.25) *in dimension d with a constant C depending only on g, d, V, s_0, s, and N, but not on ε.*

The near-conservation of actions improves to $C\varepsilon$ in dimension one ($d = 1$). □

This result is very similar to [29, Theorem 1], but there the conservation of actions was shown to be of size $C\varepsilon^{\frac{3}{2}}$ taking into account that the nonlinearity in the considered nonlinear Schrödinger equation is cubic. Here, we applied our general result for Hamiltonian partial differential equations with quadratic nonlinearity. A similar result was also obtained by Bambusi and Grébert [4, Theorem 3.26] in a slightly weaker form as explained in Section 2.2.

Besides the results from Sections 2.2 and 2.4 we can also apply the results on the long-time energy distribution of Section 2.5 to the nonlinear Schrödinger equation with a potential of convolution type (2.25). For the situations (2.22a) of a finite band initial value and (2.22b) of a double mode initial value we can apply Corollaries 2.13 and 2.14 since we already verified the assumptions of Theorem 2.5. However, we can prove even stronger results taking into account the cubic nonlinearity (instead of quadratic nonlinearity as in our general framework) in the nonlinear Schrödinger equation (2.25).

Corollary 2.16 (Long-Time Energy Distribution (a) for Nonlinear Schrödinger Equations (2.25))**.** *Let $0 < \mu \leq 1$. Under the assumptions of Corollary 2.15 and for small initial values*

$$\|\xi(0)\|_s \leq \varepsilon \quad \textit{with } (2.22a)$$

we have for any ε, such that ε^μ satisfies the smallness assumption of Corollary 2.15, the energy distribution

$$\sum_{(2m-1)B<|l|\leq(2m+1)B} |l|^{2s} I_l(\xi(t), \overline{\xi(t)}) \leq C\varepsilon^{2(2m+1)(1-\mu)+\frac{5}{2}\mu}$$

for $m \geq 1$ *over long times*

$$0 \leq t \leq \varepsilon^{-N\mu}$$

with the constant C *of Corollary 2.15.*

The estimates improve by a factor $\varepsilon^{\frac{1}{2}\mu}$ *in dimension one* ($d = 1$).

Proof. We repeat the proof of Corollary 2.13 but with a new scaling function

$$e(l) = 2\left\lceil \frac{|l|}{2B} + \frac{1}{2} \right\rceil - 1$$

adapted to the cubic nonlinearity. Indeed $e(\cdot)$ also satisfies the triangle inequality if we have at least three summands,

$$e(l + j + k) = 2\left\lceil \frac{|l + j + k|}{2B} + \frac{1}{2} \right\rceil - 1 = 2\left\lceil \frac{|l + j + k|}{2B} + \frac{3}{2} \right\rceil - 3 \leq e(l) + e(j) + e(k).$$

The statement then follows from Theorem 2.12 as in the proof of Corollary 2.13. □

Corollary 2.17 (Long-Time Energy Distribution (b) for Nonlinear Schrödinger Equations (2.25))**.** *Let* $0 < \mu \leq 1$. *Under the assumptions of Corollary 2.15 and for small initial values*

$$\|\xi(0)\|_s \leq \varepsilon \quad \textit{with } (2.22\text{b})$$

we have for any ε, *such that* ε^μ *satisfies the smallness assumption of Corollary 2.15, the energy distribution*

$$|m\tilde{j}|^{2s} I_{m\tilde{j}}(\xi(t), \overline{\xi(t)}) \leq C\varepsilon^{2|m|(1-\mu)+\frac{5}{2}\mu}$$

for odd $m \in \mathbb{Z}$ *with* $m \neq \pm 1$ *over long times*

$$0 \leq t \leq \varepsilon^{-N\mu}$$

with the constant C *of Corollary 2.15. If* $l \notin \{m\tilde{j} : m \in \mathbb{Z} \textit{ odd}\}$, *then* $\xi_l(t) = 0$ *for all times* t.

The estimates improve by a factor $\varepsilon^{\frac{1}{2}\mu}$ *in dimension one* ($d = 1$).

Proof. We repeat the proof of Corollary 2.14 and note in addition that $\xi_l(t) = 0$ for all times t if $l = m\tilde{j}$ with an even $m \in \mathbb{Z}$ by analysing the nonlinearity as in this proof. □

One could think about another initial energy distribution, where a single mode $\xi_{\tilde{j}}$ is excited. This situation, however, is not interesting in many examples. For the nonlinear Schrödinger equation (2.25) for instance one easily verifies that

$$\xi_j(t) = \begin{cases} e^{-i(\omega_j + |\xi_j(0)|^2)t}\xi_j(0), & \text{for } j = \tilde{j}, \\ 0, & \text{else} \end{cases}$$

is the solution for such initial values. In particular, the initial energy distribution is exactly conserved for such initial values for all times and not distributed among other modes.

2.7 Example — Schrödinger–Poisson Equations

We now consider the Schrödinger–Poisson equation

$$\begin{aligned} i\frac{\partial}{\partial t}\psi(x,t) &= -\Delta\psi(x,t) + V(x) * \psi(x,t) + W(x,t)\psi(x,t), \\ -\Delta W(x,t) &= |\psi(x,t)|^2 - \frac{1}{(2\pi)^d}\int_{\mathbb{T}^d} |\psi(x,t)|^2\,dx, \\ \int_{\mathbb{T}^d} W(x,t)\,dx &= 0 \end{aligned} \tag{2.28}$$

on $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$ as in Section 1.4, equation (1.11).

Verification of the Assumptions 2.1, 2.2, 2.3, and 2.4. *Assumptions 2.1, 2.2, and 2.3 are fulfilled for potentials $V \in \mathcal{S}$ with $\mathcal{S}$ from the previous Section 2.6 with constants depending only on V, d, s_0, s, and N. Assumption 2.4 is fulfilled in one dimension ($d = 1$).*

Comparing the Hamiltonian equations of motion (1.12) of the Schrödinger–Poisson equation with the ones of the nonlinear Schrödinger equation with a potential of convolution type and a nonlinearity $g(|\psi|^2) = |\psi|^2$ (2.25) and (2.26), we see that the moduli of the coefficients $P_{j,k,l}$ (see Assumption 2.1) in the Schrödinger–Poisson equation are all smaller or equal than the ones of the coefficients in the nonlinear Schrödinger equation with a potential of convolution type. Hence, the regularity assumption 2.1 is also satisfied for the Schrödinger–Poisson equation for $s \geq s_0 > \frac{d}{2}$ with constants depending only on d, s_0, and s, see Section 2.6.

Moreover, the condition of zero momentum (2.9b) in Assumption 2.2 is satisfied for the Schrödinger–Poisson equation.

Since the frequencies of the Schrödinger–Poisson equation are the same as the frequencies of the nonlinear Schrödinger equation with a potential of convolution type, also the non-resonance conditions 2.3 and 2.4 are satisfied for the Schrödinger–Poisson equation in the same way as for the nonlinear Schrödinger equation with a potential of convolution type, see Section 2.6.

We have thus proven the following corollary.

Corollary 2.18 (Long-Time Analysis of Schrödinger–Poisson Equations (2.28))**.** *Fix N, $s \geq 2s_0 > d$, and assume $V \in \mathcal{S}$. Then for any ε sufficiently small compared to the dimension d, the potential V, s_0, s, and N and for small initial values*

$$\|\psi(\cdot,0)\|_s = \|\xi(0)\|_s = \Big(\sum_{j\in\mathcal{N}} |j|^{2s}|\xi_j(0)|^2\Big)^{\frac{1}{2}} \leq \varepsilon$$

we have

- *near-conservation of actions* (2.12)*,*
- *exact conservation of energy, mass, and momentum,*

- *and regularity* (2.19)

over long times

$$0 \le t \le \varepsilon^{-N}$$

along any solution $\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t) e^{i(j\cdot x)}$ *of the Schrödinger–Poisson equation* (2.28) *in dimension* d *with a constant* C *depending only on* d, V, s_0, s, *and* N, *but not on* ε.

The near-conservation of actions improves to $C\varepsilon$ *in dimension one* ($d = 1$). □

To our knowledge, there have been no similar results for Schrödinger–Poisson equations so far. As for the nonlinear Schrödinger equation with a potential of convolution type (2.25) of Section 2.6 we get results on the long-time energy distribution for the Schrödinger–Poisson equation, and Corollaries 2.16 and 2.17 are also true for solutions of the Schrödinger–Poisson equation.

2.8 Example — Nonlinear Schrödinger Equations

In this section we apply the theoretical results of Sections 2.2 and 2.4 to the nonlinear Schrödinger equation

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x)\psi(x,t) + g(|\psi(x,t)|^2)\psi(x,t) \tag{2.29}$$

with Dirichlet boundary conditions $\psi(x,t) = 0$ for x on the boundary of $[0,\pi]$, where g is assumed to be real-valued and analytic in a neighbourhood of zero and the potential $V(x)$ also satisfies Dirichlet boundary conditions. The Hamiltonian structure of this equation was established in Section 1.4.

Verification of the Regularity Assumption 2.1. *The regularity assumption 2.1 is fulfilled for* $s \ge s_0 > \frac{1}{2}$, $g(0) = 0$, *and even potential* $V(x)$. *The constants* C_1, C_{s_0}, C_s, *and* $C_{L,s}$ *depend only on* g, V, s_0, *and* s *(and* L*).*

The requirement $g(0) = 0$ ensures (2.5) in Assumption 2.1, namely that $P_{j,k,l} = 0$ for $j \in \mathcal{N} = \mathbb{N}\setminus\{0\}$, $k \in \mathcal{N}^m$, and $l \in \mathcal{N}^{m'}$ with $m + m' < 2$, see also Section 2.6. We note for later purposes that $P_{j,k,l} = 0$ whenever $m \ne m' + 1$, in particular whenever $m + m'$ is even.

For the verification of (2.6a) we modify the proof of the corresponding result for the nonlinear Schrödinger equation with a potential of convolution type in Section 2.6. The main difficulty arises from the fact that $\frac{\partial P}{\partial \eta_j}$ does not only contain nonzero terms for $k^1 + \dots + k^m - l^1 - \dots - l^{m'} = j$ but for (in general) all $j \in \mathcal{N}$, $k \in \mathcal{N}^m$, and $l \in \mathcal{N}^{m'}$. However, a result by Craig and Wayne [19] ensures that this situation is sufficiently close to the situation of Section 2.6.

We imitate the estimates from Section 2.6 using that the coefficients $P_{j,k,l}$ introduced in Section 1.4 satisfy

$$P_{j,k,l} = \sum_{r\in\mathcal{N}} P_{j,(k^1,k^2),(r)} P_{r,(k^3,\dots,k^m),l}$$

for $j \in \mathcal{N}$, $k \in \mathcal{N}^m$, and $l \in \mathcal{N}^{m'}$ by the orthonormality of the eigenfunctions φ_j. We have for odd $m + m'$ (and $m = m' + 1$).

$$|||P|^{m,m'}(\xi^1, \dots, \xi^m, \eta^1, \dots, \eta^{m'})\|_s^2 = \frac{|g^{(m')}(0)|^2}{(m'!)^2} \sum_{j\in\mathcal{N}} |j|^{2s} \Big| \sum_{k^1,k^2,r\in\mathcal{N}} P_{j,(k^1,k^2),(r)} \xi^1_{k^1} \xi^2_{k^2} \sum_{k^3,\dots,k^m\in\mathcal{N}} \sum_{l\in\mathcal{N}^{m'}} P_{r,(k^3,\dots,k^m),l} \xi^3_{k^3} \cdots \xi^m_{k^m} \eta^1_{l^1} \cdots \eta^{m'}_{l^{m'}} \Big|^2.$$

The Cauchy–Schwarz inequality implies

$$|||P|^{m,m'}(\xi^1, \dots, \xi^m, \eta^1, \dots, \eta^{m'})\|_s^2 \le \frac{|g^{(m')}(0)|^2}{(m'!)^2} \sum_{j\in\mathcal{N}} \Big(\sum_{k^1,k^2,r\in\mathcal{N}} \frac{|P_{j,(k^1,k^2),(r)}||j|^{2s}}{|k^1|^{2s}|k^2|^{2s}|r|^{2s}} \Big) \Big(\sum_{k^1,k^2,r\in\mathcal{N}} |P_{j,(k^1,k^2),(r)}||k^1|^{2s}|\xi^1_{k^1}|^2 |k^2|^{2s} |\xi^2_{k^2}|^2 |r|^{2s} \Big| \sum_{k^3,\dots,k^m\in\mathcal{N}} \sum_{l\in\mathcal{N}^{m'}} P_{r,(k^3,\dots,k^m),l} \xi^3_{k^3} \cdots \xi^m_{k^m} \eta^1_{l^1} \cdots \eta^{m'}_{l^{m'}} \Big|^2 \Big).$$

We finally show that for $s > \frac{1}{2}$

$$\sup_{j\in\mathcal{N}} \sum_{k^1,k^2,r\in\mathcal{N}} \frac{|P_{j,(k^1,k^2),(r)}||j|^{2s}}{|k^1|^{2s}|k^2|^{2s}|r|^{2s}} \le C \quad \text{and} \quad \sup_{k^1,k^2,r\in\mathcal{N}} \sum_{j\in\mathcal{N}} |P_{j,(k^1,k^2),(r)}| \le C \tag{2.30}$$

with a constant C depending only on V and s. These two estimates imply inductively

$$|||P|^{m,m'}(\xi^1, \dots, \xi^m, \eta^1, \dots, \eta^{m'})\|_s \le C^{m'} \frac{|g^{(m')}(0)|}{m'!} \|\xi^1_{k^1}\|_s \cdots \|\xi^m_{k^m}\|_s \|\eta^1_{l^1}\|_s \cdots \|\eta^{m'}_{l^{m'}}\|_s,$$

i.e., (2.6a) in Assumption 2.1 is satisfied with constants $C_{m,m',s}$ depending only on g, V, and s. The second estimate (2.6b) needed in this assumption then follows as in Section 2.6.

In order to verify the estimates (2.30) we use [19, Proposition 6.4]. This result states that the eigenfunctions φ_n, $n \in \mathcal{N} = \mathbb{N} \setminus \{0\}$, of $-\Delta + V(x)$ admit — suitably ordered — an expansion

$$\varphi_n(x) = \sum_{\tilde n\in\mathcal{N}} \varphi_{n,\tilde n} \sin(\tilde n x) \quad \text{with} \quad |\varphi_{n,\tilde n}| \le C e^{-\sigma|n-\tilde n|}, \tag{2.31}$$

where C and σ depend only on the regularity of V (more precisely, they depend on the width of the strip around the real axis where V is analytic and periodic). This means that the eigenfunctions $\varphi_n(x)$ of $-\Delta + V(x)$ are close to the eigenfunctions $\sin(nx)$ of the unperturbed Laplacian $-\Delta$. This implies for the coefficients $P_{j,(k^1,k^2),(r)}$ arising in (2.30)

$$P_{j,(k^1,k^2),(r)} = \sum_{\tilde j,\tilde k^1,\tilde k^2,\tilde r\in\mathcal{N}} \varphi_{j,\tilde j} \varphi_{k^1,\tilde k^1} \varphi_{k^2,\tilde k^2} \varphi_{r,\tilde r} \frac{1}{\pi} \int_0^\pi \sin(\tilde j x) \sin(\tilde k^1 x) \sin(\tilde k^2 x) \sin(\tilde r x)\, dx.$$

Obviously $|\frac{1}{\pi}\int_0^\pi \sin(\tilde{j}x)\sin(\tilde{k}^1x)\sin(\tilde{k}^2x)\sin(\tilde{r}x)\,dx| \le 1$, and using $\sin(jx) = \frac{1}{2i}(e^{ijx} - e^{-ijx})$ we see that $\frac{1}{\pi}\int_0^\pi \sin(\tilde{j}x)\sin(\tilde{k}^1x)\sin(\tilde{k}^2x)\sin(\tilde{r}x)\,dx = 0$ unless $\tilde{j} = \pm\tilde{k}^1 \pm \tilde{k}^2 \pm \tilde{r}$. For the latter statement the fact that the integral of an even number of sines is computed is crucial; for this reason we apply in the above estimates the Cauchy–Schwarz inequality to the sum over k^1, k^2, and r (and not only k^1 and r as in Section 2.6). Using the result by Craig and Wayne (2.31) we get

$$|P_{j,(k^1,k^2),(r)}| \le C^4 \sum_{m\in\mathbb{N}} e^{-\sigma m} \sum_{\substack{\tilde{k}^1,\tilde{k}^2,\tilde{r}\in\mathcal{N}:\\ |j-(\pm\tilde{k}^1\pm\tilde{k}^2\pm\tilde{r})|+|k^1-\tilde{k}^1|+\\ +|k^2-\tilde{k}^2|+|r-\tilde{r}|=m}} 1.$$

This implies in particular

$$\sup_{k^1,k^2,r\in\mathcal{N}} \sum_{j\in\mathcal{N}} |P_{j,(k^1,k^2),(r)}| \le 8C^4 \sum_{m\in\mathbb{N}} e^{-\sigma m}(2m+1)^3,$$

and the second estimate in (2.30) is shown. Concerning the first estimate in (2.30), we get

$$\sum_{k^1,k^2,r\in\mathcal{N}} \frac{|P_{j,(k^1,k^2),(r)}||j|^{2s}}{|k^1|^{2s}|k^2|^{2s}|r|^{2s}} \le C^4 \sum_{m\in\mathbb{N}} e^{-\sigma m} \sum_{\substack{k^1,k^2,r,\tilde{k}^1,\tilde{k}^2,\tilde{r}\in\mathcal{N}:\\ |j-(\pm\tilde{k}^1\pm\tilde{k}^2\pm\tilde{r})|+|k^1-\tilde{k}^1|+\\ +|k^2-\tilde{k}^2|+|r-\tilde{r}|=m}} \frac{|j|^{2s}}{|k^1|^{2s}|k^2|^{2s}|r|^{2s}}.$$

The denominator $|k^1|$ in the latter sum can be estimated by $\max(|\tilde{k}^1|-m,1)^{2s}$, and doing the same for the other terms in the denominator the summands become independent of k^1, k^2, and r. This yields

$$\sum_{k^1,k^2,r\in\mathcal{N}} \frac{|P_{j,(k^1,k^2),(r)}||j|^{2s}}{|k^1|^{2s}|k^2|^{2s}|r|^{2s}} \le C^4 \sum_{m\in\mathbb{N}} e^{-\sigma m}(2m+1)^3 \sum_{\substack{\tilde{k}^1,\tilde{k}^2,\tilde{r}\in\mathcal{N}:\\ |j-(\pm\tilde{k}^1\pm\tilde{k}^2\pm\tilde{r})|\le m}} \frac{|j|^{2s}}{\max(|\tilde{k}^1|-m,1)^{2s}\max(|\tilde{k}^2|-m,1)^{2s}\max(|\tilde{r}|-m,1)^{2s}}.$$

Now we can proceed similarly as in Section 2.6, where we estimated $\sum_{k^1+r=j}\frac{|j|^{2s}}{|k^1|^{2s}|r|^{2s}}$. If for instance $|\tilde{k}^1| \ge |\tilde{k}^2|$ and $|\tilde{k}^1| \ge |\tilde{r}|$, then $|\tilde{k}^1| \ge \frac{|j|-m}{3}$, and the numerator $|j|^{2s}$ cancels out. We get a constant depending polynomially on m, and this remains true if we omit the summation over $\tilde{k}^1$. We get

$$\sum_{k^1,k^2,r\in\mathcal{N}} \frac{|P_{j,(k^1,k^2),(r)}||j|^{2s}}{|k^1|^{2s}|k^2|^{2s}|r|^{2s}} \le C^4 \sum_{m\in\mathbb{N}} e^{-\sigma m}p(m) \sum_{\tilde{k}^2,\tilde{r}\in\mathcal{N}} \frac{1}{|\tilde{k}^2|^{2s}|\tilde{r}|^{2s}}$$

with a polynomial p whose degree can be bounded in terms of s. Using (1.9) we finally get the first estimate of (2.30). This concludes the verification of the regularity assumption 2.1 for the nonlinear Schrödinger equation (2.29).

Verification of the Condition of Small Dimension or of Zero Momentum 2.2. *Assumption 2.2 is fulfilled if* $\frac{1}{2} < s_0 \leq 2$ *and* $s \geq N+3+3s_0$ *with* $\sigma = 2$ *and constants* c_2 *and* C_2 *depending only on* V*. The condition of zero momentum* (2.9b) *in this assumption is not fulfilled.*

By (1.6) the asymptotics of the frequencies (2.8) in Assumption 2.2 is fulfilled with $\sigma = 2$. The condition of small dimension (2.9a) is then fulfilled for $\frac{1}{2} < s_0 \leq \sigma = 2$ and $s \geq N+3+3s_0$. The condition of zero momentum (2.9b) is not fulfilled in general since $P_{j,k,l} \neq 0$ generically for $j \neq k^1 + \cdots + k^m - l^1 - \cdots - l^{m'}$.

Verification of the Non-Resonance Condition 2.3. *For* $\sigma_0 > 0$ *and* $R > 0$ *let*

$$\mathcal{V}_R = \Big\{ V(x) = \sum_{j\in\mathcal{N}} V_j \cos(jx) : |V_j| e^{\sigma_0 j}/R \leq \frac{1}{2} \Big\}$$

be a set of potentials endowed with the product probability measure. Then for any N *there exists* $R > 0$ *and a subset* $\mathcal{S} \subseteq \mathcal{V}_R$ *of full measure, such that the non-resonance condition 2.3 is fulfilled for any potential* $V \in \mathcal{S}$ *with a constant* C_0 *depending only on* V*,* s_0*, and* N*.*

This statement follows from Lemma 2.8 and [4, Theorem 3.18], where it is shown that the non-resonance condition (2.16) is fulfilled for any V in a suitable subset $\mathcal{S} \subseteq \mathcal{V}_R$ provided that R is chosen large enough compared to r'.

Having verified the Assumptions 2.1, 2.2, and 2.3 we can apply Theorem 2.5 and obtain near-conservation of actions over long times. Recall from Section 1.4 that energy and mass are exactly conserved along solutions of (2.29) and from Corollary 2.11 in Section 2.4 that the momentum is nearly conserved on a long time interval. The following corollary of Theorem 2.5 is now proven.

Corollary 2.19 (Long-Time Analysis of Nonlinear Schrödinger Equations (2.29))**.** *Fix* N*,* $s \geq N+3+3s_0$*,* $4 \geq 2s_0 > 1$*, and assume* $g(0) = 0$ *and* $V \in \mathcal{S}$*. Then for any* ε *sufficiently small compared to the nonlinearity* g*, the potential* V*,* s_0*,* s*, and* N *and for small initial values*

$$\|\psi(\cdot,0)\|_s = \|\xi(0)\|_s = \Big(\sum_{j\in\mathcal{N}} |j|^{2s} |\xi_j(0)|^2\Big)^{\frac{1}{2}} \leq \varepsilon$$

we have

- *near-conservation of actions* (2.12),
- *exact conservation of energy and mass,*
- *near-conservation of momentum* (2.21),
- *and regularity* (2.19)

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

along any solution $\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t) e^{i(j\cdot x)}$ *of the nonlinear Schrödinger equation* (2.29) *with a constant* C *depending only on* g*,* V*,* s_0*,* s*, and* N*, but not on* ε*.* □

A similar result was obtained by Bambusi and Grébert in [4] with slightly weaker estimates. Concerning the energy distribution for initial values with only finitely many nonzero coefficients $\xi_j(0)$ as discussed in Section 2.5, we cannot apply the theory developed there to the nonlinear Schrödinger equation (2.29) since the condition of zero momentum is not fulfilled. However, similar results to Corollaries 2.13 and 2.14 are expected to hold true also for (2.29) since the nonlinearity behaves as the nonlinearity discussed in Section 2.5 up to exponentially decaying terms; this was also crucial for the above verification of the regularity assumption 2.1.

2.9 Example — Nonlinear Wave Equations with Periodic Boundary Conditions

We consider the nonlinear wave equation (1.14) from Section 1.5

$$\frac{\partial^2}{\partial t^2} u(x,t) = \Delta u(x,t) - \rho u(x,t) + g(u(x,t)) \tag{2.32}$$

with a nonnegative real number ρ and a real-valued and analytic function g. We impose in this section periodic boundary conditions on $[-\pi,\pi]$, i.e., we consider this equation on $\mathbb{T} = \mathbb{R}/(2\pi\mathbb{Z})$ $(d=1)$.

The frequencies

$$\omega_j = \sqrt{j^2+\rho}, \quad j \in \mathcal{N} = \mathbb{Z},$$

of this nonlinear wave equation are partially resonant in the sense of the non-resonance condition 2.6 since $\omega_j = \omega_{-j}$. Therefore we aim for an application of Theorem 2.7 on the long-time near-conservation of sums of actions suited for this situation.

Verification of the Regularity Assumption 2.1. *The regularity assumption 2.1 is fulfilled for $s \geq s_0 > \frac{1}{2}$ and $g(0) = g'(0) = 0$. The constants C_1, C_{s_0}, C_s, and $C_{L,s}$ depend only on g, ρ, s_0, and s (and L).*

The nonlinearity in the nonlinear wave equation (1.15) is similar to the one in the nonlinear Schrödinger equation with a potential of convolution type (1.8). Therefore the verification of its regularity as required by Assumption 2.1 is a slight modification of the verification of the regularity of the nonlinearity in the nonlinear Schrödinger equation carried out in Section 2.6.

The coefficients $P_{j,k,l}$ take the form

$$P_{j,k,l} = \begin{cases} \frac{g^{(m+m')}(0)}{(m+m')!} \frac{-1}{2^{\frac{m+m'}{2}} (\omega_j \omega_{k^1} \cdots \omega_{k^m} \omega_{l^1} \cdots \omega_{l^{m'}})^{\frac{1}{2}}} \binom{m+m'}{m}, & k^1 + \cdots + k^m - l^1 - \cdots - l^{m'} = j, \\ 0, & \text{else} \end{cases}$$

for $j \in \mathcal{N}$, $k \in \mathcal{N}^m$, and $l \in \mathcal{N}^{m'}$. They satisfy (2.5) if $g(0) = g'(0) = 0$ as we require from now on. This condition leads to a nonlinearity in (2.32) that is at least quadratic.

Since $c_2|j| \le \omega_j \le C_2|j|$ with positive constants c_2 and C_2 depending only on ρ, we have for $|P|^{m,m'}$

$$\begin{aligned}\||P|^{m,m'}(\xi^1,\dots,\xi^m,\eta^1,\dots,\eta^{m'})\|_{s+1} \\ \le \frac{|g^{(m+m')}(0)|2^{-\frac{m+m'}{2}}\binom{m+m'}{m}}{\sqrt{c_2}(m+m')!}\Big\|\Big(\sum_{\substack{k^1+\dots+k^m\\ -l^1-\dots-l^{m'}=j}} \frac{\xi^1_{k^1}}{\sqrt{\omega_{k^1}}}\cdots\frac{\xi^m_{k^m}}{\sqrt{\omega_{k^m}}}\frac{\eta^1_{l^1}}{\sqrt{\omega_{l^1}}}\cdots\frac{\eta^{m'}_{l^{m'}}}{\sqrt{\omega_{l^{m'}}}}\Big)_{j\in\mathcal{N}}\Big\|_{s+\frac12}.\end{aligned}$$

Provided that $s \ge s_0 > \frac{d}{2} = \frac12$ the latter norm can be estimated by $C^{m+m'}\|\xi^1\|_s\cdots\|\xi^m\|_s\cdot\|\eta^1\|_s\cdots\|\eta^{m'}\|_s$ with a constant C depending only on ρ and s as was shown in Section 2.6. In particular, (2.6a) from Assumption 2.1 is satisfied with

$$C_{m,m',s} = \frac{|g^{(m+m')}(0)|}{\sqrt{c_2}(m+m')!}\,2^{-\frac{m+m'}{2}}\binom{m+m'}{m}C^{m+m'}.$$

Note that we have shown more than needed in Assumption 2.1 since we estimated $|P|^{m,m'}$ in the l^2_{s+1}-norm instead of the l^2_s-norm. Indeed, the nonlinearity in the nonlinear wave equation (2.32) is more regular than we actually need. This additional regularity is used in [17], [34], and [16].

In order to verify (2.6b) in the same assumption we first note that

$$\sum_{m+m'=2}^{\infty} C_{m+m',s}|z|^{m+m'-2} = |z|^{-2}\sum_{n=2}^{\infty}\frac{|g^{(n)}(0)|}{\sqrt{c_2}n!}\,|2^{-\frac12}Cz|^n\sum_{m=0}^{n}\binom{m+m'}{m}.$$

Since $\sum_{m=0}^{n}\binom{m+m'}{m} = 2^n$, the latter sum converges towards a constant C_s if g is analytic and if $|z|$ is sufficiently small compared to g and s. The constant C_s depends only on g, ρ, and s. This verifies (2.6b).

Verification of the Condition of Small Dimension or of Zero Momentum 2.2. *Assumption 2.2 is fulfilled with $\sigma = 1$ and constants c_2 and C_2 depending only on ρ. The condition of zero momentum* (2.9b) *in this assumption is fulfilled.*

The coefficients $P_{j,k,l}$ in the nonlinear wave equation clearly satisfy the condition of zero momentum (2.9b) in Assumption 2.1. We mention that in dimension one ($d = 1$) as considered here the alternative condition of small dimension (2.9a) is also satisfied since $\sigma = 1$ in the asymptotics of the frequencies (2.8) for the nonlinear wave equation and $s_0 > \frac{d}{2} = \frac12$ in order to satisfy the Assumption 2.1.

Verification of the Non-Resonance Condition 2.6 for Completely Resonant Frequencies. *For any $D > 0$ there exists a subset $\mathcal{S} \subseteq [0, D]$ of full measure, such that the non-resonance condition 2.6 is fulfilled for any $\rho \in \mathcal{S}$ with a constant C_0 depending only on ρ, s_0, and N.*

While the previous conditions could also be verified in higher dimensions, the fact that we work in dimension one ($d = 1$) is crucial for the verification of the non-resonance condition. Due to the partial resonances in the nonlinear wave equation we consider the non-resonance condition 2.6 instead of 2.3. We reduce here the non-resonance condition 2.6 once again to the non-resonance condition (2.16) used by Bambusi and Grébert by means of Lemma 2.8. It is shown in [4, Theorem 3.12] (see also [3, Theorem 6.5]) that there exists a subset $\mathcal{S}$ of $[0, D]$ of full measure such that for any $\rho \in \mathcal{S}$ the non-resonance condition (2.16) holds for all $\widetilde{\mathbf{k}} \in \mathbb{Z}^{\mathcal{N}}$ with the properties in (2.16) and in addition

$$\widetilde{k}_l = 0 \quad \text{if} \quad l < 0. \tag{2.33}$$

In dimension one, an arbitrary $\mathbf{k} \in \mathbb{Z}^{\mathcal{N}}$ can be decomposed as $\mathbf{k} = \widetilde{\mathbf{k}} + \mathbf{l}$ such that $\widetilde{\mathbf{k}}$ satisfies (2.33) and

$$l_0 = 0 \quad \text{and} \quad \sum_{j \in \mathcal{N}: |j| = m} l_j = 0 \quad \text{for any } m \in \mathbb{N}.$$

Then $\mathbf{k} \cdot \boldsymbol{\omega} = \widetilde{\mathbf{k}} \cdot \boldsymbol{\omega}$ since $\omega_j = \omega_{-j}$ for all $j \in \mathcal{N} = \mathbb{Z}$. Applying the non-resonance condition (2.16) for $\widetilde{\mathbf{k}} \neq \mathbf{0}$ yields in particular that $\mathbf{k} \cdot \boldsymbol{\omega} = \widetilde{\mathbf{k}} \cdot \boldsymbol{\omega} \neq 0$ for $\rho \in \mathcal{S}$, and hence $\mathbf{k} \notin \mathcal{M}$ unless $\widetilde{\mathbf{k}} = \mathbf{0}$. This verifies the structure of the resonance module $\mathcal{M}$ as required by (2.14) in Assumption 2.6.

We finally verify the non-resonance condition (2.10) for near-resonant indices $(j, \mathbf{k})$ with $\mathbf{k} - \langle j \rangle \notin \mathcal{M}$. Decomposing $\mathbf{k} - \langle j \rangle = \widetilde{\mathbf{k}} + \mathbf{l}$ as above we have $\widetilde{\mathbf{k}} \neq \mathbf{0}$ and $|\mathbf{k} \cdot \boldsymbol{\omega} - \omega_j| = |\widetilde{\mathbf{k}} \cdot \boldsymbol{\omega}|$. Lemma 2.8 then shows that $(j, \mathbf{k})$ satisfies the non-resonance condition (2.10) as required in Assumption 2.6.

Verification of the Additional Non-Resonance Condition 2.4. *The additional non-resonance condition 2.4 is fulfilled with a constant C_3 depending only on ρ.*

This can be verified in the same way as for the nonlinear Schrödinger equation in Section 2.6.

We are now in the position to apply Theorem 2.7 and its corollaries. Recall from Section 1.5 that energy and momentum are exactly conserved along solutions of the nonlinear wave equation (2.32).

Corollary 2.20 (Long-Time Analysis of Nonlinear Wave Equations (2.32) with Periodic Boundary Conditions)**.** *Fix N, $s \geq 2s_0 > 1$, and assume $g(0) = g'(0) = 0$ and $\rho \in \mathcal{S}$. Then for any ε sufficiently small compared to the nonlinearity g, ρ, s_0, s, and N and for small initial values*

$$\|\xi(0)\|_s = \Big(\sum_{j \in \mathcal{N}} |j|^{2s} \Big(\frac{\omega_j}{2} |u_j(0)|^2 + \frac{1}{2\omega_j} |v_j(0)|^2 \Big) \Big)^{\frac{1}{2}} \leq \varepsilon$$

we have

- *near-conservation of sums of actions* (2.15) *with $C\varepsilon$ instead of $C\varepsilon^{\frac{1}{2}}$,*
- *exact conservation of energy and momentum,*
- *near-conservation of mass* (2.20) *with $C\varepsilon$ instead of $C\varepsilon^{\frac{1}{2}}$,*
- *and regularity* (2.19)

over long times

$$0 \le t \le \varepsilon^{-N}$$

along any solution $u(x,t) = \sum_{j\in\mathcal{N}} u_j(t)e^{i(j\cdot x)}$ *and* $v(x,t) = \sum_{j\in\mathcal{N}} v_j(t)e^{i(j\cdot x)}$ *with* $\xi_j = (\omega_j^{\frac{1}{2}} u_j + i\omega_j^{-\frac{1}{2}} v_j)/\sqrt{2}$ *of the nonlinear wave equation* (2.32) *with periodic boundary conditions with a constant* C *depending only on* g, ρ, s_0, s, *and* N, *but not on* ε. □

This result was proven in [17]. Now we apply the results 2.13 and 2.14 on the long-time energy distribution of Section 2.5 to the nonlinear wave equation (2.32). To our knowledge, similar results for nonlinear wave equations do not exist.

Corollary 2.21 (Long-Time Energy Distribution (a) for Nonlinear Wave Equations (2.32) with Periodic Boundary Conditions)**.** *Let* $0 < \mu \le 1$. *Under the assumptions of Corollary 2.20 and for small initial values*

$$\|\xi(0)\|_s \le \varepsilon \quad \textit{with } (2.22\text{a})$$

we have for any ε, *such that* ε^μ *satisfies the smallness assumption of Corollary 2.20, the energy distribution*

$$\sum_{(m-1)B<|l|\le mB} |l|^{2s} I_l(\xi(t), \overline{\xi(t)}) \le C\varepsilon^{2m(1-\mu)+3\mu}$$

for $m \ge 2$ *over long times*

$$0 \le t \le \varepsilon^{-N\mu}$$

with the constant C *of Corollary 2.20.* □

Corollary 2.22 (Long-Time Energy Distribution (b) for Nonlinear Wave Equations (2.32) with Periodic Boundary Conditions)**.** *Let* $0 < \mu \le 1$. *Under the assumptions of Corollary 2.20 and for small initial values*

$$\|\xi(0)\|_s \le \varepsilon \quad \textit{with } (2.22\text{b})$$

we have for any ε, *such that* ε^μ *satisfies the smallness assumption of Corollary 2.20, the energy distribution*

$$I_0(\xi(t), \overline{\xi(t)}) \le C\varepsilon^{4(1-\mu)+3\mu},$$
$$|m\tilde{j}|^{2s} I_{m\tilde{j}}(\xi(t), \overline{\xi(t)}) \le C\varepsilon^{2|m|(1-\mu)+3\mu}$$

for $m \in \mathbb{Z}$ *with* $m \ne \pm 1$ *over long times*

$$0 \le t \le \varepsilon^{-N\mu}$$

with the constant C *of Corollary 2.15. If* $l \notin \{\, m\tilde{j} : m \in \mathbb{Z} \,\}$, *then* $\xi_l(t) = 0$ *for all times* t. □

2.10 Example — Nonlinear Wave Equations with Dirichlet Boundary Conditions

We finally apply the results from Sections 2.2 and 2.4 to the nonlinear wave equation

$$\frac{\partial^2}{\partial t^2} u(x,t) = \Delta u(x,t) - \rho u(x,t) + g(u(x,t)) \tag{2.34}$$

with Dirichlet boundary conditions $u(x,t) = v(x,t) = 0$ for x on the boundary of $[0,\pi]$ and with an odd nonlinearity g, $g(u) = -g(-u)$. The Hamiltonian structure of this equation was established in Section 1.5.

Using the first Hamiltonian formulation (1.16) of this equation, which is the same as in the case of periodic boundary conditions, we have already verified the assumptions needed for Theorem 2.7 and its corollaries and directly get that Corollaries 2.20, 2.21, and 2.22 are also valid along solutions of (2.34) with appropriate notions of actions, mass, and momentum, see Section 1.5. Note that the sums of actions in Corollary 2.20 are just multiples of the actions since $I_j = I_{-j}$, see also Section 1.5. This implies that we have indeed long-time near-conservation of actions and not only of sums of actions.

Concerning the second Hamiltonian formulation (1.18) of (2.34), we mention that its actions are just multiples of the actions for the first formulation since $\widetilde{u}_j = -2iu_j$ and $\widetilde{v}_j = -2iv_j$. In this way, the long-time near-conservation of actions, mass, and momentum with respect to the second formulation follows from the long-time near-conservation of actions with respect to the first formulation.

For the case of Dirichlet boundary conditions we assumed an odd nonlinearity g. This helped us to apply the theory developed for periodic boundary conditions also in the case of Dirichlet boundary conditions. But this property of the nonlinearity is indeed crucial since we are not able to verify the regularity assumption 2.1 with a general nonlinearity.

3 Modulated Fourier Expansions of Hamiltonian Partial Differential Equations

In this chapter we prove Theorem 2.5 on the long-time near-conservation of actions along solutions of the Hamiltonian equations of motion (2.2) corresponding to the Hamiltonian function (2.1) in a weakly nonlinear setting. This is done in Sections 3.1, 3.2, 3.3, 3.4, and 3.5 using the technique of modulated Fourier expansions. The proof mainly relies on a generalization of the corresponding proofs in [17] and in particular [29], where the examples of nonlinear wave and Schrödinger equations are treated. In Sections 3.6 and 3.7 we finally comment on the modifications needed for the proof of the slightly more general Theorems 2.7 and 2.12 on the long-time near-conservation of sums of actions in the case of partial resonances and the long-time near-conservation of scaled actions, respectively.

We fix N, and we assume the assumptions in Theorem 2.5 to be satisfied. The considered Hamiltonian equations of motion (2.2) then take the form

$$\begin{aligned} i\frac{d}{dt}\xi_j(t) &= \omega_j\xi_j(t) + \frac{\partial P}{\partial \eta_j}(\xi(t),\overline{\xi(t)}) \\ &= \omega_j\xi_j(t) + \sum_{m+m'=2}^{\infty}\sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l}\xi_{k^1}(t)\cdots\xi_{k^m}(t)\overline{\xi_{l^1}(t)\cdots\xi_{l^{m'}}(t)}. \end{aligned} \tag{3.1}$$

We study the weakly nonlinear situation where the initial value $\xi(0)$ is small of size $\varepsilon \le \varepsilon_0$,

$$\|\xi(0)\|_s \le \varepsilon.$$

Here, ε_0 is the constant appearing in the non-resonance condition 2.3, and we aim for a near-conservation of actions on a time interval of length ε^{-N} as stated in Theorem 2.5. We will also use the various other constants from the assumptions of Theorem 2.5. Assumption 2.1 on the regularity of the nonlinearity P yields constants C_1, $s_0 \le s$, C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$. Constants c_2, C_2, and σ result from Assumption 2.2 on the dimension or the zero momentum, and Assumption 2.3 on the non-resonance of the frequencies yields a constant C_0 apart from ε_0.

3.1 Modulated Fourier Expansions

The Idea of Modulated Fourier Expansions. In the absence of the nonlinearity ($P = 0$) the functions $e^{-i\omega_j t}$ are solutions of (3.1). Since the nonlinearity introduces products, the idea in the theory of modulated Fourier expansions is to expand solutions of (3.1) in terms of products of these exponentials,

$$\prod_{l\in\mathcal{N}}(e^{-i\omega_l t})^{k_l} = e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$$

for sequences $\mathbf{k} = (k_l)_{l\in\mathcal{N}} \in \mathbb{Z}^{\mathcal{N}}$ of integers with finitely many nonzero entries and with $\mathbf{k}\cdot\boldsymbol{\omega} = \sum_{l\in\mathcal{N}} k_l\omega_l$. We hence make the ansatz

$$\widetilde{\xi}_j(t) = \sum_{\mathbf{k}} z_j^{\mathbf{k}}(\varepsilon t)e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t} \tag{3.2}$$

for the solution of (3.1), where the sum runs over all sequences $\mathbf{k} \in \mathbb{Z}^{\mathcal{N}}$ of integers with finitely many nonzero entries indexed by $\mathcal{N}$. This is called a *modulated Fourier expansion* of $\xi_j(t)$. It separates the timescale t and the timescale $\tau = \varepsilon t$ on which the coefficients of the products $e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$, the *modulation functions* $z_j^{\mathbf{k}} = z_j^{\mathbf{k}}(\tau)$, evolve. For an overview on the short but lively history of modulated Fourier expansions we refer the reader to the Introduction of the present thesis.

The Modulation System. Inserting the ansatz (3.2) in the equations of motion (3.1) and comparing the coefficients of the exponentials $e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$ results in the *modulation system*

$$i\varepsilon\dot{z}_j^{\mathbf{k}} + (\mathbf{k}\cdot\boldsymbol{\omega})z_j^{\mathbf{k}} = \omega_j z_j^{\mathbf{k}} + \sum_{m+m'=2}^{\infty} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l} z_{k^1}^{\mathbf{k}^1}\cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1}\cdots z_{l^{m'}}^{\mathbf{l}^{m'}}} \tag{3.3a}$$

for the modulation functions $z_j^{\mathbf{k}}$ of the modulated Fourier expansion (3.2). Here and in the following, a dot $\dot{}$ symbolises the derivative with respect to the slow timescale $\tau = \varepsilon t$. The initial condition for $\xi(t)$ further yields

$$\sum_{\mathbf{k}} z_j^{\mathbf{k}}(0) = \xi_j(0). \tag{3.3b}$$

Comparison with the Modulated Fourier Expansion of Nonlinear Wave Equations in [17]. In [17], a modulated Fourier expansion for the nonlinear wave equation (1.14) of Section 1.5 is used to prove Corollary 2.20 on the long-time near-conservation of actions along solutions of (1.14).

In this reference, the function $u = u(x,t)$ and its Fourier coefficients $u_j(t)$ are expanded as a modulated Fourier expansion. The modulated Fourier expansion (3.2) for the general class of Hamiltonian partial differential equations considered here yields a different modulated Fourier expansion for the nonlinear wave equation. Indeed, we expand the complex coefficients

$$\xi_j(t) = \frac{\omega_j^{\frac{1}{2}}u_j(t) + i\omega_j^{-\frac{1}{2}}v_j(t)}{\sqrt{2}}$$

as introduced in Section 1.5 which involve not only the Fourier coefficients $u_j(t)$ but also their time derivatives $v_j(t) = \frac{d}{dt}u_j(t)$, both scaled with the corresponding frequency ω_j.

Formal Analysis of the Modulation System. Formally, (3.3a) are the equations of motion of a Hamiltonian system on a phase space of sequences $\mathbf{z} = (z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}$ with

Hamiltonian function

$$\begin{aligned}\mathbf{H}(\mathbf{z},\mathbf{w}) &= \varepsilon^{-1} \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} (\omega_j - \mathbf{k}\cdot\boldsymbol{\omega}) z_j^{\mathbf{k}} w_j^{\mathbf{k}} \\ &\quad + \varepsilon^{-1} \sum_{m,m'=0}^{\infty} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'+1}=0}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'+1}} P_{k,l} z_{k^1}^{\mathbf{k}^1}\cdots z_{k^m}^{\mathbf{k}^m} w_{l^1}^{\mathbf{l}^1}\cdots w_{l^{m'+1}}^{\mathbf{l}^{m'+1}}\end{aligned} \tag{3.4}$$

with the same coefficients $P_{k,l}$ as in the Hamiltonian function $H(\xi,\eta)$. In particular, the Hamiltonian function $\mathbf{H}$ also satisfies the condition $\overline{\mathbf{H}(\mathbf{z},\mathbf{w})} = \mathbf{H}(\overline{\mathbf{w}},\overline{\mathbf{z}})$, that we imposed in Section 1.1 on Hamiltonian functions.

Since the sum in the Hamiltonian function $\mathbf{H}$ is over all $\mathbf{k}^1,\dots,\mathbf{k}^m,\mathbf{l}^1,\dots,\mathbf{l}^{m'+1}$ with $\mathbf{k}^1+\cdots+\mathbf{k}^m-\mathbf{l}^1-\cdots-\mathbf{l}^{m'+1} = \mathbf{0}$, $\mathbf{H}(\mathbf{z},\overline{\mathbf{z}})$ is invariant under the transformation $z_j^{\mathbf{k}} \mapsto e^{i\theta k_l} z_j^{\mathbf{k}}$ for $l \in \mathcal{N}$. According to Proposition 1.4 this implies the conservation of the corresponding component of the momentum

$$\mathbf{K}_l(\mathbf{z},\mathbf{w}) = \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} k_l z_j^{\mathbf{k}} w_j^{\mathbf{k}}$$

along any solution of (3.3a).

Studying modulated Fourier expansions can hence be seen as blowing up the phase space of the original Hamiltonian function while preserving the Hamiltonian structure of the equations of motion. This blow-up introduces many conserved quantities $\mathbf{K}_l$ which give much insight into the original system.

Outline of the Analysis of the Modulation System. In the following Section 3.2, we will construct an approximate solution of the modulation system (3.3) in an iterative way. The iterated modulation functions constructed in this way will be estimated in Section 3.3 where also the defect of these iterated modulation functions in the modulation system is analysed. In Section 3.4, we will show that the modulated Fourier expansion corresponding to the iterated modulation functions describes the exact solution $\xi(t)$ of the Hamiltonian equations of motion (3.1) up to a very small error.

However, the complete analysis is valid only on a (rather) short time interval $0 \le \tau = \varepsilon t \le 1$. The extension to a long time interval $0 \le \tau = \varepsilon t \le \varepsilon^{-N+1}$ is the subject of Section 3.5. It is done with the help of the formal invariants $\mathbf{K}_l$ of the modulation system. These turn out to be almost invariants (up to ε^{N+2}) along our approximate solution of the modulation system, which are close to the actions I_j (up to $\varepsilon^{\frac{5}{2}}$) along the exact solution of (3.1). We repeat the construction of iterated modulation functions on time intervals $1 \le \tau \le 2$, $2 \le \tau \le 3$, and so on. The almost invariants will allow us to put ε^{-N+1} of them together yielding a long time interval $0 \le \tau \le \varepsilon^{-N+1}$ on which the almost invariants are nearly conserved (up to ε^3) and close to the actions (up to $\varepsilon^{\frac{5}{2}}$). This finally completes the proof of Theorem 2.5.

3.2 Iterative Solution of the Modulation System

In order to make the formal analysis of the preceding section rigorous, we construct iteratively an approximate solution of the modulation system (3.3) in this section. This construction is valid on a short time interval $0 \le \tau = \varepsilon t \le 1$.

Cut-Off. We do not cut off terms with high frequencies but instead work with all frequencies. However, we cut off terms in which a large number of frequencies is accumulated, i.e., terms with a large index $\mathbf{k}$ (recall that $z_j^{\mathbf{k}}$ is the coefficient of $e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$). We set

$$z_j^{\mathbf{k}} = 0 \quad \text{if } \|\mathbf{k}\| > L \tag{3.5}$$

with

$$L = 2N + 4 + 4s_0$$

depending only on N and s_0. Since the modulation functions decrease with increasing $\|\mathbf{k}\|$, we will be able to handle this cut-off.

Moreover, we cut off summands of the nonlinearity in (3.1), namely those with $m + m' > L$, and consider only

$$\sum_{m+m'=2}^{L} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l}\, z_{k^1}^{\mathbf{k}^1}\cdots z_{k^m}^{\mathbf{k}^m}\, \overline{z_{l^1}^{\mathbf{l}^1}\cdots z_{l^{m'}}^{\mathbf{l}^{m'}}}.$$

Again, the size of the modulation functions will enable us to control this cut-off.

The Iteration. We aim for an iterative solution of the modulation system (3.3) on the time interval $0 \le \tau \le 1$. We only consider indices $\mathbf{k}$ with $\|\mathbf{k}\| \le L$ since otherwise $z_j^{\mathbf{k}} = 0$ by (3.5). Initially we set on $0 \le \tau \le 1$

$$\left[z_j^{\langle j\rangle}\right]^0 = \xi_j(0) \quad \text{and} \quad \left[z_j^{\mathbf{k}}\right]^0 = 0 \quad \text{for } \mathbf{k} \ne \langle j\rangle.$$

Our iteration is motivated by an isolation of the dominant terms in (3.3a). We distinguish three different terms in the modulation system (3.3a).

• The nonlinear term is expected to be of size $\mathcal{O}(\varepsilon)\mathbf{z}$ since the nonlinearity is quadratic and since we expect $\mathbf{z}$ to be of size ε.

• The term $i\varepsilon\dot{z}_j^{\mathbf{k}}$ is of size $\varepsilon\dot{\mathbf{z}}$.

• The size of $(\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)z_j^{\mathbf{k}}$ depends on $\mathbf{k}$ and j. It vanishes for $\mathbf{k} = \langle j\rangle$ and is of size $\Omega(\varepsilon^{\frac{1}{2}})\mathbf{z}$ for not near-resonant indices; for near-resonant indices it is of size $\mathcal{O}(\varepsilon^{\frac{1}{2}})\mathbf{z}$.

For the indices $(j,\mathbf{k})$ with $\mathbf{k} \ne \langle j\rangle$ that are not near-resonant, the term $(\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)$ is considered dominant in (3.3a). We collect those indices (and the indices $(j,\mathbf{k})$ where $|j|$ is not too small if the condition of small dimension (2.9a) is satisfied in Assumption 2.2) in the set $\mathcal{S}_\varepsilon$,

$$\begin{aligned}\mathcal{S}_\varepsilon = \{\, (j,\mathbf{k}) \in \mathcal{N}\times\mathbb{Z}^{\mathcal{N}} : \mathbf{k} \ne \langle j\rangle,\ \|\mathbf{k}\| \le L,\ |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| \ge \varepsilon^{\frac{1}{2}},\\ |j| > \varepsilon|l| \text{ for all } l \in \mathcal{N} \text{ with } k_l \ne 0 \,\}\end{aligned}$$

if the condition of small dimension (2.9a) is satisfied in Assumption 2.2 and

$$\mathcal{S}_\varepsilon = \{\, (j,\mathbf{k}) \in \mathcal{N} \times \mathbb{Z}^{\mathcal{N}} : \mathbf{k} \neq \langle j \rangle,\ \|\mathbf{k}\| \leq L,\ |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| \geq \varepsilon^{\frac{1}{2}} \,\}$$

if the condition of zero momentum is satisfied in Assumption 2.2. The reason for these different definitions will become clear later. Since the term $(\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)$ is dominant in (3.3a) for indices $(j,\mathbf{k}) \in \mathcal{S}_\varepsilon$, we determine for those indices algebraically the $(n+1)$th iterate of the modulation function $z_j^{\mathbf{k}}$ on $0 \leq \tau \leq 1$ by

$$\Big[z_j^{\mathbf{k}}\Big]^{n+1} = \frac{1}{\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j}\Big[-i\varepsilon \dot{z}_j^{\mathbf{k}} + \sum_{m+m'=2}^{L} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l}\, z_{k^1}^{\mathbf{k}^1}\cdots z_{k^m}^{\mathbf{k}^m}\, \overline{z_{l^1}^{\mathbf{l}^1}\cdots z_{l^{m'}}^{\mathbf{l}^{m'}}}\Big]^n. \tag{3.6a}$$

The notation $[\cdot]^n$ means that the nth iterate of all modulation functions within the brackets is taken.

For $\mathbf{k} = \langle j \rangle$ the $(n+1)$th iterate of $z_j^{\langle j \rangle}$ is defined on $0 \leq \tau \leq 1$ by the differential equation

$$\Big[\dot{z}_j^{\langle j \rangle}\Big]^{n+1} = -i\varepsilon^{-1}\Big[\sum_{m+m'=2}^{L} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\langle j \rangle}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l}\, z_{k^1}^{\mathbf{k}^1}\cdots z_{k^m}^{\mathbf{k}^m}\, \overline{z_{l^1}^{\mathbf{l}^1}\cdots z_{l^{m'}}^{\mathbf{l}^{m'}}}\Big]^n \tag{3.6b}$$

with initial value

$$\Big[z_j^{\langle j \rangle}(0)\Big]^{n+1} = \xi_j(0) - \Big[\sum_{\mathbf{k}\neq\langle j \rangle} z_j^{\mathbf{k}}(0)\Big]^n \tag{3.6c}$$

motivated by (3.3b).

We are not able to identify the dominant term in (3.3a) for near-resonant indices with $|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| < \varepsilon^{\frac{1}{2}}$. For this reason we set for $n \geq 0$

$$\Big[z_j^{\mathbf{k}}\Big]^{n+1} = 0 \tag{3.6d}$$

on $0 \leq \tau \leq 1$ for near-resonant indices with the firm expectation that the non-resonance condition 2.3 allows us to control the induced error. Moreover, if the condition of small dimension (2.9a) is satisfied in Assumption 2.2 and if $|j| \leq \varepsilon |l|$ for an $l \in \mathcal{N}$ with $k_l \neq 0$, we set on $0 \leq \tau \leq 1$ for $n \geq 0$

$$\Big[z_j^{\mathbf{k}}\Big]^{n+1} = 0. \tag{3.6e}$$

We collect the indices for which we set all the iterates to zero in the set $\mathcal{R}_\varepsilon$,

$$\mathcal{R}_\varepsilon = \{\, (j,\mathbf{k}) \in \mathcal{N} \times \mathbb{Z}^{\mathcal{N}} : \mathbf{k} \neq \langle j \rangle,\ \|\mathbf{k}\| \leq L,\\ |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| < \varepsilon^{\frac{1}{2}} \text{ or } |j| \leq \varepsilon|l| \text{ for an } l \in \mathcal{N} \text{ with } k_l \neq 0 \,\}$$

if the condition of small dimension (2.9a) is satisfied in Assumption 2.2, and

$$\mathcal{R}_\varepsilon = \{\, (j,\mathbf{k}) \in \mathcal{N} \times \mathbb{Z}^{\mathcal{N}} : \mathbf{k} \neq \langle j \rangle,\ \|\mathbf{k}\| \leq L,\ |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| < \varepsilon^{\frac{1}{2}} \,\}$$

if the condition of zero momentum (2.9b) is satisfied in Assumption 2.2.

Summarising we have algebraic equations for modulation functions $z_j^{\mathbf{k}}$ belonging to indices $(j,\mathbf{k}) \in \mathcal{S}_\varepsilon$, differential equations modulation functions belonging to $(j,\langle j\rangle)$, and we set $z_j^{\mathbf{k}}$ to zero for $(j,\mathbf{k}) \in \mathcal{R}_\varepsilon$.

Single-wave Modulation Functions. If the condition of zero momentum (2.9b) is satisfied in Assumption 2.2, then for given $\mathbf{k}$ only one modulation function is nonzero,

$$\left[z_j^{\mathbf{k}}\right]^n = 0 \quad \text{for all } j \in \mathcal{N} \text{ with } j \neq j(\mathbf{k}) \text{ and all } n \text{ on } 0 \leq \tau \leq 1. \tag{3.7}$$

Recall that $j(\mathbf{k}) = \sum_{l\in\mathcal{N}} k_l l$. We refer to this phenomenon as *single-wave modulation functions*. Indeed, the index $\mathbf{k}$ corresponds to a temporal evolution $e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$, while in our examples in Sections 2.6, 2.7, and 2.9 the index j corresponds to a (spatial) wave $e^{i(j\cdot x)}$. The property (3.7) states that the evolution $e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$ consists of a single wave $e^{i(j(\mathbf{k})\cdot x)}$.

The proof of (3.7) is done by induction on n. The case $n = 0$ is clear, so let $n > 0$ and consider the iteration (3.6a) for $j \neq j(\mathbf{k})$. Inductively only those terms in the nonlinearity are nonzero with

$$k^1 = j(\mathbf{k}^1), \ldots, k^m = j(\mathbf{k}^m), l^1 = j(\mathbf{l}^1), \ldots, l^{m'} = j(\mathbf{l}^{m'}).$$

Due to the condition of zero momentum (2.9b) only those terms in the nonlinearity are nonzero where

$$j = k^1 + \cdots + k^m - l^1 - \cdots - l^{m'}.$$

This implies

$$j = j(\mathbf{k}^1) + \cdots + j(\mathbf{k}^m) - j(\mathbf{l}^1) - \cdots - j(\mathbf{l}^{m'}) = j(\mathbf{k})$$

and concludes the proof of (3.7).

Abstract Formulation of the Iteration I. We set

$$[[\mathbf{k}]] = \begin{cases} \frac{1}{2}(\|\mathbf{k}\| + 1), & \mathbf{k} \neq \mathbf{0}, \\ \frac{3}{2}, & \mathbf{k} = \mathbf{0}, \end{cases}$$

and rescale the modulation functions with corresponding powers of ε,

$$c_j^{\mathbf{k}} = \varepsilon^{-[[\mathbf{k}]]} z_j^{\mathbf{k}}.$$

This takes into account the powers of ε accumulating in the modulation functions $z_j^{\mathbf{k}}$. Moreover, we split the rescaled variables in the "diagonal" part $c_j^{\langle j\rangle}$ and the off-diagonal part $c_j^{\mathbf{k}}$ with $(j,\mathbf{k}) \in \mathcal{S}_\varepsilon$, i.e.

$$a_j^{\mathbf{k}} = \begin{cases} 0, & (j,\mathbf{k}) \in \mathcal{S}_\varepsilon, \\ c_j^{\mathbf{k}}, & \mathbf{k} = \langle j\rangle, \\ 0, & (j,\mathbf{k}) \in \mathcal{R}_\varepsilon \text{ or } \|\mathbf{k}\| > L \end{cases} \qquad \text{and} \qquad b_j^{\mathbf{k}} = \begin{cases} c_j^{\mathbf{k}}, & (j,\mathbf{k}) \in \mathcal{S}_\varepsilon, \\ 0, & \mathbf{k} = \langle j\rangle, \\ 0, & (j,\mathbf{k}) \in \mathcal{R}_\varepsilon \text{ or } \|\mathbf{k}\| > L. \end{cases}$$

Note that entries belonging to indices $(j,\mathbf{k}) \in \mathcal{R}_\varepsilon$ or to indices with $\|\mathbf{k}\| > L$ are set to zero in the iteration. Therefore, we have indeed $[\mathbf{c}]^n = [\mathbf{a}]^n + [\mathbf{b}]^n$, where $\mathbf{a} = (a_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}$, $\mathbf{b} = (b_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}$, and $\mathbf{c} = (c_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}$.

In these variables the nonlinearity reads

$$\mathbf{F}(\mathbf{c})_j^{\mathbf{k}} = \sum_{m+m'=2}^{L} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \frac{\varepsilon^{[[\mathbf{k}^1]]+\cdots+[[\mathbf{k}^m]]+[[\mathbf{l}^1]]+\cdots+[[\mathbf{l}^{m'}]]}}{\varepsilon^{[[\mathbf{k}]]}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l}\, c_{k^1}^{\mathbf{k}^1}\cdots c_{k^m}^{\mathbf{k}^m}\, \overline{c_{l^1}^{\mathbf{l}^1}\cdots c_{l^{m'}}^{\mathbf{l}^{m'}}},$$

and the iteration (3.6) becomes

$$\begin{aligned} \Big[b_j^{\mathbf{k}}\Big]^{n+1} &= \frac{1}{\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j}\Big[-i\varepsilon\dot b_j^{\mathbf{k}} + \mathbf{F}(\mathbf{c})_j^{\mathbf{k}}\Big]^n \quad \text{for } (j,\mathbf{k})\in\mathcal{S}_\varepsilon, \\ \Big[\dot a_j^{\langle j\rangle}\Big]^{n+1} &= -i\varepsilon^{-1}\Big[\mathbf{F}(\mathbf{c})_j^{\langle j\rangle}\Big]^n, \quad \Big[a_j^{\langle j\rangle}(0)\Big]^{n+1} = \varepsilon^{-1}\xi_j(0) - \Big[\sum_{\mathbf{k}\neq\langle j\rangle}\varepsilon^{[[\mathbf{k}]]-1} b_j^{\mathbf{k}}(0)\Big]^n. \end{aligned} \tag{3.8}$$

Abstract Formulation of the Iteration II. A second rescaling also takes into account the frequencies accumulating in the modulation functions. We set

$$\hat a_j^{\mathbf{k}} = \mathbf{j}^{(s-s_0)|\mathbf{k}|} a_j^{\mathbf{k}}, \quad \hat b_j^{\mathbf{k}} = \mathbf{j}^{(s-s_0)|\mathbf{k}|} b_j^{\mathbf{k}}, \quad \hat c_j^{\mathbf{k}} = \mathbf{j}^{(s-s_0)|\mathbf{k}|} c_j^{\mathbf{k}},$$

and

$$\hat{\mathbf{F}}(\hat{\mathbf{c}})_j^{\mathbf{k}} = \sum_{m+m'=2}^{L} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \frac{\varepsilon^{[[\mathbf{k}^1]]+\cdots+[[\mathbf{k}^m]]+[[\mathbf{l}^1]]+\cdots+[[\mathbf{l}^{m'}]]}}{\varepsilon^{[[\mathbf{k}]]}} \frac{\mathbf{j}^{(s-s_0)|\mathbf{k}|}}{\mathbf{j}^{(s-s_0)(|\mathbf{k}^1|+\cdots+|\mathbf{k}^m|+|\mathbf{l}^1|+\cdots+|\mathbf{l}^{m'}|)}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l}\, \hat c_{k^1}^{\mathbf{k}^1}\cdots \hat c_{k^m}^{\mathbf{k}^m}\, \overline{\hat c_{l^1}^{\mathbf{l}^1}\cdots \hat c_{l^{m'}}^{\mathbf{l}^{m'}}}.$$

The iteration for $\hat{\mathbf{b}}$ then becomes

$$\Big[\hat b_j^{\mathbf{k}}\Big]^{n+1} = \frac{1}{\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j}\Big[-i\varepsilon\dot{\hat b}_j^{\mathbf{k}} + \hat{\mathbf{F}}(\hat{\mathbf{c}})_j^{\mathbf{k}}\Big]^n \quad \text{for } (j,\mathbf{k})\in\mathcal{S}_\varepsilon. \tag{3.9}$$

3.3 Estimating the Iterated Modulation Functions

In this section we estimate the iterated modulation functions $[\mathbf{z}]^n$ constructed in the previous section. We use the norm

$$|||\mathbf{z}|||_s = \Big\|\Big(\sum_{\mathbf{k}}|z_j^{\mathbf{k}}|\Big)_{j\in\mathcal{N}}\Big\|_s = \Big(\sum_{j\in\mathcal{N}}|j|^{2s}\Big(\sum_{\mathbf{k}}|z_j^{\mathbf{k}}|\Big)^2\Big)^{\frac12}.$$

This is the norm used in [29] and [30]. In contrast to the norm used in [17], [16], and [34], namely $(\sum_{j\in\mathcal{N}}|j|^{2s}\sum_{\mathbf{k}}|z_j^{\mathbf{k}}|^2)^{\frac12}$, this norm is not completely l^2-based but mixes an

l^2- with an l^1-framework. The indices $\mathbf{k}$ are treated in the l^1-framework, whereas the indices j are treated in the l^2-framework. It turns out to be an appropriate norm to handle the Hamiltonian systems considered in this thesis, see also the comment following the estimate (3.10) and Section 3.4. The additional regularity of the nonlinearity in the nonlinear wave equation (see Section 1.5) allows the authors of [17], [34], and [16] to use a completely l^2-based norm.

Size of the Iterated Modulation Functions. In order to estimate the size of the iterated modulation functions we estimate in the following lemma the nonlinearities $\mathbf{F}$ and $\hat{\mathbf{F}}$ generalizing (2.7). This is done using the regularity assumption 2.1.

Lemma 3.1. *Denoting by* $\cdot^{(\ell)}$ *the* ℓ*th derivative with respect to* τ*, we have for* $\mathbf{c} = \mathbf{c}(\tau)$

$$|||\mathbf{F}(\mathbf{c})^{(\ell)}|||_s \le C\varepsilon^{\frac{1}{2}}$$

with a constant C *depending only on* $\max_{\tilde{\ell}=0,\dots,\ell} |||\mathbf{c}^{(\tilde{\ell})}|||_s$*,* $C_{L,s}$*,* ℓ*, and* L*. Moreover, for the diagonal elements and near-diagonal elements of* $\mathbf{F}(\mathbf{c})$ *we have*

$$\Big|\Big|\Big| \Big(\mathbf{F}(\mathbf{c})_j^{\langle j\rangle}\Big)^{(\ell)}_{j\in\mathcal{N}} \Big|\Big|\Big|_s \le C\varepsilon \quad \text{and} \quad \Big|\Big|\Big| \Big(\mathbf{F}(\mathbf{c})_j^{\mathbf{k}}\Big)^{(\ell)}_{j\in\mathcal{N},\|\mathbf{k}\|=1} \Big|\Big|\Big|_s \le C\varepsilon$$

with the same constant.

The same estimates hold true if $\mathbf{c}$*,* $\mathbf{F}$*, and* s *are replaced by* $\hat{\mathbf{c}}$*,* $\hat{\mathbf{F}}$*, and* s_0*, respectively.*

Proof. We first restrict our attention to the case $\ell = 0$. Note that for $\mathbf{k}^1 + \dots + \mathbf{k}^m - \mathbf{l}^1 - \dots - \mathbf{l}^{m'} = \mathbf{k}$ and $m + m' \ge 2$

$$\begin{aligned}[[\mathbf{k}^1]] + \dots + [[\mathbf{k}^m]] + [[\mathbf{l}^1]] + \dots + [[\mathbf{l}^{m'}]] &\ge \max\Big(\frac{1}{2}\|\mathbf{k}\| + \frac{m+m'}{2}, m+m'\Big) \\ &\ge [[\mathbf{k}]] + \frac{m+m'-1}{2}.\end{aligned}$$

Therefore we have

$$\begin{aligned}\sum_{\mathbf{k}} |\mathbf{F}(\mathbf{c})_j^{\mathbf{k}}| &\le \sum_{m+m'=2}^{L} \varepsilon^{\frac{m+m'-1}{2}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} |P_{j,k,l}| \\ &\qquad \Big(\sum_{\mathbf{k}^1} |c_{k^1}^{\mathbf{k}^1}|\Big) \cdots \Big(\sum_{\mathbf{k}^m} |c_{k^m}^{\mathbf{k}^m}|\Big) \Big(\sum_{\mathbf{l}^1} |c_{l^1}^{\mathbf{l}^1}|\Big) \cdots \Big(\sum_{\mathbf{l}^{m'}} |c_{l^{m'}}^{\mathbf{l}^{m'}}|\Big) \\ &= \sum_{m+m'=2}^{L} \varepsilon^{\frac{m+m'-1}{2}} |P|_j^{m,m'}(\xi,\dots,\xi)\end{aligned}$$

with $\xi = (\sum_{\mathbf{k}} |c_j^{\mathbf{k}}|)_{j\in\mathcal{N}}$ and $|P|_j^{m,m'}$ from Assumption 2.1. Using (2.6a) from the regularity assumption 2.1 we finally get

$$|||\mathbf{F}(\mathbf{c})|||_s = \Big\| \Big(\sum_{\mathbf{k}} |\mathbf{F}(\mathbf{c})_j^{\mathbf{k}}|\Big)_{j\in\mathcal{N}} \Big\|_s \le \varepsilon^{\frac{1}{2}} \sum_{m+m'=2}^{L} C_{m,m',s} \|\xi\|_s^{m+m'} \le \varepsilon^{\frac{1}{2}} C_{L,s} \sum_{m+m'=2}^{L} |||\mathbf{c}|||_s^{m+m'}$$

as claimed.

To handle the case $\ell > 0$ we have to differentiate $\mathbf{F}(\mathbf{c})$ using the product rule. Then the proof is very similar to the case $\ell = 0$. Pick one resulting summand where $c^{\mathbf{k}^1}$ is differentiated ℓ_1 times, $c^{\mathbf{k}^2}$ is differentiated ℓ_2 times, ..., and $c^{\mathbf{l}^{m'}}$ is differentiated $\ell_{m+m'}$ times. With the above calculation, this summand can be estimated using (2.6) by $\varepsilon^{\frac{1}{2}} C_{m,m',s} |||\mathbf{c}^{(\ell_1)}|||_s \cdots |||\mathbf{c}^{(\ell_{m+m'})}|||_s \leq \varepsilon^{\frac{1}{2}} C_{m,m',s} \max_{\tilde{\ell}=0,\dots,\ell} |||\mathbf{c}^{(\tilde{\ell})}|||_s^{m+m'}$. A crude estimate of the number of such summands for fixed ℓ, m, and m' is $(\ell+1)^{m+m'}$. This yields the result as stated in the lemma.

The estimate for the diagonal elements and near-diagonal elements of $\mathbf{F}$ is obtained in the same way using

$$[[\mathbf{k}^1]] + \cdots + [[\mathbf{k}^m]] + [[\mathbf{l}^1]] + \cdots + [[\mathbf{l}^{m'}]] \geq m + m' \geq [[\mathbf{k}]] + 1$$

for $[[\mathbf{k}]] = 1$, i.e., $\|\mathbf{k}\| = 1$. In order to estimate $|||\hat{\mathbf{F}}(\hat{\mathbf{c}})|||_{s_0}$ and its derivatives, we just notice that

$$\frac{\mathbf{j}^{(s-s_0)|\mathbf{k}|}}{\mathbf{j}^{(s-s_0)(|\mathbf{k}^1|+\cdots+|\mathbf{k}^m|+|\mathbf{l}^1|+\cdots+|\mathbf{l}^{m'}|)}} \leq 1$$

for $\mathbf{k}^1 + \cdots + \mathbf{k}^m - \mathbf{l}^1 - \cdots - \mathbf{l}^{m'} = \mathbf{k}$. The same calculations as above then yield the result. □

The estimates of the nonlinearity from Lemma 3.1 at hand, we are now able to control the size of the iterated (and rescaled) modulation functions $[\mathbf{c}]^n = [\mathbf{a}]^n + [\mathbf{b}]^n$ determined by the iteration (3.8).

Proposition 3.2 (Size of the Iterated Modulation Functions)**.** *We have on* $0 \leq \tau \leq 1$

$$|||[\mathbf{c}^{(\ell)}]^n|||_s \leq C$$

with a constant C *depending only on* $C_{L,s}$ *from the regularity assumption 2.1, the number of derivatives* ℓ*, the number of iterations* n*, and* L*.*

The same estimate holds true if $\mathbf{c}$ *and* s *are replaced by* $\hat{\mathbf{c}}$ *and* s_0*, respectively, with a constant depending in addition on* C_{L,s_0}*.*

Proof. We have from (3.6c)

$$|||[\mathbf{a}(0)]^{n+1}|||_s = \Big(\sum_{j\in\mathcal{N}} |j|^{2s} |[a_j^{\langle j\rangle}(0)]^{n+1}|^2\Big)^{\frac{1}{2}} \leq \varepsilon^{-1}\|\xi(0)\|_s + |||[\mathbf{b}(0)]^n|||_s. \tag{3.10}$$

Note that for this estimate, it is crucial to work with the norm $|||\cdot|||_s$ as defined above. The l^2-norm used in [17], [16], and [34] does not allow such an estimate and requires additional terms which are not present in our general setting. In combination with Lemma 3.1 we conclude on $0 \leq \tau = \varepsilon t \leq 1$

$$|||[\mathbf{a}(\tau)]^{n+1}|||_s \leq |||[\mathbf{a}(0)]^{n+1}|||_s + \sup_{0\leq\theta\leq 1} |||[\dot{\mathbf{a}}(\theta)]^{n+1}|||_s \leq \varepsilon^{-1}\|\xi(0)\|_s + |||[\mathbf{b}(0)]^n|||_s + C$$

with a constant $C = C(\sup_{0\le\theta\le 1} |||[\mathbf{c}(\theta)]^n|||_s, C_{L,s}, L)$. In addition, Lemma 3.1 together with the non-resonance condition 2.3 allows to estimate on this time interval

$$|||[\mathbf{b}]^{n+1}|||_s \le \varepsilon^{\frac{1}{2}} |||[\dot{\mathbf{b}}]^n|||_s + C$$

with the same constant C as in the above estimate of $|||[\mathbf{a}]^{n+1}|||_s$. Due to the appearance of $\dot{\mathbf{b}}$ in the latter estimate, we also have to control derivatives with respect to τ denoted by $\cdot^{(\ell)}$ in order to estimate the size of $[\mathbf{a}]^{n+1}$ and $[\mathbf{b}]^{n+1}$. This also can be done by means of Lemma 3.1 resulting in the estimates

$$\begin{aligned} |||[\mathbf{b}^{(\ell)}]^{n+1}|||_s &\le C\Big(\sup_{0\le\theta\le 1} \max_{\tilde\ell=0,\dots,\ell+1} |||[\mathbf{c}^{(\tilde\ell)}(\theta)]^n|||_s, C_{L,s}, \ell, L\Big), \\ |||[\mathbf{a}^{(\ell)}]^{n+1}|||_s &\le \varepsilon^{-1}\|\xi(0)\|_s + C\Big(\sup_{0\le\theta\le 1} \max_{\tilde\ell=0,\dots,\ell-1} |||[\mathbf{c}^{(\tilde\ell)}(\theta)]^n|||_s, C_{L,s}, \ell, L\Big) \end{aligned}$$

for $\ell \ge 1$. Initially we have $|||[\mathbf{a}]^0|||_s = \varepsilon^{-1}\|\xi(0)\|_s \le 1$, $|||[\mathbf{b}]^0|||_s = 0$, and $|||[\mathbf{c}^{(\ell)}]^0|||_s = 0$ for all $\ell > 0$. We conclude that

$$|||[\mathbf{c}^{(\ell)}]^n|||_s \le C$$

with a constant C depending only on $C_{L,s}$, ℓ, n, and L.

For the rescaled variables $\hat{\mathbf{a}}$, $\hat{\mathbf{b}}$, and $\hat{\mathbf{c}}$ we have

$$|||[\hat{\mathbf{a}}^{(\ell)}]^n|||_{s_0} = |||[\mathbf{a}^{(\ell)}]^n|||_s,$$

and the iteration (3.9) yields for $[\hat{\mathbf{b}}^{(\ell)}]^{n+1}$ the same estimate as for $[\mathbf{b}^{(\ell)}]^{n+1}$ with s replaced by s_0. This proves the proposition on the size of the iterated modulation functions. □

Defect of the Iterated Modulation Functions. After n steps of the iteration the defect in the modulation system (3.3a) is

$$\Big[d_j^{\mathbf{k}}\Big]^n = \Big[i\varepsilon\dot{z}_j^{\mathbf{k}} + (\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)z_j^{\mathbf{k}} - \sum_{m+m'=2}^{\infty} \sum_{\substack{\mathbf{k}^1+\dots+\mathbf{k}^m \\ -\mathbf{l}^1-\dots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l} z_{k^1}^{\mathbf{k}^1}\cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1}\cdots z_{l^{m'}}^{\mathbf{l}^{m'}}}\Big]^n,$$

whereas the defect in the initial condition (3.3b) reads

$$\Big[\widetilde{d}_j^{\langle j\rangle}(0)\Big]^n = \Big[\sum_{\mathbf{k}} z_j^{\mathbf{k}}(0)\Big]^n - \xi_j(0)$$

with $\widetilde{\mathbf{d}}(0)$ consisting only of diagonal entries. We write

$$\Big[d_j^{\mathbf{k}}\Big]^n = \Big[i\varepsilon e_j^{\mathbf{k}} + (\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)f_j^{\mathbf{k}} + g_j^{\mathbf{k}} + h_j^{\mathbf{k}} + p_j^{\mathbf{k}}\Big]^n$$

with

$$\begin{aligned}
&\Big[e_j^{\mathbf{k}}\Big]^n \quad \text{has only nonzero entries for } \mathbf{k} = \langle j \rangle, \\
&\Big[f_j^{\mathbf{k}}\Big]^n \quad \text{has only nonzero entries for } (j, \mathbf{k}) \in \mathcal{S}_\varepsilon, \\
&\Big[g_j^{\mathbf{k}}\Big]^n \quad \text{has only nonzero entries for } (j, \mathbf{k}) \in \mathcal{R}_\varepsilon, \\
&\Big[h_j^{\mathbf{k}}\Big]^n \quad \text{has only nonzero entries for } \|\mathbf{k}\| > L, \\
&\Big[p_j^{\mathbf{k}}\Big]^n = \Big[- \sum_{m+m'=L+1}^{\infty} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l} z_{k^1}^{\mathbf{k}^1} \cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1} \cdots z_{l^{m'}}^{\mathbf{l}^{m'}}}\Big]^n .
\end{aligned}$$

The defects $\mathbf{g}$, $\mathbf{h}$, and $\mathbf{p}$ result from the various cut-offs made in the construction of the iteration. They can be controlled as follows.

Proposition 3.3 (Defects from the Cut-Offs). *For ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, n, and L we have on $0 \le \tau \le 1$*

$$|||[\mathbf{g}]^n|||_s \le C\varepsilon^{\frac{L}{2}+2}, \quad |||[\mathbf{h}]^n|||_s \le C\varepsilon^{\frac{L}{2}+\frac{3}{2}}, \quad |||[\mathbf{p}]^n|||_s \le C\varepsilon^{\frac{L}{2}}$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 2.1, C_0 from the non-resonance condition 2.3, the number of iterations n, and L.

The estimates for $\mathbf{h}$ and $\mathbf{p}$ also hold true for $\hat{\mathbf{h}}$, $\hat{\mathbf{p}}$, and s_0 instead of $\mathbf{h}$, $\mathbf{p}$, and s.

Proof. The defect $\mathbf{g}$ in the indices $(j, \mathbf{k}) \in \mathcal{R}_\varepsilon$ is the effect of setting $[z_j^{\mathbf{k}}]^n = 0$ for those indices in (3.6d) and (3.6e). We control this effect using the non-resonance condition 2.3 which is assumed for the near-resonant indices in $\mathcal{R}_\varepsilon$ with $\varepsilon \le \varepsilon_0$. If the condition of small dimension (2.9a) is satisfied in Assumption 2.2, then the set $\mathcal{R}_\varepsilon$ also contains indices $(j, \mathbf{k})$ with $|j| \le \varepsilon |l|$ for an $l \in \mathcal{N}$ with $k_l \ne 0$. But for those indices the non-resonance condition (2.10) is also satisfied with $C_0 = 1$ provided that $s \ge N + 3 + 3s_0$ as required in (2.9a) since

$$\frac{|j|^{s-s_0}}{\mathbf{j}^{(s-s_0)|\mathbf{k}|}} \le \varepsilon^{s-s_0}$$

for such indices. In this way, we get for the defect $\mathbf{g}$ using the non-resonance condition 2.3

$$\begin{aligned}
|||[\mathbf{g}]^n|||_s^2 &= \sum_{j\in\mathcal{N}} |j|^{2s} \Big(\sum_{\mathbf{k}:(j,\mathbf{k})\in\mathcal{R}_\varepsilon} \Big| \Big[g_j^{\mathbf{k}}\Big]^n \Big| \Big)^2 = \sum_{j\in\mathcal{N}} |j|^{2s} \Big(\sum_{\mathbf{k}:(j,\mathbf{k})\in\mathcal{R}_\varepsilon} \varepsilon^{[[\mathbf{k}]]} \mathbf{j}^{-(s-s_0)|\mathbf{k}|} |\hat{\mathbf{F}}([\hat{\mathbf{c}}]^n)_j^{\mathbf{k}}| \Big)^2 \\
&\le \sup_{(j,\mathbf{k})\in\mathcal{R}_\varepsilon} \Big(\frac{|j|^{s-s_0} \varepsilon^{[[\mathbf{k}]]}}{\mathbf{j}^{(s-s_0)|\mathbf{k}|}} \Big)^2 |||\hat{\mathbf{F}}([\hat{\mathbf{c}}]^n)|||_{s_0}^2 \le (C\varepsilon^{N+4+2s_0})^2 = (C\varepsilon^{\frac{L}{2}+2})^2
\end{aligned}$$

with a constant C depending on C_{L,s_0}, $C_{L,s}$, C_0, n, and L by Lemma 3.1 and Proposition 3.2. Note that the non-resonance condition 2.3 is indeed only needed for near-resonant indices with $j = j(\mathbf{k})$ if the condition of zero momentum (2.9b) in Assumption 2.2 is satisfied due to $z_j^{\mathbf{k}} = 0$ for $j \neq j(\mathbf{k})$ by (3.7). Moreover, note that the above estimate of $[\mathbf{g}]^n$ does not hold for the rescaled variables $\hat{\mathbf{g}} = (\hat{g}_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} = (\mathbf{j}^{(s-s_0)|\mathbf{k}|} g_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}$ and s replaced by s_0.

$\mathbf{h}$ comprises the effect of setting $z_j^{\mathbf{k}} = 0$ for $\|\mathbf{k}\| > L$. We can control this defect on $0 \le \tau \le 1$ by

$$\begin{aligned} |||[\mathbf{h}]^n|||_s^2 &= \sum_{j\in\mathcal{N}} |j|^{2s} \Big(\sum_{\|\mathbf{k}\|>L} \Big| \Big[h_j^{\mathbf{k}} \Big]^n \Big| \Big)^2 = \sum_{j\in\mathcal{N}} |j|^{2s} \Big(\sum_{\|\mathbf{k}\|>L} \varepsilon^{[[\mathbf{k}]]} |\mathbf{F}([\mathbf{c}]^n)_j^{\mathbf{k}}|^2 \Big)^2 \\ &\le \varepsilon^{L+2} |||\mathbf{F}([\mathbf{c}]^n)|||_s^2 \le (C\varepsilon^{\frac{L}{2}+\frac{3}{2}})^2 \end{aligned}$$

with a constant C depending on $C_{L,s}$, n, and L by Lemma 3.1 and Proposition 3.2. The same estimate holds true in the rescaled variables $\hat{\mathbf{h}}$ and s replaced by s_0 with the same arguments and a constant depending in addition on C_{L,s_0}.

The consequences of cutting off the expansion of the nonlinearity are collected in $\mathbf{p}$. As in the proof of Lemma 3.1 we get using the regularity assumption 2.1 on $0 \le \tau \le 1$

$$\begin{aligned} |||[\mathbf{p}]^n|||_s &= \Big\| \Big(\sum_{\mathbf{k}} \Big| \Big[p_j^{\mathbf{k}} \Big]^n \Big| \Big)_{j\in\mathcal{N}} \Big\|_s \le \sum_{m+m'=L+1}^{\infty} \varepsilon^{\frac{m+m'-1}{2}} |||P|^{m,m'}(\xi,\dots,\xi)\|_s \\ &\le \varepsilon^{\frac{L}{2}} \sum_{m+m'=L+1}^{\infty} \varepsilon^{\frac{m+m'-L-1}{2}} C_{m,m',s} \|\xi\|_s^{m+m'} \end{aligned}$$

with $\xi = (\sum_{\mathbf{k}} |[c_j^{\mathbf{k}}]^n|)_{j\in\mathcal{N}}$. Note that by Proposition 3.2 $\|\xi\|_s = |||[\mathbf{c}]^n|||_s \le C$ with a constant depending only on $C_{L,s}$, n, and L. Thus, for ε sufficiently small compared to C_1, $C_{L,s}$, n, and L the latter sum converges by (2.6b), and we conclude

$$|||[\mathbf{p}]^n|||_s \le C\varepsilon^{\frac{L}{2}}$$

with a constant C depending only on C_s, $C_{L,s}$, n, and L. The same estimate holds true in the rescaled variables $\hat{\mathbf{p}}$, $\hat{\xi} = (\sum_{\mathbf{k}} |[\hat{c}_j^{\mathbf{k}}]^n|)_{j\in\mathcal{N}}$, and s replaced by s_0 with a constant depending in addition on C_{s_0} and C_{L,s_0}. We have thus proven for the cut-off defects $\mathbf{g}$, $\mathbf{h}$, and $\mathbf{p}$ the above proposition. □

The defects $\mathbf{e} + \mathbf{f}$ and $\widetilde{\mathbf{d}}$ are indeed the defects resulting from the iteration itself. For their study we introduce rescalings of the nonlinearity

$$\widetilde{\mathbf{F}}(\mathbf{c})_j^{\mathbf{k}} = \varepsilon^{[[\mathbf{k}]]} \mathbf{F}(\mathbf{c})_j^{\mathbf{k}} \quad \text{and} \quad \hat{\widetilde{\mathbf{F}}}(\hat{\mathbf{c}})_j^{\mathbf{k}} = \varepsilon^{[[\mathbf{k}]]} \hat{\mathbf{F}}(\hat{\mathbf{c}})_j^{\mathbf{k}},$$

for which Lipschitz estimates are provided by the following lemma.

Lemma 3.4. *Denoting by* $\cdot^{(\ell)}$ *the* ℓ*th derivative with respect to* τ*, we have for* $\mathbf{c} = \mathbf{c}(\tau)$ *and* $\widetilde{\mathbf{c}} = \widetilde{\mathbf{c}}(\tau)$

$$|||\widetilde{\mathbf{F}}(\mathbf{c})^{(\ell)} - \widetilde{\mathbf{F}}(\widetilde{\mathbf{c}})^{(\ell)}|||_s \le C\varepsilon \max_{\tilde{\ell}=0,\dots,\ell} |||\mathbf{z}^{(\tilde{\ell})} - \widetilde{\mathbf{z}}^{(\tilde{\ell})}|||_s$$

with a constant C depending only on $\max_{\tilde\ell=0,\dots,\ell}|||\mathbf{c}^{(\tilde\ell)}|||_s$, $\max_{\tilde\ell=0,\dots,\ell}|||\widetilde{\mathbf{c}}^{(\tilde\ell)}|||_s$, C_{L,s_0}, $C_{L,s}$, ℓ, *and* L. *Moreover, for the diagonal elements of* $\mathbf{F}(\mathbf{c})$ *we have*

$$\left|\left|\left|\left(\widetilde{\mathbf{F}}(\mathbf{c})_j^{\langle j\rangle}-\widetilde{\mathbf{F}}(\widetilde{\mathbf{c}})_j^{\langle j\rangle}\right)^{(\ell)}_{j\in\mathcal{N}}\right|\right|\right|_s \le C\varepsilon^{\frac{3}{2}}\max_{\tilde\ell=0,\dots,\ell}\left|\left|\left|\left(z_j^{\langle j\rangle}-\widetilde{z}_j^{\langle j\rangle}\right)^{(\tilde\ell)}_{j\in\mathcal{N}}\right|\right|\right|_s + C\varepsilon\max_{\tilde\ell=0,\dots,\ell}\left|\left|\left|\left(z_j^{\mathbf{k}}-\widetilde{z}_j^{\mathbf{k}}\right)^{(\tilde\ell)}_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}\right|\right|\right|_s$$

with the same constant.

The same estimates hold true if $\mathbf{c}$, $\widetilde{\mathbf{c}}$, $\mathbf{F}$, $\widetilde{\mathbf{F}}$, *and* s *are replaced by* $\hat{\mathbf{c}}$, $\hat{\widetilde{\mathbf{c}}}$, $\hat{\mathbf{F}}$, $\hat{\widetilde{\mathbf{F}}}$, *and* s_0, *respectively.*

Proof. The proof is similar to the proof of Lemma 3.1, and we start once again with the case $\ell=0$. Here, in order to estimate the powers of ε in $\widetilde{\mathbf{F}}$, we use

$$[[\mathbf{k}^1]]+\cdots+[[\mathbf{k}^m]]+[[\mathbf{l}^1]]+\cdots+[[\mathbf{l}^{m'}]]\ge[[\mathbf{l}]]+1 \tag{3.11}$$

for any $\mathbf{l}=\mathbf{k}^1,\dots,\mathbf{k}^m,\mathbf{l}^1,\dots,\mathbf{l}^{m'}$ if $m+m'\ge 2$. Moreover, we note the following equality for a difference of products, which is easily shown by induction on m using $2(a_1a_2-b_1b_2)=(a_1+b_1)(a_2-b_2)+(a_1-b_1)(a_2+b_2)$,

$$a_1\cdots a_m-b_1\cdots b_m=\sum_{l=1}^m(a_1+b_1)\cdots(a_{l-1}+b_{l-1})(a_l-b_l)(a_{l+1}\cdots a_m+b_{l+1}\cdots b_m)2^{-l}. \tag{3.12}$$

In a similar way as for $\mathbf{F}$ we then get

$$\sum_{\mathbf{k}}|\widetilde{\mathbf{F}}(\mathbf{c})_j^{\mathbf{k}}-\widetilde{\mathbf{F}}(\widetilde{\mathbf{c}})_j^{\mathbf{k}}|\le\varepsilon\sum_{m+m'=2}^{L}\sum_{l=1}^{m+m'}\Big(|P|_j^{m,m'}(\overbrace{\xi+\widetilde{\xi},\dots,\xi+\widetilde{\xi}}^{l-1},\eta,\xi,\dots,\xi) +|P|_j^{m,m'}(\underbrace{\xi+\widetilde{\xi},\dots,\xi+\widetilde{\xi}}_{l-1},\eta,\widetilde{\xi},\dots,\widetilde{\xi})\Big)2^{-l}$$

with $\xi=(\sum_{\mathbf{k}}|c_j^{\mathbf{k}}|)_{j\in\mathcal{N}}$, $\widetilde{\xi}=(\sum_{\mathbf{k}}|\widetilde{c}_j^{\mathbf{k}}|)_{j\in\mathcal{N}}$, and $\eta=(\sum_{\mathbf{l}}|z_j^{\mathbf{l}}-\widetilde{z}_j^{\mathbf{l}}|)_{j\in\mathcal{N}}$. Finally, we get using (2.6a) from the regularity assumption 2.1

$$|||\widetilde{\mathbf{F}}(\mathbf{c})-\widetilde{\mathbf{F}}(\widetilde{\mathbf{c}})|||_s\le\varepsilon\sum_{m+m'=2}^{L}\sum_{l=1}^{m+m'}C_{m,m',s}(\|\xi\|_s+\|\widetilde{\xi}\|_s)^{l-1}\|\eta\|_s(\|\xi\|_s^{m+m'-l}+\|\widetilde{\xi}\|_s^{m+m'-l})2^{-l},$$

which yields the result, since $\|\xi\|_s=|||\mathbf{c}|||_s$, $\|\widetilde{\xi}\|_s=|||\widetilde{\mathbf{c}}|||_s$, and $\|\eta\|_s=|||\mathbf{z}-\widetilde{\mathbf{z}}|||_s$.

In order to estimate the diagonal elements we just note that the above estimate (3.11) improves for $\mathbf{l}=\langle\tilde{j}\rangle$ to

$$[[\mathbf{k}^1]]+\cdots+[[\mathbf{k}^m]]+[[\mathbf{l}^1]]+\cdots+[[\mathbf{l}^{m'}]]\ge[[\mathbf{l}]]+\frac{3}{2}$$

if $\mathbf{k}^1+\cdots+\mathbf{k}^m-\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\langle j\rangle$ and $m+m'\ge 2$. The extension to higher derivatives as well as for $\hat{\mathbf{F}}(\hat{\mathbf{c}})-\hat{\widetilde{\mathbf{F}}}(\hat{\widetilde{\mathbf{c}}})$ is done as explained in the proof of Lemma 3.1. □

This lemma enables us to estimate the defects $\mathbf{e}$ and $\mathbf{f}$ from the iteration.

Proposition 3.5 (Defects from the Iteration). *For ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, n, and L we have on $0 \le \tau \le 1$*

$$
|||[\mathbf{e}^{(\ell)}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{4}}, \quad |||[\mathbf{f}^{(\ell)}]^n|||_s \le C\varepsilon^{\frac{n}{4}+1}, \quad |||((\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j)f_j^{\mathbf{k}})^{(\ell)}_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{2}},
$$
$$
|||[\widetilde{\mathbf{d}}(0)]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{4}}, \quad |||[\mathbf{d}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{2}} + C\varepsilon^{\frac{L}{2}}, \quad |||[\mathbf{d}]^n - [\mathbf{g}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{2}} + C\varepsilon^{\frac{L}{2}}
$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 2.1, C_0 from the non-resonance condition 2.3, the number of derivatives ℓ, the number of iterations n, and L.

The estimates for $\mathbf{e}$, $\mathbf{f}$, $\widetilde{\mathbf{d}}$, and $\mathbf{d}-\mathbf{g}$ also hold true for $\hat{\mathbf{e}}$, $\hat{\mathbf{f}}$, $\hat{\widetilde{\mathbf{d}}}$, $\hat{\mathbf{d}}-\hat{\mathbf{g}}$, and s_0 instead of $\mathbf{e}$, $\mathbf{f}$, $\widetilde{\mathbf{d}}$, $\mathbf{d}-\mathbf{g}$, and s.

Proof. We have

$$
\begin{aligned}
\Big[f_j^{\mathbf{k}}\Big]^n &= \Big[z_j^{\mathbf{k}}\Big]^n - \Big[z_j^{\mathbf{k}}\Big]^{n+1} \quad \text{for } (j,\mathbf{k}) \in \mathcal{S}_\varepsilon,\\
\Big[e_j^{\langle j\rangle}\Big]^n &= \Big[\dot z_j^{\langle j\rangle}\Big]^n - \Big[\dot z_j^{\langle j\rangle}\Big]^{n+1}, \quad \Big[\widetilde{d}_j^{\langle j\rangle}(0)\Big]^n = \Big[z_j^{\langle j\rangle}(0)\Big]^n - \Big[z_j^{\langle j\rangle}(0)\Big]^{n+1}.
\end{aligned}
$$

Inserting the iteration, we have for $n > 0$

$$
\begin{aligned}
\Big[f_j^{\mathbf{k}}\Big]^n &= \frac{-i\varepsilon}{\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j}\Big(\Big[\dot z_j^{\mathbf{k}}\Big]^{n-1} - \Big[\dot z_j^{\mathbf{k}}\Big]^n\Big) + \frac{1}{\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j}\Big(\widetilde{\mathbf{F}}([\mathbf{c}]^{n-1})_j^{\mathbf{k}} - \widetilde{\mathbf{F}}([\mathbf{c}]^n)_j^{\mathbf{k}}\Big),\\
\Big[e_j^{\langle j\rangle}\Big]^n &= -i\varepsilon^{-1}\Big(\widetilde{\mathbf{F}}([\mathbf{c}]^{n-1})_j^{\langle j\rangle} - \widetilde{\mathbf{F}}([\mathbf{c}]^n)_j^{\langle j\rangle}\Big),\\
\Big[\widetilde{d}_j^{\langle j\rangle}(0)\Big]^n &= -\sum_{\mathbf{k}\ne\langle j\rangle}\Big(\Big[z_j^{\mathbf{k}}(0)\Big]^{n-1} - \Big[z_j^{\mathbf{k}}(0)\Big]^n\Big).
\end{aligned}
$$

Note that on $0 \le \tau \le 1$

$$
\Big|\Big[z_j^{\langle j\rangle}\Big]^{n-1} - \Big[z_j^{\langle j\rangle}\Big]^n\Big| \le \Big|\Big[\widetilde{d}_j^{\langle j\rangle}(0)\Big]^{n-1}\Big| + \sup_{0\le\theta\le1}\Big|\Big[e_j^{\langle j\rangle}(\theta)\Big]^{n-1}\Big|.
$$

Using this estimate together with the Lipschitz estimates of Lemma 3.4 and Proposition 3.2 on the size of the iterated modulation functions $[\mathbf{c}]^n$ we get on $0 \le \tau \le 1$ for $n > 0$ and $\ell \ge 0$

$$
\begin{aligned}
\varepsilon^{-\frac14}|||[\mathbf{f}^{(\ell)}]^n|||_s &\le C\varepsilon^{\frac14}|||[\widetilde{\mathbf{d}}(0)]^{n-1}|||_s + C\varepsilon^{\frac14}\sup_{0\le\theta\le1}\max_{\tilde\ell=0,\dots,\ell}|||[\mathbf{e}^{(\tilde\ell)}(\theta)]^{n-1}|||_s\\
&\quad + C\varepsilon^{\frac12}\varepsilon^{-\frac14}\max_{\tilde\ell=0,\dots,\ell+1}|||[\mathbf{f}^{(\tilde\ell)}]^{n-1}|||_s,\\
|||[\mathbf{e}^{(\ell)}]^n|||_s &\le C\varepsilon^{\frac12}|||[\widetilde{\mathbf{d}}(0)]^{n-1}|||_s + C\varepsilon^{\frac12}\sup_{0\le\theta\le1}\max_{\tilde\ell=0,\dots,\ell}|||[\mathbf{e}^{(\tilde\ell)}(\theta)]^{n-1}|||_s\\
&\quad + C\varepsilon^{\frac14}\varepsilon^{-\frac14}\max_{\tilde\ell=0,\dots,\ell}|||[\mathbf{f}^{(\tilde\ell)}]^{n-1}|||_s
\end{aligned}
$$

with a constant C depending only on C_{L,s_0}, $C_{L,s}$, ℓ, n, and L. Here we used again the non-resonance condition 2.3 to avoid small denominators $|\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j| < \varepsilon^{\frac{1}{2}}$. Moreover we have

$$|||[\widetilde{\mathbf{d}}(0)]^n|||_s \le \varepsilon^{\frac{1}{4}}\varepsilon^{-\frac{1}{4}}|||[\mathbf{f}(0)]^{n-1}|||_s. \tag{3.13}$$

This implies that any of the quantities $\varepsilon^{-\frac{1}{4}}|||[\mathbf{f}^{(\ell)}]^n|||_s$, $|||[\mathbf{e}^{(\ell)}]^n|||_s$, and $|||[\widetilde{\mathbf{d}}(0)]^n|||_s$ reduces by a factor $\varepsilon^{\frac{1}{4}}$ per iteration. For $n=0$ we have $|||[\mathbf{f}^{(\ell)}]^0|||_s \le |||[\mathbf{z}^{(\ell)}]^0|||_s + |||[\mathbf{z}^{(\ell)}]^1|||_s \le C\varepsilon$, $|||[\mathbf{e}^{(\ell)}]^0|||_s \le |||[\mathbf{z}^{(\ell+1)}]^0|||_s + |||[\mathbf{z}^{(\ell+1)}]^1|||_s \le C\varepsilon$ for all $\ell \ge 0$, and $\|[\widetilde{\mathbf{d}}(0)]^0\|_s \le |||[\mathbf{z}(0)]^0|||_s + |||[\mathbf{z}(0)]^1|||_s \le C\varepsilon$ by Proposition 3.2. This yields

$$|||[\mathbf{e}^{(\ell)}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{4}}, \quad \varepsilon^{-\frac{1}{4}}|||[\mathbf{f}^{(\ell)}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{4}}, \quad |||[\widetilde{\mathbf{d}}(0)]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{4}}$$

with a constant C depending only on C_{L,s_0}, $C_{L,s}$, ℓ, n, and L.

For the rescaled variables $\hat{\mathbf{e}}$, $\hat{\mathbf{f}}$, and $\hat{\widetilde{\mathbf{d}}}$ we have

$$|||[\hat{\mathbf{e}}^{(\ell)}]^n|||_{s_0} = |||[\mathbf{e}^{(\ell)}]^n|||_s \quad \text{and} \quad |||[\hat{\widetilde{\mathbf{d}}}]^n|||_{s_0} = |||[\widetilde{\mathbf{d}}]^n|||_s;$$

moreover we get the same estimate for $|||[\hat{\mathbf{f}}^{(\ell)}]^n|||_{s_0}$ as for $|||[\mathbf{f}^{(\ell)}]^n|||_s$ using the iteration (3.9) for $[\hat{\mathbf{f}}]^n$. Considering finally $(\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j)[f_j^{\mathbf{k}}]^n$, which appears in the defect $d_j^{\mathbf{k}}$ instead of $[f_j^{\mathbf{k}}]^n$, yields an additional factor $\varepsilon^{\frac{1}{2}}$ in the estimate. We have thus shown the proposition. □

3.4 The Modulated Fourier Expansion and the Exact Solution

In the preceding sections, we constructed iteratively an approximate solution $[\mathbf{z}]^n$ of the modulation system (3.3) and estimated this solution on a short time interval $0 \le \tau = \varepsilon t \le 1$. These iterated modulation functions yield a modulated Fourier expansion

$$[\widetilde{\xi}(t)]^n = ([\widetilde{\xi}_j(t)]^n)_{j\in\mathcal{N}} \quad \text{with} \quad [\widetilde{\xi}_j(t)]^n = \sum_{\mathbf{k}} [z_j^{\mathbf{k}}(\varepsilon t)]^n e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t} \quad \text{for } j \in \mathcal{N}.$$

In this section we show that this modulated Fourier expansion indeed describes the exact solution $\xi(t)$ of the Hamiltonian equations of motion (3.1) with small initial values $\|\xi(0)\|_s \le \varepsilon$ up to a small error.

Size of the Exact Solution. We first study the size of the exact solution $\xi(t)$ of (3.1). The variation-of-constants formula yields

$$\xi_j(t) = e^{-i\omega_j t}\xi_j(0) - i\int_0^t e^{-i\omega_j(t-\theta)}\frac{\partial P}{\partial \eta_j}(\xi(\theta), \overline{\xi(\theta)})\, d\theta.$$

While $\|\xi(\theta)\|_s \le 2\varepsilon$ and if $2\varepsilon \le C_1$, we get with the estimate (2.7)

$$\|\xi(t)\|_s \le \|\xi(0)\|_s + C_s t \sup_{0\le\theta\le t}\|\xi(\theta)\|_s^2 \le \varepsilon + 4C_s t\varepsilon^2.$$

We conclude that

$$\|\xi(t)\|_s \le 2\varepsilon \quad \text{for } 0 \le t \le \frac{1}{4C_s}\varepsilon^{-1}, \tag{3.14}$$

i.e., for initial values of size ε the solution of (3.1) stays of size 2ε on an interval of length $\mathcal{O}(\varepsilon^{-1})$. This argument is referred to as a bootstrap argument, see for example [51, Proposition 1.21]. In this way, the influence of the nonlinearity can be studied on a time interval of length $\mathcal{O}(\varepsilon^{-1})$ as indicated in Section 2.1.

Size of the Iterated Modulated Fourier Expansion. The l_s^2-norm of $[\widetilde{\xi}(t)]^n$ can easily be estimated by the $|||\cdot|||_s$-norm of the iterated modulation function $[\mathbf{z}]^n$,

$$\|[\widetilde{\xi}(t)]^n\|_s^2 = \sum_{j\in\mathcal{N}} |j|^{2s} \Big|\sum_{\mathbf{k}} [z_j^{\mathbf{k}}(\varepsilon t)]^n e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}\Big|^2 \le \sum_{j\in\mathcal{N}} |j|^{2s} \Big(\sum_{\mathbf{k}} |[z_j^{\mathbf{k}}(\varepsilon t)]^n|\Big)^2 = |||[\mathbf{z}(\varepsilon t)]^n|||_s^2.$$

This estimate suggests the use of the norm $|||\cdot|||_s$ since this norm of the modulation function $\mathbf{z}$ is directly linked to the l_s^2-norm of the modulated Fourier expansion ξ. Proposition 3.2 on the size of the iterated modulation functions then allows us to control the size of the modulated Fourier expansion $[\widetilde{\xi}(t)]^n$,

$$\|[\widetilde{\xi}(t)]^n\|_s \le C\varepsilon \quad \text{for } 0 \le t \le \varepsilon^{-1} \tag{3.15}$$

with a constant C depending only on $C_{L,s}$, n, and L.

Relating the Exact Solution and the Iterated Modulated Fourier Expansion. Similar to Lemma 3.4 we obtain the following Lipschitz estimate of the nonlinearity $\frac{\partial P}{\partial \eta_j}$. In contrast to there, we take here all terms of the nonlinearity into account without any cut-off.

Lemma 3.6. *We have for* $\|\xi\|_s + \|\widetilde{\xi}\|_s \le C_1$

$$\Big\|\Big(\frac{\partial P}{\partial \eta_j}(\xi,\overline{\xi}) - \frac{\partial P}{\partial \eta_j}(\widetilde{\xi},\overline{\widetilde{\xi}})\Big)_{j\in\mathcal{N}}\Big\|_s \le C_s(\|\xi\|_s + \|\widetilde{\xi}\|_s)\|\xi - \widetilde{\xi}\|_s.$$

Proof. As in the proof of Lemma 3.4 we get using (3.12)

$$\begin{aligned}\Big|\frac{\partial P}{\partial \eta_j}(\xi,\overline{\xi}) - \frac{\partial P}{\partial \eta_j}(\widetilde{\xi},\overline{\widetilde{\xi}})\Big| \le \sum_{m+m'=2}^{\infty} \sum_{l=1}^{m+m'} \Big(&|P|_j^{m,m'}(\overbrace{|\xi|+|\widetilde{\xi}|,\dots,|\xi|+|\widetilde{\xi}|}^{l-1}, |\xi-\widetilde{\xi}|, |\xi|,\dots,|\xi|) \\ &+ |P|_j^{m,m'}(\underbrace{|\xi|+|\widetilde{\xi}|,\dots,|\xi|+|\widetilde{\xi}|}_{l-1}, |\xi-\widetilde{\xi}|, |\widetilde{\xi}|,\dots,|\widetilde{\xi}|)\Big)2^{-l}\end{aligned}$$

with $|\xi| = (|\xi_j|)_{j\in\mathcal{N}}$ and

$$\begin{aligned}\Big\|\Big(\frac{\partial P}{\partial \eta_j}(\xi,\overline{\xi}) - \frac{\partial P}{\partial \eta_j}(\widetilde{\xi},\overline{\widetilde{\xi}})\Big)_{j\in\mathcal{N}}\Big\|_s \le \sum_{m+m'=2}^{\infty} \sum_{l=1}^{m+m'} &C_{m,m',s}(\|\xi\|_s + \|\widetilde{\xi}\|_s)^{l-1} \\ &\|\xi-\widetilde{\xi}\|_s(\|\xi\|_s^{m+m'-l} + \|\widetilde{\xi}\|_s^{m+m'-l})2^{-l}\end{aligned}$$

The assumption $\|\xi\|_s + \|\widetilde{\xi}\|_s \le C_1$ together with $\sum_{l=1}^{m+m'} 2^{-l} \le 1$ and the regularity assumption 2.1 yield the result. □

We are now able to prove the following theorem.

Theorem 3.7. *Let $\xi(t)$ be the exact solution of the Hamiltonian equations of motion* (3.1)*, and let*

$$[\widetilde{\xi}(t)]^n = ([\widetilde{\xi}_j(t)]^n)_{j\in\mathcal{N}} \quad \text{with} \quad [\widetilde{\xi}_j(t)]^n = \sum_{\mathbf{k}} [z_j^{\mathbf{k}}(\varepsilon t)]^n e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t} \quad \text{for } j \in \mathcal{N}$$

be its iterated modulated Fourier expansions with the approximate solution $[\mathbf{z}]^n$ of the modulation system (3.3) *constructed in Section 3.2. Under the regularity assumption 2.1 and the non-resonance condition 2.3 we have for ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, n, and L*

$$\|\xi(t) - [\widetilde{\xi}(t)]^n\|_s \le C\varepsilon^{\frac{n}{4}+\frac{1}{2}} + C\varepsilon^{\frac{L}{2}-1} \quad \text{for } 0 \le t \le \varepsilon^{-1}\min\Big(\frac{1}{4C_s}, 1\Big)$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 2.1, C_0 from the non-resonance condition 2.3, the number of iterations n, and L.

Proof. We omit the index n. For the difference $\xi - \widetilde{\xi}$ we have

$$\xi_j(0) - \widetilde{\xi}_j(0) = -\widetilde{d}_j^{\langle j\rangle}(0),$$

and $\xi - \widetilde{\xi}$ satisfies the differential equation

$$i\frac{d}{dt}(\xi_j(t)-\widetilde{\xi}_j(t)) = \omega_j(\xi_j(t)-\widetilde{\xi}_j(t))+\Big(\frac{\partial P}{\partial\eta_j}(\xi(t),\overline{\xi(t)})-\frac{\partial P}{\partial\eta_j}(\widetilde{\xi}(t),\overline{\widetilde{\xi}(t)})\Big)-\sum_{\mathbf{k}} d_j^{\mathbf{k}}(\varepsilon t)e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}.$$

The variation-of-constants formula yields

$$\begin{aligned}\xi_j(t) - \widetilde{\xi}_j(t) = e^{-i\omega_j t}(\xi_j(0) - \widetilde{\xi}_j(0)) &- i\int_0^t e^{-i\omega_j(t-\theta)}\Big(\frac{\partial P}{\partial\eta_j}(\xi(\theta),\overline{\xi(\theta)}) - \frac{\partial P}{\partial\eta_j}(\widetilde{\xi}(\theta),\overline{\widetilde{\xi}(\theta)})\Big)\,d\theta\\ &+ i\int_0^t \sum_{\mathbf{k}} e^{-i\omega_j(t-\theta)} d_j^{\mathbf{k}}(\varepsilon\theta)e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})\theta}\,d\theta.\end{aligned}$$

Taking the l_s^2-norm we get

$$\begin{aligned}\|\xi(t) - \widetilde{\xi}(t)\|_s \le |||\widetilde{\mathbf{d}}(0)|||_s + \int_0^t \Big\|\Big(\frac{\partial P}{\partial\eta_j}(\xi(\theta),\overline{\xi(\theta)}) - \frac{\partial P}{\partial\eta_j}(\widetilde{\xi}(\theta),\overline{\widetilde{\xi}(\theta)})\Big)_{j\in\mathcal{N}}\Big\|_s\,d\theta&\\ + t\sup_{0\le\theta\le t}|||\mathbf{d}(\theta)|||_s.&\end{aligned}$$

The defects $\widetilde{\mathbf{d}}$ and $\mathbf{d}$ can be estimated with Proposition 3.5. For ε sufficiently small, (3.14) and (3.15) ensure $\|\xi\|_s + \|\widetilde{\xi}\|_s \le C\varepsilon \le C_1$ on $0 \le t \le \varepsilon^{-1}\min(\frac{1}{4C_s}, 1)$, and hence Lemma 3.6 can be used to estimate the integrand. This yields on this time interval

$$\|\xi(t) - \widetilde{\xi}(t)\|_s \le C\varepsilon^{\frac{n}{4}+\frac{1}{2}} + C\varepsilon^{\frac{L}{2}-1} + C\varepsilon\int_0^t \|\xi(\theta) - \widetilde{\xi}(\theta)\|_s\,d\theta$$

with a constant C depending only on C_{s_0}, C_s, $C_{L,s}$, C_{L,s_0}, C_0, n, and L, and the Gronwall lemma can be used to show the estimate stated in the theorem. □

3.5 The Modulated Fourier Expansion on Long Time Intervals

So far, the rigorous analysis of the modulated Fourier expansion carried out in Sections 3.2, 3.3, and 3.4 is valid on a time interval of length $\mathcal{O}(\varepsilon^{-1})$. This is the time interval on which results on the exact solution can be obtained by standard arguments, see Section 3.4. However, with the help of modulated Fourier expansions we are able to study the exact solution on much longer time intervals of length ε^{-N} for arbitrary N. The extension to such long time intervals is the topic of this section.

Putting Together Modulated Fourier Expansions. Let

$$c_0 = \min\Big(\frac{1}{4C_s}, 1\Big),$$

such that Theorem 3.7, which links the exact solution and its iterated modulated Fourier expansion, is valid on the time interval $0 \le t \le c_0\varepsilon^{-1}$ as well as the estimates of the iterated modulation functions shown in the previous sections.

A first step towards longer time intervals is done by repeating the iterative construction presented in Section 3.2 on the time interval $c_0 \le \tau \le 2c_0$. This yields iterated modulation function $[\widetilde{\mathbf{z}}]^n$ on $c_0 \le \tau \le 2c_0$. The iterations (3.6a) for non-diagonal indices $(j,\mathbf{k}) \in \mathcal{S}_\varepsilon$, (3.6b) for diagonal indices $\mathbf{k} = \langle j\rangle$, and (3.6d) and (3.6e) for indices $(j,\mathbf{k}) \in \mathcal{R}_\varepsilon$ remain unchanged but are now performed for $c_0 \le \tau \le 2c_0$, whereas the iteration (3.6c) for the initial value in diagonal indices becomes

$$\Big[\widetilde{z}_j^{\langle j\rangle}(c_0)e^{-i\omega_j c_0\varepsilon^{-1}}\Big]^{n+1} = \xi_j(c_0\varepsilon^{-1}) - \Big[\sum_{\mathbf{k}\neq\langle j\rangle} \widetilde{z}_j^{\mathbf{k}}(c_0)e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})c_0\varepsilon^{-1}}\Big]^n, \tag{3.16}$$

and we set

$$[\widetilde{z}_j^{\langle j\rangle}e^{-i\omega_j c_0\varepsilon^{-1}}]^0 = \xi_j(c_0\varepsilon^{-1}) \quad \text{and} \quad [\widetilde{z}_j^{\mathbf{k}}]^0 = 0 \quad \text{for } \mathbf{k}\neq\langle j\rangle$$

initially on $c_0 \le \tau \le 2c_0$. In other words, we repeat the iterative procedure starting again on the exact solution $\xi(c_0\varepsilon^{-1})$.

Since $\|\xi(c_0\varepsilon^{-1})\|_s \le 2\varepsilon$ by (3.14), $\xi(c_0\varepsilon^{-1})$ also satisfies the smallness condition with 2ε instead of ε, and hence Propositions 3.2, 3.3, 3.5, and Theorem 3.7 are also valid for $[\widetilde{\mathbf{z}}]^n$ and its rescaling $[\hat{\widetilde{\mathbf{z}}}]^n$ on the time interval $c_0 \le \tau \le 2c_0$ with new constants depending only on C_{s_0}, C_s, C_{L,s_0}, $C_{L,s}$, C_0, ℓ, n, and L.

We can not expect $[\mathbf{z}]^n$ and $[\widetilde{\mathbf{z}}]^n$ to agree at the interface c_0. However, we are able to bound the difference $[\mathbf{z}(c_0)]^n - [\widetilde{\mathbf{z}}(c_0)]^n$.

Proposition 3.8. *For ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, n, and L we have*

$$|||[\mathbf{z}(c_0)]^n - [\widetilde{\mathbf{z}}(c_0)]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{1}{2}} + C\varepsilon^{\frac{L}{2}-1}$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 2.1, C_0 from the non-resonance condition 2.3, the number of iterations n, and L.

The same estimate holds true if $\mathbf{z}$, $\widetilde{\mathbf{z}}$, and s are replaced by $\hat{\mathbf{z}}$, $\hat{\widetilde{\mathbf{z}}}$, and s_0, respectively.

Proof. We have using the iteration (3.16) for $\widetilde{z}_j^{\langle j\rangle}(c_0)$

$$\Big[z_j^{\langle j\rangle}(c_0)\Big]^{n+1} - \Big[\widetilde{z}_j^{\langle j\rangle}(c_0)\Big]^{n+1} = \Big[z_j^{\langle j\rangle}(c_0)\Big]^{n+1} - \Big[z_j^{\langle j\rangle}(c_0)\Big]^{n} + \Big[\sum_{\mathbf{k}} z_j^{\mathbf{k}}(c_0)e^{-i(\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j)c_0\varepsilon^{-1}}\Big]^n$$
$$- \Big[\sum_{\mathbf{k}\neq\langle j\rangle}(z_j^{\mathbf{k}}(c_0)-\widetilde{z}_j^{\mathbf{k}}(c_0))e^{-i(\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j)c_0\varepsilon^{-1}}\Big]^n - \xi_j(c_0\varepsilon^{-1})e^{i\omega_j c_0\varepsilon^{-1}}$$

Splitting $\mathbf{z}-\widetilde{\mathbf{z}} = \mathbf{u}+\mathbf{v}$ in its diagonal entries $\mathbf{u}$ and off-diagonal entries $\mathbf{v}$, i.e., $u_j^{\mathbf{k}}=0$ for $\mathbf{k}\neq\langle j\rangle$ and $v_j^{\mathbf{k}}=0$ for $(j,\mathbf{k})\notin\mathcal{S}_\varepsilon$ (note that $z_j^{\mathbf{k}}-\widetilde{z}_j^{\mathbf{k}}=0$ for $(j,\mathbf{k})\in\mathcal{R}_\varepsilon$ or $\|\mathbf{k}\|>L$), we get

$$|||[\mathbf{u}(c_0)]^{n+1}|||_s \le |||[\widetilde{\mathbf{d}}(0)]^n|||_s + c_0 \sup_{0\le\theta\le c_0} |||[\mathbf{e}(\theta)]^n|||_s$$
$$+ \|[\widetilde{\xi}(c_0\varepsilon^{-1})]^n - \xi(c_0\varepsilon^{-1})\|_s + \varepsilon^{\frac14}\varepsilon^{-\frac14}|||[\mathbf{v}(c_0)]^n|||_s.$$

Moreover, the iteration (3.6b) for higher derivatives of $\mathbf{u}$ yields

$$\Big[(u_j^{\langle j\rangle})^{(\ell+1)}(c_0)\Big]^{n+1} = -i\varepsilon^{-1}\Big[\Big(\widetilde{\mathbf{F}}(\mathbf{c})_j^{\langle j\rangle} - \widetilde{\mathbf{F}}(\widetilde{\mathbf{c}})_j^{\langle j\rangle}\Big)^{(\ell)}(c_0)\Big]^n$$

for $\ell\ge 0$, and the iteration (3.6a) for $(j,\mathbf{k})\in\mathcal{S}_\varepsilon$ yields

$$\Big[(v_j^{\mathbf{k}})^{(\ell)}(c_0)\Big]^{n+1} = \frac{-i\varepsilon}{\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j}\Big[(v_j^{\mathbf{k}})^{(\ell+1)}(c_0)\Big]^n + \frac{1}{\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j}\Big[\Big(\widetilde{\mathbf{F}}(\mathbf{c})_j^{\mathbf{k}} - \widetilde{\mathbf{F}}(\widetilde{\mathbf{c}})_j^{\mathbf{k}}\Big)^{(\ell)}(c_0)\Big]^n$$

for $\ell\ge 0$. Estimating the right-hand sides with the help of the Lipschitz estimates of Lemma 3.4 in combination with Proposition 3.2 shows

$$|||[\mathbf{u}^{(\ell+1)}(c_0)]^{n+1}|||_s \le C\varepsilon^{\frac12}\max_{\tilde\ell=0,\dots,\ell}|||[\mathbf{u}^{(\tilde\ell)}(c_0)]^n|||_s + C\varepsilon^{\frac14}\varepsilon^{-\frac14}\max_{\tilde\ell=0,\dots,\ell}|||[\mathbf{v}^{(\tilde\ell)}(c_0)]^n|||_s,$$
$$\varepsilon^{-\frac14}|||[\mathbf{v}^{(\ell)}(c_0)]^{n+1}|||_s \le C\varepsilon^{\frac14}\max_{\tilde\ell=0,\dots,\ell}|||[\mathbf{u}^{(\tilde\ell)}(c_0)]^n|||_s + C\varepsilon^{\frac12}\varepsilon^{-\frac14}\max_{\tilde\ell=0,\dots,\ell+1}|||[\mathbf{v}^{(\tilde\ell)}(c_0)]^n|||_s$$

with a constant C depending only on C_{L,s_0}, $C_{L,s}$, ℓ, n, and L.

Initially we have $|||[\mathbf{u}(c_0)]^0|||_s + |||[\mathbf{v}(c_0)]^0|||_s \le C\varepsilon$ by Proposition 3.2 and for the derivatives of the initial values $|||[\mathbf{u}^{(\ell)}(c_0)]^0|||_s = |||[\mathbf{v}^{(\ell)}(c_0)]^0|||_s = 0$ for $\ell>0$. Together with the estimates of $\widetilde{\mathbf{d}}$ and $\mathbf{e}$ from Proposition 3.5 and of $\|[\widetilde{\xi}]^n-\xi\|_s$ from Theorem 3.7 we conclude

$$|||[\mathbf{u}^{(\ell)}(c_0)]^n|||_s \le C\varepsilon^{\frac n4+\frac12} + C\varepsilon^{\frac L2-1}, \quad \varepsilon^{-\frac14}|||[\mathbf{v}^{(\ell)}(c_0)]^n|||_s \le C\varepsilon^{\frac n4+\frac12} + C\varepsilon^{\frac L2-1}$$

with a constant C depending on C_{s_0}, C_s, C_{L,s_0}, $C_{L,s}$, C_0, ℓ, n, and L. This proves the estimate stated in the proposition. For the proof of the same estimate in the rescaled variables we proceed as usual noting $|||\hat{\mathbf{u}}|||_{s_0} = |||\mathbf{u}|||_s$ and using the rescaled iteration (3.9) for $\hat{\mathbf{v}}$ as for $\mathbf{v}$. □

Almost Invariants of the Iterated Modulation Functions. In principle, we can repeat the procedure of constructing new modulated Fourier expansions on time intervals $2c_0 \le \tau \le 3c_0$, $3c_0 \le \tau \le 4c_0$, and so on. So far, however, we are not able to control the exact solution on these intervals, or more precisely at the boundary of these intervals, better than $\|\xi(2c_0\varepsilon^{-1})\|_s \le 4\varepsilon$, $\|\xi(3c_0\varepsilon^{-1})\|_s \le 8\varepsilon$, and so on, having in mind the short-time estimate (3.14). But this would imply an explosion of the constants in the estimates of the iterated modulation functions of Sections 3.3 and 3.4 and in particular a heavy dependence on ε on time intervals of length ε^{-N}.

The tool to control the exact solution in l_s^2 is provided by the structure of the modulation system (3.3). As discussed in Section 3.1 the modulation system is a Hamiltonian system with Hamiltonian function $\mathbf{H}(\mathbf{z},\mathbf{w})$, see (3.4). Many components of its momentum, namely

$$\mathbf{K}_l(\mathbf{z},\overline{\mathbf{z}}) = \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} k_l |z_j^{\mathbf{k}}|^2 \quad \text{for } l \in \mathcal{N},$$

are conserved along any solution of the modulation system due to the invariance of $\mathbf{H}(\mathbf{z},\overline{\mathbf{z}})$ under the transformation $g_\theta(\mathbf{z}) = (e^{i\theta k_l} z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}$, see Noether's Theorem 1.2, Proposition 1.4 on the conservation of the momentum, and the formal analysis in Section 3.1.

However, the rigorous treatment of the modulation system in Sections 3.2 and 3.3 only yields an approximate solution of the modulation system which satisfies the modulation system (i.e., the Hamiltonian equations of motion for (3.3)) up to a small defect $\mathbf{d}$

$$i\frac{d}{d\tau} z_j^{\mathbf{k}}(\tau) = \frac{\partial \mathbf{H}}{\partial w_j^{\mathbf{k}}}(\mathbf{z}(\tau),\overline{\mathbf{z}(\tau)}) + \varepsilon^{-1} d_j^{\mathbf{k}}(\tau),$$

where we omit the index n denoting the number of iterations used to compute $\mathbf{z}$ for convenience. Repeating the calculation of the proof of Noether's Theorem 1.2 taking into account this defect yields with $iA\mathbf{z} = \frac{d}{d\theta}|_{\theta=0} g_\theta(\mathbf{z}) = (ik_l z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}$

$$0 = \frac{d}{d\tau}\mathbf{K}_l(\mathbf{z}(\tau),\overline{\mathbf{z}(\tau)}) - 2\varepsilon^{-1}\,\mathrm{Re}\Big(\sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} ik_l z_j^{\mathbf{k}}(\tau)\overline{d_j^{\mathbf{k}}(\tau)}\Big). \tag{3.17}$$

Hence, we are able to control the (non-)conservation of the momentum by means of the defect in the equation. In order to control the derivative of $\mathbf{K}_l$ in (3.17) we need the following lemma, where we write

$$\mathbf{\Omega}\hat{\mathbf{z}} = \big((\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)\hat{z}_j^{\mathbf{k}}\big)_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} = \big((\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)\,\mathbf{j}^{(s-s_0)|\mathbf{k}|} z_j^{\mathbf{k}}\big)_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}.$$

Lemma 3.9. *Let* $\mathbf{z}$ *and* $\mathbf{d} = \mathbf{q}+\mathbf{g}$ *with* $z_j^{\mathbf{k}} = q_j^{\mathbf{k}} = 0$ *for* $(j,\mathbf{k}) \in \mathcal{R}_\varepsilon$ *or* $\|\mathbf{k}\| > L$ *and* $g_j^{\mathbf{k}} = 0$ *for* $(j,\mathbf{k}) \notin \mathcal{R}_\varepsilon$. *If the condition of zero momentum* (2.9b) *is satisfied in Assumption 2.2, we assume moreover* $z_j^{\mathbf{k}} = 0$ *for* $j \ne j(\mathbf{k})$. *Then, we have for* $s \ge 2s_0$

$$\sum_{l\in\mathcal{N}} |l|^{2s} \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} |k_l||z_j^{\mathbf{k}}||d_j^{\mathbf{k}}| \le C\varepsilon^{-2s_0} |||\hat{\mathbf{z}}|||_{s_0} |||\hat{\mathbf{q}}|||_{s_0},$$

$$\sum_{l\in\mathcal{N}} |l|^{2s} \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} |k_l||z_j^{\mathbf{k}}||d_j^{\mathbf{k}}| \le C|||\hat{\mathbf{z}}|||_{s_0} |||\hat{\mathbf{q}}|||_{s_0} + C|||\mathbf{\Omega}\hat{\mathbf{z}}|||_{s_0} |||\mathbf{\Omega}\hat{\mathbf{q}}|||_{s_0}$$

with a constant C depending only on c_2, C_2, σ, and L. The term $C|||\mathbf{\Omega}\hat{\mathbf{z}}|||_{s_0}|||\mathbf{\Omega}\hat{\mathbf{q}}|||_{s_0}$ only appears if the condition of zero momentum is not fulfilled in Assumption 2.2.

Proof. Let c_2, C_2, and σ be the constants from Assumption 2.2 describing the asymptotics of the frequencies, and let $K = \max(2L, (2C_2L/c_2)^{1/\sigma})$. Since $z_j^{\mathbf{k}} = 0$ for $(j, \mathbf{k}) \in \mathcal{R}_\varepsilon$, we can write

$$\sum_{l\in\mathcal{N}}|l|^{2s}\sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}|k_l||z_j^{\mathbf{k}}||d_j^{\mathbf{k}}| = \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}|j|^{2s_0}\frac{\sum_{l\in\mathcal{N}}|k_l||l|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}}|\hat{z}_j^{\mathbf{k}}||\hat{q}_j^{\mathbf{k}}|.$$

Estimating $\sum_{l\in\mathcal{N}}|k_l||l|^{2s}$ by $\|\mathbf{k}\||\bar{l}|^{2s}$, where $\bar{l} = \bar{l}(\mathbf{k}) \in \mathcal{N}$ denotes the largest index with respect to $|\cdot|$ with $k_{\bar{l}} \neq 0$, we get

$$\begin{aligned}\sum_{l\in\mathcal{N}}|l|^{2s}\sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}|k_l||z_j^{\mathbf{k}}||d_j^{\mathbf{k}}| \le &\sum_{\substack{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}\\ \mathbf{j}^{|\mathbf{k}|}\ge\frac{1}{K}|\bar{l}|^2 \text{ or } |j|\ge\frac{1}{K}|\bar{l}|}}|j|^{2s_0}\frac{\|\mathbf{k}\||\bar{l}|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}}|\hat{z}_j^{\mathbf{k}}||\hat{q}_j^{\mathbf{k}}| \\ &+\sum_{\substack{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}\\ \mathbf{j}^{|\mathbf{k}|}<\frac{1}{K}|\bar{l}|^2\\ \text{and } |j|<\frac{1}{K}|\bar{l}|}}|j|^{2s_0}\frac{\|\mathbf{k}\||\bar{l}|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}}|\hat{z}_j^{\mathbf{k}}||\hat{q}_j^{\mathbf{k}}|.\end{aligned} \tag{3.18}$$

Clearly, since $4(s - s_0) \ge 2s$, the first term in (3.18) can be estimated by $C|||\hat{\mathbf{z}}|||_{s_0}|||\hat{\mathbf{q}}|||_{s_0}$ using the Cauchy–Schwarz inequality. For the second term in (3.18) we distinguish two cases, depending on whether the condition of small dimension (2.9a) or the condition of zero momentum (2.9b) is fulfilled in Assumption 2.2.

(a) If the condition of small dimension (2.9a) is satisfied, then we proceed as follows in order to estimate the second term in (3.18). In this case, $\mathcal{R}_\varepsilon$ contains all indices with $|j| \le \varepsilon|l|$ for an $l \in \mathcal{N}$ with $k_l \neq 0$, in particular we have in the second term $|j| > \varepsilon|\bar{l}|$ and hence

$$\frac{\|\mathbf{k}\||\bar{l}|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}} \le \frac{\|\mathbf{k}\||\bar{l}|^{2s}}{|\bar{l}|^{2(s-s_0)|k_{\bar{l}}|}\cdots}\cdot\frac{1}{\varepsilon^{2s_0}|\bar{l}|^{2s_0}} \le \|\mathbf{k}\|\varepsilon^{-2s_0}$$

for all $(j, \mathbf{k})$ with $\hat{q}_j^{\mathbf{k}} \neq 0$.[4] Using the Cauchy–Schwarz inequality, this proves the first estimate of the lemma since $z_j^{\mathbf{k}} = 0$ for $\|\mathbf{k}\| > L$.

To avoid the dependence on ε in the second estimate stated in the lemma, more careful considerations are necessary taking into account $\mathbf{\Omega}$. We rewrite the second term in (3.18) as

$$\sum_{\substack{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}\\ \mathbf{j}^{|\mathbf{k}|}<\frac{1}{K}|\bar{l}|^2\\ \text{and } |j|<\frac{1}{K}|\bar{l}|}}|j|^{2s_0}\frac{\|\mathbf{k}\||\bar{l}|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}|\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j|^2}|(\mathbf{\Omega}\hat{\mathbf{z}})_j^{\mathbf{k}}||(\mathbf{\Omega}\hat{\mathbf{q}})_j^{\mathbf{k}}|$$

[4] This is actually the reason why we set the iterated modulation functions to zero in (3.6e) if $|j| \le \varepsilon|l|$ for an $l \in \mathcal{N}$ with $k_l \neq 0$ provided that the condition of small dimension is satisfied. If the condition of zero momentum is satisfied, we can use other arguments, see below.

and make use of $|\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j|^2$ in the denominator. Using the asymptotics of the frequencies in Assumption 2.2 we get

$$|\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j| = \Big|k_{\bar l}\omega_{\bar l} + \sum_{\bar l\neq l\in\mathcal{N}} k_l\omega_l - \omega_j\Big| \geq c_2|k_{\bar l}||\bar l|^\sigma - C_2\sum_{\bar l\neq l\in\mathcal{N}}|k_l||l|^\sigma - C_2|j|^\sigma.$$

The condition $\mathbf{j}^{|\mathbf{k}|} < \frac{1}{K}|\bar l|^2$ implies $|k_{\bar l}| = 1$ and $|l| \leq \frac{1}{K}|\bar l|$ for all $\bar l \neq l \in \mathcal{N}$ with $k_l \neq 0$. Together with $|j| < \frac{1}{K}|\bar l|$ and $\|\mathbf{k}\| \leq L$ this implies

$$|\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j| \geq c_2|\bar l|^\sigma - C_2L\frac{1}{K^\sigma}|\bar l|^\sigma = \frac{c_2}{2}|\bar l|^\sigma.$$

Using the condition of small dimension $\sigma \geq s_0$ (2.9a), we get for the denominator

$$\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}|\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j|^2 \geq |\bar l|^{2(s-s_0)}\frac{c_2}{2}|\bar l|^{2\sigma} \geq \frac{c_2}{2}|\bar l|^{2s}.$$

The Cauchy–Schwarz inequality then yields an estimate $C|||\boldsymbol{\Omega}\hat{\mathbf{z}}|||_{s_0}|||\boldsymbol{\Omega}\hat{\mathbf{q}}|||_{s_0}$ for the second term in (3.18) proving the second estimate of the lemma.

(b) Now, we consider the case that the zero momentum condition (2.9b) is satisfied. We show that in this case the second term in (3.18) is not present proving both estimates of the lemma. Pick one nonzero summand of this term. Then by hypothesis $j = j(\mathbf{k})$. Moreover, $\mathbf{j}^{|\mathbf{k}|} < \frac{1}{K}|\bar l|^2$ implies $|k_{\bar l}| = 1$ and $|l| \leq \frac{1}{K}|\bar l|$ for all $\bar l \neq l \in \mathcal{N}$ with $k_l \neq 0$. The triangle inequality together with $|j| < \frac{1}{K}|\bar l|$ yields

$$|\bar l| = \Big|j(\mathbf{k}) - \sum_{l\neq\bar l} k_l l\Big| \leq |j| + \frac{\|\mathbf{k}\|}{K}|\bar l| < |\bar l|,$$

a contradiction. □

We remark that the proof of the preceding Lemma 3.9 is the only place where we need Assumption 2.2. This lemma is used in the following proposition to study rigorously

- the conservation of $\mathbf{K}_l$ along our approximate solution $[\mathbf{z}]^n$ of the modulation system (3.3),
- the relationship between $\mathbf{K}_l$ along our approximate solution $[\mathbf{z}]^n$ of the modulation system (3.3) and the actions $I_l(\xi,\overline{\xi}) = |\xi_l|^2$ along the exact solution of the Hamiltonian equations of motion (3.1),
- and the difference of $\mathbf{K}_l$ at the interface of two iterated modulation functions $[\mathbf{z}]^n$ and $[\widetilde{\mathbf{z}}]^n$.

Proposition 3.10. *For $s \geq 2s_0$ and for ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, $n \geq 6$, and $L \geq 6$ we have on $0 \leq \tau = \varepsilon t \leq c_0$*

$$\sum_{l\in\mathcal{N}}|l|^{2s}\Big|\frac{d}{d\tau}\mathbf{K}_l([\mathbf{z}(\tau)]^n,[\overline{\mathbf{z}(\tau)}]^n)\Big| \leq C\varepsilon^{\frac{n}{4}+\frac{3}{2}-2s_0} + C\varepsilon^{\frac{L}{2}-2s_0},$$

$$\sum_{l\in\mathcal{N}}|l|^{2s}\Big|\mathbf{K}_l([\mathbf{z}(c_0)]^n,[\overline{\mathbf{z}(c_0)}]^n) - \mathbf{K}_l([\widetilde{\mathbf{z}}(c_0)]^n,[\overline{\widetilde{\mathbf{z}}(c_0)}]^n)\Big| \leq C\varepsilon^{\frac{n}{4}+\frac{3}{2}-2s_0} + C\varepsilon^{\frac{L}{2}-2s_0},$$

$$\sum_{l\in\mathcal{N}}|l|^{2s}\Big|\mathbf{K}_l([\mathbf{z}(\tau)]^n,[\overline{\mathbf{z}(\tau)}]^n) - I_l(\xi(t),\overline{\xi(t)})\Big| \leq C\varepsilon^{\frac{5}{2}}$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 2.1, c_2, C_2, and σ describing the asymptotics of the frequencies in Assumption 2.2, C_0 from the non-resonance condition 2.3, the number of iterations n, and L.

The third estimate improves to $C\varepsilon^3$ if the additional non-resonance condition 2.4 is satisfied with a constant C depending in addition on C_3 from the additional non-resonance condition 2.4.

Proof. The first estimate follows from equation (3.17), Lemma 3.9 applied to $\mathbf{z} = [\mathbf{z}]^n$,

$$\mathbf{q} = [\mathbf{d}]^n - [\mathbf{g}]^n = i\varepsilon[\mathbf{e}]^n + [((\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j)f_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}]^n + [\mathbf{h}]^n + [\mathbf{p}]^n,$$

and $\mathbf{g} = [\mathbf{g}]^n$, Proposition 3.2 on the size of $\mathbf{z}$, and Propositions 3.3 and 3.5 on the defects in $\mathbf{q}$.

For the second estimate we note that

$$\sum_{l\in\mathcal{N}} |l|^{2s} \Big| \mathbf{K}_l(\mathbf{z},\overline{\mathbf{z}}) - \mathbf{K}_l(\widetilde{\mathbf{z}},\overline{\widetilde{\mathbf{z}}}) \Big| \le \sum_{l\in\mathcal{N}} |l|^{2s} \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} |k_l| \Big| |z_j^{\mathbf{k}}|^2 - |\widetilde{z}_j^{\mathbf{k}}|^2 \Big|$$

and $\big||z_j^{\mathbf{k}}|^2 - |\widetilde{z}_j^{\mathbf{k}}|^2\big| \le |z_j^{\mathbf{k}} - \widetilde{z}_j^{\mathbf{k}}||z_j^{\mathbf{k}} + \widetilde{z}_j^{\mathbf{k}}|$. Hence, the result follows from Lemma 3.9, Proposition 3.2 on the size of $[\mathbf{z}]^n$ and $[\widetilde{\mathbf{z}}]^n$, and Proposition 3.8 on the error $[\mathbf{z}]^n - [\widetilde{\mathbf{z}}]^n$ at the interface c_0.

Let's turn finally to the third estimate. On the one hand, we have by the second estimate of Lemma 3.9

$$\begin{aligned} \sum_{l\in\mathcal{N}} |l|^{2s} \Big| \mathbf{K}_l(\mathbf{z},\overline{\mathbf{z}}) - |z_l^{\langle l\rangle}|^2 \Big| &\le \sum_{l\in\mathcal{N}} |l|^{2s} \sum_{\substack{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}} \\ (j,\mathbf{k})\neq(l,\langle l\rangle)}} |k_l||z_j^{\mathbf{k}}|^2 \\ &\le C|||(\hat{z}_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_{s_0}^2 + C|||\boldsymbol{\Omega}(\hat{z}_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_{s_0}^2, \end{aligned} \tag{3.19}$$

where we omit the index n of $\mathbf{z}$, and $\mathbf{z}$ is evaluated at time $\tau = \varepsilon t$. On the other hand, we have using the Cauchy–Schwarz inequality

$$\sum_{l\in\mathcal{N}} |l|^{2s} \Big| |z_l^{\langle l\rangle}|^2 - |\xi_l|^2 \Big| \le \Big(|||(z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_s + \|\widetilde{\xi} - \xi\|_s \Big) \Big(\varepsilon|||\mathbf{a}|||_s + \|\xi\|_s \Big)$$

since

$$\Big| |z_l^{\langle l\rangle}|^2 - |\xi_l|^2 \Big| \le |z_l^{\langle l\rangle} e^{-i\omega_l t} - \xi_l||z_l^{\langle l\rangle} e^{-i\omega_l t} + \xi_l| \le (|z_l^{\langle l\rangle} e^{-i\omega_l t} - \widetilde{\xi}_l| + |\widetilde{\xi}_l - \xi_l|)(|z_l^{\langle l\rangle}| + |\xi_l|),$$

where we omit again the index n of $\mathbf{z}$, $\mathbf{a}$, $\mathbf{b}$, and $\widetilde{\xi}$, and all quantities are evaluated at time $\tau = \varepsilon t$ and t, respectively. Note that $|||\mathbf{a}|||_s \le C$ by Proposition 3.2, $\|\xi\|_s \le C\varepsilon$ by (3.14), and $\|\widetilde{\xi} - \xi\|_s \le C\varepsilon^{\frac{n}{4}+\frac{1}{2}} + C\varepsilon^{\frac{L}{2}-1}$ by Theorem 3.7 with constants depending only on C_{s_0}, C_s, C_{L,s_0}, $C_{L,s}$, C_0, n, and L. Hence,

$$\sum_{l\in\mathcal{N}} |l|^{2s} \Big| |z_l^{\langle l\rangle}|^2 - |\xi_l|^2 \Big| \le C\varepsilon(|||(z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_s + \varepsilon^{\frac{n}{4}+\frac{1}{2}} + \varepsilon^{\frac{L}{2}-1}). \tag{3.20}$$

In order to control the right-hand sides of (3.19) and (3.20) we study $|||(z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_s$. A direct application of Proposition 3.2 yields an estimate $C\varepsilon$ since $\varepsilon^{[[\mathbf{k}]]} \le \varepsilon$ but we can do better. We consider the iteration (3.8) for $b_j^{\mathbf{k}}$ if $[[\mathbf{k}]] = 1$. The estimate of the near-diagonal entries of $\mathbf{F}$ in Lemma 3.1 together with Proposition 3.2 yields the estimate

$$|||([b_j^{\mathbf{k}}]^n)_{j\in\mathcal{N},\|\mathbf{k}\|=1}|||_s \le \varepsilon^{\frac12}|||[\dot{\mathbf{b}}]^{n-1}|||_s + C\varepsilon^{\frac12},$$

and hence we have

$$|||(z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_s \le \varepsilon|||([b_j^{\mathbf{k}}]^n)_{j\in\mathcal{N},\|\mathbf{k}\|=1}|||_s + \varepsilon^{\frac32}|||([b_j^{\mathbf{k}}]^n)_{j\in\mathcal{N},\|\mathbf{k}\|\neq1}|||_s \le C\varepsilon^{\frac32}. \qquad (3.21)$$

The same is true in the rescaled variables $\hat{\mathbf{z}}$ with s replaced by s_0. Moreover, in order to control the influence of $\mathbf{\Omega}$ in (3.19), we note that the iteration (3.9) for $\hat{\mathbf{b}}$ yields

$$\left[(\mathbf{\Omega}\hat{\mathbf{b}})_j^{\mathbf{k}}\right]^n = \left[-i\varepsilon\dot{\hat{b}}_j^{\mathbf{k}} + \hat{\mathbf{F}}(\hat{\mathbf{c}})_j^{\mathbf{k}}\right]^{n-1},$$

and hence $|||[\mathbf{\Omega}\hat{\mathbf{b}}]^n|||_{s_0} \le \varepsilon|||[\dot{\hat{\mathbf{b}}}]^{n-1}|||_{s_0} + |||[\hat{\mathbf{F}}(\hat{\mathbf{c}})]^{n-1}|||_{s_0}$. Proposition 3.2 on the size of $\hat{\mathbf{c}}$ and Lemma 3.1 then imply $|||[\mathbf{\Omega}\hat{\mathbf{b}}]^n|||_{s_0} \le C\varepsilon^{\frac12}$ with a constant C depending only on C_{L,s_0}, $C_{L,s}$, n, and L, and hence

$$|||\mathbf{\Omega}(\hat{z}_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_{s_0} \le C\varepsilon^{\frac32},$$

where we omit again the index n. Using these estimates for $z_j^{\mathbf{k}}$ in (3.19) and (3.20) finally yield the third estimate of the proposition.

If the optional non-resonance condition 2.4 is satisfied, the estimate (3.21) of $z_j^{\mathbf{k}}$ with $\mathbf{k} \neq \langle j\rangle$ improves to $C\varepsilon^2$ instead of $C\varepsilon^{\frac32}$ as we show next. Recall once again the iteration (3.8) for $\mathbf{b}$ where we divide by $\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j$. By the condition of zero momentum, only indices $(j,\mathbf{k})$ with $j = j(\mathbf{k})$ yield nonzero modulation functions (3.7), and therefore only denominators of the form $\mathbf{k}\cdot\boldsymbol{\omega} - \omega_{j(\mathbf{k})}$ need to be taken into account. But for $\|\mathbf{k}\| \le 2$ such denominators can be estimated independently of ε using (2.11) from the optional non-resonance condition 2.4. That means that we don't loose a factor $\varepsilon^{\frac12}$ in the estimate of those $b_j^{\mathbf{k}}$ with $\|\mathbf{k}\| \le 2$. For them we hence get a factor $\varepsilon^{\frac12}\varepsilon^{[[\mathbf{k}]]} = \varepsilon^2$ and for the other indices $\varepsilon^{[[\mathbf{k}]]} \le \varepsilon^2$. In this way we get $|||(z_j^{\mathbf{k}})_{j\in\mathcal{N},\mathbf{k}\neq\langle j\rangle}|||_s \le C\varepsilon^2$ with a constant C depending in addition on C_3 from Assumption 2.4. This proves the improved third estimate of the proposition. □

From Short to Long Time Intervals — Proof of Theorem 2.5. Recall that, in order to put many modulated Fourier expansions together, we have to ensure the regularity of ξ at the boundary of the intervals. This is done with the help of Proposition 3.10 as indicated in Figure 4 and explained below.

The third estimate of Proposition 3.10 indeed yields an estimate for the exact solution $\|\xi(t)\|_s^2 = \sum_{l\in\mathcal{N}}|l|^{2s}I_l(\xi(t),\overline{\xi(t)})$ in terms of the almost invariants

$$\sum_{l\in\mathcal{N}}|l|^{2s}|\mathbf{K}_l([\mathbf{z}(\varepsilon t)]^n, [\overline{\mathbf{z}(\varepsilon t)}]^n)|.$$

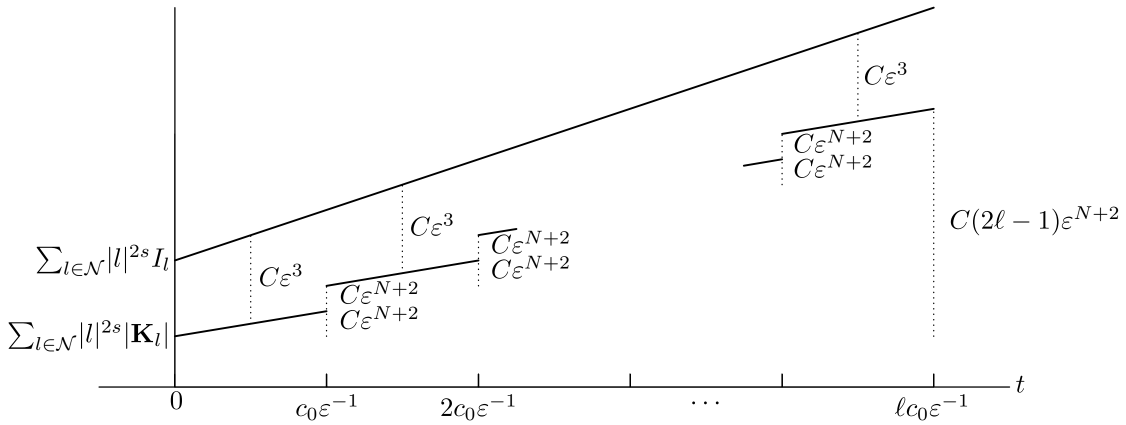

Figure 4: From short to long time intervals

They are $\mathcal{O}(\varepsilon^{\frac{5}{2}})$ (or even $\mathcal{O}(\varepsilon^3)$ if Assumption 2.4 is fulfilled) close to each other. In particular, $\|\xi(t)\|_s$ can be bounded by 2ε as long as

$$\begin{aligned}\Big|\sum_{l\in\mathcal{N}}|l|^{2s}|\mathbf{K}_l([\mathbf{z}(\varepsilon t)]^n,[\overline{\mathbf{z}(\varepsilon t)}]^n)| - \sum_{l\in\mathcal{N}}|l|^{2s}|\mathbf{K}_l([\mathbf{z}(0)]^n,[\overline{\mathbf{z}(0)}]^n)|\Big| \\ \leq \sum_{l\in\mathcal{N}}|l|^{2s}\Big|\mathbf{K}_l([\mathbf{z}(\varepsilon t)]^n,[\overline{\mathbf{z}(\varepsilon t)}]^n) - \mathbf{K}_l([\mathbf{z}(0)]^n,[\overline{\mathbf{z}(0)}]^n)\Big|\end{aligned} \tag{3.22}$$

is bounded by $C\varepsilon^3$ provided that ε is sufficiently small compared to C.

The first two estimates of Proposition 3.10 allow us to control (3.22) by $C\varepsilon^3$: We let the number of iteration n equal $4N+8s_0+2$ (depending only on N and s_0). Then we can put $c_0^{-1}\varepsilon^{-N+1}$ intervals of length $c_0\varepsilon^{-1}$ together still ensuring inductively $\|\xi(t)\|_s \leq 2\varepsilon$ as explained above. Using the third estimate of Proposition 3.10 in (3.22), this proves the statement of Theorem 2.5. Note that $C_{L,s} \leq C_1^{-L+2}C_s$ and that L depends only on N and s_0.

3.6 The Modulated Fourier Expansion for Partially Resonant Frequencies

Now, we turn to the proof of Theorem 2.7 where the non-resonance condition 2.3 used in Theorem 2.5 is replaced by the weaker non-resonance condition 2.6 allowing completely resonant frequencies up to certain extent. Recall that the resonance module was defined as

$$\mathcal{M} = \{\, \mathbf{k} \in \mathbb{Z}^{\mathcal{N}} : \mathbf{k}\cdot\boldsymbol{\omega} = 0 \,\}.$$

We use the ideas described for finite dimensional Hamiltonian systems with resonant frequencies in [15].

Resonant Modulated Fourier Expansions. We are not able anymore to distinguish temporal waves $e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$ and $e^{-i(\mathbf{l}\cdot\boldsymbol{\omega})t}$ if $\mathbf{k}-\mathbf{l} \in \mathcal{M}$. For this reason, the summation in the modulated Fourier expansion (3.2) is not over all $\mathbf{k} \in \mathbb{Z}^{\mathcal{N}}$ but only over all residue classes $[\mathbf{k}] = \mathbf{k} + \mathcal{M} \in \mathbb{Z}^{\mathcal{N}}/\mathcal{M}$ in the case of a nontrivial resonance module,

$$\widetilde{\xi}_j(t) = \sum_{[\mathbf{k}]} z_j^{[\mathbf{k}]}(\varepsilon t) e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}. \tag{3.23}$$

We call this a *resonant modulated Fourier expansion.*

The Choice of a Representative. The resonant modulated Fourier expansion (3.23) does not depend on the choice of the representative $\mathbf{k}$ of the residue class $[\mathbf{k}]$. Here and in the following, we choose as a representative always a member $\mathbf{k}$ of the residue class with minimal

$$\sum_{l\in\mathcal{N}:|l|=m} |k_l|$$

for all $m \in \mathbb{N}$. The linearity of the resonance module $\mathcal{M}$ and the condition (2.14) in Assumption 2.6 ensure the existence of a representative (not necessarily unique) that minimizes $\sum_{l\in\mathcal{N}:|l|=m}|k_l|$ for all $m \in \mathbb{N}$ simultaneously. Indeed, (2.14) implies that $\mathcal{M}$ is generated by those $\mathbf{k} \in \mathbb{Z}^{\mathcal{N}}$ with nonzero entries only for indices $l \in \mathcal{N}$ with $|l| = m$ for a single $m \in \mathbb{N}$. Choosing the representative in this way also implies that it is minimal with respect to $\|\mathbf{k}\|$, $[[\mathbf{k}]]$, and $\mathbf{j}^{(s-s_0)|\mathbf{k}|}$.

The Modulation System. In the same way as in Section 3.1, we are now able to derive a modulation system (3.3), where the summation in the modulation system (3.3a) is now over all residue classes $[\mathbf{k}^1], \dots, [\mathbf{k}^m], [\mathbf{l}^1], \dots, [\mathbf{l}^{m'}]$ with

$$[\mathbf{k}^1] + \cdots + [\mathbf{k}^m] - [\mathbf{l}^1] - \cdots - [\mathbf{l}^{m'}] = [\mathbf{k}],$$

and the summation in the Hamiltonian function (3.4) of the modulation system is over all residue classes $[\mathbf{k}^1], \dots, [\mathbf{k}^m], [\mathbf{l}^1], \dots, [\mathbf{l}^{m'+1}]$ with

$$[\mathbf{k}^1] + \cdots + [\mathbf{k}^m] - [\mathbf{l}^1] - \cdots - [\mathbf{l}^{m'+1}] = [\mathbf{0}] = \mathcal{M}.$$

Because of the form of the latter summation, the new Hamiltonian for the resonant modulation system is not invariant under the transformation $z_j^{[\mathbf{k}]} \mapsto e^{i\theta k_l} z_j^{[\mathbf{k}]}$ for $l \in \mathcal{N}$ anymore. However, due to the condition (2.14) in Assumption 2.6, which ensures that $\mathcal{M}$ is rather small, this new Hamiltonian is invariant under the transformation $z_j^{[\mathbf{k}]} \mapsto e^{i\theta \sum_{l\in\mathcal{N}:|l|=m} k_l} z_j^{[\mathbf{k}]}$ for $m \in \mathbb{N}$, and this invariance leads to formal invariants

$$\mathbf{K}_m(\mathbf{z}, \overline{\mathbf{z}}) = \sum_{j\in\mathcal{N},[\mathbf{k}]\in\mathbb{Z}^{\mathcal{N}}/\mathcal{M}} \Big(\sum_{l\in\mathcal{N}:|l|=m} k_l \Big) |z_j^{[\mathbf{k}]}|^2 \tag{3.24}$$

for $m \in \mathbb{N}$ and with $\mathbf{z} = (z_j^{[\mathbf{k}]})_{j\in\mathcal{N},[\mathbf{k}]\in\mathbb{Z}^{\mathcal{N}}/\mathcal{M}}$.

Iterative Solution of the Resonant Modulation System. We use the iteration described in Section 3.2 to construct an approximate solution for the resonant modulation system. The estimates of Section 3.3 are also valid for this iteration if we define $[[[\mathbf{k}]]]$ and $\mathbf{j}^{(s-s_0)|[\mathbf{k}]|}$ by their values for the representative of the residue class $[\mathbf{k}]$ as chosen above. Indeed, this choice ensures that all the inequalities used for

$$[[\mathbf{k}^1]] + \cdots + [[\mathbf{k}^m]] + [[\mathbf{l}^1]] + \cdots + [[\mathbf{l}^{m'}]] \quad \text{and} \quad \mathbf{j}^{(s-s_0)|\mathbf{k}^1|+\cdots+|\mathbf{k}^m|+|\mathbf{l}^1|+\cdots+|\mathbf{l}^{m'}|}$$

are also valid for the residue classes. Then, the relation between the exact solution and its iterated modulated Fourier expansion as stated in Theorem 3.7 is also shown as in Section 3.4.

From Short to Long Time Intervals — Proof of Theorem 2.7. Also the extension to long time intervals is done as in Section 3.5. However, since the "new" formal invariants (3.24) not only contain $|z_l^{\langle l\rangle}|^2$ as a leading term (with respect to powers of ε) like the invariants $\mathbf{K}_l$ in Section 3.5 but the sum $\sum_{l\in\mathcal{N}:|l|=m}|z_l^{[\langle l\rangle]}|^2$, we cannot expect the third inequality of Proposition 3.10 relating $\mathbf{K}_l$ and the action I_l to be true anymore. But we can show its variant

$$\sum_{m\in\mathbb{N}} m^{2s}\Big|\mathbf{K}_m([\mathbf{z}(\tau)]^n, [\overline{\mathbf{z}(\tau)}]^n) - \sum_{l\in\mathcal{N}:|l|=m} I_l(\xi(t),\overline{\xi(t)})\Big| \le C\varepsilon^{\frac{5}{2}},$$

and the regularity of the exact solution $\xi(t)$ can once again be ensured by

$$\|\xi(t)\|_s^2 = \sum_{l\in\mathcal{N}}|l|^{2s} I_l(\xi(t),\overline{\xi(t)}) = \sum_{m\in\mathbb{N}} m^{2s} \sum_{l\in\mathcal{N}:|l|=m} I_l(\xi(t),\overline{\xi(t)}).$$

In this way, the extension to long time intervals is done as in Section 3.5 yielding near-conservation of the sums of actions

$$\sum_{l\in\mathcal{N}:|l|=m} I_l(\xi(t),\overline{\xi(t)})$$

over long times $0 \le t \le \varepsilon^{-N}$ as stated in Theorem 2.7.

3.7 The Modulated Fourier Expansion with Scaled Norms

In this section we comment on the modifications needed in the previous proofs of Theorems 2.5 and 2.7 in order to prove Theorem 2.12 where scaled actions are studied and scaled norms

$$\|\xi\|_{s,e} = \Big(\sum_{j\in\mathcal{N}} \varepsilon^{-2e(j)(1-\mu)}|j|^{2s}|\xi_j|^2\Big)^{\frac{1}{2}}$$

are used.

A New Norm for Modulation Functions. In principle we can repeat the proofs of the preceding sections. Since the initial value is now of size ε^μ in the norm $\|\cdot\|_{s,e}$ instead of size ε in the norm $\|\cdot\|_s$, any ε appearing in the estimates has to be replaced by ε^μ, and the scaling by $\varepsilon^{[[\mathbf{k}]]}$ is replaced by $\varepsilon^{\mu[[\mathbf{k}]]}$. Moreover, the norm $|||\cdot|||_s$ for modulation functions has to be adapted. We replace this norm by

$$|||\mathbf{z}|||_{s,e} = \Big\| \Big(\sum_{\mathbf{k}} \varepsilon^{-e(\mathbf{k})(1-\mu)} |z_j^{\mathbf{k}}| \Big)_{j\in\mathcal{N}} \Big\|_s ,$$

where

$$e(\mathbf{k}) = \sum_{l\in\mathcal{N}} |k_l| e(l)$$

for $\mathbf{k} \in \mathbb{Z}^{\mathcal{N}}$.

Properties of the Scaling Function e. The main properties we need for adapting the arguments of the preceding sections are

$$\varepsilon^{-e(\mathbf{k})(1-\mu)} \le \varepsilon^{-e(\mathbf{k}^1)(1-\mu)} \cdots \varepsilon^{-e(\mathbf{k}^m)(1-\mu)} \varepsilon^{-e(\mathbf{l}^1)(1-\mu)} \cdots \varepsilon^{-e(\mathbf{l}^{m'})(1-\mu)} \tag{3.25}$$

for $\mathbf{k} = \mathbf{k}^1 + \cdots + \mathbf{k}^m - \mathbf{l}^1 - \cdots - \mathbf{l}^{m'}$,

$$\varepsilon^{-e(j^1+j^2)(1-\mu)} \le \varepsilon^{-e(j^1)(1-\mu)} \varepsilon^{-e(j^2)(1-\mu)} \quad \text{and} \quad \varepsilon^{-e(j)(1-\mu)} \le \varepsilon^{-e(\mathbf{k})(1-\mu)} \tag{3.26}$$

for $j = j(\mathbf{k})$ due to the triangle inequality of $e(\cdot)$, and

$$\varepsilon^{-e(l)(1-\mu)} \le \varepsilon^{-e(\mathbf{k})(1-\mu)} \tag{3.27}$$

if $k_l \neq 0$.

The first property (3.25) ensures that the estimates of the nonlinearity in Lemma 3.1 and Lemma 3.4 are also true in the norm $|||\cdot|||_{s,e}$ (with ε^μ instead of ε as mentioned above).

The first part of the second property (3.26) ensures the validity of the estimates (2.6a) in the regularity assumption and (2.7) with $\|\cdot\|_{s,e}$ instead of $\|\cdot\|_s$. The second part ensures that

$$\Big\| \Big(\sum_{\mathbf{k}} |z_j^{\mathbf{k}}| \Big)_{j\in\mathcal{N}} \Big\|_{s,e} = \Big\| \Big(\varepsilon^{-e(j)(1-\mu)} \sum_{\mathbf{k}} |z_j^{\mathbf{k}}| \Big)_{j\in\mathcal{N}} \Big\|_s \le |||\mathbf{z}|||_{s,e}.$$

This is needed when replacing the norms $\|\cdot\|_s$ and $|||\cdot|||_s$ by $\|\cdot\|_{s,e}$ and $|||\cdot|||_{s,e}$ for the estimates (3.10), (3.13), (3.15), and the estimate of $\mathbf{u}$ in the proof of Proposition 3.8.

The third property (3.27) is needed when adapting Section 3.5 to the new situation. In order to have regularity in the norm $\|\cdot\|_{s,e}$ we should prove Proposition 3.10 with $\sum_{l\in\mathcal{N}} \varepsilon^{-2e(l)(1-\mu)} |l|^{2s} \ldots$ instead of $\sum_{l\in\mathcal{N}} |l|^{2s} \ldots$. This is done by adapting Lemma 3.9 to this situation using (3.27) and replacing $|||\cdot|||_{s_0}$ by $|||\cdot|||_{s_0,e}$ on the right-hand sides of the estimates of Lemma 3.9.

The Case of a Cubic Nonlinearity. If the nonlinearity is (at least) cubic and if the coefficients $P_{j,k,l}$ of the nonlinearity are nonzero only if $k \in \mathcal{N}^{m+1}$ and $l \in \mathcal{N}^m$, then the triangle inequality for $e(\cdot)$ is assumed in Theorem 2.12 only for sums of three or more indices (recall that the triangle inequality was used to prove (3.26)). Indeed, for a cubic nonlinearity the first inequality of (3.26) is only needed for sums of (at least) three indices. If in addition $P_{j,k,l}$ is nonzero only for $k \in \mathcal{N}^{m+1}$ and $l \in \mathcal{N}^m$, the same calculation as for the verification of the single wave property (3.7) shows that

$$\left[z_j^{\mathbf{k}}\right]^n = 0 \quad \text{for all } \mathbf{k} \text{ with } \sum_{l \in \mathcal{N}} k_l \neq 1 \text{ or } j \neq j(\mathbf{k}).$$

In particular, $[z_j^{\mathbf{k}}]^n = 0$ if $\mathbf{k} \neq \langle j \rangle$ and $\|\mathbf{k}\| \leq 2$. This implies that the second inequality of (3.26) is only needed for $\mathbf{k} = \langle j \rangle$ and $\|\mathbf{k}\| > 2$. In particular, the triangle inequality for $e(\cdot)$ with three or more summands is sufficient for the second inequality of (3.26).

The same modifications can also be done in the partially resonant situation combining the above changes with Section 3.6. In this way, the proof of Theorem 2.12 is a modification of the proofs of Theorems 2.5 and 2.7.

4 Long-Time Analysis of Spatial Semi-Discretizations of Hamiltonian Partial Differential Equations

In this chapter we study spatial semi-discretizations of the Hamiltonian partial differential equations of Chapter 2 on a long time interval (see the last column in Figure 1).

4.1 Spatial Semi-Discretizations of Hamiltonian Partial Differential Equations

As in the previous chapters we focus here again on weakly nonlinear Hamiltonian partial differential equations with Hamiltonian function (2.1),

$$H(\xi,\eta)=\sum_{j\in\mathcal{N}}\omega_j\xi_j\eta_j+P(\xi,\eta), \tag{4.1}$$

where ω_j, $j\in\mathcal{N}$, are real frequencies and P is a function with a zero of order (at least) three at the origin and with $\overline{P(\xi,\eta)}=P(\overline{\eta},\overline{\xi})$. We study spatial semi-discretizations of such equations.

Spatial Semi-Discretizations. Standard methods for discretizing a partial differential equation in space are spectral methods, finite differences, or finite elements. They all reduce the partial differential equation to an ordinary differential equation in time. We consider here spatial semi-discretizations of Hamiltonian partial differential equations which preserve the Hamiltonian structure, i.e., which result in *Hamiltonian* ordinary differential equations. Various examples can be found in Sections 4.4, 4.5, and 4.6.

The Hamiltonian function of the semi-discretization in space is assumed to have the form

$$H^M(\xi,\eta)=\sum_{j\in\mathcal{N}}\omega_j^M\xi_j\eta_j+P^M(\xi,\eta), \tag{4.2}$$

where M denotes the spatial discretization parameter, and (by a slight abuse of notation) we denote again by ξ and η the variables belonging now to a finite dimensional phase space $l_s^2=l_s^2(\mathbb{C}^{\mathcal{N}_M})$ with a *finite* set of indices $\mathcal{N}_M\subseteq\mathbb{Z}^d$. We usually choose a full grid

$$\mathcal{N}_M=\{-M,\dots,M\}^d \quad \text{or} \quad \mathcal{N}_M=\{-M,\dots,M-1\}^d.$$

We assume again that P^M has a zero of order at least three at the origin and that $\overline{P^M(\xi,\eta)}=P^M(\overline{\eta},\overline{\xi})$. Moreover, we assume for the discrete frequencies ω_j^M as for ω_j in the continuous Hamiltonian function (4.1) that they are real.

The variables ξ used in the semi-discrete Hamiltonian function (4.2) are related to the variables in the underlying Hamiltonian function (4.1) by an embedding

$$\iota: l_0^2(\mathbb{C}^{\mathcal{N}_M})\to l_0^2(\mathbb{C}^{\mathcal{N}})$$

of the finite dimensional space $l_0^2(\mathbb{C}^{\mathcal{N}_M})$ of the spatial semi-discretization in the infinite dimensional space $l_0^2(\mathbb{C}^{\mathcal{N}})$ of the underlying partial differential equation. This map reproduces from the semi-discrete numerical solution ξ a function $\iota(\xi)$ in the phase space of the underlying equation. It is given in a natural way by the semi-discretization and can be thought of as an interpolation. Often, we have a natural embedding $\iota = \mathrm{id}$ ($\iota(\xi)_j = \xi_j$ for $j \in \mathcal{N}_M$ and $\iota(\xi)_j = 0$ for $j \in \mathcal{N} \setminus \mathcal{N}_M$).

Problem Setting. Long-time investigations of Hamiltonian ordinary differential equations such as (4.2) date back to Poincaré, Lindstedt, and Birkhoff in the 19th and early 20th century and are famous and well-known nowadays, see for example [36, Chapter X]. In the context of spatial semi-discretizations of partial differential equations however, it is important to understand the influence of the spatial discretization parameter M in the Hamiltonian function (4.2) on such results. Even more, one is interested in results which do not depend on this parameter M. In order to tackle such questions it seems to be necessary to take the underlying infinite dimensional problem (4.1) into account, and first results for nonlinear wave equations [34] and nonlinear Schrödinger equations [29] have been obtained only recently. Here, we generalise these results.

4.2 Long-Time Near-Conservation of Actions

From Theorem 2.5 (or Theorem 2.7 in the case of partial resonances) we know that under suitable assumptions we have long-time near-conservation of actions along the exact solution of a Hamiltonian partial differential equation. Is this still true along a spatial semi-discretization of a Hamiltonian partial differential equation with constants independent of the spatial discretization parameter M?

For the semi-discrete Hamiltonian function (4.2) we have two different notions of actions. The first one is the notion of discrete actions I_j^M associated to the discrete Hamiltonian function H^M (4.2), and we are interested in the behaviour of these actions along the numerical solution $\xi(t)$,

$$I_j^M(\xi(t), \overline{\xi(t)}) - I_j^M(\xi(0), \overline{\xi(0)}).$$

The second notion of actions arises naturally in the numerical context. We solve a semi-discretization in order to have an approximation to the exact solution. Therefore, we are interested in the behaviour of the actions I_j of the continuous Hamiltonian function (4.1) along the numerical solution $\iota(\xi(t))$ embedded to the space of the Hamiltonian partial differential equation underlying the spatial semi-discretization,

$$I_j(\iota(\xi(t)), \overline{\iota(\xi(t))}) - I_j(\iota(\xi(0)), \overline{\iota(\xi(0))}).$$

Of course, in the often encountered situation of a natural embedding $\iota = \mathrm{id}$ both notions of actions agree,

$$I_j(\iota(\xi), \overline{\iota(\xi)}) = I_j^M(\xi, \overline{\xi}). \tag{4.3}$$

Theorems 2.5 and 2.7 have been formulated in such a way that they also cover the finite dimensional case where the set of indices is finite. If we are able to verify the assumptions of these theorems for the semi-discrete situation (4.2) with constants independent of M, we get long-time near-conservation of discrete actions I_j^M along a spatial semi-discretization of a Hamiltonian partial differential equation with constants independent of M. Concerning the continuous actions I_j, we impose the following assumption relating them to the discrete actions.

Assumption 4.1. If the non-resonance condition 2.3 is fulfilled for the discrete frequencies ω_j^K, $j \in \mathcal{N}_M$, we assume that there exist constants c_l, $l \in \mathcal{N}_M$, such that

$$I_l(\iota(\xi), \overline{\iota(\xi)}) = \begin{cases} c_l I_l^M(\xi, \overline{\xi}), & l \in \mathcal{N}_M \subseteq \mathcal{N}, \\ 0, & \text{else} \end{cases}$$

for all $\xi \in l_0^2(\mathbb{C}^{\mathcal{N}_M})$. By C_4 we denote the maximum of c_l, $l \in \mathcal{N}_M$.

If the non-resonance condition 2.6 is fulfilled for the discrete frequencies ω_j^K, $j \in \mathcal{N}_M$, we assume that there exist constants c_m, $m \in \mathbb{N}$, such that

$$\sum_{l \in \mathcal{N}:|l|=m} I_l(\iota(\xi), \overline{\iota(\xi)}) = \begin{cases} c_m \sum_{l \in \mathcal{N}_M:|l|=m} I_l^M(\xi, \overline{\xi}), & \text{there exists } l \in \mathcal{N}_M \text{ with } |l| = m, \\ 0, & \text{else} \end{cases}$$

for all $\xi \in l_0^2(\mathbb{C}^{\mathcal{N}_M})$. By C_4 we denote the maximum of c_m, $m \in \mathbb{N}$.

An important example is the case of the natural embedding $\iota = \mathrm{id}$ where Assumption 4.1 is fulfilled with all constants equal to one, see (4.3).

Theorem 4.2 (Long-Time Near-Conservation of Actions)**.** *Under the assumptions of Theorem 2.5 on H^M and ω_l^K, $l \in \mathcal{N}_M$, instead of H and ω_l, $l \in \mathcal{N}$, we have near-conservation of discrete actions*

$$\sum_{l \in \mathcal{N}_M} |l|^{2s} \frac{|I_l^M(\xi(t), \overline{\xi(t)}) - I_l^M(\xi(0), \overline{\xi(0)})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{4.4}$$

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

with the constant C of Theorem 2.5.

If in addition Assumption 4.1 is satisfied, we also have near-conservation of continuous actions

$$\sum_{l \in \mathcal{N}} |l|^{2s} \frac{|I_l(\iota(\xi(t)), \overline{\iota(\xi(t))}) - I_l(\iota(\xi(0)), \overline{\iota(\xi(0))})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{4.5}$$

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

with a constant C depending in addition on C_4.

The near-conservation of actions improves to $C\varepsilon$ with a constant depending in addition on C_3 if in addition the non-resonance condition 2.4 is satisfied.

Proof. The long-time near-conservation of discrete actions (4.4) follows immediately from Theorem 2.5. Concerning the continuous actions, we note that

$$\sum_{l\in\mathcal{N}} |l|^{2s} |I_l(\iota(\xi(t)),\overline{\iota(\xi(t))}) - I_l(\iota(\xi(0)),\overline{\iota(\xi(0))})| \le C_4 \sum_{l\in\mathcal{N}_M} |l|^{2s} |I_l^M(\xi(t),\overline{\xi(t)}) - I_l^M(\xi(0),\overline{\xi(0)})|$$

by Assumption 4.1. □

The remarkable long-time behaviour along the exact solution is thus transferred to the numerical solution. In the case of completely resonant frequencies we get the following theorem whose proof is the same as the proof of Theorem 4.2.

Theorem 4.3 (Long-Time Near-Conservation of Sums of Actions)**.** *Under the assumptions of Theorem 2.7 on H^M and ω_l^K, $l \in \mathcal{N}_M$, instead of H and ω_l, $l \in \mathcal{N}$, we have near-conservation of sums of discrete actions*

$$\sum_{m\in\mathbb{N}} m^{2s} \frac{|\sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi(t),\overline{\xi(t)}) - \sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi(0),\overline{\xi(0)})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{4.6}$$

and, if in addition Assumption 4.1 is satisfied, also near-conservation of sums of continuous actions

$$\sum_{m\in\mathbb{N}} m^{2s} \frac{|\sum_{l\in\mathcal{N}:|l|=m} I_l(\iota(\xi(t)),\overline{\iota(\xi(t))}) - \sum_{l\in\mathcal{N}:|l|=m} I_l(\iota(\xi(0)),\overline{\iota(\xi(0))})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{4.7}$$

over long times

$$0 \le t \le \varepsilon^{-N}$$

with the corresponding constant C of Theorem 4.2.

The near-conservation of actions improves to $C\varepsilon$ with a constant depending in addition on C_3 if in addition the non-resonance condition 2.4 is satisfied. □

4.3 Long-Time Regularity and Long-Time Analysis of Energy, Mass, and Momentum

As for the actions in the previous Section 4.2 we have two different notions of regularity and of the other possibly conserved quantities energy, mass, and momentum. The first one is the notion of regularity of $\xi(t)$ and the notion of discrete energy H^M, discrete mass m^M, and discrete momentum K^M originating from the discrete Hamiltonian function H^M. The second one is the notion of regularity of $\iota(\xi(t))$ and the notion of continuous energy H, continuous mass m, and continuous momentum K along $\iota(\xi(t))$. The second notion is in particular important from a numerical point of view.

The following corollaries on the regularity of the semi-discrete solution and on long-time near-conservation of mass and momentum along the semi-discrete solution follow from Theorems 4.2 and 4.3 as their continuous counterparts 2.9, 2.10, and 2.11.

Corollary 4.4 (Long-Time Regularity). *Under the assumptions of Theorem 4.2 or Theorem 4.3 we have regularity*

$$\|\xi(t)\|_s \leq 2\varepsilon \tag{4.8}$$

and, if in addition Assumption 4.1 is satisfied, also regularity

$$\|\iota(\xi(t))\|_s \leq 2\varepsilon \tag{4.9}$$

over long times

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

□

The discrete mass m^M is exactly conserved along a semi-discrete solution provided that the discrete Hamiltonian function H^M is invariant under some transformation as required in Proposition 1.3. If it is not an exact invariant, we have the following corollary.

Corollary 4.5 (Long-Time Near-Conservation of Mass). *Under the assumptions of Theorem 4.2 or Theorem 4.3 we have near-conservation of discrete mass*

$$\frac{|m^M(\xi(t), \overline{\xi(t)}) - m^M(\xi(0), \overline{\xi(0)})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{4.10}$$

and, if in addition Assumption 4.1 is satisfied, also near-conservation of continuous mass

$$\frac{|m(\iota(\xi(t)), \overline{\iota(\xi(t))}) - m(\iota(\xi(0)), \overline{\iota(\xi(0))})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{4.11}$$

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

with the corresponding constant C of Theorem 4.2.

As there, the estimate improves to $C\varepsilon$ if in addition the non-resonance condition 2.4 is satisfied. □

Also for the discrete momentum K^M we have either exact conservation by Proposition 1.4 or long-time near-conservation as stated in the following corollary. Note that exact conservation of momentum along exact solutions does not necessarily imply its exact conservation along semi-discrete solutions, see Section 4.5.

Corollary 4.6 (Long-Time Near-Conservation of Momentum). *Under the assumptions of Theorem 4.2 and for $s \geq \frac{1}{2}$ we have near-conservation of discrete momentum*

$$\frac{|K_l^M(\xi(t), \overline{\xi(t)}) - K_l^M(\xi(0), \overline{\xi(0)})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{4.12}$$

and, if in addition Assumption 4.1 is satisfied, also near-conservation of continuous momentum

$$\frac{|K_l(\iota(\xi(t)), \overline{\iota(\xi(t))}) - K_l(\iota(\xi(0)), \overline{\iota(\xi(0))})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{4.13}$$

for $l = 1, \dots, d$ over long times

$$0 \le t \le \varepsilon^{-N}$$

with the corresponding constant C of Theorem 4.2.

As there, the estimate improves to $C\varepsilon$ if in addition the non-resonance condition 2.4 is satisfied. □

Discrete and Continuous Energy. Of course, the discrete energy H^M is exactly conserved along any solution of the semi-discrete system (4.2) by Proposition 1.1. Since the discrete energy H^M is conserved along the semi-discrete solution, the question on the behaviour of H along the embedding of the semi-discrete solution reduces to the question on the size of the difference

$$H(\iota(\xi), \overline{\iota(\xi)}) - H^M(\xi, \bar{\xi}).$$

We will estimate this difference for our examples taking the special structure of H and H^M into account.

In the same way as the long-time estimates for actions, mass, and momentum, we can transfer the results on energy distribution in Theorem 2.12 and its Corollaries 2.13 and 2.14 also to the semi-discrete situation.

4.4 Example — A Spectral Galerkin Method for Nonlinear Schrödinger Equations of Convolution Type

We first consider a spatial semi-discretization of the nonlinear Schrödinger equation with a potential of convolution type

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x) * \psi(x,t) + g(|\psi(x,t)|^2)\psi(x,t) \qquad (4.14)$$

as studied in Sections 1.4 and 2.6, see equations (1.7) and (2.25). Recall from Section 2.6 that along any solution of such a nonlinear Schrödinger equation we have under suitable assumptions long-time near-conservation of actions, long-time regularity, and exact conservation of energy, mass, and momentum by Corollary 2.15.

The Spectral Galerkin Method. A simple approach for a spatial semi-discretization of the nonlinear Schrödinger equation (4.14) is a *spectral Galerkin method*. As an ansatz for the solution $\psi = \psi(x,t)$ of the nonlinear Schrödinger equation (4.14) we choose a truncated spectral representation

$$\psi^M(x,t) = \sum_{j \in \mathcal{N}_M} \xi_j(t) e^{i(j\cdot x)}$$

in the finite dimensional approximation space $\langle e^{i(j\cdot x)} : j \in \mathcal{N}_M \rangle$ with a finite set $\mathcal{N}_M \subseteq \mathcal{N} = \mathbb{Z}^d$. A typical choice of the set $\mathcal{N}_M$, that will be investigated here, is a full grid

$$\mathcal{N}_M = \{ -M, \dots, M \}^d$$

with a spatial discretization parameter M. In view of the condition of zero momentum in Assumption 2.2 we define the addition of indices from this set as the usual addition in $\mathbb{Z}^d$; in particular, $\mathcal{N}_M$ is not closed under this addition. The embedding ι relating the semi-discrete setting with the continuous one is in the light of $\psi(x,t) = \sum_{j\in\mathcal{N}} \xi_j(t)e^{i(j\cdot x)}$ the natural embedding $\iota = \mathrm{id}$.

In a Galerkin method we require that the residual of the ansatz $\psi^M(x,t)$, when inserted in the nonlinear Schrödinger equation (4.14), is orthogonal to the above approximation space with respect to the $L^2(\mathbb{R}^d)$ scalar product. Due to the orthonormality of the basis functions $e^{i(j\cdot x)}$ this results in the equations

$$i\frac{d}{dt}\xi_j(t) = \omega_j\xi_j(t) + \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!}\sum_{\substack{j^1+\cdots+j^{m+1}\\ -j^{m+2}-\cdots-j^{2m+1}=j}} \xi_{j^1}(t)\cdots\xi_{j^{m+1}}(t)\overline{\xi_{j^{m+2}}(t)\cdots\xi_{j^{2m+1}}(t)} \tag{4.15}$$

for $j \in \mathcal{N}_M$. These are the same equations as for the Fourier coefficients of the exact solution (1.8), but the set of indices is restricted to $\mathcal{N}_M$ (and implicitly $\xi_j(t) = 0$ for $j \notin \mathcal{N}_M$). The above semi-discrete equations (4.15) are again Hamiltonian with Hamiltonian function

$$H^M(\xi,\eta) = \sum_{j\in\mathcal{N}_M}\omega_j\xi_j\eta_j + \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!(m+1)}\sum_{\substack{j^1+\cdots+j^{m+1}\\ -j^{m+1}-\cdots-j^{2m+2}=0}} \xi_{j^1}\cdots\xi_{j^{m+1}}\eta_{j^{m+2}}\cdots\eta_{j^{2m+2}}$$

defined on a subset of the finite dimensional phase space $l_s^2(\mathbb{C}^{\mathcal{N}_M}) \times l_s^2(\mathbb{C}^{\mathcal{N}_M})$. In terms of the ansatz ψ^M the equations (4.15) read

$$i\frac{\partial}{\partial t}\psi^M(x,t) = -\Delta\psi^M(x,t) + V(x) * \psi^M(x,t) + \mathcal{P}(g(|\psi^M(x,t)|^2)\psi^M(x,t)) \tag{4.16a}$$

with the $L^2(\mathbb{R}^d)$-orthonormal projection $\mathcal{P}$ on the approximation space $\langle e^{i(j\cdot x)} : j \in \mathcal{N}_M\rangle$,

$$\mathcal{P}\Big(\sum_{j\in\mathcal{N}}\varphi_j e^{i(j\cdot x)}\Big) = \sum_{j\in\mathcal{N}_M}\varphi_j e^{i(j\cdot x)}.$$

The initial value $\psi^M(\cdot,0)$ is defined by

$$\psi^M(\cdot,0) = \mathcal{P}(\psi(\cdot,0)). \tag{4.16b}$$

Verification of the Assumptions 2.1, 2.2, 2.3, 2.4, and 4.1. *The Assumptions 2.1, 2.2, 2.3, and 2.4 are satisfied under the same conditions and with the same constants (in particular independent of M) as for the continuous nonlinear Schrödinger equation with a potential of convolution type in Section 2.6. Assumption 4.1 is fulfilled with $C_4 = 1$.*

The semi-discrete nonlinearity P^M is just a truncation of the nonlinearity P in the continuous nonlinear Schrödinger equation (4.14), where the summation is only over the indices in $\mathcal{N}_M$. The nonlinearity P satisfied the regularity assumption 2.1 as was shown in

Section 2.6, and hence the regularity assumption 2.1 is also fulfilled for the semi-discrete nonlinearity P^M with constants independent of the spatial discretization parameter M. This also implies that the condition of zero momentum is satisfied in Assumption 2.2.

Moreover the semi-discrete frequencies ω_j^M are the same as the continuous frequencies ω_j, and hence the non-resonance condition 2.3 is also satisfied in the semi-discrete situation with constants independent of M. The same is true for the additional non-resonance condition 2.4 in dimension one ($d = 1$). Assumption 4.1 is fulfilled with a constant $C_4 = 1$ since we have a natural embedding $\iota = \mathrm{id}$ and hence $I_j(\iota(\xi), \overline{\xi}) = I_j^M(\xi, \overline{\xi})$ by (4.3).

We get the following corollary corresponding to Corollary 2.15 in the continuous situation.

Corollary 4.7 (Long-Time Analysis of the Spectral Galerkin Discretization of Nonlinear Schrödinger Equations (4.14))**.** *Under the assumptions of Corollary 2.15 with smallness of* $\psi^M(\cdot, 0)$ *instead of* $\psi(\cdot, 0)$ *we have*

- *near-conservation of discrete actions* (4.4) *and continuous actions* (4.5)*,*
- *exact conservation of discrete and continuous energy, discrete and continuous mass, and discrete and continuous momentum,*
- *and regularity* (4.8) *and* (4.9)

over long times

$$0 \le t \le \varepsilon^{-N}$$

along any solution $\psi^M(x,t) = \sum_{j \in \mathcal{N}_M} \xi_j(t) e^{i(j \cdot x)}$ *of the semi-discrete nonlinear Schrödinger equation* (4.16) *in dimension* d *with the constant* C *of Corollary 2.15 independent of* ε *and the spatial discretization parameter* M*.*

The near-conservation of actions improves to $C\varepsilon$ *in dimension one* ($d = 1$)*.*

Proof. All assumptions of Theorem 4.2 are fulfilled. Long-time near-conservation of discrete and continuous actions then follows from this theorem, and regularity follows from Corollary 4.4.

Along solutions of the semi-discrete equation (4.15) the energies H and H^M agree,

$$H(\iota(\xi(t)), \overline{\iota(\xi(t))}) = H^M(\xi(t), \overline{\xi(t)}),$$

and hence we have exact conservation of $H = H^M$ along such solutions.

Since the discrete Hamiltonian function H^M is, as the continuous one, invariant under the transformations $\xi \mapsto e^{i\theta}\xi$ and $\xi_j \mapsto e^{i\theta j_l}\xi_j$ for $l = 1, \dots, d$, discrete mass m^M and discrete momentum K^M are also exact invariants of the semi-discrete system (4.15). Along semi-discrete solutions $\xi(t)$ they agree with the mass m and the momentum K of (4.1) along $\iota(\xi(t))$ since we have a natural embedding $\iota = \mathrm{id}$. Hence the continuous quantities m and K are also conserved exactly along $\iota(\xi(t))$. □

This corollary shows that we can expect the same behaviour along the semi-discrete solution as along the exact solution on a long time interval: near-conservation of actions and exact conservation of energy, mass, and momentum. Note that the smallness

$\|\xi(0)\|_s \le \varepsilon$ of the discrete initial value $\psi^M(\cdot,0) = \mathcal{P}(\psi(\cdot,0))$, as required in Corollary 4.7, is implied by the smallness of the initial value $\psi(\cdot,0)$ for the exact solution as required in Corollary 2.15.

We now study the energy distribution along the Galerkin semi-discretization (4.16) in the case of finite band initial values (2.22a) and initial values consisting only of a pair of modes (2.22b). For the exact solution of the nonlinear Schrödinger equation (4.14) we have studied the energy distribution in Corollaries 2.16 and 2.17. As there we get the following semi-discrete counterparts using $\iota = \mathrm{id}$.

Corollary 4.8 (Long-Time Energy Distribution (a) for the Spectral Galerkin Discretization of Nonlinear Schrödinger Equations (4.14))**.** *Let $0 < \mu \le 1$. Under the assumptions of Corollary 2.15 and for small initial values*

$$\|\xi(0)\|_s \le \varepsilon \quad \textit{with } (2.22\mathrm{a})$$

we have for any ε, such that ε^μ satisfies the smallness assumption of Corollary 2.15, the energy distribution

$$\sum_{(2m-1)B<|l|\le(2m+1)B} |l|^{2s} I_l^M(\xi(t),\overline{\xi(t)}) \le C\varepsilon^{2(2m+1)(1-\mu)+\frac{5}{2}\mu}$$

for $m \ge 1$ over long times

$$0 \le t \le \varepsilon^{-N\mu}$$

along any solution $\psi^M(x,t) = \sum_{j\in\mathcal{N}_M} \xi_j(t) e^{i(j\cdot x)}$ of the semi-discrete nonlinear Schrödinger equation (4.16) in dimension d with the constant C of Corollary 2.15.

The same energy distribution holds for the continuous actions $I_l(\iota(\xi(t)),\overline{\iota(\xi(t))})$. The estimates improve by a factor $\varepsilon^{\frac{1}{2}\mu}$ in dimension one ($d=1$). □

Corollary 4.9 (Long-Time Energy Distribution (b) for the Spectral Galerkin Discretization of Nonlinear Schrödinger Equations (4.14))**.** *Let $0 < \mu \le 1$. Under the assumptions of Corollary 2.15 and for small initial values*

$$\|\xi(0)\|_s \le \varepsilon \quad \textit{with } (2.22\mathrm{b})$$

we have for any ε, such that ε^μ satisfies the smallness assumption of Corollary 2.15, the energy distribution

$$|m\tilde{j}|^{2s} I_{m\tilde{j}}^M(\xi(t),\overline{\xi(t)}) \le C\varepsilon^{2|m|(1-\mu)+\frac{5}{2}\mu}$$

for odd $m \in \mathbb{Z}$ with $m \ne \pm 1$ and $m\tilde{j} \in \mathcal{N}_M$ over long times

$$0 \le t \le \varepsilon^{-N\mu}$$

along any solution $\psi^M(x,t) = \sum_{j\in\mathcal{N}_M} \xi_j(t) e^{i(j\cdot x)}$ of the semi-discrete nonlinear Schrödinger equation (4.16) in dimension d with the constant C of Corollary 2.15. If $l \notin \{m\tilde{j} : m \in \mathbb{Z} \text{ odd}\}$, then $\xi_l(t) = 0$ for all times t.

The same energy distribution holds for the continuous actions $I_l(\iota(\xi(t)),\overline{\iota(\xi(t))})$. The estimates improve by a factor $\varepsilon^{\frac{1}{2}\mu}$ in dimension one ($d=1$). □

The same discretization can be applied to the Schrödinger–Poisson equation as studied in Section 1.4 and 2.7, see equations (1.11) and (2.28). Corollaries 4.7, 4.9, and 4.8 are also true for the spectral Galerkin method applied to this equation.

4.5 Example — A Spectral Collocation Method for Nonlinear Schrödinger Equations of Convolution Type

We consider another spatial semi-discretization of the nonlinear Schrödinger equation with a potential of convolution type (4.14) by a *spectral collocation method.* This semi-discretization is well suited for a subsequent discretization in time by a splitting integrator, see Section 5.6.

The Spectral Collocation Method. As for the spectral Galerkin method of Section 4.4 we choose a truncated spectral representation

$$\psi^M(x,t) = \sum_{j\in\mathcal{N}_M} \xi_j(t) e^{i(j\cdot x)}$$

as an ansatz for the solution of the nonlinear Schrödinger equation (4.14). The set $\mathcal{N}_M \subseteq \mathcal{N} = \mathbb{Z}^d$ is chosen as a full grid

$$\mathcal{N}_M = \{\, -M, \dots, M-1 \,\}^d,$$

but this time the addition of indices from this set is defined modulo $2M$ in each entry in such a way that $\mathcal{N}_M$ is closed under the addition. It is clear that $|\cdot|$, as defined in Section 1.1, satisfies the triangle inequality with respect to this addition. Again, the embedding ι is the natural embedding id.

We insert the ansatz ψ^M in the nonlinear Schrödinger equation (4.14). We then evaluate the residual at the *collocation points*

$$x_k = \frac{\pi}{M} k \quad \text{for } k \in \mathcal{N}_M$$

and require it to be zero,

$$i\frac{\partial}{\partial t}\psi^M(x_k,t) = -\Delta\psi^M(x,t)|_{x=x_k} + V(x) * \psi^M(x,t)|_{x=x_k} + g(|\psi^M(x_k,t)|^2)\psi^M(x_k,t)$$

and

$$\psi^M(x_k,0) = \psi(x_k,0)$$

for all $k \in \mathcal{N}_M$. Using the discrete orthogonality

$$\frac{1}{(2M)^d} \sum_{k\in\mathcal{N}_M} e^{-i(l\cdot x_k)} e^{i(j\cdot x_k)} = \begin{cases} 1, & j \equiv l \bmod 2M, \text{ i.e., } j-k=0 \text{ in } \mathcal{N}_M, \\ 0, & \text{else} \end{cases}$$

this can be rewritten in terms of the coefficients ξ_j of ψ^M as

$$i\frac{d}{dt}\xi_j(t) = \omega_j \xi_j(t) + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{\substack{j^1+\cdots+j^{m+1} \\ -j^{m+2}-\cdots-j^{2m+1}=j}} \xi_{j^1}(t)\cdots\xi_{j^{m+1}}(t)\overline{\xi_{j^{m+2}}(t)\cdots\xi_{j^{2m+1}}(t)} \tag{4.17}$$

for $j \in \mathcal{N}_M$. These equations are formally the same as for the spectral Galerkin method (4.15) but the condition $j^1 + \cdots + j^{m+1} - j^{m+2} - \cdots - j^{2m+1} = j$ in the nonlinearity is now computed with the addition in $\mathcal{N}_M$, i.e., modulo $2M$ in each entry. They are the Hamiltonian equations of motion of the Hamiltonian function

$$H^M(\xi,\eta) = \sum_{j\in\mathcal{N}_M} \omega_j \xi_j \eta_j + \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{\substack{j^1+\cdots+j^{m+1} \\ -j^{m+2}-\cdots-j^{2m+2}=0}} \xi_{j^1}\cdots\xi_{j^{m+1}}\eta_{j^{m+2}}\cdots\eta_{j^{2m+2}}, \tag{4.18}$$

where again the indices are summed up in $\mathcal{N}_M$ modulo $2M$. We can write the Hamiltonian equations of motion (4.17) in terms of ψ^M as

$$i\frac{\partial}{\partial t}\psi^M(x,t) = -\Delta\psi^M(x,t) + V(x) * \psi^M(x,t) + \mathcal{Q}(g(|\psi^M(x,t)|^2)\psi^M(x,t)) \tag{4.19a}$$

with the trigonometric interpolation

$$\mathcal{Q}\Big(\sum_{j\in\mathcal{N}} \varphi_j e^{i(j\cdot x)}\Big) = \sum_{j\in\mathcal{N}_M} \Big(\sum_{l\in\mathcal{N}:l\equiv j \bmod 2M} \varphi_l \Big) e^{i(j\cdot x)}.$$

This trigonometric interpolation is defined in such a way that $\mathcal{Q}(\varphi)(x_k) = \varphi(x_k)$ for all $k \in \mathcal{N}_M$ and hence the name. The initial value then satisfies

$$\psi^M(\cdot,0) = \mathcal{Q}(\psi(\cdot,0)). \tag{4.19b}$$

Verification of the Assumptions 2.1, 2.2, 2.3, 2.4, and 4.1. *The Assumptions 2.1, 2.2, 2.3, and 2.4 are satisfied under the same conditions and with constants depending on the same parameters (in particular independent of M) as for the continuous nonlinear Schrödinger equation with a potential of convolution type in Section 2.6. Assumption 4.1 is fulfilled with $C_4 = 1$.*

The coefficients $P^M_{j,k,l}$ of the discrete nonlinearity are given by (2.26) as in the continuous situation, but where the sum of indices is computed in $\mathcal{N}_M$, i.e.

$$P^M_{j,k,l} = \sum_{\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} P_{\tilde{j},k,l}.$$

In particular, we have using the Cauchy–Schwarz inequality

$$\begin{aligned}
&\| |P^M|^{m,m'}(\xi^1,\ldots,\xi^m,\eta^1,\ldots,\eta^{m'}) \|_s^2 \\
&\quad \le \sum_{j\in\mathcal{N}_M} |j|^{2s} \Big(\sum_{\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} |P|_{\tilde{j}}^{m,m'}(|\xi^1|,\ldots,|\xi^m|,|\eta^1|,\ldots,|\eta^{m'}|) \Big)^2 \\
&\quad \le \sum_{j\in\mathcal{N}_M} \Big(\sum_{\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} \frac{|j|^{2s}}{|\tilde{j}|^{2s}} \Big) \Big(\sum_{\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} |\tilde{j}|^{2s} |P|_{\tilde{j}}^{m,m'}(|\xi^1|,\ldots,|\xi^m|,|\eta^1|,\ldots,|\eta^{m'}|)^2 \Big) \\
&\quad \le \sup_{j\in\mathcal{N}_M} \Big(\sum_{\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} \frac{|j|^{2s}}{|\tilde{j}|^{2s}} \Big) \| |P|^{m,m'}(|\xi^1|,\ldots,|\xi^m|,|\eta^1|,\ldots,|\eta^{m'}|) \|_s^2.
\end{aligned}$$

The sum $\sum_{\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} \frac{|j|^{2s}}{|\tilde{j}|^{2s}}$ can be bounded for $s > \frac{d}{2}$ and $j \in \mathcal{N}_M$ (and hence $|j| \le \sqrt{d}M$) by a constant depending only on d and s using Lemma 4.10 below. In this way the regularity assumption 2.1 for P^M reduces to the one for P with constants depending on the same quantities.

The relation of the coefficients $P_{j,k,l}$ and $P_{j,k,l}^M$ also shows that the discrete nonlinearity P^M satisfies the condition of zero momentum in Assumption 2.2 (with the addition in $\mathcal{N}_M$). Since the discrete frequencies are the same as the frequencies in the continuous situation, the non-resonance condition 2.3 is also satisfied in the discrete situation, and the same is true for the additional non-resonance condition 2.4 in dimension one ($d = 1$). Assumption 4.1 is fulfilled since we have a natural embedding $\iota = \mathrm{id}$.

We finally give the proof of the lemma that we used in the above estimates.

Lemma 4.10. *We have for any* $j \in \mathcal{N}_M$ *and any* $s > \frac{d}{2}$

$$M^{2s} \sum_{j\neq\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} \frac{1}{|\tilde{j}|^{2s}} \le C$$

with a constant C *depending only on* d *and* s.

Proof. We have

$$M^{2s} \sum_{j\neq\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} \frac{1}{|\tilde{j}|^{2s}} \le \sum_{0\neq\tilde{j}\in\mathcal{N}} \frac{M^{2s}}{|j+2M\tilde{j}|_\infty^{2s}} \le \sum_{0\neq\tilde{j}\in\mathcal{N}} \frac{1}{(2|\tilde{j}|_\infty - 1)^{2s}} \le \sum_{0\neq\tilde{j}\in\mathcal{N}} \frac{d^s}{|\tilde{j}|^{2s}},$$

where $|\cdot|_\infty$ denotes the supremum norm in $\mathbb{R}^d$. The latter sum converges for $s > \frac{d}{2}$ as was shown in (1.9). □

The following corollary corresponds to Corollary 2.15 in the continuous situation. It was first proven in [29].

Corollary 4.11 (Long-Time Analysis of the Spectral Collocation Discretization of Nonlinear Schrödinger Equations (4.14))**.** *Under the assumptions of Corollary 2.15 with smallness of* $\psi^M(\cdot,0)$ *instead of* $\psi(\cdot,0)$ *we have*

- *near-conservation of discrete actions* (4.4) *and continuous actions* (4.5)*,*
- *exact conservation of discrete energy,*
- *near-conservation of continuous energy*

$$\frac{|H(\iota(\xi(t)),\overline{\iota(\xi(t))}) - H(\iota(\xi(0)),\overline{\iota(\xi(0))})|}{\varepsilon^2} \le CM^{-s}\varepsilon^2,$$

- *exact conservation of discrete and continuous mass,*
- *near-conservation of discrete momentum* (4.12) *and continuous momentum* (4.13)*,*
- *and regularity* (4.8) *and* (4.9)

over long times

$$0 \le t \le \varepsilon^{-N}$$

along any solution $\psi^M(x,t) = \sum_{j\in\mathcal{N}_M} \xi_j(t)e^{i(j\cdot x)}$ *of the semi-discrete nonlinear Schrödinger equation* (4.19) *in dimension* d *with a constant* C *depending on the same parameters as the constant of Corollary 2.15, but not on* ε *and the spatial discretization parameter* M*.*

The near-conservation of actions and momentum improves to $C\varepsilon$ *in dimension one* ($d = 1$)*.*

Proof. We can apply Theorem 4.2 and Corollary 4.4 to obtain long-time near-conservation of discrete and continuous actions and long-time regularity.

Both, the Hamiltonian function H^M for the spatial semi-discretization and the Hamiltonian function H of the nonlinear Schrödinger equation (4.14), are invariant under the transformation $\xi \mapsto e^{i\theta}\xi$. This implies exact conservation of discrete mass m^M along the semi-discrete solution. Since $\iota = \mathrm{id}$, we have $m^M(\xi,\overline{\xi}) = m(\iota(\xi),\iota(\overline{\xi}))$ and hence also exact conservation of continuous mass.

Note that the momentum K^M is not an exact invariant of the semi-discrete solution, whereas the momentum K is an exact invariant along the exact solution. This is due to the fact that H^M is not invariant under the transformations $\xi_j \mapsto e^{i\theta j_l}\xi_j$ for $l = 1,\dots,d$ anymore, since the summation of indices in its nonlinearity is done in $\mathcal{N}_M$, i.e., modulo $2M$. However, Corollary 2.11 ensures at least near-conservation of discrete and continuous momentum over long times along the semi-discrete solution.

In contrast to the situation in Section 4.4, where we studied a spectral Galerkin discretization, the discrete energy H^M is not the same as the energy H of the nonlinear Schrödinger equation. We thus cannot expect exact conservation of H along semi-discrete solutions, but a bound on the difference $H^M - H$ can help us to understand the long-time behaviour of H along the semi-discrete solution, see Section 4.3 (recall that H^M is exactly conserved by Proposition 1.1). We have

$$H^M(\xi,\overline{\xi}) - H(\iota(\xi),\overline{\iota(\xi)}) = \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{\substack{0\ne\tilde{j}\in\mathcal{N}:\\ \tilde{j}\equiv 0 \bmod 2M}} \sum_{\substack{j^1+\dots+j^{m+1}\\ -j^{m+2}-\dots-j^{2m+2}=\tilde{j}}} \xi_{j^1}\cdots\xi_{j^{m+1}}\overline{\xi_{j^{m+2}}\cdots\xi_{j^{2m+2}}},$$

where the indices belonging to $\mathcal{N}_M$ are now summed up with the addition in $\mathcal{N} = \mathbb{Z}^d$. Writing

$$P^m_{\tilde{j}} = \sum_{\substack{j^1+\cdots+j^{m+1}\\ -j^{m+2}-\cdots-j^{2m+2}=\tilde{j}}} \xi_{j^1}\cdots\xi_{j^{m+1}}\overline{\xi_{j^{m+2}}\cdots\xi_{j^{2m+2}}}$$

we get using the Cauchy–Schwarz inequality

$$\begin{aligned}|H^M(\xi,\overline{\xi}) - H(\iota(\xi),\overline{\iota(\xi)})| &\le \sum_{m=0}^{\infty}\frac{|g^{(m)}(0)|}{m!(m+1)} \sum_{\substack{0\neq\tilde{j}\in\mathcal{N}:\\ \tilde{j}\equiv 0 \bmod 2M}} |P^m_{\tilde{j}}| \\ &\le \sum_{m=0}^{\infty}\frac{|g^{(m)}(0)|}{m!(m+1)}\Big(\sum_{\substack{0\neq\tilde{j}\in\mathcal{N}:\\ \tilde{j}\equiv 0 \bmod 2M}} \frac{1}{|\tilde{j}|^{2s}}\Big)^{\frac12}\Big(\sum_{\substack{0\neq\tilde{j}\in\mathcal{N}:\\ \tilde{j}\equiv 0 \bmod 2M}} |\tilde{j}|^{2s}|P^m_{\tilde{j}}|^2\Big)^{\frac12}.\end{aligned}$$

By Lemma 4.10 we have $\sum_{0\neq\tilde{j}\in\mathcal{N}:\tilde{j}\equiv 0 \bmod 2M}\frac{1}{|\tilde{j}|^{2s}} \le CM^{-2s}$ with a constant C depending only on d and s. Using the arguments of Section 2.6 and $g(0)=0$ we then get

$$|H^M(\xi,\overline{\xi}) - H(\iota(\xi),\overline{\iota(\xi)})| \le CM^{-s}\|\xi\|_s^4$$

provided that $\|\xi\|_s$ is sufficiently small with a constant C depending only on g, d, and s. Combining this estimate with the long-time regularity and the exact conservation of H^M finally yields the long-time near-conservation of energy along the semi-discrete solution with a constant C independent of M,

$$|H(\iota(\xi(t)),\overline{\iota(\xi(t))}) - H(\iota(\xi(0)),\overline{\iota(\xi(0))})| \le CM^{-s}\varepsilon^4$$

for $0 \le t \le \varepsilon^{-N}$. □

For the actions we have proven the same kind of long-time near-conservation as for the exact solution in Corollary 2.15. For energy and momentum, which are exactly conserved along the exact solution, we have proven that they are at least almost conserved over long times.

Concerning the energy distribution for finite band initial values (2.22a), we get the same long-time behaviour along the solution of the spectral collocation method as for the exact solution in Corollary 2.16 and the spectral Galerkin method in Corollary 4.8.

Corollary 4.12 (Long-Time Energy Distribution (a) for the Spectral Collocation Discretization of Nonlinear Schrödinger Equations (4.14))**.** *Let* $0 < \mu \le 1$. *Under the assumptions of Corollary 2.15 and for small initial values*

$$\|\xi(0)\|_s \le \varepsilon \quad \textit{with } (2.22a)$$

we have for any ε*, such that* ε^μ *satisfies the smallness assumption of Corollary 2.15, the energy distribution*

$$\sum_{(2m-1)B<|l|\le(2m+1)B} |l|^{2s} I^M_l(\xi(t),\overline{\xi(t)}) \le C\varepsilon^{2(2m+1)(1-\mu)+\frac52\mu}$$

for $m \geq 1$ *over long times*

$$0 \leq t \leq \varepsilon^{-N\mu}$$

along any solution $\psi^M(x,t) = \sum_{j\in\mathcal{N}_M} \xi_j(t) e^{i(j\cdot x)}$ *of the semi-discrete nonlinear Schrödinger equation* (4.19) *in dimension* d *with the constant* C *of Corollary 4.11.*

The same energy distribution holds for the continuous actions $I_l(\iota(\xi(t)), \overline{\iota(\xi(t))})$*. The estimates improve by a factor* $\varepsilon^{\frac{1}{2}\mu}$ *in dimension one* ($d = 1$). □

Concerning the situation (2.22b) of an initial value with (only) a pair $\xi_{\tilde{j}}$ and $\xi_{-\tilde{j}}$ of initially excited modes, we get the following corollary. It differs from Corollaries 2.16 for the exact solution and 4.8 for the spectral Galerkin discretization since indices are added modulo $2M$ in the spectral collocation discretization. According to Corollary 2.14 we expect $\xi_l(t)$ to be nonzero for $l = m\tilde{j}$ with $m \in \mathbb{Z}$, where $m\tilde{j}$ is computed with the addition of $\mathcal{N}_M$, i.e., modulo $2M$ in each component. Hence, the energy will be distributed among all modes l that are multiples of $\tilde{j}$ modulo $2M$. This is an aliasing effect due to the aliasing formula, and we will see this effect also in the numerical experiments of Section 5.6 for the full discretization. We have the following result.

Corollary 4.13 (Long-Time Energy Distribution (b) for the Spectral Collocation Discretization of Nonlinear Schrödinger Equations (4.14))**.** *Let* $0 < \mu \leq 1$*. Under the assumptions of Corollary 2.15 and for small initial values*

$$\|\xi(0)\|_s \leq \varepsilon \quad \textit{with } (2.22\text{b})$$

we have for any ε*, such that* ε^μ *satisfies the smallness assumption of Corollary 2.15, the energy distribution*

$$|l|^{2s} I_l^M(\xi(t), \overline{\xi(t)}) \leq C\varepsilon^{2|m(l)|(1-\mu)+\frac{5}{2}\mu}$$

for $0, \pm\tilde{j} \neq l \in \{\, m\tilde{j} : m \in \mathbb{Z}$ *odd*$\}$*, where* $m\tilde{j} \in \mathcal{N}_M$ *is computed in* $\mathcal{N}_M$ *(i.e., modulo* $2M$*), over long times*

$$0 \leq t \leq \varepsilon^{-N\mu}$$

along any solution $\psi^M(x,t) = \sum_{j\in\mathcal{N}_M} \xi_j(t) e^{i(j\cdot x)}$ *of the semi-discrete nonlinear Schrödinger equation* (4.19) *in dimension* d *with the constant* C *of Corollary 4.11. If* $l \notin \{\, m\tilde{j} :$ $m \in \mathbb{Z}$ *odd*$\}$*, then* $\xi_l(t) = 0$ *for all times* t*.*

The same energy distribution holds for the continuous actions $I_l(\iota(\xi(t)), \overline{\iota(\xi(t))})$*. The estimates improve by a factor* $\varepsilon^{\frac{1}{2}\mu}$ *in dimension one* ($d = 1$). □

Again, the spectral collocation method can be applied also to Schrödinger–Poisson equations, see Sections 1.4 and 2.7, and Corollaries 4.11, 4.12, and 4.13 are also true for this method applied to these equations.

4.6 Example — A Spectral Collocation Method for Nonlinear Wave Equations

The nonlinear wave equation

$$\frac{\partial^2}{\partial t^2} u(x,t) = \Delta u(x,t) - \rho u(x,t) + g(u(x,t)) \tag{4.20}$$

in dimension one ($d = 1$) with periodic boundary conditions was studied in Sections 1.5 and 2.9, see equations (1.14) and (2.32). In this section we study a spatial semi-discretization of this equation with a spectral collocation method as for the nonlinear Schrödinger equation in Section 4.5.

The Spectral Collocation Method. As an ansatz for the solution of (4.20) we choose again a spectral representation

$$u^M(x,t) = \sum_{|j|\le M}{}' u_j(t)e^{i(j\cdot x)} \quad \text{and} \quad v^M(x,t) = \sum_{|j|\le M}{}' v_j(t)e^{i(j\cdot x)}$$

with a spatial discretization parameter M. The symbol $\sum'$ means that the first and the last summand are taken with a factor $\frac{1}{2}$. We require that this ansatz fulfills the nonlinear wave equation in the collocation points $x_k = k\frac{\pi}{M}$, $k \in \mathcal{N}_M$, where we choose again a full grid $\mathcal{N}_M = \{-M, \dots, M-1\}$ equipped with the addition modulo $2M$. This yields an ordinary differential equation

$$\frac{\partial^2}{\partial t^2}u^M(x_k,t) = \Delta u^M(x,t)|_{x=x_k} - \rho u^M(x_k,t) + g(u^M(x_k,t))$$

with initial values

$$u^M(x_k,0) = u(x_k,0) \quad \text{and} \quad v^M(x_k,0) = v(x_k,0)$$

for all $k \in \mathcal{N}_M$. Due to $e^{i(Mx_k)} = e^{i(-Mx_k)}$ these equations only determine $\frac{1}{2}(u_{-M} + u_M)$ and $\frac{1}{2}(v_{-M} + v_M)$, and we therefore require in addition

$$u_{-M}(t) = u_M(t) \quad \text{and} \quad v_{-M}(t) = v_M(t).$$

Using the trigonometric interpolation $\mathcal{Q}'$ defined similarly as in Section 4.5 we can rewrite the equations as

$$\frac{\partial^2}{\partial t^2}u^M(x,t) = \Delta u^M(x,t) - \rho u^M(x,t) + \mathcal{Q}'(g(u^M(x,t))) \tag{4.21a}$$

with initial values

$$u^M(\cdot,0) = \mathcal{Q}'(u(\cdot,0)) \quad \text{and} \quad v^M(\cdot,0) = \mathcal{Q}'(v(\cdot,0)), \tag{4.21b}$$

where now

$$\mathcal{Q}'\Big(\sum_{j\in\mathcal{N}=\mathbb{Z}^d} \varphi_j e^{i(j\cdot x)}\Big) = \sum_{|j|\le M}{}'\Big(\sum_{l\in\mathcal{N}:l\equiv j \bmod 2M} \varphi_l\Big)e^{i(j\cdot x)}.$$

This is the spectral collocation method applied to the nonlinear wave equation. The primes ensure that for real initial values $u(\cdot,0)$ and $v(\cdot,0)$ as considered in Section 1.5 the initial values $u^M(\cdot,0)$ and $v^M(\cdot,0)$ for the spectral collocation method are also real-valued leading to real-valued solutions u^M and v^M.

In order to establish the Hamiltonian structure of the equation (4.21) we introduce as in Section 1.5 variables

$$\xi_j = \frac{\omega_j^{\frac{1}{2}} u_j + i\omega_j^{-\frac{1}{2}} v_j}{\sqrt{2}}$$

for $j \in \mathcal{N}_M$. The embedding $\iota : l_0^2(\mathbb{C}^{\mathcal{N}_M}) \to l_0^2(\mathbb{C}^{\mathcal{N}})$ is thus not the natural embedding but

$$\iota(\xi)_j = \begin{cases} \xi_j, & |j| < M, \\ \frac{1}{2}\xi_{-M}, & |j| = M, \\ 0, & |j| > M. \end{cases}$$

Assuming real-valued solutions $u^M(x,t)$ we can rewrite (4.21a) as in Section 1.5 in terms of ξ as

$$i\frac{d}{dt}\xi_j(t) = \omega_j\xi_j(t) - \frac{1}{\sqrt{2\omega_j}} \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{j^1+\cdots+j^m=j} \frac{\xi_{j^1} + \overline{\xi_{-j^1}}}{\sqrt{2\omega_{j^1}}} \cdots \frac{\xi_{j^m} + \overline{\xi_{-j^m}}}{\sqrt{2\omega_{j^m}}}, \tag{4.22}$$

where the summation of indices from $\mathcal{N}_M$ is in $\mathcal{N}_M$, i.e., modulo $2M$, and we use the convention $\xi_M = \xi_{-M}$. Hence, the semi-discrete nonlinear wave equation (4.21) is a Hamiltonian ordinary differential equation with Hamiltonian function

$$H^M(\xi,\eta) = \sum_{j\in\mathcal{N}_M} \omega_j\xi_j\eta_j - \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{j^1+\cdots+j^{m+1}=0} \frac{\xi_{j^1} + \eta_{-j^1}}{\sqrt{2\omega_{j^1}}} \cdots \frac{\xi_{j^{m+1}} + \eta_{-j^{m+1}}}{\sqrt{2\omega_{j^{m+1}}}}$$

with summation again in $\mathcal{N}_M$ and the convention $\eta_M = \eta_{-M}$.

Verification of the Assumptions 2.1, 2.2, 2.4, 2.6, and 4.1. *The Assumptions 2.1, 2.2, 2.4, and 2.6 are satisfied under the same conditions and with constants depending on the same parameters (in particular independent of M) as for the continuous nonlinear wave equation in Section 2.9. Assumption 4.1 is fulfilled with $C_4 = 1$.*

The Assumptions 2.1, 2.2, 2.4, and 2.6 follow from the corresponding assumptions for the continuous situation in the same way as in Section 4.5 for the spectral collocation method applied to the nonlinear Schrödinger equation. Concerning Assumption 4.1, we note that

$$I_j(\iota(\xi), \overline{\iota(\xi)}) = \begin{cases} I_j^M(\xi,\overline{\xi}), & |j| < M, \\ \frac{1}{4} I_{-M}^M(\xi,\overline{\xi}), & |j| = M, \\ 0, & |j| > M \end{cases}$$

due to the definition of ι. This implies that Assumption 4.1 is fulfilled with $c_m = 1$ for $m < M$ and $c_M = \frac{1}{2}$.

We get the following corollary stating long-time near-conservation of actions, energy, mass, and momentum along semi-discrete solutions. Such a result can also be found in [34], where slightly better estimates for energy and momentum are proven (with additional factors M^{-1} and M^{-2} by exploiting the frequencies in the denominator of the nonlinearity of the nonlinear wave equation). The proof of the near-conservation of energy and momentum, that we present here, is the same as in [34].

Corollary 4.14 (Long-Time Analysis of the Spectral Collocation Discretization of Nonlinear Wave Equations (4.20))**.** *Under the assumptions of Corollary 2.20 we have*

- *near-conservation of sums of discrete actions* (4.6) *and continuous actions* (4.7) *with* $C\varepsilon$ *instead of* $C\varepsilon^{\frac{1}{2}}$*,*
- *exact conservation of discrete energy,*
- *near-conservation of continuous energy*

$$\frac{|H(\iota(\xi(t)),\overline{\iota(\xi(t))}) - H(\iota(\xi(0)),\overline{\iota(\xi(0))})|}{\varepsilon^2} \leq CM^{-s}\varepsilon,$$

- *near-conservation of discrete mass* (4.10) *and continuous mass* (4.11) *with* $C\varepsilon$ *instead of* $C\varepsilon^{\frac{1}{2}}$*,*
- *near-conservation of continuous momentum*

$$\frac{|K(\iota(\xi(t)),\overline{\iota(\xi(t))}) - K(\iota(\xi(0)),\overline{\iota(\xi(0))})|}{\varepsilon^2} \leq CM^{-s+1}\varepsilon t,$$

- *and regularity* (4.8) *and* (4.9)

over long times

$$0 \leq t \leq \varepsilon^{-N}$$

along any solution $u^M(x,t) = \sum'_{|j|\leq M} u_j(t)e^{i(j\cdot x)}$ *and* $v^M(x,t) = \sum'_{|j|\leq M} v_j(t)e^{i(j\cdot x)}$ *with* $\xi_j = (\omega_j^{\frac{1}{2}}u_j + i\omega_j^{-\frac{1}{2}}v_j)/\sqrt{2}$ *for* $j \in \mathcal{N}_M$ *of the semi-discrete nonlinear wave equation* (4.21) *with a constant* C *depending on the same parameters as the constant of Corollary 2.20, but not on* ε *and the spatial discretization parameter* M*.*

Proof. Long-time near-conservation of sums of discrete and continuous actions is ensured by Theorem 4.3. Corollaries 4.4 and 4.5 imply regularity and long-time near-conservation of discrete and continuous mass.

Exact conservation of discrete energy H^M is ensured by Proposition 1.1. The near-conservation of continuous energy H can be shown similarly as in the proof of Corollary 4.11 in Section 4.5 for the spectral collocation method applied to the nonlinear Schrödinger equation. However, the difference $H^M(\xi,\overline{\xi}) - H(\iota(\xi),\overline{\iota(\xi)})$ not only contains a nonlinear term as in this proof but also a term

$$\sum_{j\in\mathcal{N}_M} \omega_j I_j^M(\xi,\overline{\xi}) - \sum_{j\in\mathcal{N}} \omega_j I_j(\iota(\xi),\overline{\iota(\xi)}) = \frac{1}{2}\omega_M I_{-M}^M(\xi,\overline{\xi})$$

due to the difference of discrete and continuous actions. By the long-time near-conservation of sums of discrete actions (4.6) we have

$$\left|\omega_M I_{-M}^M(\xi(t),\overline{\xi(t)}) - \omega_M I_{-M}^M(\xi(0),\overline{\xi(0)})\right| \leq CM^{-2s+1}\varepsilon^3$$

for $0 \leq t \leq \varepsilon^{-N}$. The nonlinearity in the difference can be estimated similar as in the proof mentioned above, and we get long-time near-conservation of energy as stated in the corollary.

The momentum is not an exact invariant of the semi-discrete solution since the summation of indices in the Hamiltonian function H^M is modulo $2M$. In order to prove at least its near-conservation we cannot apply Corollary 4.6 due to the resonances in the nonlinear wave equation. We proceed as in [34, Section 6] choosing $\widetilde{\xi}$ as a solution of the Hamiltonian equations of motion of (4.1) for the exact solution with initial value $\iota(\xi(0))$. Along $\widetilde{\xi}(t)$ the momentum K is exactly conserved by Corollary 2.20. Since $\|\iota(\xi)\|_s \le \|\xi\|_s \le \varepsilon$, we have by (3.14)

$$\|\widetilde{\xi}(t)\|_s \le C\varepsilon \quad \text{and} \quad \|\iota(\xi(t))\|_s \le \|\xi(t)\|_s \le C\varepsilon \tag{4.23}$$

for $0 \le t \le c_0\varepsilon^{-1}$ with constants c_0 and C depending only on g, ρ, and s. The equations of motion for $\widetilde{\xi}$ take the form

$$i\frac{d}{dt}\widetilde{\xi}_j = \omega_j\widetilde{\xi}_j + \frac{\partial P}{\partial \eta_j}(\widetilde{\xi}, \overline{\widetilde{\xi}}).$$

For semi-discrete solution $\xi(t)$ we have

$$\begin{aligned} i\frac{d}{dt}\iota(\xi)_j &= \omega_j\iota(\xi)_j + \iota(\nabla_\eta P^M(\xi, \overline{\xi}))_j \\ &= \omega_j\iota(\xi)_j + \frac{\partial P}{\partial \eta_j}(\iota(\xi), \overline{\iota(\xi)}) + \iota(\kappa(\nabla_\eta P(\iota(\xi), \overline{\iota(\xi)})))_j - (\nabla_\eta P(\iota(\xi), \overline{\iota(\xi)}))_j \end{aligned}$$

with $\kappa : l_0^2(\mathbb{C}^{\mathcal{N}}) \to l_0^2(\mathbb{C}^{\mathcal{N}_M})$ defined by

$$\kappa(\xi)_j = \sum_{l\in\mathcal{N}:l\equiv j \bmod 2M} \xi_l$$

for $j \in \mathcal{N}$. This is similar to the trigonometric interpolation $\mathcal{Q}'$. Proceeding as in the proof of Theorem 3.7 and using the smallness of $\widetilde{\xi}$ and $\iota(\xi)$ (4.23), we get for $\frac{1}{2} < s' \le s$ and $0 \le t \le \varepsilon^{-1}$

$$\|\widetilde{\xi} - \iota(\xi)\|_{s'} \le C\varepsilon \int_0^t \|\widetilde{\xi}(\theta) - \iota(\xi(\theta))\|_{s'}\, d\theta + t \sup_{0\le\theta\le t} \|\eta(\theta) - \iota(\kappa(\eta(\theta)))\|_{s'} \tag{4.24}$$

with $\eta = \nabla_\eta P(\iota(\xi), \overline{\iota(\xi)})$. We now estimate $\eta - \iota(\kappa(\eta))$ which is just the error of the trigonometric interpolation $\mathcal{Q}'$. This can be estimated following [34, Lemma 4.2]. The Cauchy–Schwarz inequality implies

$$\begin{aligned} \|\eta - \iota(\kappa(\eta))\|_{s'} &\le \Big(\sum_{|j|\ge M} |j|^{2s'}|\eta_j|^2\Big)^{\frac{1}{2}} + \Big(\sum_{|j|\le M} |j|^{2s'}\Big(\sum_{j\ne\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} |\eta_{\tilde{j}}|\Big)^2\Big)^{\frac{1}{2}} \\ &\le CM^{-(s-s')}\|\eta\|_s + \Big(\sum_{|j|\le M} CM^{-2(s-s')}\Big(\sum_{j\ne\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} |\tilde{j}|^{2s}|\eta_{\tilde{j}}|^2\Big)\Big)^{\frac{1}{2}} \end{aligned}$$

with $CM^{-2(s-s')} \ge \sum_{j\ne\tilde{j}\in\mathcal{N}:\tilde{j}\equiv j \bmod 2M} \frac{|j|^{2s'}}{|\tilde{j}|^{2s}}$ by Lemma 4.10 with a constant C depending only on d, ρ, s', and s. This implies $\|\eta - \iota(\kappa(\eta))\|_{s'} \le CM^{-(s-s')}\|\eta\|_s$ with a constant depending only on d, ρ, s', and s. Using (2.7) and (4.23) for $\eta = \nabla_\eta P(\iota(\xi), \overline{\iota(\xi)})$ we get

$$\|\eta - \iota(\kappa(\eta))\|_{s'} \le CM^{-(s-s')}\varepsilon^2$$

on $0 \le t \le c_0\varepsilon^{-1}$ with a constant depending in addition on $C_{s'}$. Using this estimate in (4.24), the Gronwall inequality implies for $0 \le t \le c_0\varepsilon^{-1}$

$$\|\widetilde{\xi}(t) - \iota(\xi(t))\|_{s'} \le CM^{-(s-s')}\varepsilon^2 t.$$

This finally yields using the Cauchy–Schwarz inequality

$$|K(\widetilde{\xi}(t), \overline{\widetilde{\xi}(t)}) - K(\iota(\xi(t)), \overline{\iota(\xi(t))})| \le \|\widetilde{\xi}(t) - \iota(\xi(t))\|_1 (\|\widetilde{\xi}(t)\|_0 + \|\iota(\xi(t))\|_0) \le CM^{-(s-1)}\varepsilon^3 t$$

for $0 \le t \le c_0\varepsilon^{-1}$. The exact conservation of the momentum K along $\widetilde{\xi}$ finally yields the short-time estimate

$$|K(\iota(\xi(t)), \overline{\iota(\xi(t))}) - K(\iota(\xi(0)), \overline{\iota(\xi(0))})| \le CM^{-(s-1)}\varepsilon^3 t, \tag{4.25}$$

which is valid for $0 \le t \le c_0\varepsilon^{-1}$. We repeat this procedure on $c_0\varepsilon^{-1} \le t \le 2c_0\varepsilon^{-2}$ with initial value $\iota(\xi(c_0\varepsilon^{-1}))$ for $\widetilde{\xi}(t)$, on $2c_0\varepsilon^{-1} \le t \le 3c_0\varepsilon^{-2}$ with initial value $\iota(\xi(2c_0\varepsilon^{-1}))$, and so on. The long-time regularity of $\iota(\xi(t))$ ensures that all the initial values satisfy the smallness condition $\|\iota(\xi(nc_0\varepsilon^{-1}))\|_s \le 2\varepsilon$ for $0 \le nc_0\varepsilon^{-1} \le \varepsilon^{-N}$, and (4.25) is valid on this time interval with constants independent of the particular time interval. Putting together the time intervals proves the long-time near-conservation of momentum as stated in the corollary. □

As for the exact solution we can study the problem of energy distribution along solutions of the semi-discrete equations (4.21). From Corollaries 2.13 and 2.14 we get the following results.

Corollary 4.15 (Long-Time Energy Distribution (a) for the Spectral Collocation Discretization of Nonlinear Wave Equations (4.20))**.** *Let* $0 < \mu \le 1$. *Under the assumptions of Corollary 2.20 and for small initial values*

$$\|\xi(0)\|_s \le \varepsilon \quad \textit{with } (2.22\text{a})$$

we have for any ε, *such that* ε^μ *satisfies the smallness assumption of Corollary 2.20, the energy distribution*

$$\sum_{(m-1)B<|l|\le mB} |l|^{2s} I_l^M(\xi(t), \overline{\xi(t)}) \le C\varepsilon^{2m(1-\mu)+3\mu}$$

for $m \ge 2$ *over long times*

$$0 \le t \le \varepsilon^{-N\mu}$$

with the constant C *of Corollary 4.14.*

The same energy distribution holds for the continuous actions $I_l(\iota(\xi(t)), \overline{\iota(\xi(t))})$. □

Corollary 4.16 (Long-Time Energy Distribution (b) for the Spectral Collocation Discretization of Nonlinear Wave Equations (4.20))**.** *Let* $0 < \mu \le 1$. *Under the assumptions of Corollary 2.20 and for small initial values*

$$\|\xi(0)\|_s \le \varepsilon \quad \textit{with } (2.22\text{b})$$

we have for any ε, such that ε^{μ} satisfies the smallness assumption of Corollary 2.20, the energy distribution

$$I_0^M(\xi(t),\overline{\xi(t)}) \le C\varepsilon^{4(1-\mu)+3\mu},$$
$$|l|^{2s} I_l^M(\xi(t),\overline{\xi(t)}) \le C\varepsilon^{2|m(l)|(1-\mu)+3\mu}$$

for $0,\pm\tilde{j} \neq l \in \{\, m\tilde{j} : m \in \mathbb{Z}\,\}$, where $m\tilde{j} \in \mathcal{N}_M$ is computed in $\mathcal{N}_M$ (i.e., modulo $2M$), over long times

$$0 \le t \le \varepsilon^{-N\mu}$$

with the constant C of Corollary 4.14. If $l \notin \{\, m\tilde{j} : m \in \mathbb{Z}\,\}$, then $\xi_l(t) = 0$ for all times t.

The same energy distribution holds for the continuous actions $I_l(\iota(\xi(t)),\overline{\iota(\xi(t))})$. □

In the latter corollary we observe again aliasing effects as for the spectral collocation method applied to the nonlinear Schrödinger equation in Section 4.5.

5 Long-Time Analysis of Full Discretizations of Hamiltonian Partial Differential Equations

In this chapter we transfer the results from Chapters 2 and 4 on exact and spatially discrete solutions of Hamiltonian partial differential equations to full discretizations (see the last column in Figure 1).

5.1 Full Discretizations of Hamiltonian Partial Differential Equations

In Chapter 4 we considered spatial semi-discretizations of Hamiltonian partial differential equations with Hamiltonian function

$$H(\xi,\eta) = \sum_{j\in\mathcal{N}} \omega_j \xi_j \eta_j + P(\xi,\eta) \tag{5.1}$$

in a weakly nonlinear setting with real frequencies ω_j, $j \in \mathcal{N}$, where P is a function with a zero of order (at least) three at the origin and with $\overline{P(\xi,\eta)} = P(\overline{\eta},\overline{\xi})$. The studied spatial semi-discretization was a (finite dimensional) Hamiltonian system with Hamiltonian function of the form

$$H^M(\xi,\eta) = \sum_{j\in\mathcal{N}_M} \omega_j^M \xi_j \eta_j + P^M(\xi,\eta), \tag{5.2}$$

where M denotes the spatial discretization parameter. The embedding $\iota : l_0^2(\mathbb{C}^{\mathcal{N}_M}) \to l_0^2(\mathbb{C}^{\mathcal{N}})$ is used to relate the finite dimensional phase space of the semi-discrete Hamiltonian function with the phase space of the continuous Hamiltonian function. In this chapter we finally discretize this ordinary differential equation in time.

Splitting Integrators. For a full discretization of the Hamiltonian equations of motion of (5.1) we use a *splitting integrator* (*split-step method*) for the time discretization of the spatially discrete Hamiltonian equations of motion of (5.2), see for example [36, Chapter II.5]. The idea of such a discretization is to split the Hamiltonian function (5.2) into two Hamiltonian functions

$$H_0^{M,h}(\xi,\eta) = \sum_{j\in\mathcal{N}_M} \omega_j^{M,h} \xi_j \eta_j \quad \text{and} \quad P^{M,h}(\xi,\eta),$$

which are related to $\sum_{j\in\mathcal{N}_M} \omega_j^M \xi_j\eta_j$ and $P^M(\xi,\eta)$, and solving their Hamiltonian equations of motion

$$i\frac{d}{dt}\xi_j(t) = \frac{\partial H_0^{M,h}}{\partial \eta_j}(\xi(t),\overline{\xi(t)}) = \omega_j^{M,h}\xi_j(t) \tag{5.3a}$$

and

$$i\frac{d}{dt}\xi_j(t) = \frac{\partial P^{M,h}}{\partial \eta_j}(\xi(t), \overline{\xi(t)}) \tag{5.3b}$$

one after another over short times h (or $\frac{h}{2}$, ...). The benefit is that these equations are often easy to solve: The first equation (5.3a) is a decoupled linear equation, and in all our applications the second equation (5.3b) is also easy to solve, see Sections 5.6 and 5.7.

The function $P^{M,h}$ is assumed to be a Hamiltonian function such that (5.3b) are Hamiltonian equations of motion. Often $\omega_j^{M,h} = \omega_j$ and $P^{M,h} = P^M$ are independent of the time step-size h as in Section 5.6 for the nonlinear Schrödinger equation and also in Section 5.7 for the nonlinear wave equation. However, they may depend on h (and are not the same as in the semi-discretization) for instance due to a filter function as in Section 5.7 for the mollified impulse method applied to the nonlinear wave equation. Here and in the following, we omit the indices M and h of the frequencies $\omega_j^{M,h}$ and write again ω_j.

Examples of Splitting Integrators. For the (first order) *Lie–Trotter splitting* we perform first a time step h with the flow of the equation (5.3b), and take the result as an initial value for a time step h with the flow of the equation (5.3a). Denoting by $\Phi_t^{H_0}$ and Φ_t^P the flows of the Hamiltonian equations of motion (5.3a) and (5.3b), respectively, i.e., $\xi(h) = \Phi_h^{H_0}(\xi^0)$ if $\xi(t)$ is a solution of (5.3a) with initial value ξ^0 and similar for P, the Lie–Trotter splitting reads

$$\xi^{n+1} = \Phi_h^{H_0} \circ \Phi_h^P(\xi^n) \quad \text{for } n = 0, 1, 2, \dots \tag{5.4}$$

with given initial value ξ^0. ξ^n is supposed to approximate the exact solution $\xi(t_n)$ at time $t_n = nh$.

The symmetric (second order) variant of the Lie–Trotter splitting is the *Strang splitting* which reads

$$\xi^{n+1} = \Phi_{h/2}^P \circ \Phi_h^{H_0} \circ \Phi_{h/2}^P(\xi^n) \quad \text{for } n = 0, 1, 2, \dots. \tag{5.5}$$

Of course, in an implementation of a sequence of time steps of the Strang splitting (5.5) we use that

$$\xi^n = \Phi_{h/2}^P \circ \left(\Phi_h^{H_0} \circ \Phi_h^P\right)^n \circ \Phi_{-h/2}^P(\xi^0). \tag{5.6}$$

For more informations on splitting integrators we refer to [36, Chapter II.5].

Problem Setting. In Chapters 2 and 4 we studied the long-time behaviour of the exact solution of (5.1) and its spatial semi-discretization (5.2). We have shown that under suitable assumptions the actions are nearly conserved along both, the exact as well as the semi-discrete solution, on a remarkably long time interval. This enabled us to study conserved quantities of the exact solution, such as energy, mass, and momentum, along the semi-discrete solution. Indeed, they are (at least) nearly conserved on a long time interval.

In this chapter we investigate the long-time behaviour of a fully discrete solution of the Hamiltonian partial differential equation with Hamiltonian function (5.1). More precisely, we study exact invariants (such as energy) and almost invariants (such as actions) of the exact solution along the fully discrete solution. Our aim is to prove that the behaviour of the exact solution is well reproduced by the numerical solution. In particular, we want to show that all these quantities are at least nearly conserved on a long time interval similar as we did for the semi-discretization in space.

In principle, the backward error analysis arguments of [36, Chapters IX and X] could be applied to the time discretization of the finite dimensional Hamiltonian system (5.2) from the semi-discretization in space. However, the constants then would depend on the spatial discretization parameter M whereas we seek for results that are independent of M as in Chapter 4. Moreover, backward error analysis requires $h\omega_{\max}$ to be very small, where $\omega_{\max}$ denotes the largest frequency of the semi-discretized system, see [36, Chapters IX and XIII] and [32]. We would like to avoid such a severe step-size restriction.

5.2 Long-Time Near-Conservation of Actions

Near-conservation of actions turned out to be a good starting point for the long-time analysis of the exact and the spatially discrete solution of a Hamiltonian partial differential equation. In this section we formulate a corresponding result for the fully discrete solution of such a partial differential equation. We recover the long-time near-conservation of actions along the exact and the spatially discrete solution also along the fully discrete solution. This is done under suitable assumptions which are formulated next.

In order to study the numerical solution over long times we need a regularity assumption on the flow of the nonlinearity $P^{M,h}$. This is different to the continuous situation where the regularity assumption 2.1 was imposed on the nonlinearity itself. This is due to the modulated Fourier expansion of the numerical solution that we will study in Chapter 6. There, we use the numerical solution itself (and in particular for the splitting integrators (5.4) and (5.5) the flow of $P^{M,h}$) for the derivation of the modulation system for the modulated Fourier expansion, whereas we used in Chapter 3 the differential equation determining the exact solution (and not the exact solution itself) in order to determine the modulation system.

Assumption 5.1 (Regularity Assumption on the Flow of $P^{M,h}$)**.** We denote by $\xi(t)$ the solution of (5.3b) with initial value ξ^0 and assume that there exists an expansion

$$\begin{aligned} \Phi_t^P(\xi^0)_j = \xi_j(t) &= \sum_{\ell=0}^{\infty} \frac{t^\ell}{\ell!} \frac{d^\ell}{dt^\ell} \xi_j(0) \\ &= \xi_j^0 + \sum_{m+m'=2}^{\infty} \sum_{k\in\mathcal{N}_M^m,\, l\in\mathcal{N}_M^{m'}} t\widehat{P}_{j,k,l} \xi_{k^1}^0 \cdots \xi_{k^m}^0 \overline{\xi_{l^1}^0 \cdots \xi_{l^{m'}}^0} \end{aligned} \tag{5.7}$$

of the flow Φ_t^P of the nonlinearity $P^{M,h}$ with coefficients $\widehat{P}_{j,k,l} = \widehat{P}_{j,k,l}(t)$ depending on t. This expansion is obtained formally by differentiating the equations of motion (5.3b) which are assumed to be of the form

$$i\frac{d}{dt}\xi_j(t) = \sum_{m+m'=2}^{\infty} \sum_{k\in\mathcal{N}_M^m,\, l\in\mathcal{N}_M^{m'}} P_{j,k,l}\xi_{k^1}(t)\cdots\xi_{k^m}(t)\overline{\xi_{l^1}(t)\cdots\xi_{l^{m'}}(t)} \tag{5.8}$$

similar to (2.4) in Assumption 2.1. The coefficients $\widehat{P}_{j,k,l}$ are hence sums of products of the coefficients $P_{j,k,l}$ multiplied with $(-it)^\ell/l!$.

We assume that the expansion (5.7) indeed converges by requiring regularity as in Assumption 2.1, estimate (2.6), of

$$|\widehat{P}|_j^{m,m'}(\xi^1,\dots,\xi^m,\eta^1,\dots,\eta^{m'}) = \sum_{k\in\mathcal{N}_M^m,\, l\in\mathcal{N}_M^{m'}} |\widehat{P}_{j,k,l}|\xi_{k^1}^1\cdots\xi_{k^m}^m\eta_{l^1}^1\cdots\eta_{l^{m'}}^{m'}$$

for $t\le 1$ with constants $C_{m,m',s}$, $C_{L,s}$, C_s, and C_1 independent of ε, M, h, and t.

The regularity of the flow of $P^{M,h}$ as required in Assumption 5.1 is usually implied by the regularity assumption 2.1 for the nonlinearity P as we will see in our examples in Sections 5.6 and 5.7.

In the continuous situation of Chapter 2 we imposed in Assumption 2.2 alternatively a condition of small dimension (2.9a) or of zero momentum (2.9b). In the fully discrete situation we necessarily need in our proofs the condition of zero momentum and therefore leave the condition of small dimension aside.

Assumption 5.2 (Condition of Zero Momentum)**.** We assume that the frequencies $\omega_j = \omega_j^{M,h}$ grow like a power of $|j|$, i.e., there exist positive constants c_2, C_2, and σ such that

$$c_2|j|^\sigma \le |\omega_j| \le C_2|j|^\sigma \quad \text{for all } j\in\mathcal{N}_M.$$

Moreover, we assume that

$$\widehat{P}_{j,k,l}\neq 0 \text{ implies } j = k^1+\cdots+k^m-l^1-\cdots-l^{m'}$$

for $j\in\mathcal{N}_M$, $k\in\mathcal{N}_M^m$, and $l\in\mathcal{N}_M^{m'}$. In the latter assumption the addition $+$ of indices is not necessarily the addition in $\mathbb{Z}^d$. Any addition such that the triangle inequality for $|\cdot|$ is fulfilled can be considered.

The derivation of the coefficients $\widehat{P}_{j,k,l}$ from the coefficients $P_{j,k,l}$ in Assumption 5.1 shows that this zero momentum condition is implied by the zero momentum condition

$$P_{j,k,l}\neq 0 \text{ implies } j = k^1+\cdots+k^m-l^1-\cdots-l^{m'}$$

for $j\in\mathcal{N}$, $k\in\mathcal{N}^m$, and $l\in\mathcal{N}^{m'}$ on the coefficients $P_{j,k,l}$ of $P^{M,h}$ in (5.8), which we imposed on the nonlinearity $\frac{\partial P}{\partial\eta_j}$ in Assumption 2.2 for the exact solution.

As in the continuous situation we need a non-resonance condition on the (discrete) frequencies $\omega_j=\omega_j^{M,h}$, $j\in\mathcal{N}_M$. This non-resonance condition, however, also includes the time step-size h, a parameter of the discretization, suggesting the possibility of numerical resonances. We will discuss this topic and also the validity of the non-resonance condition in Section 5.3.

Assumption 5.3 (Non-Resonance Condition)**.** Let $\varepsilon \leq \varepsilon_0$ for fixed $\varepsilon_0 \leq 1$. We define an *(ε-)near-resonant* index $(j, \mathbf{k})$ as an index with

$$j = j(\mathbf{k}), \quad \|\mathbf{k}\| \leq 2N + 4 + 4s_0, \quad \mathbf{k} \neq \langle j \rangle, \quad \text{and} \quad \frac{|e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1|}{h} < \varepsilon^{\frac{1}{2}},$$

where again $\langle j \rangle = (\delta_{jl})_{l \in \mathcal{N}_M}$ with Kronecker's delta. For given N and $s \geq s_0$ from the regularity assumption 5.1 we impose the non-resonance condition

$$\frac{|j|^{s-s_0}}{\mathbf{j}^{(s-s_0)|\mathbf{k}|}} \varepsilon^{\frac{1}{2}\|\mathbf{k}\|} \leq C_0 \varepsilon^{N+3+2s_0} \quad \text{for any } (\varepsilon\text{-})\text{near-resonant index } (j, \mathbf{k}) \tag{5.9a}$$

and the non-resonance condition

$$\frac{\sum_{l \in \mathcal{N}_M} |k_l| |l|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|} |j|^{2s_0}} \leq C_0 \varepsilon^N \quad \text{for any } (\varepsilon\text{-})\text{near-resonant index } (j, \mathbf{k}) \tag{5.9b}$$

for any $\varepsilon \leq \varepsilon_0 \leq 1$ on the frequencies ω_l, $l \in \mathcal{N}_M$, with a constant C_0 independent of ε, M, h, and $(j, \mathbf{k})$.

A non-resonance condition of the form (5.9a) was also used in the continuous situation in Assumption 2.3. A non-resonance condition (5.9b) was not needed there but turns out to be closely related to (5.9a). We will show in Section 5.3 that it is indeed fulfilled in many situations.

Under these assumptions we have the following theorem. It states that we have long-time near-conservation of actions as in Theorem 2.5 not only for the exact solution of the Hamiltonian equations of motion but also for the fully discrete schemes (5.4) and (5.5). As in the semi-discrete situation of Section 4.2 we distinguish between discrete actions I_j^M related to the semi-discrete Hamiltonian function H^M (5.2) and the continuous actions I_j related to the underlying continuous Hamiltonian function H (5.1).

Theorem 5.4 (Long-Time Near-Conservation of Actions)**.** *Fix N and let the regularity assumption 5.1, the condition of zero momentum 5.2, and the non-resonance condition 5.3 be satisfied. Then for any ε sufficiently small compared to C_1, C_{s_0}, C_s, and $s \geq 2s_0$ from 5.1, c_2, C_2, and σ from 5.2, C_0 and ε_0 from 5.3, and N and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon$$

we have near-conservation of discrete actions

$$\sum_{l \in \mathcal{N}_M} |l|^{2s} \frac{|I_l^M(\xi^n, \overline{\xi^n}) - I_l^M(\xi^0, \overline{\xi^0})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{5.10}$$

over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N}$$

along any numerical solution ξ^n of the Hamiltonian equations of motion defined by the Lie–Trotter splitting (5.4) *or the Strang splitting* (5.5) *with a constant C depending only* *on C_1, C_{s_0}, C_s, s_0, s, c_2, C_2, σ, C_0, and N, but not on ε, the spatial discretization parameter M, and the time step-size $h \le 1$.*

If in addition Assumption 4.1 is satisfied, we also have near-conservation of continuous actions

$$\sum_{l\in\mathcal{N}} |l|^{2s} \frac{|I_l(\iota(\xi^n),\overline{\iota(\xi^n)}) - I_l(\iota(\xi^0),\overline{\iota(\xi^0)})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{5.11}$$

over long times

$$0 \le t_n = nh \le \varepsilon^{-N}$$

with a constant C depending in addition on C_4.

The proof of this theorem will be given in Chapter 6 following the proof of Theorem 2.5 in Chapter 3. Similar results have been obtained recently and independently by Faou, Grébert, and Paturel [25] and [26] with a different proof based on normal form theory.

In the same way as for the exact solution in Section 2.2, we can handle the case of partially resonant frequencies, which occur for instance in the nonlinear wave equation with periodic boundary conditions, see Sections 1.5 and 2.9, if we replace the non-resonance condition 5.3 by the following condition.

Assumption 5.5 (Non-Resonance Condition in the Presence of Completely Resonant Frequencies)**.** The non-resonance conditions (5.9a) and (5.9b) are fulfilled for any near-resonant index $(j,\mathbf{k})$ such that $\mathbf{k} - \langle j\rangle$ does not belong to the resonance module

$$\mathcal{M} = \{\, \mathbf{k} \in \mathbb{Z}^{\mathcal{N}_M} : \mathbf{k}\cdot\boldsymbol{\omega} = 0 \,\}.$$

This resonance module is assumed to fulfill

$$\text{if } \mathbf{k}\in\mathcal{M}, \text{ then } \sum_{j\in\mathcal{N}_M : |j|=m} k_j = \sum_{j\in\mathcal{N}_M : |j|=m} k_j\omega_j = 0.$$

Theorem 5.6 (Long-Time Near-Conservation of Sums of Actions)**.** *Under the assumptions of Theorem 5.4 but with the non-resonance condition 5.3 replaced by the non-resonance condition 5.5 we have near-conservation of sums of discrete actions*

$$\sum_{m\in\mathbb{N}} m^{2s} \frac{|\sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi^n,\overline{\xi^n}) - \sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi^0,\overline{\xi^0})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{5.12}$$

and, if in addition Assumption 4.1 is satisfied, also near-conservation of sums of continuous actions

$$\sum_{m\in\mathbb{N}} m^{2s} \frac{|\sum_{l\in\mathcal{N}:|l|=m} I_l(\iota(\xi^n),\overline{\iota(\xi^n)}) - \sum_{l\in\mathcal{N}:|l|=m} I_l(\iota(\xi^0),\overline{\iota(\xi^0)})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{5.13}$$

over long times

$$0 \le t_n = nh \le \varepsilon^{-N}$$

with the corresponding constant C of Theorem 5.4.

The proof of this theorem is given in Chapter 6.

5.3 On the Non-Resonance Condition and on Numerical Resonances

In the non-resonance condition 5.3 the near-resonant indices are defined essentially by

$$\frac{|e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1|}{h} < \varepsilon^{\frac{1}{2}},$$

whereas they are defined by

$$|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| < \varepsilon^{\frac{1}{2}}$$

in the non-resonance condition 2.3 for the continuous situation. In the continuous situation we have shown in Section 2.3 that the non-resonance condition is valid in many situations. Here, we study the validity of the non-resonance condition 5.3 for the discrete setting in the case that the discrete frequencies $\omega_j^{M,h}$ agree with the continuous ones.

The Possibility of Numerical Resonances. We first note that the definition of near-resonant indices in 5.3 includes the step-size h, a numerical parameter. This suggests the possibility of *numerical resonances*, i.e., resonances that are not present in the equation itself but simply due to the numerical discretization or more precisely a bad choice of the step-size h.

Indeed, the non-resonance condition in the discrete setting has to control all indices $(j, \mathbf{k})$ where $|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j|h$ is close to an integer multiple of 2π, whereas the non-resonance condition in the continuous situation only has to control indices with $|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j|$ close to zero. In particular, if the step-size h is chosen as $2\pi m/|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j|$ with a positive integer m and $(j, \mathbf{k})$ not satisfying (5.9a), then the non-resonance condition 5.3 is not satisfied, and we cannot apply our Theorem 5.4, although the frequencies themselves may be non-resonant in the sense of Assumption 2.3 and Theorem 2.5 is applicable. As our numerical experiments show, we encounter indeed numerical resonances in such situations and Theorem 5.4 is not valid, see Section 5.6.

There are at least two general situations where the discrete non-resonance condition 5.3 is valid. We emphasize that neither of them is necessary for the discrete non-resonance condition to be fulfilled.

Restriction of the Time Step-Size h in Terms of the Spatial Discretization Parameter M. Note that in the limit $h \to 0$ the definition of near-resonant indices in the discrete setting reduces to the one for the continuous setting. This suggests to use a step-size restriction in order to reduce the discrete non-resonance condition to the continuous one which is fulfilled in many situations. Note that $|e^{ix} - 1| = 2|\sin(x/2)|$, and hence

$$\frac{2}{\pi}|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| \le \frac{|e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1|}{h} \le |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| \quad \text{for} \quad |\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j|h \le \pi.$$

Since only indices with $\|\mathbf{k}\| \le 2N + 4 + 4s_0$ can be near-resonant, we conclude that under the step-size restriction

$$h\omega_{\max} \le \frac{\pi}{2N + 5 + 4s_0} \tag{5.14}$$

the sets of near-resonant indices are the same for the discrete and the continuous situation (up to factor $\pi/2$ in front of $\varepsilon^{\frac{1}{2}}$, which does not change the non-resonance condition qualitatively). Here we denote by $\omega_{\max}$ the largest frequency which is present in $H_0^{M,h}$. Typically $\omega_{\max} \le C_2\sqrt{d^\sigma}M^\sigma$ with the spatial discretization parameter M and C_2 and σ from Assumption 5.2. Note that (5.14) implies $N \le \frac{C}{h\omega_{\max}}$, and hence the length of the time interval $0 \le t \le \varepsilon^{-N}$ depends on the smallness of $h\omega_{\max}$.

We now show that no numerical resonances occur under the step-size restriction (5.14). More precisely, we show that under the above step-size restriction (5.14) the non-resonance condition (2.16) on the frequencies used by Bambusi and Grébert (in the continuous situation) implies our non-resonance condition 5.3 used in the discrete setting. The main point is to handle the additional non-resonance condition (5.9b) used in the discrete but not in the continuous setting. Recall that we have shown in Lemma 2.8 that the non-resonance condition (2.16) used by Bambusi and Grébert implies our non-resonance condition 2.3 used in the continuous situation.

Lemma 5.7. *If the asymptotics of the frequencies in Assumption 5.2 is valid and if $\varepsilon \le 1$, then we have the following result.*

If the step-size restriction (5.14) *is fulfilled and if the non-resonance condition* (2.16) *is fulfilled for $\widetilde{\mathbf{k}} = \mathbf{k} - \langle j \rangle$ with a near-resonant index $(j, \mathbf{k})$ as in 5.3, then this near-resonant index also satisfies the non-resonance conditions* (5.9a) *and* (5.9b) *in Assumption 5.3 for $s \ge 2\alpha(N+3+2s_0)+2s_0$ and a constant C_0 depending only on α, γ, s_0, s, c_2, C_2, σ, and N, where α and γ are chosen in* (2.16) *for $r' = 2N+3+4s_0$.*

In particular, the step-size restriction (5.14) *and the non-resonance condition* (2.16) *imply the non-resonance condition 5.3.*

Proof. Under the step-size restriction (5.14) we have

$$\frac{2}{\pi}|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j| \le \frac{|e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1|}{h} \tag{5.15}$$

as explained above, and hence Lemma 2.8 ensures that the first part (5.9a) of the non-resonance condition 5.3 is fulfilled.

We now turn to the second condition (5.9b) in the non-resonance condition 5.3, i.e., we have to control

$$\frac{\sum_{l\in\mathcal{N}_M}|k_l||l|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}}.$$

We combine the ideas of the proofs of Lemma 2.8 and Lemma 3.9. The numerator can be estimated by $\|\mathbf{k}\||\bar{l}|^{2s}$ where $\bar{l} \in \mathcal{N}_M$ denotes the largest index with respect to $|\cdot|$ with $k_{\bar{l}} \ne 0$. As in the proof of Lemma 2.8 we choose $r \in \mathbb{N}$ minimal such that $\sum_{|l|>r}|k_l| \le 1$. In order to estimate the denominator we distinguish two cases as in the proof of Lemma 3.9 and make use of the condition of zero momentum 5.2.

(a) If $|l| > \frac{1}{2\|\mathbf{k}\|}|\bar{l}|$ for $\bar{l} \ne l \in \mathcal{N}_M$ with $k_l \ne 0$, then

$$\mathbf{j}^{2(s-s_0)|\mathbf{k}|} \ge \frac{1}{(2\|\mathbf{k}\|)^{2(s-s_0)}}|\bar{l}|^{4(s-s_0)} \ge \frac{1}{(2\|\mathbf{k}\|)^{2(s-s_0)}}|\bar{l}|^{2s}r^{2s-4s_0}.$$

(b) On the contrary, if $|l| \leq \frac{1}{2\|\mathbf{k}\|}|\bar{l}|$ for all $\bar{l} \neq l \in \mathcal{N}_M$ with $k_l \neq 0$, then due to the condition of zero momentum 5.2

$$|j| = |j(\mathbf{k})| \geq \Big|\sum_{l\in\mathcal{N}_M} k_l l\Big| \geq |\bar{l}| - \sum_{\bar{l}\neq l\in\mathcal{N}_M} |k_l||l| \geq \frac{1}{2}|\bar{l}|.$$

We conclude that

$$\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0} \geq |\bar{l}|^{2(s-s_0)} r^{2(s-s_0)} \frac{1}{2^{2s_0}}|\bar{l}|^{2s_0}.$$

As in the proof of Lemma 2.8 and using (5.15) we get for (numerically) near-resonant indices $(j, \mathbf{k})$ that $1/r^\alpha \leq \pi\varepsilon^{\frac{1}{2}}/(2\gamma)$ with α and γ from (2.16). Using this in the above estimates of the denominator we get

$$\frac{\sum_{l\in\mathcal{N}_M}|k_l||l|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|}|j|^{2s_0}} \leq C_0\varepsilon^{\frac{2s-4s_0}{2\alpha}}$$

with a constant C_0 depending only on α, γ, s_0, s, and N. The second non-resonance condition (5.9b) in 5.3 is thus fulfilled provided that $s \geq \alpha N + 2s_0$. □

Restriction of the Spatial Discretization Parameter M in Terms of ε. Instead of imposing a step-size restriction as in Lemma 5.7, we can impose a restriction on the spatial discretization in terms of ε in the spirit of [25]. In that paper a non-resonance condition of the form

$$\frac{|e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1|}{h} \geq \frac{\gamma^*}{M^{\alpha^*}} \tag{5.16}$$

for $\mathbf{k} \neq \langle j\rangle$ is used, see [25, Hypothesis 3.4], where M denotes the spatial discretization parameter. It is shown that there exists a step-size h_0 such that this non-resonance condition is fulfilled for all time step-sizes h in a dense subset of $(0, h_0)$ provided that the frequencies satisfy a (continuous) non-resonance condition in the spirit of (2.16) and in the case of a typical spatial discretization where $\omega_{\max} \leq C_2\sqrt{d^\sigma}M^\sigma$.

The non-resonance condition (5.16) is clearly weaker than our non-resonance condition 5.3 if $1/M^{\alpha^*} \geq \varepsilon^{\frac{1}{2}}$ since this excludes any near-resonance. In other words, our non-resonance condition 5.3 is an empty condition in this situation, and we have the following lemma.

Lemma 5.8. *If the non-resonance condition* (5.16) *holds and if* $M \leq \varepsilon^{-\frac{1}{2\alpha^*}}$*, then the non-resonance condition 5.3 holds for any s and any constant C_0.* □

We note that α^* grows with N, and hence M has to be small for large N. This is the situation studied in [25] where $M \leq \varepsilon^{-\sigma}$ with $1/\sigma$ growing with N is assumed. We have here in Lemma 5.8 an explicit bound for σ in terms of the non-resonance condition, whereas it seems to be difficult to bound σ in [25] explicitly, see Remark 4.3 therein.

A study of resonances in the numerical integration of weakly nonlinear Hamiltonian partial differential equations is given in [24] as well as a possible way to avoid such resonances by truncating the linear part of the equation.

5.4 Long-Time Regularity and Long-Time Near-Conservation of Energy, Mass, and Momentum

In the same way as in Sections 2.4 and 4.3, we get from Theorems 5.4 and 5.6 the following corollaries on the long-time regularity of the numerical solution ξ^n and on the near-conservation of discrete mass m^M, continuous mass m, discrete momentum K^M, and continuous momentum K over long times along the numerical solution.

Corollary 5.9 (Long-Time Regularity). *Under the assumptions of Theorem 5.4 or Theorem 5.6 we have regularity*

$$\|\xi^n\|_s \leq 2\varepsilon \tag{5.17}$$

and, if in addition Assumption 4.1 is satisfied, also regularity

$$\|\iota(\xi^n)\|_s \leq 2\varepsilon \tag{5.18}$$

over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N}.$$

□

Corollary 5.10 (Long-Time Near-Conservation of Mass). *Under the assumptions of Theorem 5.4 or Theorem 5.6 we have near-conservation of discrete mass*

$$\frac{|m^M(\xi^n, \overline{\xi^n}) - m^M(\xi^0, \overline{\xi^0})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{5.19}$$

and, if in addition Assumption 4.1 is satisfied, also near-conservation of continuous mass

$$\frac{|m(\iota(\xi^n), \overline{\iota(\xi^n)}) - m(\iota(\xi^0), \overline{\iota(\xi^0)})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{5.20}$$

over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N}$$

with the corresponding constant C of Theorem 5.4. □

Corollary 5.11 (Long-Time Near-Conservation of Momentum). *Under the assumptions of Theorem 5.4 and for $s \geq \frac{1}{2}$ we have near-conservation of discrete momentum*

$$\frac{|K_l(\xi^n, \overline{\xi^n}) - K_l(\xi^0, \overline{\xi^0})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{5.21}$$

and, if in addition Assumption 4.1 is satisfied, also near-conservation of continuous momentum

$$\frac{|K_l(\iota(\xi^n), \overline{\iota(\xi^n)}) - K_l(\iota(\xi^0), \overline{\iota(\xi^0)})|}{\varepsilon^2} \leq C\varepsilon^{\frac{1}{2}} \tag{5.22}$$

for $l = 1, \dots, d$ over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N}$$

with the corresponding constant C of Theorem 5.4. □

Note that mass and momentum may also be exact invariants along the numerical solution provided that both Hamiltonian functions $H_0^{M,h}$ and $P^{M,h}$ are invariant under the transformations needed to apply Propositions 1.3 and 1.4. Another possibility is that mass (or momentum) is an exact invariant of the exact solution but not of the numerical solution. In this situation Corollary 5.10 (or Corollary 5.11) ensures at least near-conservation of mass (or momentum) over long times.

Long-Time Near-Conservation of Energy. The semi-discrete energy H^M is exactly conserved along the spatial semi-discretization, but this is typically not true along the fully discrete solution. Accordingly, we cannot proceed as described in Section 4.3 in order to study the continuous energy H along the fully discrete solution. However, the energy H can be written in terms of the actions I_j as

$$H(\iota(\xi),\overline{\iota(\xi)}) = \sum_{j\in\mathcal{N}} \omega_j I_j(\iota(\xi),\overline{\iota(\xi)}) + P(\iota(\xi),\overline{\iota(\xi)}),$$

and Theorems 5.4 and 5.6 provide near-conservation of actions over long times. In order to show near-conservation of continuous energy

$$\frac{|H(\iota(\xi^n),\overline{\iota(\xi^n)}) - H(\iota(\xi^0),\overline{\iota(\xi^0)})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{5.23}$$

over long times $0 \le t_n = nh \le \varepsilon^{-N}$, it suffices therefore to control the nonlinearity

$$|P(\iota(\xi),\overline{\iota(\xi)})| \le C\varepsilon^{\frac{5}{2}}$$

on this time interval. Since this nonlinearity is cubic, and since we have by Corollary 5.9 long-time regularity $\|\xi(t)\|_s \le 2\varepsilon$, the nonlinearity can usually be bounded in this way ensuring the long-time near-conservation of energy along the fully discrete solution.

In the same way, one can obtain near-conservation of discrete energy

$$\frac{|H^M(\xi^n,\overline{\xi^n}) - H^M(\xi^0,\overline{\xi^0})|}{\varepsilon^2} \le C\varepsilon^{\frac{1}{2}} \tag{5.24}$$

over long times $0 \le t_n = nh \le \varepsilon^{-N}$ by controlling the semi-discrete nonlinearity P^M.

5.5 Long-Time Energy Distribution

In Section 2.5 we studied the energy distribution along solutions of Hamiltonian partial differential equations in situations where the energy is located initially in a finite number of modes (2.22a) and (2.22b). We have shown that the energy is then distributed among the other modes as expected, and that this distribution is preserved on a remarkably long time interval. In this section we give corresponding results for the fully discrete solution showing again that the behaviour of the exact solution is well reproduced.

The key for the results of Section 2.5 was an extension of Theorems 2.5 and 2.7 to the case of a scaled norm. The corresponding result for the fully discrete solution is the following theorem whose proof is given in Chapter 6.

Theorem 5.12 (Long-Time Near-Conservation of Scaled Actions)**.** *Let $e : \mathcal{N}_M \to \mathbb{R}_+$ satisfy the triangle inequality and let $0 < \mu \leq 1$. (If the nonlinearity $\frac{\partial P}{\partial \eta_j}$ is at least cubic for all $j \in \mathcal{N}_M$ and $P_{j,k,l} \neq 0$ only for $k \in \mathcal{N}_M^{m+1}$ and $l \in \mathcal{N}_M^m$, then the triangle inequality needs to be satisfied only for sums of at least three indices.)*

Under the assumptions of Theorem 5.4 and for small initial values

$$\|\xi^0\|_{s,e} \leq \varepsilon^\mu$$

instead of $\|\xi^0\|_s \leq \varepsilon$ with ε^μ satisfying the smallness assumption of Theorem 5.4 we have near-conservation of scaled discrete actions

$$\sum_{l \in \mathcal{N}_M} |l|^{2s} \frac{|I_l^M(\xi^n, \overline{\xi^n}) - I_l^M(\xi^0, \overline{\xi^0})|}{\varepsilon^{2e(l)(1-\mu)+2\mu}} \leq C \varepsilon^{\frac{1}{2}\mu}$$

over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N\mu}$$

with the constant C of Theorem 5.4.

In the situation of partial resonances as in Theorem 5.6 we have near-conservation of sums of scaled discrete actions

$$\sum_{m \in \mathbb{N}} m^{2s} \frac{|\sum_{l \in \mathcal{N}_M : |l| = m} I_l^M(\xi^n, \overline{\xi^n}) - \sum_{l \in \mathcal{N}_M : |l| = m} I_l^M(\xi^0, \overline{\xi^0})|}{\varepsilon^{2e(m)(1-\mu)+2\mu}} \leq C \varepsilon^{\frac{1}{2}\mu}$$

over long times $0 \leq t_n = nh \leq \varepsilon^{-N\mu}$ if $e(l) = e(|l|)$ depends only on $|l|$.

The same energy distribution holds for the continuous actions $I_l(\iota(\xi^n), \overline{\iota(\xi^n)})$ with the corresponding constant of Theorem 5.4 if in addition Assumption 4.1 is satisfied.

The following corollaries treat the cases of initial values with a finite band of initially excited modes (2.22a) and a pair of initially excited modes (2.22b). They follow from Theorem 5.12 in the same way as the corollaries of Section 2.5 follow from Theorem 2.12 using a scaling function $e(\cdot)$ that represents the expected energy distribution.

Corollary 5.13 (Long-Time Energy Distribution (a))**.** *Let $0 < \mu \leq 1$. Under the assumptions of Theorem 5.4 or Theorem 5.6 and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon \quad \text{with (2.22a)}$$

we have for any ε, such that ε^μ satisfies the smallness assumption of Theorem 5.4 or 5.6, the energy distribution

$$\sum_{(m-1)B < |l| \leq mB} |l|^{2s} I_l^M(\xi^n, \overline{\xi^n}) \leq C \varepsilon^{2m(1-\mu)+\frac{5}{2}\mu}$$

for $m \geq 2$ over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N\mu}$$

with the constant C of Theorem 5.4.

The same energy distribution holds for the continuous actions $I_l(\iota(\xi^n), \overline{\iota(\xi^n)})$ with the corresponding constant of Theorem 5.4 if in addition Assumption 4.1 is satisfied. □

In the following corollary we denote as in Section 2.5 for $l \in \{\, m\tilde{j} : m \in \mathbb{Z} \,\} \cap \mathcal{N}_M$ by $m(l)$ the minimal integer with respect to $|\cdot|$ such that $l = m(l)\tilde{j}$. Note that we consider here finite sets $\mathcal{N}_M$ of indices with a possibly different addition than in the set of indices $\mathcal{N}$ in Chapter 2. Hence, $m(l)$ in the discrete situation may defer from $m(l)$ in the continuous situation, see also Section 4.5.

Corollary 5.14 (Long-Time Energy Distribution (b))**.** *Let* $0 < \mu \le 1$. *Under the assumptions of Theorem 5.4 and for small initial values*

$$\|\xi^0\|_s \le \varepsilon \quad \textit{with } (2.22\text{b})$$

we have for any ε*, such that* ε^μ *satisfies the smallness assumption of Theorem 2.5, the energy distribution*

$$I_0^M(\xi^n, \overline{\xi^n}) \le C\varepsilon^{4(1-\mu)+\frac{5}{2}\mu},$$
$$|l|^{2s} I_l^M(\xi^n, \overline{\xi^n}) \le C\varepsilon^{2|m(l)|(1-\mu)+\frac{5}{2}\mu}$$

for $0, \pm\tilde{j} \ne l \in \{\, m\tilde{j} : m \in \mathbb{Z} \,\} \cap \mathcal{N}_M$ *over long times*

$$0 \le t_n = nh \le \varepsilon^{-N\mu}$$

with the constant C *of Theorem 5.4. If* $l \notin \{\, m\tilde{j} : m \in \mathbb{Z} \,\}$*, then* $\xi_l(t) = 0$ *for all times* t*.*

The same energy distribution holds for the continuous actions $I_l(\iota(\xi^n), \overline{\iota(\xi^n)})$ *with the corresponding constant of Theorem 5.4 if in addition Assumption 4.1 is satisfied. Moreover, the same result holds true in the situation of Theorem 5.6 in dimension one* $(d = 1)$*.* □

5.6 Example — Split-Step Fourier Methods for Nonlinear Schrödinger Equations of Convolution Type

We study a full discretization of the nonlinear Schrödinger equation with a potential of convolution type

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x) * \psi(x,t) + g(|\psi(x,t)|^2)\psi(x,t) \tag{5.25}$$

on $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$ as introduced in Section 1.4, equation (1.7). In Section 2.6 we studied the exact solution of such equations. We have shown long-time near-conservation of actions and exact conservation of energy, mass, and momentum, see Corollary 2.15. Moreover, we studied the energy distribution for special initial values in Corollaries 2.16 and 2.17. In Sections 4.4 and 4.5 we studied spatial semi-discretizations of these equations by a spectral Galerkin and a spectral collocation method and proved long-time results in Corollaries 4.7, 4.8, 4.9, 4.11, 4.12, and 4.13. In particular we proved (at least approximatively) the same behaviour of actions, energy, mass, and momentum along the semi-discrete solution as along the exact solution. In this section we study a full discretization of (5.25) and apply Theorem 5.4 on the long-time near-conservation of actions along the fully discrete solution and its corollaries to this discretization.

Split-Step Fourier Methods. In order to discretize the nonlinear Schrödinger equation (5.25) in time and space we apply a splitting integrator (5.4) or (5.5) to the semi-discretization in space by a spectral collocation method as described in Section 4.5. This is called a *split-step Fourier method* based on the Lie–Trotter splitting (5.4) or the Strang splitting (5.5) and is widely used for the numerical integration of (nonlinear) Schrödinger equations, see [41] and references therein. From the semi-discretization in space we have the embedding $\iota = \mathrm{id}$.

For the splitting integrators (5.4) and (5.5) we solve the equations of motion (5.3a) and (5.3b) with

$$H_0^{M,h}(\xi,\eta) = \sum_{j\in\mathcal{N}_M} \omega_j \xi_j \eta_j \quad \text{and} \quad P^{M,h}(\xi,\eta) = H^M(\xi,\eta) - H_0^{M,h}(\xi,\eta),$$

where H^M is the Hamiltonian function (4.18) of the semi-discretization in space by the spectral collocation method and $\mathcal{N}_M = \{-M,\dots,M-1\}^d$ is a full grid with addition modulo $2M$ as in Section 4.5. In terms of the ansatz $\psi^M(x,t) = \sum_{j\in\mathcal{N}_M} \xi_j(t) e^{i(j\cdot x)}$ the equations of motion (5.3a) and (5.3b) determining the split-step method then read

$$\begin{aligned} i\frac{d}{dt}\xi_j(t) &= \omega_j \xi_j(t) \quad \text{for } j \in \mathcal{N}_M, \\ i\frac{\partial}{\partial t}\psi^M(x_k,t) &= g(|\psi^M(x_k,t)|^2)\psi^M(x_k,t) \quad \text{for } k \in \mathcal{N}_M. \end{aligned}$$

The first equation is linear with solution

$$\xi_j(t) = e^{-i\omega_j t}\xi_j(0), \quad j \in \mathcal{N}_M.$$

For the second equation we first note that $|\psi^M(x_k,t)|^2$ is conserved along any solution as is shown by a multiplication of the equation with $\overline{\psi^M(x_k,t)}$ (g is assumed to be real-valued). Its solution can therefore be easily computed as

$$\psi^M(x_k,t) = e^{-ig(|\psi^M(x_k,0)|^2)t}\psi^M(x_k,0), \quad k \in \mathcal{N}_M. \tag{5.26}$$

Note that $\psi^M(x_k,t)$ and $\xi_j(t)$ are related by the discrete Fourier transform $\mathcal{F}_{2M} : \mathbb{C}^{2M} \to \mathbb{C}^{2M}$,

$$\mathcal{F}_{2M}(\xi_j(t))_{j\in\mathcal{N}_M} = (\psi^M(x_k,t))_{k\in\mathcal{N}_M},$$

which can be efficiently computed using the fast Fourier transform (FFT).

The Lie–Trotter Split-Step Fourier Method. One time step of the split-step Fourier method based on the Lie–Trotter splitting (5.4) starting with $\xi^n = (\xi_j^n)_{j\in\mathcal{N}_M}$ can be written as

$$\psi^{M,n} = (\psi^{M,n}(x_k))_{k\in\mathcal{N}_M} = \mathcal{F}_{2M}(\xi^n), \tag{5.27a}$$

$$\psi^{M,n,+} = (e^{-ig(|\psi^{M,n}(x_k)|^2)h}\psi^{M,n}(x_k))_{k\in\mathcal{N}_M}, \tag{5.27b}$$

$$\xi^{n,+} = (\xi_j^{n,+})_{j\in\mathcal{N}_M} = \mathcal{F}_{2M}^{-1}(\psi^{M,n,+}), \tag{5.27c}$$

$$\xi^{n+1} = (e^{-i\omega_j h}\xi_j^{n,+})_{j\in\mathcal{N}_M}. \tag{5.27d}$$

In the first equation we transform the vector ξ^n from the frequency domain to the space domain using the fast Fourier transform. In the space domain we then solve (5.3b) in the second equation by simply multiplying each component with a complex number (5.26). After having transformed the result back to the frequency domain in the third equation using again the fast Fourier transform, we finally perform a time step h with (5.3a) again simply by multiplying each component with a complex number. In this way we compute from $\xi^n \approx \xi(t_n)$ a new approximation $\xi^{n+1} \approx \xi(t_{n+1})$ at time $t_{n+1} = (n+1)h = t_n + h$, where all steps are very easy (and fast) to compute.

The Strang Split-Step Fourier Method. Similarly, the split-step Fourier method based on the Strang splitting (5.5) reads

$$\psi^{M,n} = (\psi^{M,n}(x_k))_{k\in\mathcal{N}_M} = \mathcal{F}_{2M}(\xi^n), \tag{5.28a}$$
$$\psi^{M,n,+} = (e^{-ig(|\psi^{M,n}(x_k)|^2)\frac{h}{2}}\psi^{M,n}(x_k))_{k\in\mathcal{N}_M}, \tag{5.28b}$$
$$\xi^{n,+} = (\xi_j^{n,+})_{j\in\mathcal{N}_M} = \mathcal{F}_{2M}^{-1}(\psi^{M,n,+}), \tag{5.28c}$$
$$\xi^{n,-} = (e^{-i\omega_j h}\xi_j^{n,+})_{j\in\mathcal{N}_M}, \tag{5.28d}$$
$$\psi^{M,n,-} = \mathcal{F}_{2M}(\xi^{n,-}), \tag{5.28e}$$
$$\psi^{M,n+1} = (e^{-ig(|\psi^{M,n,-}(x_k)|^2)\frac{h}{2}}\psi^{M,n,-}(x_k))_{k\in\mathcal{N}_M}, \tag{5.28f}$$
$$\xi^{n+1} = \mathcal{F}_{2M}^{-1}(\psi^{M,n+1}). \tag{5.28g}$$

In order to apply Theorem 5.4 and its corollaries to the split-step Fourier methods (5.27) and (5.28) we verify its various assumptions.

Verification of the Assumptions 5.1, 5.2, 5.3, and 4.1. *The Assumptions 5.1 and 5.2 are satisfied under the same conditions and with constants depending on the same parameters (in particular independent of M and h) as for the continuous nonlinear Schrödinger equation with a potential of convolution type in Section 2.6. Assumption 4.1 is fulfilled with $C_4 = 1$.*

Assumption 5.1 imposes a regularity condition on the flow of the nonlinearity $P^{M,h} = P^M$. From (5.26) we know that the flow can be written in terms of the function $\psi^M(x,t) = \sum_{j\in\mathcal{N}_M}\xi_j(t)e^{i(j\cdot x)}$ as

$$\psi^M(x,t) = \mathcal{Q}\Big(e^{-ig(|\psi^M(x,0)|^2)t}\psi^M(x,0)\Big) = \sum_{m=0}^{\infty}\frac{(-it)^m}{m!}\mathcal{Q}\Big(g(|\psi^M(x,0)|^2)^m\psi^M(x,0)\Big)$$

using the trigonometric interpolation $\mathcal{Q}$ as introduced in Section 4.5. Writing this equation in terms of the Fourier coefficients ξ_j, we clearly see that the flow Φ_t^P has an expansion of the form (5.7) as required in Assumption 5.1 with coefficients $\widehat{P}_{j,k,l}$ satisfying the condition of zero momentum 5.2. For the verification of (2.6) for $|\widehat{P}|^{m,m'}$ we restrict ourselves to the case of a cubic nonlinearity in (5.25), i.e., $g(|\psi|^2) = |\psi|^2$. This is done just for notational simplicity (though the formulas are still complicated ...); all the calculations can be redone for a general (real-valued and analytic) nonlinearity g. In the case of a cubic nonlinearity the expansion (5.7) of the flow of $P^{M,h} = P^M$ takes the form

$$\xi_j(t) = \xi_j^0 + \sum_{m=1}^{\infty} \frac{(-it)^m}{m!} \sum_{\substack{j^1+\cdots+j^{m+1} \\ -j^{m+2}-\cdots-j^{2m+1}=j}} \xi_{j^1}^0 \cdots \xi_{j^{m+1}}^0 \overline{\xi_{j^{m+2}}^0 \cdots \xi_{j^{2m+1}}^0}$$

for initial value ξ^0, i.e.,

$$\widehat{P}_{j,k,l} = \begin{cases} \frac{(-i)^{m'} t^{m'-1}}{m'!}, & m = m'+1 \geq 2,\ k^1 + \cdots + k^m - l^1 - \cdots - l^{m'} = j, \\ 0, & \text{else} \end{cases}$$

for $j \in \mathcal{N}_M$, $k \in \mathcal{N}_M^m$, and $l \in \mathcal{N}_M^{m'}$. This means that $|\widehat{P}|^{m,m'}$ as introduced in Assumption 5.1 equals $|P^M|^{m,m'}$ from Section 4.5 for the spectral collocation method for the nonlinear Schrödinger equation (5.25) up to a constant factor (depending on t). The estimates from Sections 4.5 and 2.6 hence imply that

$$\| |\widehat{P}|^{m,m'}(\xi^1, \ldots, \xi^m, \eta^1, \ldots, \eta^{m'}) \|_s \leq C^{m+m'} \frac{t^{m'-1}}{m'!} \|\xi^1\|_s \cdots \|\xi^m\|_s \|\eta^1\|_s \cdots \|\eta^{m'}\|_s$$

for $m = m' + 1$ with a constant depending only on d and s provided that $s > \frac{d}{2}$. This verifies (2.6a) for $|\widehat{P}|^{m,m'}$. Moreover a calculation as in Section 2.6 shows that (2.6b) is satisfied for any constant C_1 (in general, C_1 depends on the convergence radius of g). This verifies that for any $s \geq s_0 > \frac{d}{2}$ the regularity assumption 5.1 on the flow of $P^{M,h} = P^M$ is satisfied with constants depending only on g, d, s_0, and s. Moreover, the condition of zero momentum 5.2 and Assumption 4.1 are satisfied.

The non-resonance condition 2.3 used in Chapter 2 for the exact solution is satisfied for the frequencies ω_j, $j \in \mathcal{N}_M$, as we verified in Section 2.6 for "typical" potentials $V \in \mathcal{S}$. In Section 5.3 we mentioned situations where this non-resonance condition implies the non-resonance condition 5.3 needed in the fully discrete context. In other situations this non-resonance condition 5.3 stays an assumption and has to be verified.

We have the following corollary stating that the exact invariants energy and momentum of the exact solution are nearly conserved over long times along the fully discrete solution. For the actions we have the same kind of long-time near-conservation for the fully discrete solution as for the exact solution.

Corollary 5.15 (Long-Time Analysis of Split-Step Fourier Methods Applied to Nonlinear Schrödinger Equations (5.25))**.** *Fix N, $s \geq 2s_0 > d$, and assume $g(0) = 0$ and the non-resonance condition 5.3 on the frequencies and on the time step-size h. Then for any ε sufficiently small compared to the nonlinearity g, the dimension d, the potential V, s_0, s, C_0, ε_0, and N and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon$$

we have

- *near-conservation of discrete actions* (5.10) *and continuous actions* (5.11),
- *near-conservation of discrete energy* (5.24) *and continuous energy* (5.23),
- *exact conservation of discrete and continuous mass,*
- *near-conservation of discrete momentum* (5.21) *and continuous momentum* (5.22),
- *and regularity* (5.17) *and* (5.18)

over long times

$$0 \le t_n = nh \le \varepsilon^{-N}$$

along any numerical solution ξ^n of the nonlinear Schrödinger equation with a potential of convolution type (5.25) *in dimension d defined by the Lie–Trotter split-step Fourier method* (5.27) *or the Strang split-step Fourier method* (5.28) *with a constant C depending only on g, d, V, s_0, s, C_0, and N, but not on ε, the spatial discretization parameter M, and the time step-size $h \le 1$.*

Proof. Having verified the Assumptions 5.1, 5.2, and 4.1, Theorem 5.4 ensures the long-time near-conservation of actions along the fully discrete solution, and Corollary 5.9 ensures its long-time regularity.

The discrete mass m^M is an exact invariant also of the fully discrete solution since both, $H_0^{M,h} = H_0^M$ and $P^{M,h} = P^M$, are invariant under the transformation $\xi \mapsto e^{i\theta}\xi$. Hence, their flows conserve m^M by Proposition 1.3, and the numerical scheme is just a composition of these flows. This implies exact conservation of discrete mass m^M along $\xi(t)$ and also of continuous mass m along the embedded numerical solution $\iota(\xi(t))$.

The same argument is not true for the momentum, an exact invariant of the exact solution, since the nonlinearity $P^{M,h} = P^M$ does not satisfy the required invariance, see also Section 4.5. However, Corollary 5.11 ensures the long-time near-conservation of momentum along the numerical solution.

For the energy we proceed as described in Section 5.4 by estimating the nonlinearity P. Indeed, we have by (1.10) and Corollary 5.9

$$|P(\xi,\overline{\xi})| \le C\varepsilon^4,$$

for ε sufficiently small since $g(0) = 0$. This yields the long-time estimate (5.23) for the energy. The same estimate is true for the discrete nonlinearity P^M, and hence we also have long-time near-conservation of discrete energy H^M. □

This corollary was first proven in [30, Theorem 2]. Note that discrete actions $I_j^M(\xi,\overline{\xi})$ and continuous actions $I_j(\iota(\xi),\overline{\iota(\xi)})$ agree for the nonlinear Schrödinger equation since $\iota = \mathrm{id}$, and that the same is true for mass and momentum. All properties proven for nonlinear Schrödinger equations with a potential of convolution type (5.25) and their discretizations are summarised in Table 3. Split-step Fourier methods can also be applied to Schrödinger–Poisson equations, see Sections 1.4 and 2.7, and Corollary 5.15 is also true in this situation.

Besides Theorem 5.4 and its corollaries we can also apply Corollaries 5.13 and 5.14 on energy distribution to the fully discrete solution in a similar way as we did for the

	exact solution	spectral semi-discretization		full discretization
		Galerkin	Collocation	split-step Fourier
	(Corollary 2.15)	(Corollary 4.7)	(Corollary 4.11)	(Corollary 5.15)
actions	long-time near-conservation			
energy	exact conservation		long-time near-conservation	
mass	exact conservation			
momentum	exact conservation		long-time near-conservation	

Table 3: Conservation properties of nonlinear Schrödinger equations with a potential of convolution type (5.25) and their discretizations.

semi-discrete solution in Section 4.5 and for the exact solution in Section 2.6. Once again, we get the same behaviour along the fully discrete solution as along the exact and the semi-discrete solution under suitable assumptions.

Corollary 5.16 (Long-Time Energy Distribution (a) for Split-Step Fourier Methods Applied to Nonlinear Schrödinger Equations (5.25))**.** *Let* $0 < \mu \leq 1$*. Under the assumptions of Corollary 5.15 and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon \quad \textit{with } (2.22a)$$

we have for any ε*, such that* ε^μ *satisfies the smallness assumption of Corollary 5.15, the energy distribution*

$$\sum_{(2m-1)B<|l|\leq(2m+1)B} |l|^{2s} I_l^M(\xi^n, \overline{\xi^n}) \leq C\varepsilon^{2(2m+1)(1-\mu)+\frac{5}{2}\mu}$$

for $m \geq 1$ *over long times*

$$0 \leq t_n = nh \leq \varepsilon^{-N\mu}$$

with the constant C *of Corollary 5.15.*

The same energy distribution holds for the continuous actions $I_l(\iota(\xi^n), \overline{\iota(\xi^n)})$*.* □

Corollary 5.17 (Long-Time Energy Distribution (b) for Split-Step Fourier Methods Applied to Nonlinear Schrödinger Equations (5.25))**.** *Let* $0 < \mu \leq 1$*. Under the assumptions of Corollary 5.15 and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon \quad \textit{with } (2.22b)$$

we have for any ε*, such that* ε^μ *satisfies the smallness assumption of Corollary 5.15, the energy distribution*

$$|l|^{2s} I_l(\xi^n, \overline{\xi^n}) \leq C\varepsilon^{2|m(l)|(1-\mu)+\frac{5}{2}\mu}$$

for $0, \pm\tilde{j} \neq l \in \{m\tilde{j} : m \in \mathbb{Z} \text{ odd}\}$*, where* $m\tilde{j} \in \mathcal{N}_M$ *is computed in* $\mathcal{N}_M$ *(i.e., modulo* $2M$*), over long times*

$$0 \leq t_n = nh \leq \varepsilon^{-N\mu}$$

with the constant C *of Corollary 5.15. If* $l \notin \{m\tilde{j} : m \in \mathbb{Z} \text{ odd}\}$*, then* $\xi_l(t) = 0$ *for all times* t*.*

The same energy distribution holds for the continuous actions $I_l(\iota(\xi^n), \overline{\iota(\xi^n)})$*.* □

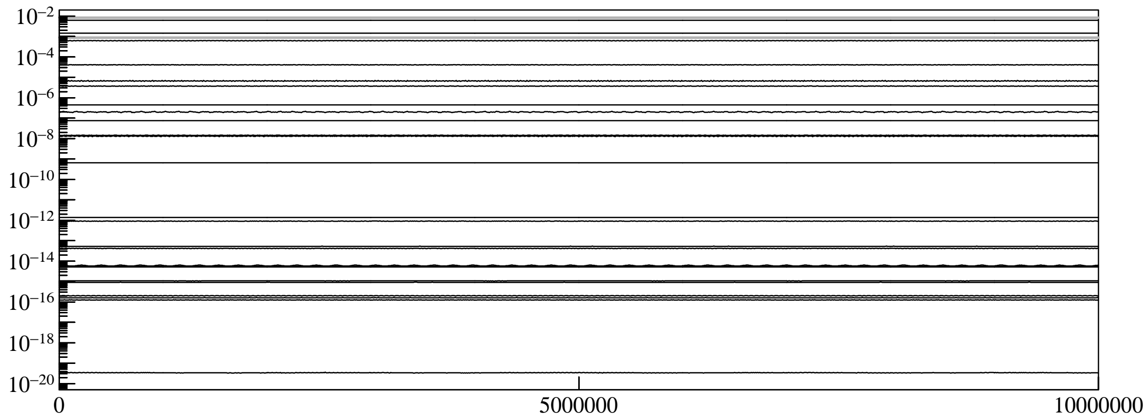

Figure 5: Numerical Experiment 5.18: Actions (black lines), discrete energy (upper grey line), and momentum (lower grey line).

In the following numerical experiments illustrating the theoretical results 5.15, 5.16, and 5.17 we restrict our attention to the *cubic nonlinear Schrödinger equation* with a potential of convolution type

$$i\frac{\partial}{\partial t}\psi(x,t) = -\Delta\psi(x,t) + V(x) * \psi(x,t) + |\psi(x,t)|^2\psi(x,t) \tag{5.29}$$

on $\mathbb{T}^d = \mathbb{R}^d/(2\pi\mathbb{Z}^d)$, i.e., we consider (5.25) with $g(|\psi|^2) = |\psi|^2$. For other numerical experiments with this nonlinear Schrödinger equation we refer to [30] and [25].

Numerical Experiment 5.18 (Long-Time Near-Conservation of Actions, Energy, and Momentum in One Dimension)**.** We apply the Lie–Trotter split-step Fourier method (5.27) to the nonlinear Schrödinger equation (5.29) in one dimension ($d = 1$) with a potential $V(x)$ such that

$$\omega_j = \sqrt{|j|^4 + r_j} \tag{5.30}$$

with $r_j = 0.5$ for $j > 0$ and $r_j = 0.8$ else. As initial value we choose

$$\psi(x,0) = \frac{1}{10}\Big(\frac{1}{2-\cos(x)} + i\Big(\frac{x}{\pi} - 1\Big)^3\Big(\frac{x}{\pi} + 1\Big)^2\Big), \tag{5.31}$$

i.e., in our numerical scheme $\psi^0 = \mathcal{Q}(\psi(\cdot,0))$. We apply the split step method (5.27) with $2M = 2^8$ collocation points and with a time step-size $h = 0.1$ on a time interval of length 10^7. The evolution of the first 11 actions and 14 other actions as well as discrete energy and momentum is plotted in Figure 5 on this time interval. All these quantities are well (though not exactly) conserved. This behaviour is explained by Corollary 5.15. We compute the discrete energy H^M instead of H for computational simplicity; the computation of the nonlinearity in H is very expensive.

Numerical Experiment 5.19 (Long-Time Near-Conservation of Actions, Energy, and Momentum in Two Dimensions)**.** We now study the cubic nonlinear Schrödinger equation

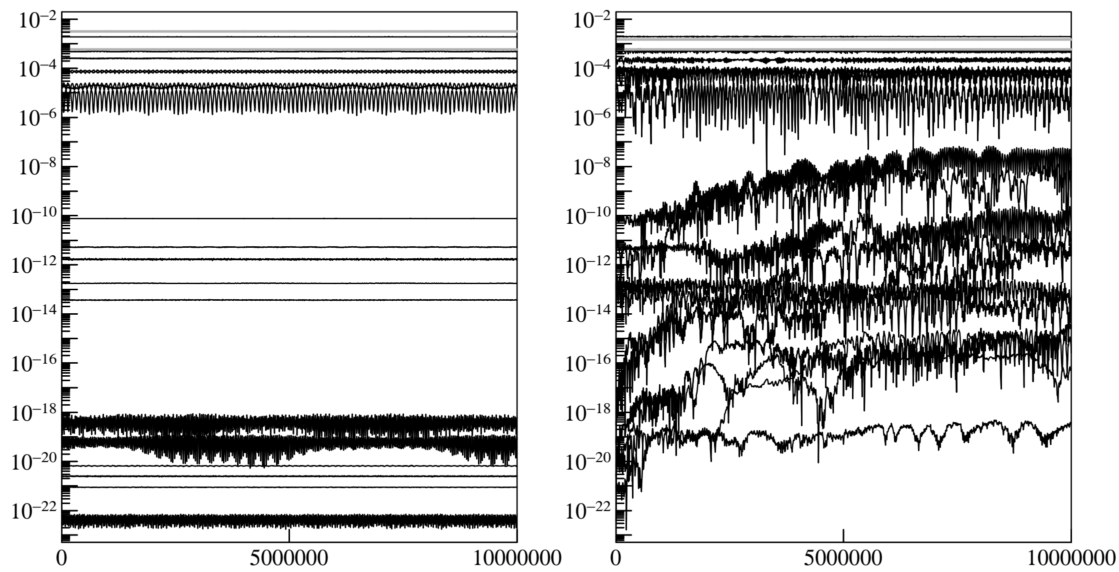

Figure 6: Numerical Experiment 5.19: Actions (black lines), discrete energy (upper grey line), and first component of momentum (lower grey line) for non-resonant frequencies (left) and for hyper-resonant frequencies (right).

(5.29) in two dimensions ($d = 2$) solved with the split-step Fourier method (5.27). We perform 10^8 steps of length $h = 0.1$ on a full grid with $(2M)^2 = 2^{10}$ grid points and with initial value

$$\psi(x,0) = \frac{1}{10}\Big(\frac{1}{(2-\cos(x_1))(2-\sin(x_2))} - i\Big(\frac{x_1^2}{\pi^2}-1\Big)^2\Big(\frac{x_2^2}{\pi^2}-1\Big)^2\Big).$$

In a first experiment the potential $V(x)$ is chosen in such a way that

$$\omega_j = \sqrt{(j_1^2+j_2^2)^2 + r_j}$$

with $r_j = 0.5$ for $j_1, j_2 \geq 0$, $r_j = 0.6$ for $j_1 \geq 0$ and $j_2 < 0$, $r_j = 0.7$ for $j_1 < 0$ and $j_2 \geq 0$, and $r_j = 0.8$ else. In Figure 6 we see on the left-hand side the near-conservation of actions, discrete energy, and the first component of the momentum as explained by Corollary 5.15. Here, the first 9 and 16 other actions are plotted.

On the right-hand side of Figure 6 the results of the same experiment without potential ($V = 0$), i.e., with hyper-resonant frequencies

$$\omega_j = j_1^2 + j_2^2,$$

are plotted. This hyper-resonant situation is not covered by Corollary 5.15.

Numerical Experiment 5.20 (Resonant Time Step-Sizes)**.** We consider again the cubic nonlinear Schrödinger equation (5.29) with frequencies (5.30) and initial value (5.31) in one dimension ($d = 1$) as in the Experiment 5.18. We apply the split-step method (5.27) with $M = 2^7$ and a time step-size

$$h = \frac{2\pi}{\omega_7 + \omega_{-3} + \omega_1 - \omega_5} \approx 0.1834.$$

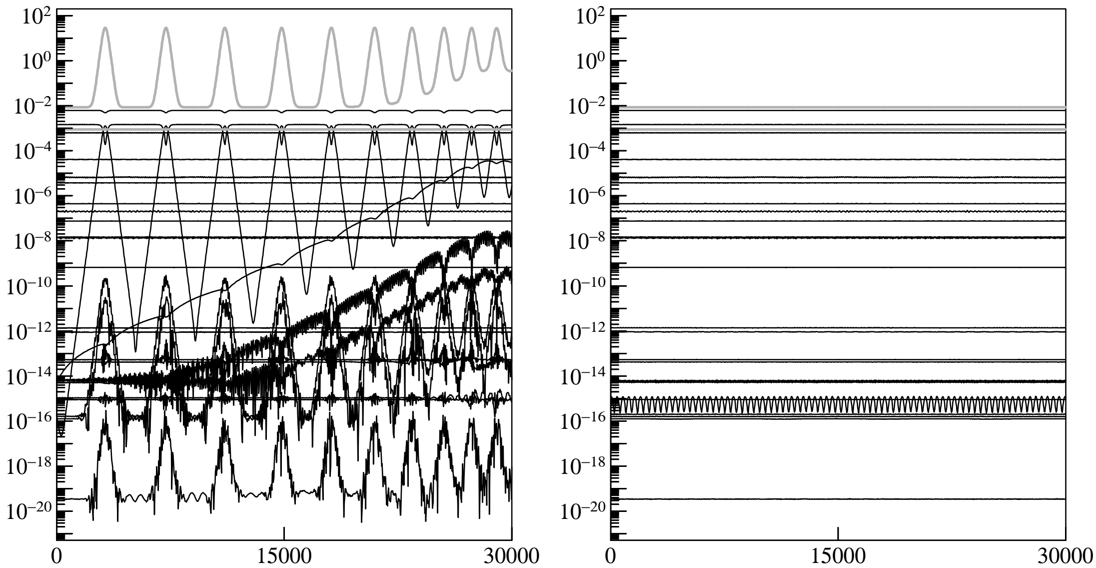

Figure 7: Numerical Experiment 5.20: Actions (black lines), discrete energy (upper grey line), and momentum (lower grey line) for a resonant time step-size $h = 2\pi/(\omega_7 + \omega_{-3} + \omega_1 - \omega_5) \approx 0.1834$ (left) and $h = 0.18$ (right).

This time step-size is of the form $2\pi m/|\mathbf{k}\cdot\boldsymbol{\omega} - \omega_{j(\mathbf{k})}|$ and therefore resonant as explained in Section 5.3. The behaviour of the first 11 actions and 14 other actions as well as energy and momentum is plotted in the left part of Figure 7 when integrated on a time interval of length $3\cdot 10^4$. The effects of the numerical resonance is clearly visible. However, if we perform the same experiment with a slightly different time step-size $h = 0.18$, we don't see these effects, see the right part of Figure 7.

This observation motivates the following study of numerical resonances in dependence of the time step-size h. We perform the above experiment for different time step-sizes $h \in [0.01, 0.2]$ on a time interval of length 5000. In Figure 8 the maximal deviation in actions, energy, and momentum is plotted. The resolution of the interval of time step-sizes is chosen as 10^{-4}.

Numerical Experiment 5.21 (Long-Time Energy Distribution (a))**.** We now solve the cubic nonlinear Schrödinger equation (5.29) with frequencies (5.30) in one dimension ($d = 1$) for a finite band initial value (2.22a)

$$\psi(x,0) = \frac{1}{100}\Big(\frac{1}{2} + \cos(x) + \cos(2x) + \cos(3x) + \cos(4x) + \cos(5x)\Big) = \frac{1}{200}\sum_{j=-5}^{5} e^{ijx} \quad (5.32)$$

using the split-step Fourier method (5.27) with a time step-size $h = 0.1$ and $2M = 2^7$ grid points. Initially, all the energy is located in a finite band of width 11 ($B = 5$ in (2.22a)). In Figure 9 the initial energy distribution is plotted with grey dots (the many nonzero but very small values are rounding errors originating from the computation of the Fourier coefficients of the initial value with the fast Fourier transform). This energy is distributed

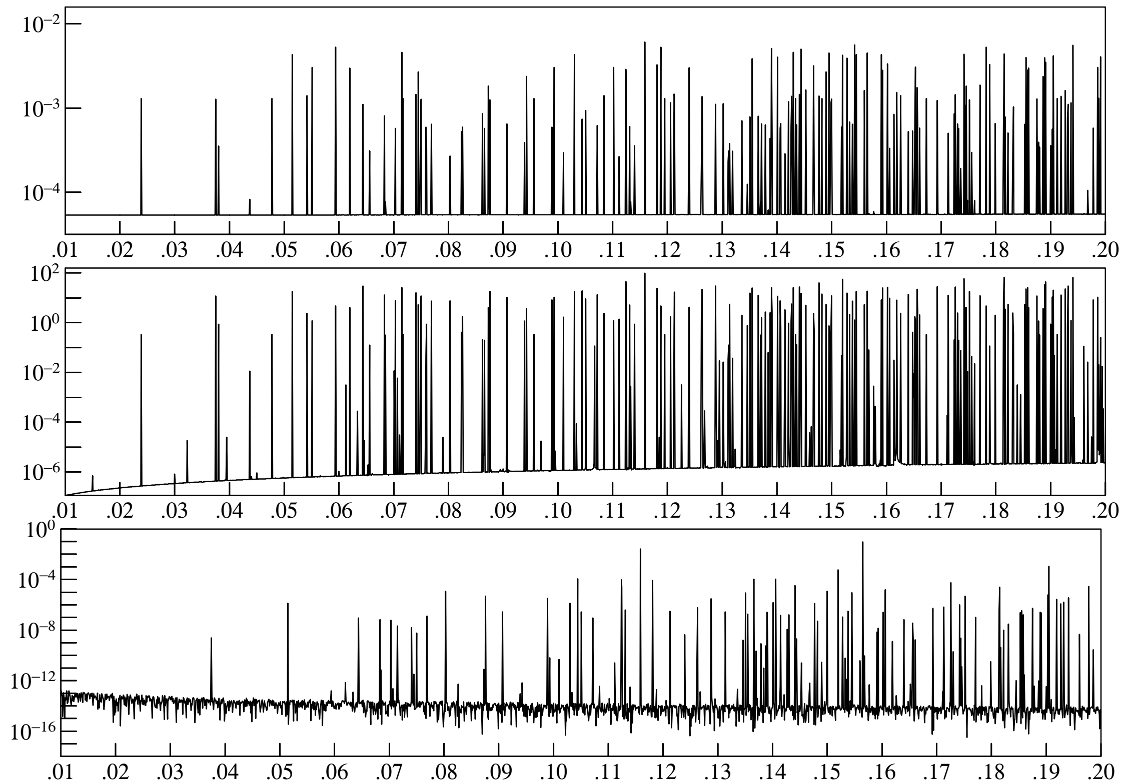

Figure 8: Numerical Experiment 5.20: Maximal deviation in actions (upper image), discrete energy (middle image), and momentum (lower image) for time step-sizes $h \in [0.01, 0.2]$.

among the other modes according to Corollary 5.16. In Figure 9 the distribution at time 10^7 is plotted with black dots and agrees with the energy distribution predicted by Corollary 5.16.

In Figure 10 the evolution of the energy distribution in time is plotted. Starting with

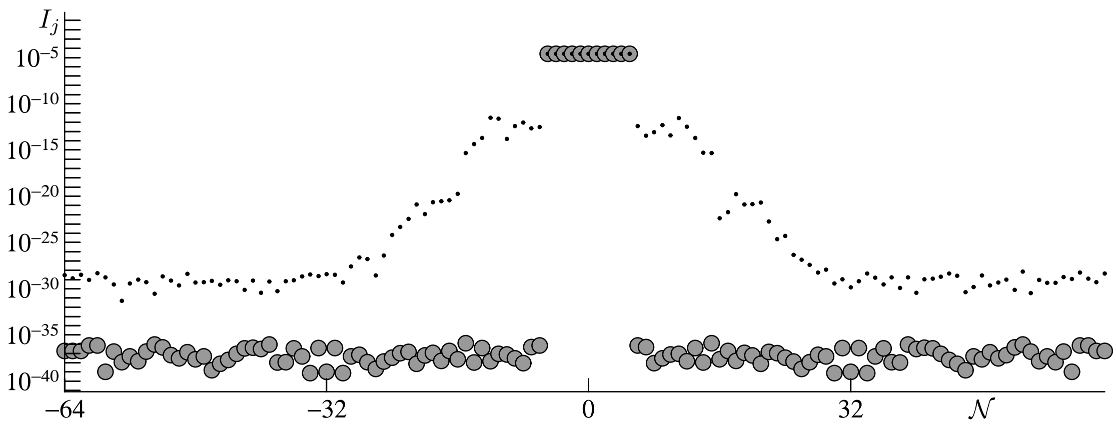

Figure 9: Numerical Experiment 5.21: Energy distribution at time $t = 0$ (grey dots) and $t = 10^7$ (black dots) for the finite band initial value (5.32).

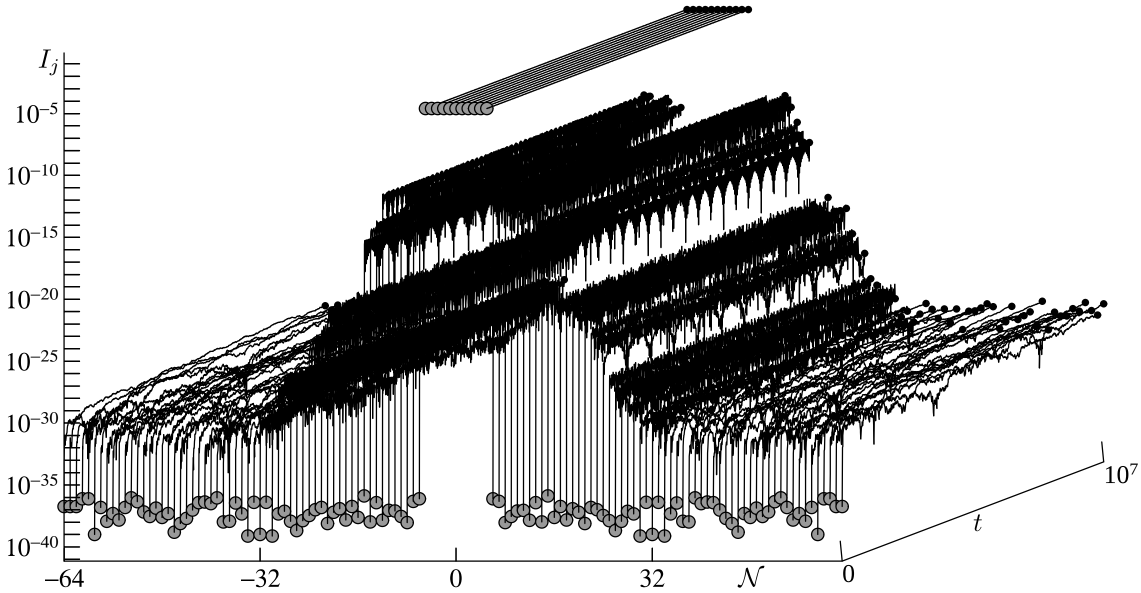

Figure 10: Numerical Experiment 5.21: Time evolution of the energy distribution for the finite band initial value (5.32).

the energy distribution in grey dots at time $t = 0$ the final energy distribution in black dots at time $t = 10^7$ is reached after very few time steps and is then approximately conserved.

Numerical Experiment 5.22 (Long-Time Energy Distribution (b))**.** Now we choose

$$\psi(x,0) = \frac{1}{10}\cos(15x) = \frac{1}{20}e^{15ix} + \frac{1}{20}e^{-15ix} \tag{5.33}$$

as initial value for (5.29). This is an example for the situation (2.22b) where all the energy is located initially in a pair of modes ($\tilde{j} = 15$ in (2.22b)) as plotted in grey dots in Figure 11. We solve the nonlinear Schrödinger equation (5.29) with frequencies (5.30) as in the Experiment 5.21 using the split-step Fourier method (5.27) with a time step-size $h = 0.1$ and $2M = 2^7$ grid points. The energy distribution at time $t = 10^7$ is plotted in Figure 11 in black dots, and the time evolution of the energy distribution on the time interval $0 \leq t \leq 10^7$ is plotted in Figure 12.

We observe the behaviour as stated in Corollary 5.17. The energy of size 10^{-3} (or more precisely $\frac{1}{4}10^{-2}$) in the modes ξ_{15} and ξ_{-15} is distributed among the modes ξ_{45} and ξ_{-45} with size $10^{-3\cdot 3}$ (up to a factor $1-\mu$), among the modes $\xi_{75} = \xi_{-53}$ and $\xi_{-75} = \xi_{53}$ with size $10^{-5\cdot 3}$, and among the modes $\xi_{105} = \xi_{-23}$ and $\xi_{-105} = \xi_{23}$ with size $10^{-7\cdot 3}$. The latter two effects are aliasing effects as explained in Section 4.5. The energy distributed among the other modes $\xi_{135} = \xi_7, \ldots$ is not distinguishable from the rounding errors in all modes.

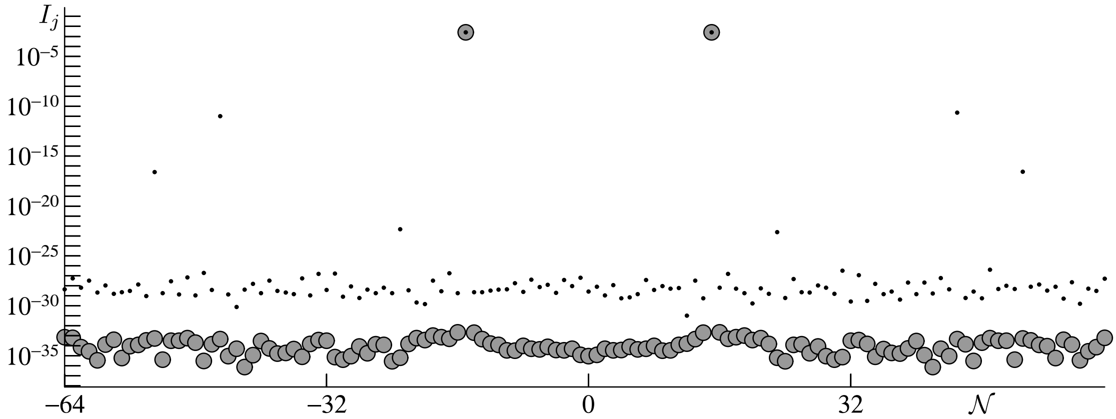

Figure 11: Numerical Experiment 5.22: Energy distribution at time $t = 0$ (grey dots) and $t = 10^7$ (black dots) for the two-mode initial value (5.33).

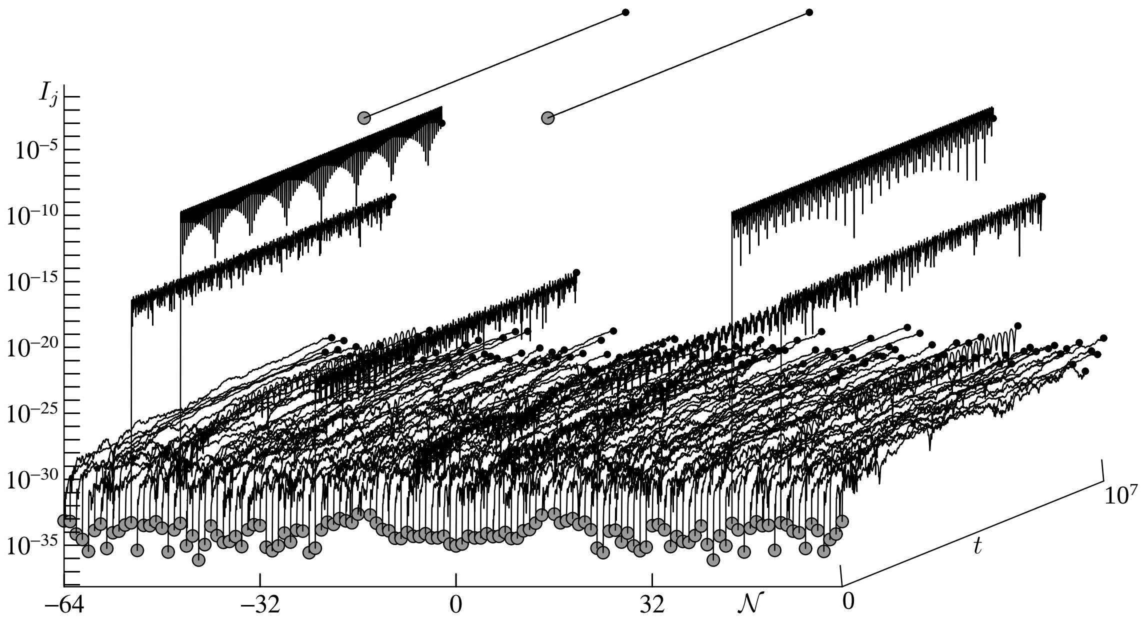

Figure 12: Numerical Experiment 5.22: Time evolution of the energy distribution for the two-mode initial value (5.33).

5.7 Example — Trigonometric Integrators for Nonlinear Wave Equations

In Section 4.6 we studied a spatial semi-discretization by a spectral collocation method of the nonlinear wave equation

$$\frac{\partial^2}{\partial t^2}u(x,t) = \Delta u(x,t) - \rho u(x,t) + g(u(x,t)) \tag{5.34}$$

in one dimension ($d = 1$) with periodic boundary conditions, see equations (1.14), (2.32), and (4.20). As explained there, the spatial semi-discretization is a Hamiltonian ordinary differential equation with Hamiltonian function (5.2), where $\omega_j^M = \omega_j = \sqrt{j^2 + \rho}$ for

$j \in \mathcal{N}_M = \{\, -M, \ldots, M-1 \,\}$ and

$$P^M(\xi,\eta) = -\sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!(m+1)} \sum_{j^1+\cdots+j^{m+1}=0} \frac{\xi_{j^1}+\eta_{-j^1}}{\sqrt{2\omega_{j^1}}} \cdots \frac{\xi_{j^{m+1}}+\eta_{-j^{m+1}}}{\sqrt{2\omega_{j^{m+1}}}}.$$

The embedding $\iota : l_0^2(\mathbb{C}^{\mathcal{N}_M}) \to l_0^2(\mathbb{C}^{\mathcal{N}})$ is given by

$$\iota(\xi)_j = \begin{cases} \xi_j, & |j| < M, \\ \frac{1}{2}\xi_{-M}, & |j| = M, \\ 0, & |j| > M, \end{cases}$$

see also Section 4.6. For the discretization in time of this spatial semi-discretization we consider the symplectic *trigonometric integrators* of [36, Chapter XIII]. They all can be interpreted as a Strang splitting (5.5) as introduced in Section 5.1.

Deuflhard's Method. We apply the Strang splitting (5.5) with

$$H_0^{M,h}(\xi,\eta) = \sum_{j\in\mathcal{N}_M} \omega_j \xi_j \eta_j \quad \text{and} \quad P^{M,h}(\xi,\eta) = P^M(\xi,\eta)$$

in (5.3a) and (5.3b) to the spatial semi-discretization. The solution of (5.3a) is

$$\xi_j(t) = e^{-i\omega_j t}\xi_j(0). \tag{5.35a}$$

The differential equation (5.3b) takes the form

$$i\frac{d}{dt}\xi_j(t) = -\frac{1}{\sqrt{2\omega_j}} \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{j^1+\cdots+j^m=j} \frac{\xi_{j^1}+\overline{\xi_{-j^1}}}{\sqrt{2\omega_{j^1}}} \cdots \frac{\xi_{j^m}+\overline{\xi_{-j^m}}}{\sqrt{2\omega_{j^m}}},$$

and a simple calculation shows that $\frac{d}{dt}(\xi_j(t) + \overline{\xi_{-j}(t)}) = 0$ along any solution of (5.3b). Hence, the solution of (5.3b) takes in this situation the simple form

$$\xi_j(t) = \xi_j(0) + \frac{it}{\sqrt{2\omega_j}} \sum_{m=0}^{\infty} \frac{g^{(m)}(0)}{m!} \sum_{j^1+\cdots+j^m=j} \frac{\xi_{j^1}(0)+\overline{\xi_{-j^1}(0)}}{\sqrt{2\omega_{j^1}}} \cdots \frac{\xi_{j^m}(0)+\overline{\xi_{-j^m}(0)}}{\sqrt{2\omega_{j^m}}}, \tag{5.35b}$$

and the numerical scheme (5.5) is indeed easy to compute.

We now write the numerical discretization (5.5) in terms of the variables u_j and v_j. Recall from Section 1.5 that for $j \in \mathcal{N}_M$

$$\xi_j = \frac{\omega_j^{\frac{1}{2}} u_j + i\omega_j^{-\frac{1}{2}} v_j}{\sqrt{2}}.$$

Hence, (5.35a) can be written as

$$u_j(t) = \cos(\omega_j t)u_j(0) + \frac{1}{\omega_j}\sin(\omega_j t)v_j(0),$$
$$v_j(t) = -\omega_j \sin(\omega_j t)u_j(0) + \cos(\omega_j t)v_j(0),$$

and (5.35b) as

$$u_j(t) = u_j(0),$$
$$v_j(t) = v_j(0) + t\sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!}\sum_{j^1+\cdots+j^m=j}\frac{u_{j^1}(0)}{\sqrt{2\omega_{j^1}}}\cdots\frac{u_{j^m}(0)}{\sqrt{2\omega_{j^m}}},$$

where the sum is over indices $j^1,\dots,j^m\in\mathcal{N}_M$ and their sum is computed in $\mathcal{N}_M$ modulo $2M$. Using these equations, the Strang splitting (5.5) reads in terms of the Fourier coefficients u_j and v_j of u^M and v^M, respectively,

$$u_j^{n+1} = \cos(\omega_j h)u_j^n + \frac{1}{\omega_j}\sin(\omega_j h)v_j^n + \frac{h}{2\omega_j}\sin(\omega_j h)g_j(u^n),$$
$$v_j^{n+1} = -\omega_j\sin(\omega_j h)u_j^n + \cos(\omega_j h)v_j^n + \frac{h}{2}\cos(\omega_j h)g_j(u^n) + \frac{h}{2}g_j(u^{n+1}),$$

where

$$g_j(u^n) = \sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!}\sum_{j^1+\cdots+j^m=j}\frac{u_{j^1}^n}{\sqrt{2\omega_{j^1}}}\cdots\frac{u_{j^m}^n}{\sqrt{2\omega_{j^m}}} = \mathcal{F}_{2M}^{-1}(g(\mathcal{F}_{2M}((u_k^n)_{k\in\mathcal{N}_M})))_j.$$

We get precisely *Deuflhard's method* which reads in a two-step formulation

$$u_j^{n+1} - 2\cos(\omega_j h)u_j^n + u_j^{n-1} = h^2\,\mathrm{sinc}(\omega_j h)g_j(u^n), \tag{5.36a}$$
$$2h\,\mathrm{sinc}(\omega_j h)v_j^n = u_j^{n+1} - u_j^{n-1}, \tag{5.36b}$$

see [21] and [36, Chapter XIII.1.2].

The Mollified Impulse Method. The *mollified impulse method* was introduced in [27], see also [36, Chapter XIII.1.4]. As Deuflhard's method, this method is a Strang splitting (5.5) but with the nonlinearity $P^M(\xi,\eta)$ replaced by $P^M(\phi(\boldsymbol{\omega}h)\xi,\phi(\boldsymbol{\omega}h)\eta)$. Here, ϕ is a real-valued filter function with $\phi(0)=1$ and bounded values $\phi(\omega_j h)$, $j\in\mathcal{N}_M$, that acts by pointwise multiplication on ξ. Usually ϕ is chosen such that $\phi(\omega_j h)\to 0$ as $\omega_j h\to\infty$, that is $\phi(\boldsymbol{\omega}h)\xi = (\phi(\omega_j h)\xi_j)_{j\in\mathcal{N}}$ filters out components of ξ corresponding to large frequencies. A typical choice for the filter function ϕ is

$$\phi = \mathrm{sinc}\,.$$

In (5.3a) and (5.3b) we have

$$H_0^{M,h}(\xi,\eta) = \sum_{j\in\mathcal{N}_M}\omega_j\xi_j\eta_j \quad\text{and}\quad P^{M,h}(\xi,\eta) = P^M(\phi(\boldsymbol{\omega}h)\xi,\phi(\boldsymbol{\omega}h)\eta).$$

If $\phi=1$, the mollified impulse method reduces to Deuflhard's method. The same calculations as for Deuflhard's method yield (5.35a) for the solution of (5.3a) and

$$\xi_j(t) = \xi_j(0) + \frac{it\phi(\omega_j h)}{\sqrt{2\omega_j}}\sum_{m=0}^{\infty}\frac{g^{(m)}(0)}{m!} \sum_{j^1+\cdots+j^m=j}\phi(\omega_{j^1}h)\frac{\xi_{j^1}(0)+\overline{\xi_{-j^1}(0)}}{\sqrt{2\omega_{j^1}}}\cdots\phi(\omega_{j^m}h)\frac{\xi_{j^m}(0)+\overline{\xi_{-j^m}(0)}}{\sqrt{2\omega_{j^m}}} \tag{5.37}$$

for the solution of (5.3b). This finally results in the same equations for u_j^{n+1} and v_j^{n+1} as for Deuflhard's method but with

$$\widetilde{g}_j(u^n) = \phi(\omega_j h) g_j(\phi(\boldsymbol{\omega} h) u^n)$$

instead of $g_j(u^n)$. In a two-step formulation this reads

$$u_j^{n+1} - 2\cos(\omega_j h) u_j^n + u_j^{n-1} = h^2 \operatorname{sinc}(\omega_j h)\phi(\omega_j h) g_j(\phi(\boldsymbol{\omega} h) u^n), \tag{5.38a}$$

$$2h \operatorname{sinc}(\omega_j h) v_j^n = u_j^{n+1} - u_j^{n-1}. \tag{5.38b}$$

Verification of the Assumptions 5.1, 5.2, 5.5, and 4.1. *The Assumptions 5.1 and 5.2 are satisfied under the same conditions and with constants depending on the same parameters (in particular independent of M and h) as for the continuous nonlinear wave equation in Section 2.9 and in addition on the bound for the filter function $\phi(\omega_j h)$, $j \in \mathcal{N}_M$. Assumption 4.1 is fulfilled with $C_4 = 1$.*

The verification of the regularity assumption 5.1 on the flow of $P^{M,h}$ is easy for Deuflhard's method (5.36), since in this case the coefficients $\widehat{P}_{j,k,l}$ from (5.7) in Assumption 5.1 agree with the coefficients $P_{j,k,l}$ from (5.8) (see (4.22) and (5.35b)). The regularity assumption 5.1 is therefore satisfied if the regularity assumption 2.1 is satisfied for $P^{M,h} = P^M$. In Section 4.6 we verified that this is the case for $g(0) = g'(0) = 0$ and $s \geq s_0 > \frac{d}{2} = \frac{1}{2}$. The requirement of a bounded filter function ϕ in the mollified impulse method (5.38) ensures that the same is true for this scheme. Note that the usual choice $\phi = \operatorname{sinc}$ is bounded by one.

The condition of zero momentum 5.2 is also satisfied since we verified it in Section 4.6 for $P_{j,k,l} = \widehat{P}_{j,k,l}$. As in Section 4.6, Assumption 4.1 can be verified with a constant $C_4 = 1$. For the non-resonance condition 5.5 we refer to the discussion in Section 5.3 and to Section 2.9, where the related non-resonance condition 2.3 was verified for many values of ρ.

The following corollary summarises the long-time behaviour of Deuflhard's method (5.36) and the mollified impulse method (5.38) when applied to nonlinear wave equations.

Corollary 5.23 (Long-Time Analysis of Deuflhard's Method and the Mollified Impulse Method Applied to Nonlinear Wave Equations (5.34))**.** *Fix N, $s \geq 2s_0 > 1$, and assume $g(0) = g'(0) = 0$ and the non-resonance condition 5.5 on the frequencies and on the time step-size h. Then for any ε sufficiently small compared to the nonlinearity g, the bound for the filter function $\phi(\omega_j h)$ ($j \in \mathcal{N}_M$), ρ, s_0, s, C_0, ε_0, and N and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon$$

we have

- *near-conservation of sums of discrete actions* (5.12) *and continuous actions* (5.13)*,*
- *near-conservation of discrete energy* (5.24) *and continuous energy* (5.23)*,*
- *near-conservation of discrete mass* (5.19) *and continuous mass* (5.20)*,*

- *near-conservation of continuous momentum*

$$\frac{|K(\iota(\xi^n),\overline{\iota(\xi^n)}) - K(\iota(\xi^0),\overline{\iota(\xi^0)})|}{\varepsilon^2} \leq CM^{-s+1}\varepsilon t_n,$$

- *and regularity* (5.17) *and* (5.18)

over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N}$$

along any numerical solution ξ^n *of the nonlinear wave equation* (5.34) *defined by Deuflhard's method* (5.36) *or the mollified impulse method* (5.38) *with a constant* C *depending only on* g*, the bound for the filter function* $\phi(\omega_j h)$ $(j \in \mathcal{N}_M)$*,* ρ*,* s_0*,* s*,* C_0*, and* N*, but not on* ε*, the spatial discretization parameter* M*, and the time step-size* $h \leq 1$*.*

Proof. Theorem 5.6 ensures long-time near-conservation of sums of actions along the fully discrete solution computed with Deuflhard's method (5.36) or the mollified impulse method (5.38). Corollaries 5.9 and 5.10 ensure the long-time regularity and the long-time near-conservation of mass. In the same way as for the nonlinear Schrödinger equation in Section 5.6, we get long-time near-conservation of energy by estimating the nonlinearities $|P(\iota(\xi^n),\overline{\iota(\xi^n)})| \leq C\varepsilon^3$ and $|P^M(\xi^n,\overline{\xi^n})| \leq C\varepsilon^3$ and using the regularity of ξ^n.

In order to study the behaviour of the momentum K along the fully discrete solution we consider separately the solutions of (5.3a) and (5.3b) which form the numerical scheme (5.5). Note that we have exact conservation of continuous momentum along any solution of the linear equations (5.3a),

$$K(\iota(\Phi_h^{H_0}(\xi)),\overline{\iota(\Phi_h^{H_0}(\xi))}) = K(\iota(\xi),\overline{\iota(\xi)}), \tag{5.39}$$

since the actions are conserved along these solutions. Concerning the steps with the nonlinear part (5.3b), we proceed as in the proof of Corollary 4.14 on the spatial semi-discretization. Besides considering $\Phi_{h/2}^P(\xi)$ we also consider a solution $\widetilde{\xi}(h/2)$ computed with the flow of the continuous nonlinearity P for the initial value $\iota(\xi)$. The proof of Corollary 4.14 then shows that

$$|K(\iota(\Phi_{h/2}^P(\xi)),\overline{\iota(\Phi_{h/2}^P(\xi))}) - K(\iota(\xi),\overline{\iota(\xi)})| \leq CM^{-(s-1)}\varepsilon^3 h. \tag{5.40}$$

Putting (5.39) and (5.40) together yields for the Strang splitting near-conservation of momentum as stated in the corollary. □

A similar result was proven in [16, Theorem 3]. There, improved near-conservation of actions and energy (with $C\varepsilon$ instead of $C\varepsilon^{\frac{1}{2}}$ on the right-hand sides of the estimates) is shown using an additional non-resonance condition. The near-conservation of momentum in [16] is of the form $C(\varepsilon + M^{-s} + M^{-s+1}\varepsilon t_n)$, whereas our analysis following the proof of Corollary 4.14 yields an estimate $CM^{-s+1}\varepsilon t_n$. The non-resonance condition used in [16] seems to be stronger than ours since our notion of a near-resonant index is weaker than the one used in [16]. Moreover, we don't need an additional non-resonance condition of the form $|\sin(\omega_j h)| \geq h\varepsilon^{\frac{1}{2}}$ as in [16] but only an additional non-resonance condition (5.9b) that is closely related to the non-resonance condition (5.9a), see Section 5.3.

Table 4 summarises the properties proven for exact and numerical solutions of nonlinear wave equations (5.34) in Corollaries 2.20, 4.14, and 5.23.

	exact solution (Corollary 2.20)	spectral semi-discretization Collocation (Corollary 4.14)	full discretization Deuflhard, mollified impulse (Corollary 5.23)
sums of actions	long-time near-conservation		
energy	exact conservation	long-time near-conservation	
mass	long-time near-conservation		
momentum	exact conservation	long-time near-conservation	

Table 4: Conservation properties of nonlinear wave equations (5.34) and their discretizations.

Applying Corollaries 5.13 and 5.14 we get the following results on the energy distribution along fully discrete solutions of the nonlinear wave equation (5.34) computed with Deuflhard's method or the mollified impulse method. We observe the same behaviour as along the exact solution 2.21 and 2.22 up to aliasing effects which were already observed for the spatial semi-discretization in Corollary 4.16.

Corollary 5.24 (Long-Time Energy Distribution (a) for Deuflhard's Method and the Mollified Impulse Method Applied to Nonlinear Wave Equations (5.34))**.** *Let* $0 < \mu \leq 1$. *Under the assumptions of Corollary 5.23 and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon \quad \textit{with } (2.22\text{a})$$

we have for any ε, *such that* ε^μ *satisfies the smallness assumption of Corollary 5.23, the energy distribution*

$$\sum_{(m-1)B<|l|\leq mB} |l|^{2s} I_l^M(\xi^n, \overline{\xi^n}) \leq C\varepsilon^{2m(1-\mu)+\frac{5}{2}\mu}$$

for $m \geq 2$ *over long times*

$$0 \leq t_n = nh \leq \varepsilon^{-N\mu}$$

with the constant C *of Corollary 5.23.*

The same energy distribution holds for the continuous actions $I_l(\iota(\xi^n), \overline{\iota(\xi^n)})$. □

Corollary 5.25 (Long-Time Energy Distribution (b) for Deuflhard's Method and the Mollified Impulse Method Applied to Nonlinear Wave Equations (5.34))**.** *Let* $0 < \mu \leq 1$. *Under the assumptions of Corollary 5.23 and for small initial values*

$$\|\xi^0\|_s \leq \varepsilon \quad \textit{with } (2.22\text{b})$$

we have for any ε, such that ε^μ satisfies the smallness assumption of Corollary 5.23, the energy distribution

$$I_0^M(\xi^n, \overline{\xi^n}) \leq C\varepsilon^{4(1-\mu)+\frac{5}{2}\mu},$$
$$|l|^{2s} I_l^M(\xi^n, \overline{\xi^n}) \leq C\varepsilon^{2|m(l)|(1-\mu)+\frac{5}{2}\mu}$$

for $0, \pm\tilde{j} \neq l \in \{\, m\tilde{j} : m \in \mathbb{Z}\,\}$, where $m\tilde{j} \in \mathcal{N}_M$ is computed in $\mathcal{N}_M$ (i.e., modulo $2M$), over long times

$$0 \leq t_n = nh \leq \varepsilon^{-N\mu}$$

with the constant C of Corollary 5.23. If $l \notin \{\, m\tilde{j} : m \in \mathbb{Z}\,\}$, then $\xi_l(t) = 0$ for all times t.

The same energy distribution holds for the continuous actions $I_l(\iota(\xi^n), \overline{\iota(\xi^n)})$. □

We conclude this section with some numerical experiments. Other experiments can be found in [16]. We consider the nonlinear wave equation with a quadratic nonlinearity and $\rho = \frac{1}{2}$

$$\frac{\partial^2}{\partial t^2} u(x,t) = \Delta u(x,t) - \frac{1}{2} u(x,t) + u(x,t)^2 \qquad (5.41)$$

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

Numerical Experiment 5.26 (Long-Time Near-Conservation of Sums of Actions, Energy, and Momentum for Deuflhard's Method)**.** We solve the quadratic nonlinear wave equation (5.41) numerically with Deuflhard's method (5.36) with $2M = 2^8$ grid points and a time step-size $h = 0.1$. As initial values for u and $\frac{\partial}{\partial t}u$ we choose

$$u(x,0) = \frac{1}{10(2-\cos(x))} \quad \text{and} \quad \frac{\partial}{\partial t} u(x,0) = \frac{1}{10(2-\sin(x))}.$$

In Figure 13 the first 20 sums of actions, discrete energy, and momentum are plotted on a time interval of length 10^7. The near-conservation of these quantities is explained by Corollary 5.23.

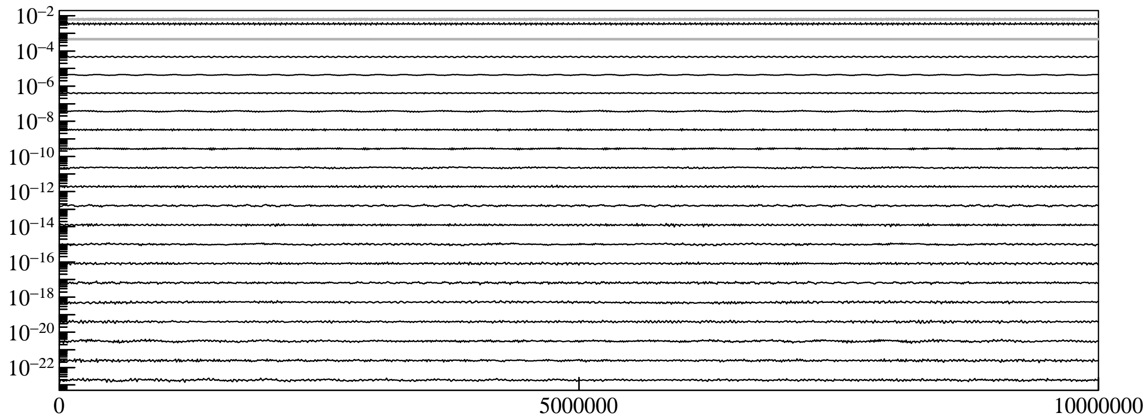

Figure 13: Numerical Experiment 5.26: Actions (black lines), discrete energy (upper grey line), and momentum (lower grey line).

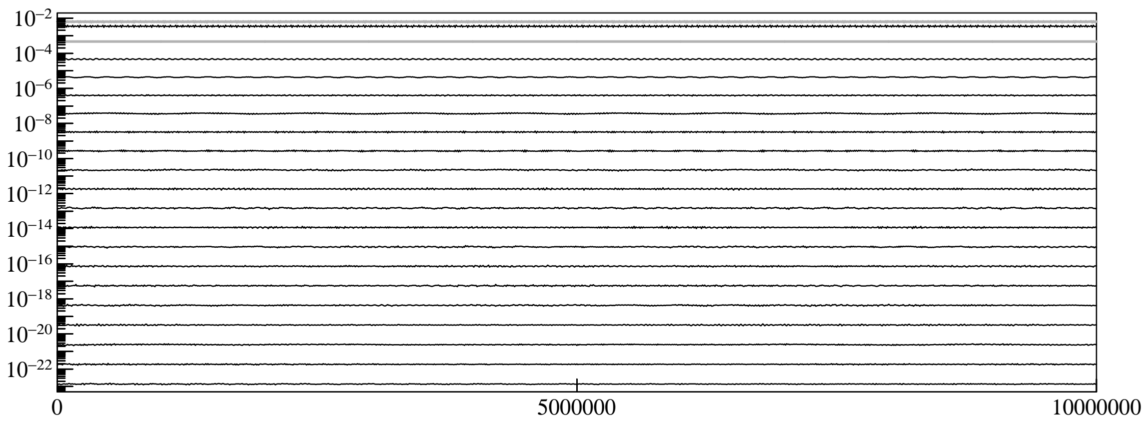

Figure 14: Numerical Experiment 5.27: Actions (black lines), discrete energy (upper grey line), and momentum (lower grey line).

Numerical Experiment 5.27 (Long-Time Near-Conservation of Sums of Actions, Energy, and Momentum for the Mollified Impulse Method)**.** We perform the same numerical experiment as in 5.26 but with the mollified impulse method (5.38) with $\phi = \mathrm{sinc}$ instead of Deuflhard's method ($\phi = 1$). Again, we observe long-time near-conservation of sums of actions, discrete energy, and momentum, see Figure 14.

Numerical Experiment 5.28 (Long-Time Energy Distribution (b) for Deuflhard's Method)**.** We choose

$$u(x,0) = \frac{\partial}{\partial t} u(x,0) = \frac{1}{20}\cos(15x) = \frac{1}{40}e^{15ix} + \frac{1}{40}e^{-15ix} \tag{5.42}$$

as initial value for (5.41), i.e., all the energy is located in a pair of modes (2.22b). This initial energy distribution is plotted in grey dots in Figure 15. For the numerical solution of (5.41) we choose Deuflhard's method (5.36) with a time step-size $h = 0.1$ and $2M = 2^7$ grid points. At time $t = 10^7$ we get the energy distribution plotted in black dots in Figure

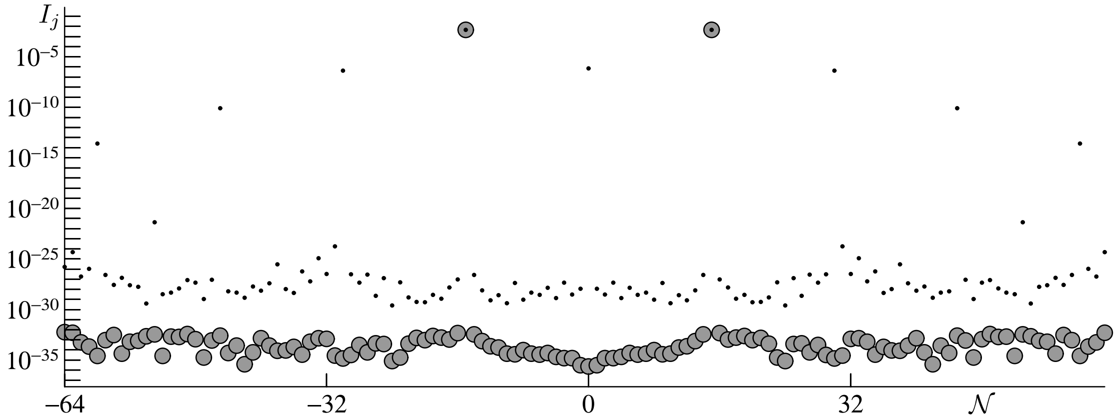

Figure 15: Numerical Experiment 5.28: Energy distribution at time $t = 0$ (grey dots) and $t = 10^7$ (black dots) for the two-mode initial value (5.42).

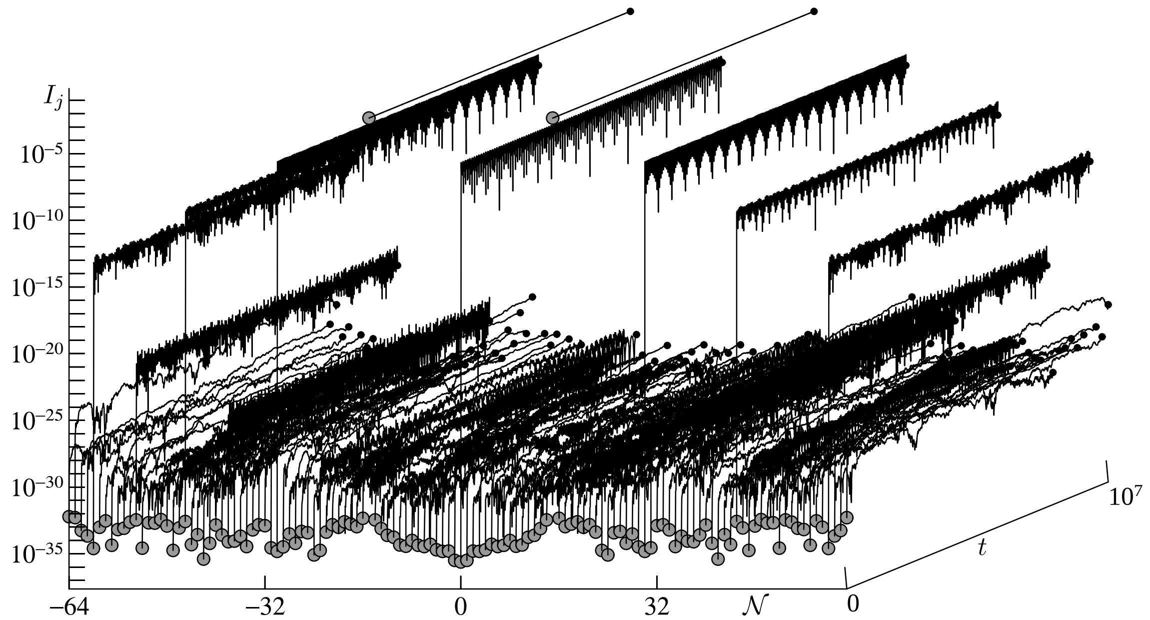

Figure 16: Numerical Experiment 5.28: Time evolution of the energy distribution for the two-mode initial value (5.42).

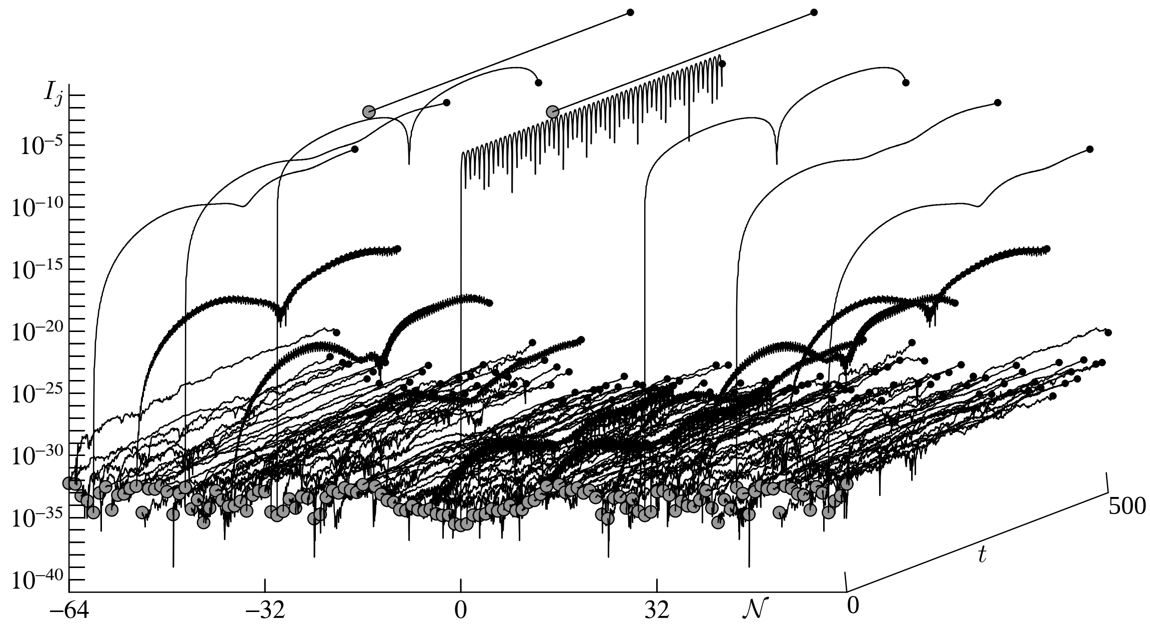

Figure 17: Numerical Experiment 5.28: Time evolution of the energy distribution for the two-mode initial value (5.42) on a short time interval.

15. The time evolution of the energy distribution on the time interval $0 \leq t \leq 10^7$ is plotted in Figure 16. The short-time evolution of the energy distribution on $0 \leq t \leq 500$ is plotted in Figure 17.

We observe the behaviour as stated in Corollary 5.24. Note that even less energy than expected is distributed. This is certainly due to the special form of the nonlinearity in the nonlinear wave equations where frequencies appear in the denominator, see also Sections 1.5 and 2.9.

In contrast to the corresponding Experiment 5.22 for the cubic nonlinear Schrödinger equation the energy is distributed not only among odd multiples of $\tilde{j} = 15$ but among all of its multiples.

Numerical Experiment 5.29 (Long-Time Energy Distribution (b) for the Mollified Impulse Method)**.** We perform the same numerical experiment as in 5.28 but use the mollified impulse method (5.38) with $\phi = \mathrm{sinc}$ instead of Deuflhard's method. We obtain an energy distribution as plotted in Figure 18.

Compared to Deuflhard's method (see Figure 15) even less energy is distributed. The reason for this behaviour is the filter function $\phi = \mathrm{sinc}$ used in the mollified impulse method which reduces the influence of the nonlinearity for large frequencies and large time step-sizes.

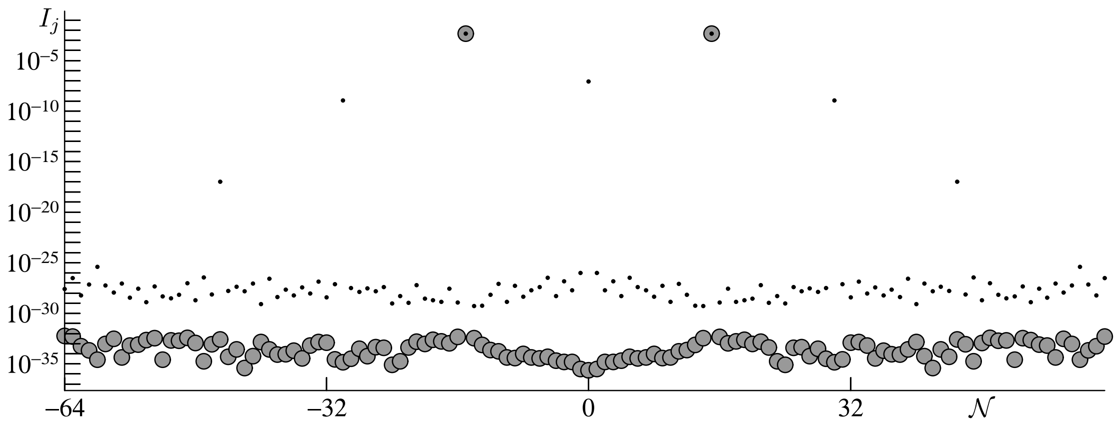

Figure 18: Numerical Experiment 5.29: Energy distribution at time $t = 0$ (grey dots) and $t = 10^7$ (black dots) for the two-mode initial value (5.42).

5.8 Example — The Störmer–Verlet Method for Nonlinear Wave Equations

In this section we consider again the nonlinear wave equation (5.34) with periodic boundary conditions, see also equations (1.14), (2.32), and (4.20). We study a full discretization of this equation by the famous *Störmer–Verlet method*. We apply this time discretization again to the spatial semi-discretization in space by a spectral Galerkin method as studied in Section 4.6.

The Störmer–Verlet Method. The Störmer–Verlet method applied to the spatial semi-discretization of the nonlinear wave equation reads

$$u_j^{n+1} - 2u_j^n + u_j^{n-1} = h^2(-\omega_j^2 u_j^n + g_j(u^n)), \tag{5.43a}$$

$$2hv_j^n = u_j^{n+1} - u_j^{n-1}. \tag{5.43b}$$

The Störmer–Verlet Method as a Trigonometric Integrator. Following [36, Chapter XIII.8] we introduce for step-sizes in the linear stability interval,

$$h\omega_j \le c < 2 \quad \text{for all } j \in \mathcal{N}_M,$$

modified frequencies $\omega_j^{M,h}$ with

$$1 - \frac{h^2\omega_j^2}{2} = \cos(\omega_j^{M,h} h) \tag{5.44}$$

and minimal $\omega_j^{M,h} \ge 0$. Moreover, we introduce new variables

$$\hat u^n = (\hat u_j^n)_{j\in\mathcal{N}} = (\operatorname{sinc}(\omega_j^{M,h}h)^{\frac12} u_j^n)_{j\in\mathcal{N}} = \operatorname{sinc}(\boldsymbol{\omega}^{M,h}h)^{\frac12} u^n \quad \text{and} \quad \hat v^n = \operatorname{sinc}(\boldsymbol{\omega}^{M,h}h)^{-\frac12} v^n.$$

Note that $\operatorname{sinc}(\omega_j^{M,h}h)$ is positive. In the new variables the Störmer–Verlet method (5.43) becomes the mollified impulse method

$$\hat u_j^{n+1} - 2\cos(\omega_j^{M,h}h)\hat u_j^n + \hat u_j^{n-1} = h^2 \operatorname{sinc}(\omega_j^{M,h}h)^{\frac12} g_j((\operatorname{sinc}(\boldsymbol{\omega}^{M,h}h)^{-\frac12}\hat u^n), \tag{5.45a}$$

$$2h\operatorname{sinc}(\omega_j h)\hat v_j^n = \hat u_j^{n+1} - \hat u_j^{n-1} \tag{5.45b}$$

with $\phi = \operatorname{sinc}^{-\frac12}$. This filter function is bounded under the restriction $h\omega_j \le c < 2$ by a constant depending only on c.

Long-Time Analysis of the Störmer–Verlet Method. As in [16], the interpretation of the Störmer–Verlet method (5.43) as a trigonometric integrator (5.45) allows us to perform a long-time analysis as for the trigonometric integrators in Section 5.7. We assume that the modified frequencies (5.44) together with the time step-size h satisfy the non-resonance condition 5.5. By Corollary 5.23 we then have long-time near-conservation of sums of actions in the new variables,

$$\sum_{m\in\mathbb{N}} m^{2s} \frac{\left|\sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\hat\xi^n, \overline{\hat\xi^n}) - \sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\hat\xi^0, \overline{\hat\xi^0})\right|}{\varepsilon^2} \le C\varepsilon^{\frac12}, \tag{5.46}$$

where

$$\hat\xi_j = \frac{(\omega_j^{M,h})^{\frac12}\hat u_j + i(\omega_j^{M,h})^{-\frac12}\hat v_j}{\sqrt{2}}.$$

This can be transferred to a result in the original variables. Note that the sums of actions read in terms of the original variables u and v

$$\sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi,\overline{\xi}) = I_l^M(\xi,\overline{\xi}) + I_{-l}^M(\xi,\overline{\xi}) = \omega_l|u_l|^2 + \omega_l^{-1}|v_l|^2$$

if $l \in \mathcal{N}_M$ with $|l| = m$. This implies

$$\sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi,\overline{\xi}) - \sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\hat\xi,\overline{\hat\xi}) = \Big(\frac{\omega_l}{\omega_l^{M,h}\operatorname{sinc}(\omega_l^{M,h}h)} - 1\Big)\omega_l^{M,h}|\hat u_l|^2 + \Big(\frac{\omega_l^{M,h}\operatorname{sinc}(\omega_l^{M,h}h)}{\omega_l} - 1\Big)(\omega_l^{M,h})^{-1}|\hat v_l|^2.$$

Using the relation (5.44), i.e., $\sin(\frac{1}{2}\omega_l^{M,h} h) = \frac{1}{2}\omega_l h$, we get

$$\frac{\omega_l}{\omega_l^{M,h}\,\mathrm{sinc}(\omega_l^{M,h} h)} = \frac{1}{\cos(\frac{1}{2}\omega_l^{M,h} h)}$$

and hence

$$\Big|\sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi,\overline{\xi}) - \sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\hat{\xi},\overline{\hat{\xi}})\Big| \le Ch^2 \sum_{l\in\mathcal{N}_M:|l|=m} |l|^2 I_l^M(\hat{\xi},\overline{\hat{\xi}})$$

with a constant C depending only on ρ and $\omega_M h = c < 2$. This finally implies with (5.46) also near-conservation of sums of discrete actions in the original variables

$$\sum_{m\in\mathbb{N}} m^{2s-2}\frac{|\sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi^n,\overline{\xi^n}) - \sum_{l\in\mathcal{N}_M:|l|=m} I_l^M(\xi^0,\overline{\xi^0})|}{\varepsilon^2} \le C(\varepsilon^{\frac{1}{2}} + h^2)$$

over long times

$$0 \le t_n = nh \le \varepsilon^{-N}.$$

The same estimate holds true for the continuous actions since Assumption 4.1 is satisfied. Note that we have in this estimate a factor m^{2s-2} instead of m^{2s} as in (5.12).

We then get regularity

$$\|\xi^n\|_{s-1} \le 2\varepsilon + C\varepsilon h$$

and near-conservation of mass

$$\frac{|m(\xi^n,\overline{\xi^n}) - m(\xi^0,\overline{\xi^0})|}{\varepsilon^2} \le C(\varepsilon^{\frac{1}{2}} + h^2)$$

over long times

$$0 \le t_n = nh \le \varepsilon^{-N}$$

along the numerical solution computed with the Störmer–Verlet method (5.43). Note that the long-time regularity is in a weaker norm than the regularity of the initial value. Applying the same arguments as for the long-time analysis of Deuflhard's method and the mollified impulse method we get near-conservation of energy

$$\frac{|H(\xi^n,\overline{\xi^n}) - H(\xi^0,\overline{\xi^0})|}{\varepsilon^2} \le C(\varepsilon^{\frac{1}{2}} + h^2)$$

and near-conservation of momentum

$$\frac{|K(\xi^n,\overline{\xi^n}) - K(\xi^0,\overline{\xi^0})|}{\varepsilon^2} \le CM^{-s+1}\varepsilon t_n,$$

over long times

$$0 \le t_n = nh \le \varepsilon^{-N}.$$

In summary we have shown similar long-time results for the Störmer–Verlet method (5.43) as in Corollary 5.23 for Deuflhard's method (5.36) and the mollified impulse method (5.38).

Numerical Experiment 5.30 (Long-Time Near-Conservation of Sums of Actions, Energy, and Momentum for the Störmer–Verlet Method)**.** We perform the same numerical experiment with the quadratic nonlinear wave equation (5.41) as in 5.26 but this time with the Störmer–Verlet method (5.43). The time step-size $h = 0.1$ does not fulfill the stability condition $h\omega_j \leq c < 2$ for all $j \in \mathcal{N}_M$, see Figure 19. Choosing a time step-size $h = 0.01$ we get again long-time near-conservation of sums of actions, discrete energy, and momentum, see Figure 19.

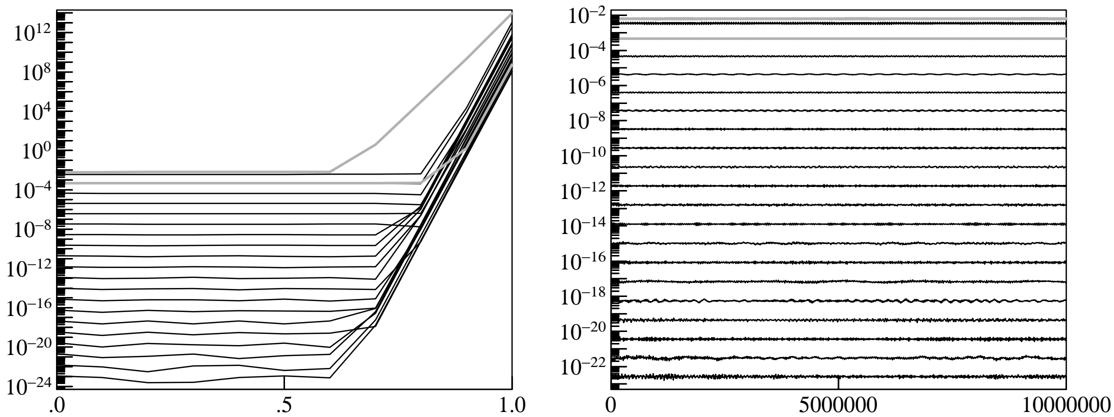

Figure 19: Numerical Experiment 5.30: Actions (black lines), discrete energy (upper grey line), and momentum (lower grey line) for $h = 0.1$ (left) and $h = 0.01$ (right).

6 Modulated Fourier Expansions of Full Discretizations of Hamiltonian Partial Differential Equations

The proof of Theorems 5.4, 5.6, and 5.12 on the long-time near-conservation of actions along fully discrete weakly nonlinear Hamiltonian partial differential equations (5.4) and (5.5) given in this chapter follows the lines of the corresponding proofs for the exact solution presented in Chapter 3. Once again, modulated Fourier expansions are the main tool. It turns out that the ideas and the techniques used in the continuous situation also apply in the fully discrete setting.

Throughout this chapter we work under the assumptions of Theorem 5.4 (and later also Theorems 5.6 and 5.12). We consider small initial values

$$\|\xi^0\|_s \leq \varepsilon.$$

For fixed N we study the numerical solution defined by the Lie–Trotter splitting (5.4) or the Strang splitting (5.5) on time intervals of length ε^{-N}. From Assumption 5.1 on the regularity of the flow of the nonlinearity $P^{M,h}$ we have constants C_1, $s_0 \leq s$, C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$, from the condition of zero momentum 5.2 we have constants c_2, C_2, and σ, and from the non-resonance condition 5.5 we have constants C_0 and ε_0. For convenience, we write in this chapter $\mathcal{N}$ instead of $\mathcal{N}_M$ and ω_j instead of $\omega_j^{M,h}$.

On the Strang Splitting. Without loss of generality we prove Theorems 5.4, 5.6, and 5.12 only for the Lie–Trotter splitting (5.4). Indeed, the results for the Strang splitting (5.5) follow immediately from the corresponding results for the Lie–Trotter splitting since the result of the Strang-splitting after n time steps differs from the one of the Lie–Trotter only by half a time step with the nonlinearity at the beginning and at the end (5.6) which of course do not affect the long-time behaviour.

The Splitting Integrator in Formulas. We now introduce rather complicated formulas for the Lie–Trotter splitting (5.4) which will be needed below.

The flow $\Phi_h^{H_0}$ of (5.3a) is readily written down,

$$\Phi_h^{H_0}(\xi) = (e^{-i\omega_j h}\xi_j)_{j\in\mathcal{N}},$$

and the regularity assumption 5.1 yields an expression for the flow Φ_h^P of (5.3b). Putting the two expressions together we get the following formula for the Lie–Trotter splitting,

$$\xi_j^{n+1} = e^{-i\omega_j h}\xi_j^n + e^{-i\omega_j h}\sum_{m+m'=2}^{\infty}\;\sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} h\widehat{P}_{j,k,l}\xi_{k^1}^n\cdots\xi_{k^m}^n\overline{\xi_{l^1}^n\cdots\xi_{l^{m'}}^n} \tag{6.1}$$

with $\widehat{P}_{j,k,l} = \widehat{P}_{j,k,l}(h)$. Due to the condition of zero momentum 5.2 the coefficients in this expression satisfy $\widehat{P}_{j,k,l} = 0$ for $j \neq k^1 + \cdots + k^m - l^1 - \cdots - l^{m'}$.

6.1 Modulated Fourier Expansions for the Full Discretization

The Modulation System. As for the exact solution of the Hamiltonian equations of motion in Section 3.1 we seek for a modulated Fourier expansion

$$\widetilde{\xi}_j(t) = \sum_{\mathbf{k}} z_j^{\mathbf{k}}(\varepsilon t) e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$$

of the fully discrete solution ξ^n, $n = 0, 1, 2, \dots$, given by the Lie–Trotter splitting (6.1). The sum in the expansion runs again over all sequences $\mathbf{k} \in \mathbb{Z}^{\mathcal{N}}$ of integers with finitely many nonzero entries indexed by $\mathcal{N}$. The requirement $\widetilde{\xi}_j(t_n) = \xi_j^n$ with $t_n = nh$ for $n = 0, 1, 2, \dots$ and a comparison of the coefficients of $e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t}$ lead to equations

$$\begin{aligned} z_j^{\mathbf{k}}(\varepsilon(t+h)) e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})h} &= e^{-i\omega_j h} z_j^{\mathbf{k}}(\varepsilon t) \\ &\quad + e^{-i\omega_j h} \sum_{m+m'=2}^{\infty} \sum_{\substack{\mathbf{k}^1+\dots+\mathbf{k}^m \\ -\mathbf{l}^1-\dots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} h\widehat{P}_{j,k,l} z_{k^1}^{\mathbf{k}^1} \cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1} \cdots z_{l^{m'}}^{\mathbf{l}^{m'}}} \end{aligned}$$

for the modulation functions $z_j^{\mathbf{k}}$ in the modulated Fourier expansion, where the modulation functions in the nonlinearity are evaluated at time εt. A Taylor expansion of $z_j^{\mathbf{k}}(\varepsilon(t+h))$ yields the modulation system

$$\begin{aligned} &\frac{e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h}-1}{h} z_j^{\mathbf{k}}(\varepsilon t) + \varepsilon \dot{z}_j^{\mathbf{k}}(\varepsilon t) e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h} + \sum_{\ell=2}^{\infty} \frac{\varepsilon^\ell h^{\ell-1}}{\ell!} (z_j^{\mathbf{k}})^{(\ell)}(\varepsilon t) e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h} \\ &\qquad = \sum_{m+m'=2}^{\infty} \sum_{\substack{\mathbf{k}^1+\dots+\mathbf{k}^m \\ -\mathbf{l}^1-\dots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} \widehat{P}_{j,k,l} z_{k^1}^{\mathbf{k}^1} \cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1} \cdots z_{l^{m'}}^{\mathbf{l}^{m'}}}, \end{aligned} \tag{6.2a}$$

where the dot and $\cdot^{(\ell)}$ denote derivatives with respect to the slow time $\tau = \varepsilon t$. The initial condition $\widetilde{\xi}(0) = \xi^0$ further yields

$$\sum_{\mathbf{k}} z_j^{\mathbf{k}}(0) = \xi_j^0. \tag{6.2b}$$

Note that the modulation system (6.2) for fully discrete Hamiltonian partial differential equations is formally very similar to the one (3.3) for the exact solution of such equations. In both systems we have the modulation function multiplied with a possibly small number $\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j$ or $(e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h} - 1)/h$, we have its derivative multiplied with ε, and we have a nonlinearity. In the modulation system for the fully discrete equation we have in addition higher derivatives of the modulation function multiplied by corresponding powers of ε.

Formal Analysis of the Modulation System. The modulation system (3.3) for the exact solution of a Hamiltonian partial differential equations is again Hamiltonian, see Section 3.1. For the modulation system of the fully discrete solution (6.2) this is — in general — not true anymore. This is the major difference in the analysis of the exact and the numerical solution.

Of course, the presence of higher derivatives is a first problem in establishing a Hamiltonian structure in the modulation system. However, for our analysis it would be sufficient to establish a Hamiltonian structure of the nonlinear term in the modulation system. But this is also impossible in general since a possible Hamiltonian function $\mathbf{P}$ for the nonlinear term in the modulation system does in general not satisfy the condition $\overline{\mathbf{P}(\mathbf{z},\mathbf{w})} = \mathbf{P}(\overline{\mathbf{w}},\overline{\mathbf{z}})$ that we imposed in Section 1.1 on Hamiltonian functions.

To exemplify this fact, let us consider the Lie–Trotter split-step Fourier method applied to the cubic nonlinear Schrödinger equation (5.29) studied in Section 5.6. We verified in Section 5.6 that the nonlinearity in the modulation system consists in this situation of terms of the form

$$\sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^{m'+1}\\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{\substack{k^1+\cdots+k^{m'+1}\\ -l^1-\cdots-l^{m'}=j}} \frac{(-i)^{m'}h^{m'-1}}{m'!} \xi_{k^1}^{\mathbf{k}^1}\cdots\xi_{k^{m'+1}}^{\mathbf{k}^{m'+1}} \overline{\xi_{l^1}^{\mathbf{l}^1}\cdots\xi_{l^{m'}}^{\mathbf{l}^{m'}}}$$

for $m' \geq 1$. In a possible Hamiltonian function this would lead to a term of the form

$$\sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^{m'+1}\\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'+1}=\mathbf{0}}} \sum_{\substack{k^1+\cdots+k^{m'+1}\\ -l^1-\cdots-l^{m'+1}=0}} \frac{(-i)^{m'}h^{m'-1}}{(m'+1)!} \xi_{k^1}^{\mathbf{k}^1}\cdots\xi_{k^{m'+1}}^{\mathbf{k}^{m'+1}} \overline{\xi_{l^1}^{\mathbf{l}^1}\cdots\xi_{l^{m'+1}}^{\mathbf{l}^{m'+1}}}.$$

But for odd m' this term does not fulfill the above condition on Hamiltonian functions. For trigonometric integrators for the nonlinear wave equation as studied in Section 5.7 this situation does not occur since the coefficients $\widehat{P}_{j,k,l}$ in the corresponding modulation system agree with the coefficients $P_{j,k,l}$ originating from the nonlinear Hamiltonian function $P^{M,h} = P^M$, see also [16].

The reason for the difference between the modulation systems for the exact and the numerical solution is the same as the reason why we impose the regularity assumption 5.1 on the flow of the nonlinearity $P^{M,h}$ instead of the nonlinearity itself as for the exact solution, see Assumption 2.1: The modulation system (6.2) was derived by considering the numerical solution itself (and not the differential equations determining this numerical solution), whereas the modulation system (3.3) for the exact solution was derived by considering the equations of motion determining the exact solution (and not the exact solution itself).

Introduction of an Auxiliary Modulation System. To overcome the problem of a missing Hamiltonian structure of the modulation system (6.2a) we consider an auxiliary modulation system related to the flow of the nonlinearity $P^{M,h}$ but based on the equations of motion determining this flow. We follow the lines of [30] and consider the auxiliary modulation system

$$i\frac{d}{dt}v_j^{\mathbf{k}} = \sum_{m+m'=2}^{\infty} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m\\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} P_{j,k,l} v_{k^1}^{\mathbf{k}^1}\cdots v_{k^m}^{\mathbf{k}^m} \overline{v_{l^1}^{\mathbf{l}^1}\cdots v_{l^{m'}}^{\mathbf{l}^{m'}}}. \tag{6.3}$$

Up to a summand $(\mathbf{k}\cdot\boldsymbol{\omega})v_j^{\mathbf{k}}$, this is the modulation system that we would obtain from the equations of motion (5.3b) and (5.8) of the nonlinearity $P^{M,h}$, i.e., from the differential equation determining the nonlinear step of the Lie–Trotter splitting (5.4). Since this modulation system is directly related to Hamiltonian equations of motion, we can detect formal invariants

$$\mathbf{K}_l(\mathbf{v},\mathbf{u}) = \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} k_l v_j^{\mathbf{k}} u_j^{\mathbf{k}} \tag{6.4}$$

as in Section 3.1 using Proposition 1.4 and the invariance of the associated Hamiltonian function

$$\mathbf{P}(\mathbf{v},\mathbf{u}) = \sum_{m,m'=0}^{\infty} \sum_{\substack{\mathbf{k}^1+\dots+\mathbf{k}^m\\ -\mathbf{l}^1-\dots-\mathbf{l}^{m'+1}=\mathbf{0}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'+1}} P_{k,l} v_{k^1}^{\mathbf{k}^1}\cdots v_{k^m}^{\mathbf{k}^m} u_{l^1}^{\mathbf{l}^1}\cdots u_{l^{m'+1}}^{\mathbf{l}^{m'+1}}$$

under the transformation $v_j^{\mathbf{k}} \mapsto e^{i\theta k_l} v_j^{\mathbf{k}}$. Here, the coefficients $P_{k,l}$ are the coefficients of the Hamiltonian nonlinearity $P^{M,h}$, and hence we have $\overline{\mathbf{P}(\mathbf{v},\mathbf{u})} = \mathbf{P}(\overline{\mathbf{u}},\overline{\mathbf{v}})$.

Outline of the Analysis of the Modulation System. In summary, we are not able to detect a Hamiltonian structure (and subsequently formal invariants) in the modulation system (6.2) originating from the Lie–Trotter splitting but we can detect a Hamiltonian structure in the modulation system (6.3) originating from the differential equations determining the individual steps of the Lie–Trotter splitting.

The modulation system (6.2) is not useless however since we use this modulation system to determine an approximate solution in Section 6.2. Due to the analogy of the modulation system (6.2) with the modulation system (3.3) of the exact solution, this can be done in a very similar way as in Section 3.2. The same is true for the estimates of the iterated modulated Fourier expansion in Section 6.3 and for the comparison of the modulated Fourier expansion with the (exact) numerical solution in Section 6.4.

The formal invariants of the modulation system (6.3) are then needed to extend the considered time intervals to long ones in Section 6.5. In order to complete the analysis, we finally relate the solutions of the two modulation systems to each other.

6.2 Iterative Solution of the Modulation System

In this section we construct as in Section 3.2 iteratively an approximate solution of the modulation system (6.2).

Cut-Off. As in Section 3.2 we cut off all summands of the nonlinearity in the modulation system (6.2) with $m+m' > L$, where again

$$L = 2N + 4 + 4s_0,$$

and we set all modulation functions $z_j^{\mathbf{k}}$ with $\|\mathbf{k}\| > L$ to zero. In contrast to the modulation system (3.3) for the exact solution, the modulation system (6.2) also contains higher derivatives of the modulation functions $z_j^{\mathbf{k}}$. We truncate all derivatives greater than $\frac{L}{2}$.

The Iteration. The iteration is constructed in exactly the same way as in Section 3.2 by isolating the dominant terms in (6.2a), but now the (possibly small) denominators are $(e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1)/h$ instead of $\mathbf{k}\cdot\boldsymbol{\omega} - \omega_j$. With the notation

$$\mathcal{S}_{\varepsilon,h} = \{\, (j,\mathbf{k}) \in \mathcal{N} \times \mathbb{Z}^{\mathcal{N}} : \mathbf{k} \neq \langle j \rangle,\ \|\mathbf{k}\| \leq L,\ |e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1|/h \geq \varepsilon^{\frac{1}{2}} \,\}$$

the iteration then reads on $0 \leq \tau \leq 1$

$$\begin{aligned} \Big[z_j^{\mathbf{k}}\Big]^{n+1} = \frac{h}{e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1} \Big[& - \sum_{\ell=1}^{L/2} \frac{\varepsilon^\ell h^{\ell-1}}{\ell!} (z_j^{\mathbf{k}})^{(\ell)} e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} \\ & + \sum_{m+m'=2}^{L} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} \widehat{P}_{j,k,l} z_{k^1}^{\mathbf{k}^1} \cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1} \cdots z_{l^{m'}}^{\mathbf{l}^{m'}}} \Big]^n \end{aligned} \tag{6.5a}$$

for $(j,\mathbf{k}) \in \mathcal{S}_{\varepsilon,h}$,

$$\begin{aligned} \Big[\dot z_j^{\langle j\rangle}\Big]^{n+1} = \varepsilon^{-1} \Big[& - \sum_{\ell=2}^{L/2} \frac{\varepsilon^\ell h^{\ell-1}}{\ell!} (z_j^{\langle j\rangle})^{(\ell)} e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} \\ & + \sum_{m+m'=2}^{L} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\langle j\rangle}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} \widehat{P}_{j,k,l} z_{k^1}^{\mathbf{k}^1} \cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1} \cdots z_{l^{m'}}^{\mathbf{l}^{m'}}} \Big]^n \end{aligned} \tag{6.5b}$$

for indices $(j, \langle j \rangle)$ with initial value

$$\Big[z_j^{\langle j\rangle}(0)\Big]^{n+1} = \xi_j^0 - \Big[\sum_{\mathbf{k}\neq\langle j\rangle} z_j^{\mathbf{k}}(0)\Big]^n, \tag{6.5c}$$

and

$$\Big[z_j^{\mathbf{k}}\Big]^{n+1} = 0 \tag{6.5d}$$

for near-resonant indices

$$(j,\mathbf{k}) \in \mathcal{R}_{\varepsilon,h} = \{\, (j,\mathbf{k}) \in \mathcal{N} \times \mathbb{Z}^{\mathcal{N}} : \mathbf{k} \neq \langle j \rangle,\ \|\mathbf{k}\| \leq L,\ |e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1|/h < \varepsilon^{\frac{1}{2}} \,\}.$$

Initially we set again $[z_j^{\mathbf{k}}]^0 = 0$ for $\mathbf{k} \neq \langle j \rangle$ and $[z_j^{\langle j\rangle}]^0 = \xi_j^0$ on $0 \leq \tau \leq 1$.

Abstract Formulation of the Iteration. We use the notation $[[\mathbf{k}]]$ and the rescalings $c_j^{\mathbf{k}} = \varepsilon^{-[[\mathbf{k}]]} z_j^{\mathbf{k}}$ and $\hat c_j^{\mathbf{k}} = \varepsilon^{-[[\mathbf{k}]]} \mathbf{j}^{(s-s_0)|\mathbf{k}|} z_j^{\mathbf{k}}$ as in Section 3.2, and we split again the rescaled variables $c_j^{\mathbf{k}} = a_j^{\mathbf{k}} + b_j^{\mathbf{k}}$ and $\hat c_j^{\mathbf{k}} = \hat a_j^{\mathbf{k}} + \hat b_j^{\mathbf{k}}$ with $a_j^{\mathbf{k}} = \hat a_j^{\mathbf{k}} = 0$ for $\mathbf{k} \neq \langle j \rangle$ and $b_j^{\mathbf{k}} = \hat b_j^{\mathbf{k}} = 0$ for $(j,\mathbf{k}) \notin \mathcal{S}_{\varepsilon,h}$. We can again reformulate the iteration for the rescaled variables leading to similar formulas as (3.8) and (3.9) containing higher derivatives of the modulation functions and other denominators.

6.3 Estimating the Iterated Modulation Functions

Since the modulation system (6.2), for which we constructed iteratively an approximate solution $[\mathbf{z}]^n$ in the preceding Section 6.2, is qualitatively the same as the modulation system (3.3), whose iterated modulation functions were estimated in Section 3.3, we can proceed as in this section to estimate the iterated modulation functions (6.5) of (6.2).

Size of the Iterated Modulation Functions. The estimates of the iterated modulation functions in Proposition 3.2 can be proven in the same way as in Section 3.3 for the new iterated modulation functions (6.5). We just mention the differences.

• The (possibly small) denominators are now $(e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h}-1)/h$ instead of $\mathbf{k}\cdot\boldsymbol{\omega}-\omega_j$ and can be controlled in the same way as in Section 3.3 using the definition of near-resonant indices in the non-resonance condition 5.5 instead of the non-resonance condition 2.3 used there.

• The nonlinearity in the modulation system (6.2) can be controlled in the same way as the nonlinearity in (3.3). Indeed, the regularity assumption 5.1 on the flow of $P^{M,h}$ corresponds exactly to the regularity assumption 2.1 when considered on the level of modulation systems (6.2) and (3.3), respectively.

• The higher derivatives appearing in the modulation system (6.2) don't affect the estimates of Section 3.3 since they only imply a stronger dependence on ℓ and L of the constants.

Keeping these arguments in mind, the same proof as in Section 3.3 yields the following proposition on the size of the iterated modulation functions.

Proposition 6.1 (Size of the Iterated Modulation Functions)**.** *We have on* $0 \le \tau \le 1$

$$|||[\mathbf{c}^{(\ell)}]^n|||_s \le C$$

with a constant C *depending only on* $C_{L,s}$ *from the regularity assumption 5.1, the number of derivatives* ℓ*, the number of iterations* n*, and* L*.*

The same estimate holds true if $\mathbf{c}$ *and* s *are replaced by* $\hat{\mathbf{c}}$ *and* s_0*, respectively, with a constant depending in addition on* C_{L,s_0}*.* □

Defect of the Iterated Modulation Functions. We now study the defect

$$\Big[d_j^{\mathbf{k}}\Big]^n = \Big[\frac{e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h}-1}{h} z_j^{\mathbf{k}}(\varepsilon t) + \sum_{\ell=1}^{\infty} \frac{\varepsilon^\ell h^{\ell-1}}{\ell!} (z_j^{\mathbf{k}})^{(\ell)}(\varepsilon t) e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h} - \sum_{m+m'=2}^{\infty} \sum_{\substack{\mathbf{k}^1+\dots+\mathbf{k}^m \\ -\mathbf{l}^1-\dots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} \widehat{P}_{j,k,l} z_{k^1}^{\mathbf{k}^1}\cdots z_{k^m}^{\mathbf{k}^m} \overline{z_{l^1}^{\mathbf{l}^1}\cdots z_{l^{m'}}^{\mathbf{l}^{m'}}}\Big]^n$$

in the modulation system (6.2a) after n iterations and the defect

$$\Big[\widetilde{d}_j^{\langle j\rangle}(0)\Big]^n = \Big[\sum_{\mathbf{k}} z_j^{\mathbf{k}}(0)\Big]^n - \xi_j^0$$

in the initial conditions (6.2b) of the modulation system.

The cut-off defects $\mathbf{g}$, $\mathbf{h}$, and $\mathbf{p}$ resulting from setting $z_j^{\mathbf{k}} = 0$ for $(j, \mathbf{k}) \in \mathcal{R}_{\varepsilon,h}$ or $\|\mathbf{k}\| > L$ and truncating the nonlinearity for $m + m' > L$ (see Section 3.3) can be estimated as in Proposition 3.3 of Section 3.3. The additional cut-off effect resulting from the truncation of the Taylor expansion of $z_j^{\mathbf{k}}(\varepsilon(t+h))$ can be estimated using the integral form of the remainder term of the Taylor expansion,

$$\sum_{\ell=1}^{\infty} \frac{(\varepsilon h)^\ell}{\ell!} (z_j^{\mathbf{k}})^{(\ell)}(\varepsilon t) - \sum_{\ell=1}^{L/2} \frac{(\varepsilon h)^\ell}{\ell!} (z_j^{\mathbf{k}})^{(\ell)}(\varepsilon t) = \int_{\varepsilon t}^{\varepsilon(t+h)} \frac{(\varepsilon(t+h) - \theta)^{L/2}}{(L/2)!} (z_j^{\mathbf{k}})^{(L/2+1)}(\theta)\, d\theta.$$

In the norm $|||\cdot|||_s$ as well as in the norm $|||\cdot|||_{s_0}$ this can be estimated by $C\varepsilon^{\frac{L}{2}+1}$ using Proposition 6.1 on the size of $\mathbf{z}$ with a constant C depending only on $C_{L,s}$, C_{L,s_0}, n, and L.

The defect from the iteration can be estimated as in Section 3.3 with the modifications as used for the estimates of the size of the iterated modulation functions. We finally get the following Proposition using the same notations for the defects from the iteration as in Section 3.3 ($\mathbf{e}$ and $\mathbf{f}$).

Proposition 6.2 (Defect of the Iterated Modulation Functions)**.** *For ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, n, and L we have on $0 \le \tau \le 1$*

$$|||[\mathbf{e}^{(\ell)}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{4}}, \ |||[\mathbf{f}^{(\ell)}]^n|||_s \le C\varepsilon^{\frac{n}{4}+1}, \ |||((e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} - 1)/h) f_j^{\mathbf{k}})^{(\ell)}_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}}|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{2}},$$
$$|||[\widetilde{\mathbf{d}}(0)]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{4}}, \quad |||[\mathbf{d}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{2}} + C\varepsilon^{\frac{L}{2}}, \quad |||[\mathbf{d}]^n - [\mathbf{g}]^n|||_s \le C\varepsilon^{\frac{n}{4}+\frac{3}{2}} + C\varepsilon^{\frac{L}{2}}$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 5.1, C_0 from the non-resonance condition 5.3, the number of derivatives ℓ, the number of iterations n, and L.

The estimates for $\mathbf{e}$, $\mathbf{f}$, $\widetilde{\mathbf{d}}$, and $\mathbf{d} - \mathbf{g}$ also hold true for $\hat{\mathbf{e}}$, $\hat{\mathbf{f}}$, $\hat{\widetilde{\mathbf{d}}}$, $\hat{\mathbf{d}} - \hat{\mathbf{g}}$, and s_0 instead of $\mathbf{e}$, $\mathbf{f}$, $\widetilde{\mathbf{d}}$, $\mathbf{d} - \mathbf{g}$, and s. □

6.4 The Modulated Fourier Expansion and the Numerical Solution

In this section we show that the iterated modulated Fourier expansion

$$[\widetilde{\xi}(t)]^n = ([\widetilde{\xi}_j(t)]^n)_{j\in\mathcal{N}} \quad \text{with} \quad [\widetilde{\xi}_j(t)]^n = \sum_{\mathbf{k}} [z_j^{\mathbf{k}}(\varepsilon t)]^n e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t} \quad \text{for } j \in \mathcal{N}$$

agrees at time $t = t_\nu = \nu h$ with the numerical solution ξ^ν after ν time steps defined by the Lie–Trotter splitting (6.1) up to a small error $\varepsilon^{\frac{n}{4}+\frac{1}{2}} + \varepsilon^{\frac{L}{2}-1}$.[5] This is done as in Section 3.4 for the exact solution.

[5]The notation ν for the number of time steps in the numerical discretization is used from now on to avoid confusion with the index n denoting the number of iterations in the iterated modulation function.

Size of the Numerical Solution. For the numerical solution defined by (6.1) we get using the regularity assumption 5.1 on the flow of $P^{M,h}$ as in the proof of (2.7)

$$\|\xi^{\nu+1}\|_s \leq \|\xi^\nu\|_s + C_s h \|\xi^\nu\|_s^2$$

provided that $\|\xi^\nu\| \leq C_1$. Inductively, we get $\|\xi^{\nu+1}\|_s \leq \|\xi^0\|_s + C_s h(\|\xi^\nu\|_s^2 + \cdots + \|\xi^0\|_s^2)$. We conclude that

$$\|\xi^\nu\|_s \leq 2\varepsilon \quad \text{for } 0 \leq t_\nu = \nu h \leq \frac{1}{4C_s}\varepsilon^{-1}. \tag{6.6}$$

Size of the Iterated Modulated Fourier Expansion. The size of the iterated modulated Fourier expansion $[\widetilde{\xi}(t)]^n$ is estimated as in Section 3.4 by

$$\|[\widetilde{\xi}(t)]^n\|_s \leq |||[\mathbf{z}(\varepsilon t)]^n|||_s \leq C\varepsilon \quad \text{for } 0 \leq t \leq \varepsilon^{-1} \tag{6.7}$$

with a constant C depending only on $C_{L,s}$, n, and L.

The numerical solution ξ^ν can then be related to the iterated modulated Fourier expansion $[\widetilde{\xi}(t_\nu)]^n$ as follows.

Theorem 6.3. *Let ξ^ν be the numerical solution defined by the Lie–Trotter splitting* (5.4)*, and let*

$$[\widetilde{\xi}(t)]^n = ([\widetilde{\xi}_j(t)]^n)_{j\in\mathcal{N}} \quad \textit{with} \quad [\widetilde{\xi}_j(t)]^n = \sum_{\mathbf{k}} [z_j^{\mathbf{k}}(\varepsilon t)]^n e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t} \quad \textit{for } j \in \mathcal{N}$$

be its iterated modulated Fourier expansions with the approximate solution $[\mathbf{z}]^n$ of the modulation system (6.2) *constructed in Section 6.2. Under the regularity assumption 5.1, the condition of zero momentum 5.2, and the non-resonance condition 5.3 we have for ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, n, and L*

$$\|\xi^\nu - [\widetilde{\xi}(t_\nu)]^n\|_s \leq C\varepsilon^{\frac{n}{4}+\frac{1}{2}} + C\varepsilon^{\frac{L}{2}-1} \quad \textit{for } 0 \leq t_\nu = \nu h \leq \varepsilon^{-1}\min\Big(\frac{1}{4C_s}, 1\Big)$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 5.1, C_0 from the non-resonance condition 5.3, the number of iterations n, and L.

Proof. For notational simplicity we omit the index n denoting the number of iterations. Note that

$$\|\xi^0 - \widetilde{\xi}(0)\|_s = |||\widetilde{\mathbf{d}}(0)|||_s$$

since $\xi_j^0 - \widetilde{\xi}_j(0) = -\widetilde{d}_j^{\langle j\rangle}(0)$. Moreover, by the definition of the defect $\mathbf{d}$

$$\begin{aligned}
e^{i\omega_j h}\widetilde{\xi}_j(t_{\nu+1}) &= \sum_{\mathbf{k}} z_j^{\mathbf{k}}(\varepsilon(t_\nu + h))e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t_\nu}e^{i(\omega_j - \mathbf{k}\cdot\boldsymbol{\omega})h} \\
&= \widetilde{\xi}_j(t_\nu) + \sum_{m+m'=2}^{\infty} \sum_{k\in\mathcal{N}^m,\, l\in\mathcal{N}^{m'}} h\widehat{P}_{j,k,l}\widetilde{\xi}_{k^1}(t_\nu)\cdots\widetilde{\xi}_{k^m}(t_\nu)\overline{\widetilde{\xi}_{l^1}(t_\nu)\cdots\widetilde{\xi}_{l^{m'}}(t_\nu)} \\
&\quad + h\sum_{\mathbf{k}} d_j^{\mathbf{k}}(\varepsilon t_\nu)e^{-i(\mathbf{k}\cdot\boldsymbol{\omega})t_\nu}.
\end{aligned}$$

Subtracting this equation from the equation (6.1) determining the splitting we get

$$\|\xi^{\nu+1} - \widetilde{\xi}(t_{\nu+1})\|_s \le \|\xi^{\nu} - \widetilde{\xi}(t_\nu)\|_s + C\varepsilon h \|\xi^{\nu} - \widetilde{\xi}(t_\nu)\|_s + h |\!|\!| \mathbf{d}(t_\nu) |\!|\!|_s,$$

where we used Lemma 3.6 applied to the nonlinearity appearing in the splitting (6.1) (note that the regularity assumption 5.1 ensures that this nonlinearity has the same properties as the nonlinearity in Lemma 3.4). This estimate is valid for $0 \le t_\nu = \nu h \le \varepsilon^{-1} \min(\frac{1}{4C_s}, 1)$, where $\|\xi^\nu\|_s + \|\widetilde{\xi}(t_\nu)\|_s \le C\varepsilon \le C_1$ by (6.6) and (6.7) for ε sufficiently small. The claimed estimate now follows inductively using Proposition 6.2 on the defects $\mathbf{d}$ and $\widetilde{\mathbf{d}}$. □

6.5 The Modulated Fourier Expansion on Long Time Intervals

In this section we extend the analysis of the (iterated) modulated Fourier expansion, which is so far only valid on short time intervals of length ε^{-1}, to long time intervals ε^{-N}. For the exact solution we used for this purpose the formal invariants of the modulation system in Section 3.5. For the numerical solution studied in this section we use the formal invariants of the auxiliary modulation system (6.3) due to the lack of formal invariants of the modulation system (6.2).

Putting Together Modulated Fourier Expansions. In Sections 6.2, 6.3, and 6.4 we constructed and analysed an iterated modulated Fourier expansion $[\mathbf{z}]^n$ on a time interval $0 \le \tau = \varepsilon t \le \min(\frac{1}{4C_s}, 1)$. We now construct and analyse in the same way an iterated modulated Fourier expansion $[\widetilde{\mathbf{z}}]^n$ on a new time interval of length $\mathcal{O}(\varepsilon^{-1})$. This is done as in Section 3.5 with the exception that we have to ensure that the lengths of the time intervals are multiples of the time step-size h. We set

$$c_0 = \varepsilon h \left\lfloor \frac{\varepsilon^{-1} \min(\frac{1}{4C_s}, 1)}{h} \right\rfloor$$

and proceed as in Section 3.5 considering the time interval $c_0 \le \tau \le 2c_0$ (but with this slightly smaller c_0). In the same way as in that section, we can bound the difference $[\mathbf{z}]^n - [\widetilde{\mathbf{z}}]^n$ as follows.

Proposition 6.4. *For ε sufficiently small compared to C_1, C_{L,s_0}, $C_{L,s}$, ε_0, n, and L we have*

$$|\!|\!| [\mathbf{z}(c_0)]^n - [\widetilde{\mathbf{z}}(c_0)]^n |\!|\!|_s \le C\varepsilon^{\frac{n}{4}+\frac{1}{2}} + C\varepsilon^{\frac{L}{2}-1}$$

with a constant C depending only on C_{s_0}, C_s, C_{L,s_0}, and $C_{L,s}$ from the regularity assumption 5.1, C_0 from the non-resonance condition 5.3, the number of iterations n, and L.

The same estimate holds true if $\mathbf{z}$, $\widetilde{\mathbf{z}}$, and s are replaced by $\hat{\mathbf{z}}$, $\hat{\widetilde{\mathbf{z}}}$, and s_0, respectively. □

Analysis of the Auxiliary Modulation System. We derive an expression for the solution of the auxiliary modulation system (6.3). Recall that we derived in Assumption

5.1 an expression for the solution of the differential equation (5.8) (which is (5.3b)). This differential equation (5.8) can be written due to the regularity assumption 5.1 and the condition of zero momentum 5.2 as

$$i\frac{d}{dt}\xi_j(t) = \sum_{m+m'=2}^{\infty} \sum_{\substack{k^1+\cdots+k^m \\ -l^1-\cdots-l^{m'}=j}} P_{j,k,l}\xi_{k^1}(t)\cdots\xi_{k^m}(t)\overline{\xi_{l^1}(t)\cdots\xi_{l^{m'}}(t)},$$

where $k=(k^1,\dots,k^m)$ and $l=(l^1,\dots,l^{m'})$. This equation is very similar to the auxiliary modulation system (6.3). Therefore, the solution of the auxiliary modulation system can be derived in the same way as the solution of this equation in Assumption 5.1. Indeed, the same calculation as in Assumption 5.1 shows that

$$v_j^{\mathbf{k}}(h) = v_j^{\mathbf{k}}(0) + \sum_{m+m'=2} \sum_{\substack{\mathbf{k}^1+\cdots+\mathbf{k}^m \\ -\mathbf{l}^1-\cdots-\mathbf{l}^{m'}=\mathbf{k}}} \sum_{\substack{k^1+\cdots+k^m \\ -l^1-\cdots-l^{m'}=j}} h\widehat{P}_{j,k,l} v_{k^1}^{\mathbf{k}^1}(0)\cdots v_{k^m}^{\mathbf{k}^1 m}(0)\overline{v_{l^1}^{\mathbf{l}^1}(0)\cdots v_{l^{m'}}^{\mathbf{l}^{m'}}(0)} \tag{6.8}$$

is a formal solution of the auxiliary modulation system (6.3) with the coefficients $\widehat{P}_{j,k,l} = \widehat{P}_{j,k,l}(h)$ from (5.7). This fact heavily relies on the condition of zero momentum 5.2, since we are not able to establish the analogy between (5.8) and (6.3) otherwise. As shown in Section 6.1, the invariants $\mathbf{K}_l(\mathbf{v},\mathbf{u})$ as defined by (6.4) are conserved along $(\mathbf{v},\overline{\mathbf{v}})$ as defined by (6.4),

$$\mathbf{K}_l(\mathbf{v}(h),\overline{\mathbf{v}(h)}) = \mathbf{K}_l(\mathbf{v}(0),\overline{\mathbf{v}(0)}). \tag{6.9}$$

Relating the Modulation System (6.2) **and the Auxiliary Modulation System** (6.3)**.** If we choose $\mathbf{v}(0)=\mathbf{z}(\varepsilon t_\nu)$ as initial value of the auxiliary modulation system, then an exact solution of the modulation system (6.2) satisfies

$$e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h} z_j^{\mathbf{k}}(\varepsilon t_{\nu+1}) = v_j^{\mathbf{k}}(h)$$

due to (6.2) and (6.8). Since we do not have an exact solution of the modulation system (6.2) at our disposal but only an approximate solution $[\mathbf{z}]^n$, we get

$$e^{i(\omega_j-\mathbf{k}\cdot\boldsymbol{\omega})h}\Big[z_j^{\mathbf{k}}(\varepsilon t_{\nu+1})\Big]^n = v_j^{\mathbf{k}}(h) + h\Big[d_j^{\mathbf{k}}(\varepsilon t_\nu)\Big]^n \quad \text{for} \quad v_j^{\mathbf{k}}(0) = \Big[z_j^{\mathbf{k}}(\varepsilon t_\nu)\Big]^n,$$

where $\mathbf{d}$ is just the defect from Section 6.3. This means that our approximate solution $[\mathbf{z}]^n$ agrees at the discrete point εt_ν and $\varepsilon t_{\nu+1}$ with the solution $\mathbf{v}$ of the auxiliary modulation system (6.3) up to a small defect and a phase factor. Equation (6.9) implies almost conservation of $\mathbf{K}_l$ along discrete points of $[\mathbf{z}]^n$,

$$\begin{aligned} &\Big|\mathbf{K}_l(\mathbf{z}(\varepsilon t_{\nu+1}),\overline{\mathbf{z}(\varepsilon t_{\nu+1})}) - \mathbf{K}_l(\mathbf{z}(\varepsilon t_\nu),\overline{\mathbf{z}(\varepsilon t_\nu)})\Big| \\ &\qquad = \Big|\sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} k_l|v_j^{\mathbf{k}}(h)+hd_j^{\mathbf{k}}(\varepsilon t_\nu)|^2 - \sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} k_l|v_j^{\mathbf{k}}(0)|^2\Big| \\ &\qquad \le 2h\sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} |k_l||z_j^{\mathbf{k}}(\varepsilon t_{\nu+1})||d_j^{\mathbf{k}}(\varepsilon t_\nu)| + 3h^2\sum_{j\in\mathcal{N},\mathbf{k}\in\mathbb{Z}^{\mathcal{N}}} |k_l||d_j^{\mathbf{k}}(\varepsilon t_\nu)|^2, \end{aligned} \tag{6.10}$$

where we omit the index n denoting the number of iterations. After a multiplication by $|l|^{2s}$ and a summation over all $l \in \mathcal{N}$ the first term on the right-hand side of the last estimate can be estimated by means of Lemma 3.9. For the second term, however, we can not use this lemma since $\mathbf{d}$ contains nonzero entries for $(j, \mathbf{k}) \in \mathcal{R}_{\varepsilon,h}$. We therefore prove the following extension of Lemma 3.9 which makes use of the non-resonance condition (5.9b) in Assumption 5.3 not needed in the continuous situation in Chapters 2 and 3. Note that we have single wave modulation functions due to the condition of zero momentum 5.2, and hence $d_j^{\mathbf{k}} = 0$ for $j \neq j(\mathbf{k})$.

Lemma 6.5. *We have for* $\mathbf{d}$ *with* $d_j^{\mathbf{k}} = 0$ *for* $j \neq j(\mathbf{k})$

$$\sum_{l \in \mathcal{N}} |l|^{2s} \sum_{(j,\mathbf{k}) \in \mathcal{R}_{\varepsilon,h}} |k_l| |d_j^{\mathbf{k}}|^2 \leq C \varepsilon^{\frac{L}{2}-2-2s_0} |||\hat{\mathbf{d}}|||_{s_0}^2$$

with a constant C *depending only on* s_0, s, C_0, *and* L.

Proof. We have

$$\sum_{l \in \mathcal{N}} |l|^{2s} \sum_{(j,\mathbf{k}) \in \mathcal{R}_{\varepsilon,h}} |k_l| |d_j^{\mathbf{k}}|^2 \leq \sum_{(j,\mathbf{k}) \in \mathcal{R}_{\varepsilon,h}} |j|^{2s_0} \frac{\sum_{l \in \mathcal{N}} |k_l| |l|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|} |j|^{2s_0}} |\hat{d}_j^{\mathbf{k}}|^2,$$

and the non-resonance condition (5.9b) ensures

$$\frac{\sum_{l \in \mathcal{N}} |k_l| |l|^{2s}}{\mathbf{j}^{2(s-s_0)|\mathbf{k}|} |j|^{2s_0}} \leq C_0 \varepsilon^{\frac{L}{2}-2-2s_0}. \qquad \square$$

Now, we are in the position to prove the analogue of Proposition 3.10 in order to control $\mathbf{K}_l$ along the iterated modulated Fourier expansion and on the interface, and to relate these almost invariants and the actions.

Proposition 6.6. *For* $s \geq 2s_0$ *and for* ε *sufficiently small compared to* C_1, C_{L,s_0}, $C_{L,s}$, ε_0, $n \geq 6$, *and* $L \geq 6$ *we have for* $0 \leq \varepsilon t_\nu = \varepsilon \nu h \leq c_0$

$$\sum_{l \in \mathcal{N}} |l|^{2s} \Big| \mathbf{K}_l([\mathbf{z}(\varepsilon t_\nu)]^n, [\overline{\mathbf{z}(\varepsilon t_\nu)}]^n) - \mathbf{K}_l([\mathbf{z}(0)]^n, [\overline{\mathbf{z}(0)}]^n) \Big| \leq C \varepsilon^{\frac{n}{4}+\frac{3}{2}-2s_0} + C \varepsilon^{\frac{L}{2}-2s_0},$$

$$\sum_{l \in \mathcal{N}} |l|^{2s} \Big| \mathbf{K}_l([\mathbf{z}(c_0)]^n, [\overline{\mathbf{z}(c_0)}]^n) - \mathbf{K}_l([\widetilde{\mathbf{z}}(c_0)]^n, [\overline{\widetilde{\mathbf{z}}(c_0)}]^n) \Big| \leq C \varepsilon^{\frac{n}{4}+\frac{3}{2}-2s_0} + C \varepsilon^{\frac{L}{2}-2s_0},$$

$$\sum_{l \in \mathcal{N}} |l|^{2s} \Big| \mathbf{K}_l([\mathbf{z}(\varepsilon t_\nu)]^n, [\overline{\mathbf{z}(\varepsilon t_\nu)}]^n) - I_l^M(\xi^\nu, \overline{\xi^\nu}) \Big| \leq C \varepsilon^{\frac{5}{2}}$$

with a constant C *depending only on* C_{s_0}, C_s, C_{L,s_0}, $C_{L,s}$, s_0, *and* s *from the regularity assumption 5.1,* c_2, C_2, *and* σ *describing the asymptotics of the frequencies in Assumption 5.2,* C_0 *from the non-resonance condition 5.3, the number of iterations* n, *and* L.

Proof. The second and the third estimate are proven in exactly the same way as the corresponding estimates in Proposition 3.10.

For the first estimate we consider (6.10) since

$$\begin{aligned}&\sum_{l\in\mathcal{N}}|l|^{2s}\Big|\mathbf{K}_l([\mathbf{z}(\varepsilon t_\nu)]^n,[\overline{\mathbf{z}(\varepsilon t_\nu)}]^n)-\mathbf{K}_l([\mathbf{z}(0)]^n,[\overline{\mathbf{z}(0)}]^n)\Big|\\&\qquad\le\sum_{\nu'=1}^{\nu}\sum_{l\in\mathcal{N}}|l|^{2s}\Big|\mathbf{K}_l([\mathbf{z}(\varepsilon t_{\nu'})]^n,[\overline{\mathbf{z}(\varepsilon t_{\nu'})}]^n)-\mathbf{K}_l([\mathbf{z}(\varepsilon t_{\nu'-1})]^n,[\overline{\mathbf{z}(\varepsilon t_{\nu'-1})}]^n)\Big|.\end{aligned}\tag{6.11}$$

The first term on the right-hand side of (6.10) can be estimated with the first estimate of Lemma 3.9, Proposition 6.1 on the size of $[\hat{\mathbf{z}}]^n$, and Proposition 6.2 on the defect $[\hat{\mathbf{d}}]^n-[\hat{\mathbf{g}}]^n$ by

$$Ch\varepsilon^{-2s_0+1+\frac{n}{4}+\frac{3}{2}}+Ch\varepsilon^{-2s_0+1+\frac{L}{2}}$$

with a constant C depending on C_{s_0}, C_s, C_{L,s_0}, $C_{L,s}$, c_2, C_2, σ, C_0, n, and L. In the second term on the right-hand side of (6.10) the sum of indices $(j,\mathbf{k})\notin\mathcal{R}_{\varepsilon,h}$ can be estimated using Lemma 3.9 and Proposition 6.1 by the same quantity. In order to estimate the indices $(j,\mathbf{k})\in\mathcal{R}_{\varepsilon,h}$ in the second term on the right-hand side of (6.10) we use Lemma 6.5. Note that by Lemma 3.1 and Proposition 6.1

$$|||[\hat{\mathbf{g}}]^n|||_{s_0}^2=\sum_{j\in\mathcal{N}}|j|^{2s_0}\Big(\sum_{\mathbf{k}}\varepsilon^{[[\mathbf{k}]]}|\hat{\mathbf{F}}([\hat{\mathbf{c}}]^n)_j^{\mathbf{k}}|\Big)^2\le\varepsilon^2|||\hat{\mathbf{F}}([\hat{\mathbf{c}}]^n)|||_{s_0}^2\le C\varepsilon^3.$$

Lemma 6.5 yields for the sum of the indices $(j,\mathbf{k})\in\mathcal{R}_{\varepsilon,h}$ on the right-hand side of (6.10) the estimate

$$Ch^2\varepsilon^{3+\frac{L}{2}-2-2s_0}$$

with a constant C depending on C_{L,s_0}, $C_{L,s}$, s_0, s, C_0, n, and L. Summing up the estimate (6.10) ν times as in (6.11) proves the first estimate in the proposition (note that $\nu\le c_0\varepsilon^{-1}h^{-1}\le\varepsilon^{-1}h^{-1}$). □

From Short to Long Time Intervals — Proof of Theorem 5.4. Proposition 6.6 at hand, the extension to long time intervals can be done as in Section 3.5 putting $c_0^{-1}\varepsilon^{-N+1}$ intervals of length $c_0\varepsilon^{-1}$ together, see also Figure 4 in that section. In this way we get long-time near-conservation of discrete actions I_l^M. This implies the long-time near-conservation of continuous actions I_l if Assumption 4.1 is satisfied as in the proof of Theorem 4.2. This finally concludes the proof of Theorem 5.4.

The Modulated Fourier Expansion for Partially Resonant Frequencies and with Scaled Norms — Proof of Theorems 5.6 and 5.12. The proofs of the extensions of Theorem 5.4 to the case of partially resonant frequencies in Theorem 5.6 and of scaled norms in Theorem 5.12 are obtained by the modifications described in Sections 3.6 and 3.7 for the continuous situation.

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