

Effective Equations in Mathematical Quantum Mechanics

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Inhaltsverzeichnis

| | |
|--|------------|
| Zusammenfassung | v |
| Abstract | vii |
| Danksagung | ix |
| 1. Introduction | 1 |
| 2. Approximation of a nonlinear Schrödinger equation on periodic quantum graphs | 5 |
| 2.1. Introduction | 5 |
| 2.2. Main result | 7 |
| 2.2.1. The periodic quantum graph | 7 |
| 2.2.2. The Floquet-Bloch spectrum | 8 |
| 2.2.3. The effective amplitude equation | 11 |
| 2.2.4. The amplitude equations at the Dirac points | 13 |
| 2.3. Local existence and uniqueness | 14 |
| 2.4. Bloch transform | 16 |
| 2.4.1. Bloch transform on the real line | 17 |
| 2.4.2. The system in Bloch space | 18 |
| 2.4.3. Bloch transform for smooth functions | 18 |
| 2.5. Estimates for the residual terms | 19 |
| 2.5.1. Derivation of the effective amplitude equation | 19 |
| 2.5.2. The improved approximation | 20 |
| 2.5.3. From Fourier space to Bloch space | 21 |
| 2.5.4. Estimates in Bloch space | 23 |
| 2.6. Estimates for the error term | 26 |
| 2.7. Discussion | 27 |
| 3. Approximation of a cubic Klein-Gordon equation on periodic quantum graphs | 31 |
| 3.1. The model | 31 |
| 3.2. Main result | 32 |
| 3.2.1. The Floquet-Bloch spectrum | 32 |
| 3.2.2. The effective amplitude equation | 34 |
| 3.3. Local existence and uniqueness | 35 |
| 3.4. Derivation of the NLS approximation | 37 |
| 3.4.1. The system in Bloch space | 37 |
| 3.4.2. Derivation of the effective amplitude equation | 38 |
| 3.5. The improved approximation and estimates for the residual terms | 39 |
| 3.5.1. The improved approximation | 39 |
| 3.5.2. From Fourier space to Bloch space | 40 |

| | |
|--|-----------|
| 3.5.3. Estimates in Bloch space | 42 |
| 3.6. Estimates for the error term | 43 |
| 4. Approximation of a two-dimensional Gross-Pitaevskii equation with a periodic potential | 45 |
| 4.1. The model | 45 |
| 4.2. The spectral situation | 47 |
| 4.2.1. Wannier function decomposition in one dimension | 47 |
| 4.2.2. Properties of the harmonic oscillator | 50 |
| 4.3. Main result | 51 |
| 4.4. Computation of the residual | 52 |
| 4.4.1. Residual of the approximate solution | 52 |
| 4.4.2. The improved approximation | 53 |
| 4.4.3. Estimates on the error term | 58 |
| 4.5. Local Existence and uniqueness | 62 |
| 4.6. Control on the error bound | 63 |
| A. Appendices to Chapter 3 | 67 |
| A.1. Computation of the spectral bands $\omega(\ell)$ | 67 |
| A.2. Calculations for the derivation of the effective amplitude equation | 69 |
| B. Appendices to Chapter 4 | 71 |
| B.1. The function space $\mathcal{H}^{1,2}$ | 71 |
| B.2. Computation of the projection $\Pi_{n,j}$ | 76 |
| Bibliography | 77 |

Zusammenfassung

Um die Dynamik von quantenmechanischen Systemen zu untersuchen, ist es oft sehr nützlich, effektive Gleichungen als eine Näherung für das ursprüngliche System zu betrachten. Solche reduzierten Modelle lassen sich aus Vielteilchensystemen ebenso herleiten wie auch aus schon bekannten partiellen Differentialgleichungen. In dieser Arbeit studieren wir physikalische Probleme, welche durch eine nichtlineare Differentialgleichung beschrieben werden und deren Dynamik mit Hilfe einer einfacheren effektiven Gleichung approximiert werden soll.

Zunächst betrachten wir eine nichtlineare Schrödingergleichung und eine kubische Klein-Gordon Gleichung auf einem periodischen Quantengraph. Für die Amplitude eines sich auf dem Graph bewegenden Wellenpakets leiten wir in beiden Fällen eine Näherungsgleichung her. Diese effektiven Gleichungen haben ebenfalls die Form einer nichtlinearen Schrödingergleichung, sind jedoch auf einem homogenen Raum definiert. Wir rechtfertigen diese Näherungen durch den Beweis, dass sich die Lösungen der effektiven Gleichungen für lange Zeiten nahe der tatsächlichen Lösungen der ursprünglichen Probleme befinden. Dafür nutzen wir einen Blochwellenansatz und schätzen den Fehler zwischen beiden Lösungen mit Hilfe eines Gronwall-Arguments ab. Im Falle der kubischen Klein-Gordon Gleichung benötigen wir noch eine zusätzliche Energieabschätzung für den Fehlerterm.

Im zweiten Teil der Arbeit konzentrieren wir uns auf eine nichtlineare Schrödingergleichung mit einem zusätzlichen Potential, der sogenannten Gross-Pitaevskii Gleichung. Diese betrachten wir auf dem zweidimensionalen homogenen Raum mit einem periodischen Potential in x -Richtung und einem harmonischen Oszillatorpotential in y -Richtung. Die Periodizität wird hier durch eine unendliche Folge von endlich hohen Potentialwänden eingeführt. Als Näherungsgleichung erhalten wir eine diskrete nichtlineare Schrödingergleichung, deren Lösungen lokalisierte Amplituden in den einzelnen Potentialtöpfen darstellen. Wir nutzen einen Ansatz aus Eigenfunktionen der entsprechenden linearen Anfangswertprobleme in beiden Raumrichtungen und beweisen einen Approximationssatz für das so hergeleitete effektive System. Erneut benötigen wir eine Energieabschätzung, um den Fehlerterm mit Hilfe des Satzes von Gronwall zu beschränken.

Abstract

In order to analyze the dynamics of quantum mechanical systems, it is often very useful to consider effective equations as an approximation for the original system. Such reduced models can be derived from many body systems as well as from partial differential equations already known. In this thesis, we study physical problems described by a nonlinear differential equation whose dynamics will be approximated by a simpler effective equation.

First we consider a nonlinear Schrödinger equation and a cubic Klein-Gordon equation on a periodic quantum graph. In both cases, we derive an approximation equation for the amplitude of a wave packet moving on the graph. These effective equations also have the form of a nonlinear Schrödinger equation but on a homogeneous space. We justify these approximations by proving that the solutions of the effective equations lie close to the true solutions of the original problem on a long time scale. For that reason, we use a Bloch wave ansatz and estimate the error between both solutions with the help of a Gronwall argument. In the case of the cubic Klein-Gordon equation, we need an additional energy estimate for the error term.

In the second part of the thesis, we concentrate on the nonlinear Schrödinger equation with an additional potential, the so-called Gross-Pitaevskii equation. We consider this equation on the two-dimensional homogeneous space with a periodic potential in x -direction and a harmonic oscillator potential in y -direction. The periodicity is introduced here by an infinite sequence of potential walls of finite height. As an approximation equation, we obtain a discrete nonlinear Schrödinger equation whose solutions represent localized amplitudes in the corresponding potential wells. We use an ansatz built with eigenfunctions of the respective linear initial value problems in both space directions and prove an approximation theorem for the derived effective system. Once more, we need an energy estimate to bound the error term with Gronwall's theorem.

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1. Introduction

In mathematical physics, it is often necessary to approximate complex physical systems by effective equations. Such simplified mathematical models often lead to a deeper understanding of the physical problem and give us solutions we are unable to obtain in the original setting. For example, in a mean-field approximation of the linear N-body Schrödinger equation the effective dynamics of a Bose gas can be described by a Gross-Pitaevskii equation. We refer to [22] for more details on this topic.

A different approach to obtain an effective equation is to consider a nonlinear partial differential equation as original system, which then will be approximated by a simpler nonlinear evolution problem. In such a situation, it is common to use a so-called multiple scaling expansion to derive an effective equation. By proving that the solutions of the original system lie close to the used multiscale ansatz, the validity of the approximation equation can be justified.

A simple application of this technique is used for the approximation of the cubic Klein-Gordon equation

$$\partial_t^2 u = \partial_x^2 u - u - u^3, \quad t \in \mathbb{R}, \quad x \in \mathbb{R},$$

where the ansatz

$$\varepsilon \Psi_{\text{nlS}}(t, x) = \varepsilon A(T, X) e^{i l_0 x} e^{i \omega_0 t} + c.c.$$

leads to the nonlinear Schrödinger equation

$$2i\omega_0 \partial_T A = (1 - c_g^2) \partial_X^2 A - 3|A|^2 A$$

as an effective equation describing the amplitude $A(T, X) \in \mathbb{C}$ of a spatially and temporarily oscillating wave packet. Here, the small perturbation parameter $0 < \varepsilon \ll 1$ and the group velocity c_g of the wave packet define the slow time variable $T = \varepsilon^2 t$ and the rescaled space variable $X = \varepsilon(x - c_g t)$. In order to obtain an approximation result of the form

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|u(t, x) - \varepsilon \Psi_{\text{nlS}}(t, x)\|_{\mathcal{B}} \leq C\varepsilon^\beta, \quad (1.1)$$

for $\beta > 1$, it is necessary to bound the error term $\varepsilon^\beta R = u - \varepsilon \Psi_{\text{nlS}}$ such that $\|R\|_{\mathcal{B}} = \mathcal{O}(1)$ in a suitable chosen Banach space \mathcal{B} . In [19], a bound of the formal order $\mathcal{O}(\varepsilon^{3/2})$ in the space $L^2(\mathbb{R})$ is proved by the use of Gronwall's theorem.

This thesis is divided into two main parts, where we use the approach introduced above to obtain effective amplitude equations in two different physical settings. In Chapter 2, we consider a nonlinear Schrödinger equation

$$i\partial_t u = -\partial_x^2 u - |u|^2 u, \quad t \in \mathbb{R}, \quad x \in \Gamma$$

as an original system acting on periodic quantum graphs Γ . An example for a such a periodic quantum graph is shown in Figure 1.1.

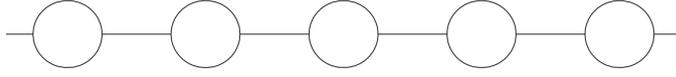


Figure 1.1.: A periodic quantum graph Γ .

For this problem, a nonlinear Schrödinger equation

$$i\partial_T A = \nu_1 \partial_X^2 A + \nu_2 |A|^2 A \quad (1.2)$$

with $T \in \mathbb{R}$, $X \in \mathbb{R}$, $\nu_1, \nu_2 \in \mathbb{R}$ and $A(T, X) \in \mathbb{C}$ occurs as an universal amplitude equation for slow modulations in time and space of an oscillating wave packet. Note that the effective equation (1.2) is now defined on a homogeneous space. Using Bloch wave analysis and adapting the approach mentioned above to periodic quantum graphs, we justify an approximation result of the form (1.1). The content of this chapter is already published in [17].

In Chapter 3, we transfer these ideas to the problem of the cubic Klein-Gordon equation as the original system on a periodic quantum graph Γ and justify a similar approximation theorem, where the effective amplitude equation is also given by (1.2).

A more detailed view on the topic of quantum graphs is given in the introduction of Chapter 2. The second part of this thesis is devoted to the Gross-Pitaevskii equation on a two-dimensional homogeneous space,

$$i\partial_t u = -\Delta u + V(r)u + \sigma|u|^2 u, \quad t \in \mathbb{R}_+, \quad r \in \mathbb{R}^2, \quad (1.3)$$

where $u(t, r) : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{C}$ and $V(r)$ is given by a periodic sequence of potential wells with a height of the formal order $\mathcal{O}(\varepsilon^{-2})$ in x -direction and a harmonic oscillator potential in y -direction. An example for such a periodic well potential is shown in Figure 1.2. Thus, the Gross-Pitaevskii equation can be seen as a nonlinear Schrödinger equation with a nonzero potential $V(r)$.

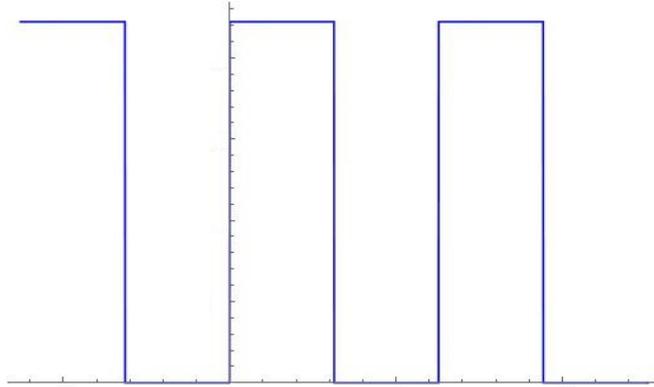


Figure 1.2.: A one-dimensional periodic well potential.

The one-dimensional Gross-Pitaevskii equation with a periodic potential of the formal order $\mathcal{O}(\varepsilon^{-2})$ is discussed in [32]. Here the authors justify that the original system can be approximated by a system of discrete nonlinear Schrödinger equations.

In Chapter 4, we transfer the analysis from [32] to our two-dimensional problem and also approximate the original solutions of (1.3) for small values of ε by solutions of infinitely many coupled discrete nonlinear Schrödinger equations

$$i\partial_T a_m = \alpha(a_{m-1} + a_{m+1}) + \sigma\beta |a_m|^2 a_m, \quad (1.4)$$

where the amplitude functions $a_m(T)$ are located in the m -th potential well and evolve in the slow time $T = \mu t$ with $\mu = \mu(\varepsilon) > 0$. In contrast to the one-dimensional problem, higher regularity is needed to control the nonlinearity of (1.3) in \mathbb{R}^2 . For this reason, we introduce the anisotropic Sobolev space $\mathcal{H}^{1,2}(\mathbb{R}^2)$ to obtain a similar justification result of the formal order $\mathcal{O}(\mu^{3/2})$ as in [32].

For a more detailed introduction into the problem and a proper definition of the Sobolev space $\mathcal{H}^{1,2}(\mathbb{R}^2)$, we refer to Section 4.1.

2. Approximation of a nonlinear Schrödinger equation on periodic quantum graphs ¹

We consider a nonlinear Schrödinger (NLS) equation on a spatially extended periodic quantum graph. With a multiple scaling expansion, an effective amplitude equation can be derived in order to describe slow modulations in time and space of an oscillating wave packet. Using Bloch wave analysis and Gronwall's inequality, we estimate the distance between the macroscopic approximation which is obtained via the amplitude equation and true solutions of the NLS equation on the periodic quantum graph. Moreover, we prove an approximation result for the amplitude equations which occur at the Dirac points of the system.

2.1. Introduction

A quantum graph is a network of bonds (or edges) connected at the vertices. Such systems appear as models for the description of free electrons in organic molecules, in the study of waveguides, photonic crystals, or Anderson localization, or as limit on shrinking thin wires [42]. Quantum graphs are used in mesoscopic physics to obtain a theoretical understanding of nanotechnological objects such as nanotubes or graphen, cf. [18, 20, 21]. A recent monograph [9] gives a good introduction to the mathematics and physics of quantum graphs.

In the linear theory, partial differential equations (PDEs) are defined on the quantum graph according to the following two ingredients. First, a differential operator acts on functions defined on the bonds. Second, certain boundary conditions are applied to the functions at the vertices. In particular, continuity of functions and conservation of flows through the vertices are expressed by the so called Kirchhoff boundary conditions.

Here we are interested in nonlinear PDEs posed on an infinitely extended periodic chain of identical quantum graphs. Nonlinear PDEs on quantum graphs have been only considered recently [26] mostly in the context of unbounded graphs with finitely many vertices. Variational results on existence of ground states on such unbounded graphs were obtained in a series of papers [2, 3, 4, 5]. It is the purpose of this chapter to derive and justify an effective amplitude equation for the description of slow modulations in time and space of an oscillating wave packet. As a PDE toy model on the periodic quantum graph, we consider a nonlinear Schrödinger (NLS) equation. The effective amplitude equation also has the form of a NLS equation but on a homogeneous space. In what follows, we refer to these two NLS equations as to the original system and to the amplitude equation.

Hence, we consider the following NLS equation on the periodic quantum graph as the original system,

$$i\partial_t u + \partial_x^2 u + |u|^2 u = 0, \quad t \in \mathbb{R}, \quad x \in \Gamma, \quad (2.1)$$

¹This chapter is a slightly modified version of the published article [17]. The contribution of the author to this article is included in all main parts of the analysis.

where Γ is the quantum graph and $u : \mathbb{R} \times \Gamma \rightarrow \mathbb{C}$. The Kirchhoff boundary conditions at the vertices are defined below in (2.2)-(2.3).

In order to explain our approach without too many technical details, we develop our subsequent presentation to one special quantum graph shown in Figure 2.1. However, our approach can be extended to other quantum graphs, as discussed in Section 2.7.

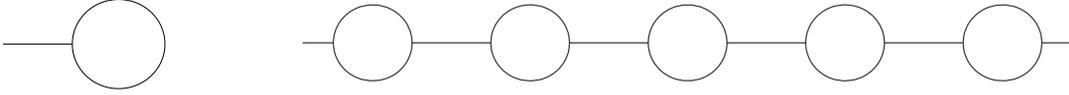


Figure 2.1.: The basic cell Γ_0 (left) of the periodic quantum graph Γ (right).

The spectral problems associated with the linear Schrödinger operator on the periodic quantum graph of Figure 2.1 and its modifications have been recently studied in the literature [20, 21, 25]. Our work is different in the sense that we are studying the time evolution (Cauchy) problem for the nonlinear version of the Schrödinger equation associated with localized initial data. In the recent work [33], the authors have studied the stationary NLS equation on the periodic quantum graph Γ and constructed two families of localized bound states by reducing the differential equations to the discrete maps.

The problem of localization in the periodic setting has been a fascinating topic of research with several effective amplitude equations appearing in this context [29]. In particular, tight-binding approximation [1, 32, 34] and coupled-mode approximation [39, 31, 13] were derived and justified in the limit of large and small periodic potentials respectively. We are addressing here the envelope approximation, which is the most universal approximation of modulated wave packets in nonlinear dispersive PDEs [19]. The envelope approximation provides a homogenization of the NLS equation (2.1) on the periodic quantum graph Γ with an effective homogeneous NLS equation derived for a given wave packet.

Justification of the homogeneous NLS equation in the context of nonlinear Klein-Gordon equations with smooth spatially periodic coefficients has been carried out in the work [10]. A modified analytical approach with a similar result was developed in Section 2.3.1 in [29] in the context of the Gross-Pitaevskii equation with a smooth periodic potential. Since the periodic quantum graph introduces singularities in the effective potential (by means of the Kirchhoff boundary conditions), it is an open question to be inspected here if the analytical techniques from [10, 29] can be made applicable to the NLS equation (2.1) on the periodic quantum graph Γ . The answer to this question turns out to be positive. With the same technique involving Bloch wave analysis and Gronwall's inequality, we prove estimates on the distance between the macroscopic approximation via the amplitude equation and the true solutions of the original system. Moreover, we explain that the same technique can also be used to prove an approximation result for the amplitude equations which occur at the Dirac points associated with the periodic graph Γ . The amplitude equations at the Dirac points take the form of the coupled-mode (Dirac) system.

The chapter is organized as follows. The main results are described in Section 2.2, after introducing the spectral problem associated with the periodic quantum graph on Figure 2.1. Local existence and uniqueness of solutions of the Cauchy problem for the NLS equation (2.1) is discussed in Section 2.3. The Bloch transform is introduced and studied in Section 2.4. In Section 2.5, we derive the effective amplitude equation, construct an improved approximation, and estimate the residual for this improved approximation. The justification of the amplitude equation is

developed in Section 2.6. Discussion of other periodic quantum graphs is given in the concluding Section 2.7.

Notation: We denote with $H^s(\mathbb{R})$ the Sobolev space of s -times weakly differentiable functions on the real line whose derivatives up to order s are in $L^2(\mathbb{R})$. The norm $\|u\|_{H^s}$ for u in the Sobolev space $H^s(\mathbb{R})$ is equivalent to the norm $\|(I - \partial_x^2)^{s/2}u\|_{L^2}$ in the Lebesgue space $L^2(\mathbb{R})$. Throughout this chapter, many different constants are denoted by C if they can be chosen independently of the small parameter $0 < \varepsilon \ll 1$.

2.2. Main result

2.2.1. The periodic quantum graph

The periodic quantum graph Γ shown on Figure 2.1 can be expressed as

$$\Gamma = \bigoplus_{n \in \mathbb{Z}} \Gamma_n, \quad \text{with} \quad \Gamma_n = \Gamma_{n,0} \oplus \Gamma_{n,+} \oplus \Gamma_{n,-},$$

where $\Gamma_{n,0}$ represents the horizontal link of length π between the circles and $\Gamma_{n,\pm}$ represent the upper and lower semicircles of the same length π , for $n \in \mathbb{Z}$. In what follows, $\Gamma_{n,0}$ is identified isometrically with the interval $I_{n,0} = [2\pi n, 2\pi n + \pi]$ and $\Gamma_{n,\pm}$ are identified with the intervals $I_{n,\pm} = [2\pi n + \pi, 2\pi(n+1)]$. For a function $u : \Gamma \rightarrow \mathbb{C}$, we denote the part on the interval $I_{n,0}$ associated to $\Gamma_{n,0}$ with $u_{n,0}$ and the parts on the intervals $I_{n,\pm}$ associated to $\Gamma_{n,\pm}$ with $u_{n,\pm}$.

The second-order differential operator ∂_x^2 appearing on the right-hand side of the NLS equation (2.1) is defined under certain boundary conditions at the vertex points $\{x = n\pi : n \in \mathbb{Z}\}$. We use so called Kirchhoff boundary conditions, which are given by the continuity of the functions at the vertices

$$\begin{cases} u_{n,0}(t, 2\pi n + \pi) = u_{n,+}(t, 2\pi n + \pi) = u_{n,-}(t, 2\pi n + \pi), \\ u_{n+1,0}(t, 2\pi(n+1)) = u_{n,+}(t, 2\pi(n+1)) = u_{n,-}(t, 2\pi(n+1)), \end{cases} \quad (2.2)$$

and the continuity of the fluxes at the vertices

$$\begin{cases} \partial_x u_{n,0}(t, 2\pi n + \pi) = \partial_x u_{n,+}(t, 2\pi n + \pi) + \partial_x u_{n,-}(t, 2\pi n + \pi), \\ \partial_x u_{n+1,0}(t, 2\pi(n+1)) = \partial_x u_{n,+}(t, 2\pi(n+1)) + \partial_x u_{n,-}(t, 2\pi(n+1)). \end{cases} \quad (2.3)$$

Remark 2.2.1. The symmetry constraint $u_{n,+}(t, x) = u_{n,-}(t, x)$ is an invariant reduction of the NLS equation (2.1) provided the initial data of the corresponding Cauchy problem satisfies the same reduction. In the case of symmetry reduction, the boundary conditions (2.2) and (2.3) can be simplified as follows:

$$\begin{cases} u_{n,0}(t, 2\pi n + \pi) = u_{n,+}(t, 2\pi n + \pi), \\ u_{n+1,0}(t, 2\pi(n+1)) = u_{n,+}(t, 2\pi(n+1)) \end{cases} \quad (2.4)$$

and

$$\begin{cases} \partial_x u_{n,0}(t, 2\pi n + \pi) = 2\partial_x u_{n,+}(t, 2\pi n + \pi), \\ \partial_x u_{n+1,0}(t, 2\pi(n+1)) = 2\partial_x u_{n,+}(t, 2\pi(n+1)). \end{cases} \quad (2.5)$$

In this way, the NLS equation (2.1) on the periodic graph Γ becomes equivalent to the NLS equation with a singular periodic potential.

The scalar PDE problem on the periodic quantum graph Γ is transferred to a vector-valued PDE problem on the real axis by introducing the functions

$$u_0(x) = \begin{cases} u_{n,0}(x), & x \in I_{n,0}, \\ 0, & x \in I_{n,\pm}, \end{cases} \quad n \in \mathbb{Z}, \quad (2.6)$$

and

$$u_{\pm}(x) = \begin{cases} u_{n,\pm}(x), & x \in I_{n,\pm}, \\ 0, & x \in I_{n,0}, \end{cases} \quad n \in \mathbb{Z}. \quad (2.7)$$

We introduce sets I_0 and I_{\pm} by

$$I_0 = \bigcup_{n \in \mathbb{Z}} I_{n,0} = \text{supp}(u_0) \quad \text{and} \quad I_{\pm} = \bigcup_{n \in \mathbb{Z}} I_{n,\pm} = \text{supp}(u_{\pm}).$$

We collect the functions u_0 and u_{\pm} in the vector $U = (u_0, u_+, u_-)$ and rewrite the evolution problem (2.1) as

$$i\partial_t U + \partial_x^2 U + |U|^2 U = 0, \quad t \in \mathbb{R}, \quad x \in \mathbb{R} \setminus \{k\pi : k \in \mathbb{Z}\}, \quad (2.8)$$

subject to the conditions (2.2)-(2.3) at the vertex points $x \in \{k\pi : k \in \mathbb{Z}\}$, where the cubic nonlinear term stands for the vector $|U|^2 U = (|u_0|^2 u_0, |u_+|^2 u_+, |u_-|^2 u_-)$.

2.2.2. The Floquet-Bloch spectrum

The spectral problem

$$\omega W = -\partial_x^2 W, \quad x \in \mathbb{R} \setminus \{k\pi : k \in \mathbb{Z}\}, \quad (2.9)$$

is obtained by inserting $U(t, x) = W(x)e^{-i\omega t}$ into the linearization associated to the NLS equation (2.8). The components of $W = (w_0, w_+, w_-)$ satisfy the conditions (2.2)-(2.3) and have their supports in (I_0, I_+, I_-) . The eigenfunctions W can be represented in the form of the so-called Bloch waves

$$W(x) = e^{i\ell x} f(\ell, x), \quad \ell, x \in \mathbb{R}, \quad (2.10)$$

where $f(\ell, \cdot) = (f_0, f_+, f_-)(\ell, \cdot)$ is a 2π -periodic function for every $\ell \in \mathbb{R}$. Since these functions satisfy the continuation conditions

$$f(\ell, x) = f(\ell, x + 2\pi), \quad f(\ell, x) = f(\ell + 1, x)e^{ix}, \quad \ell, x \in \mathbb{R}, \quad (2.11)$$

we can restrict the definition of $f(\ell, x)$ to $x \in \mathbb{T}_{2\pi} = \mathbb{R}/(2\pi\mathbb{Z})$ and $\ell \in \mathbb{T}_1 = \mathbb{R}/\mathbb{Z}$. The torus $\mathbb{T}_{2\pi}$ is isometrically parameterized with $x \in [0, 2\pi]$ and the torus \mathbb{T}_1 with $\ell \in [-1/2, 1/2]$, where the endpoints of the intervals are identified to be the same for both tori.

Hence, f can be found as solution of the eigenvalue problem

$$-(\partial_x + i\ell)^2 f = \omega(\ell) f, \quad x \in \mathbb{T}_{2\pi}, \quad (2.12)$$

subject to the boundary conditions

$$\begin{cases} f_0(\ell, \pi) = f_+(\ell, \pi) = f_-(\ell, \pi), \\ f_0(\ell, 0) = f_+(\ell, 2\pi) = f_-(\ell, 2\pi) \end{cases} \quad (2.13)$$

and

$$\begin{cases} (\partial_x + i\ell)f_0(\ell, \pi) = (\partial_x + i\ell)f_+(\ell, \pi) + (\partial_x + i\ell)f_-(\ell, \pi), \\ (\partial_x + i\ell)f_0(\ell, 0) = (\partial_x + i\ell)f_+(\ell, 2\pi) + (\partial_x + i\ell)f_-(\ell, 2\pi). \end{cases} \quad (2.14)$$

The functions $f_0(\ell, \cdot)$ and $f_{\pm}(\ell, \cdot)$ have supports in $I_{0,0} = [0, \pi] \subset \mathbb{T}_{2\pi}$ and $I_{0,\pm} = [\pi, 2\pi] \subset \mathbb{T}_{2\pi}$. The boundary conditions (2.13)-(2.14) are derived from (2.2)-(2.3) by using the 2π -periodicity of the eigenfunction $f(\ell, \cdot)$. Note that $e^{i\cdot x}f(\cdot, x)$ and $\omega(\cdot)$ are 1-periodic functions on \mathbb{T}_1 . The extended variable $U = (u_0, u_+, u_-)$ is needed to give a meaning to $e^{i\ell x}$ which is defined for $x \in \mathbb{R}$, but not for $x \in \Gamma$.

The spectrum of the spectral problem (2.9) consists of two parts [20, 21, 33]. One part is represented by the sequence of eigenvalues at $\{m^2\}_{m \in \mathbb{N}}$ of infinite multiplicity. For a fixed $m \in \mathbb{N}$, a bi-infinite sequence of eigenfunctions $(W^{m,k})_{k \in \mathbb{Z}}$ of the spectral problem (2.9) exists and is supported compactly in each circle with the explicit representation:

$$w_{n,0}^{m,k}(x) = 0, \quad w_{n,+}^{m,k}(x) = -w_{n,-}^{m,k}(x) = \delta_{nk} \sin(m(x - 2\pi k)), \quad n \in \mathbb{Z}. \quad (2.15)$$

The second part in the spectrum of the spectral problem (2.9) is represented by the union of a countable set of spectral bands, which correspond to the real roots $\rho_{1,2}$ of the transcendental equation $\rho^2 - \text{tr}(M)(\omega)\rho + 1 = 0$. Here

$$\text{tr}(M)(\omega) := \frac{1}{4} [9 \cos(2\pi\sqrt{\omega}) - 1]$$

is the trace of the monodromy matrix M associated with the linear difference equation obtained after solving the differential equation (2.9) subject to the conditions (2.2)-(2.3), cf. [14, 33]. Real roots are obtained when $\text{tr}(M)(\omega) \in [-2, 2]$.

The corresponding eigenfunctions of the spectral problem (2.9) are distributed over the entire periodic graph Γ and satisfy the symmetry constraints $w_{n,+}(x) = w_{n,-}(x)$, $n \in \mathbb{Z}$ and the constrained boundary conditions (2.4)-(2.5).

The spectral bands of the periodic eigenvalue problem (2.12) are shown on Figure 2.2. The flat bands at $\omega = m^2$, $m \in \mathbb{N}$ correspond to the eigenvalues of the spectral problem (2.9) of infinite algebraic multiplicity. It is clear from the explicit representation (2.15) that the corresponding eigenfunctions can also be written in the Bloch wave form (2.10) associated with the Bloch wave number $\ell \in \mathbb{T}_1$.

Let us confirm the spectral properties suggested by Figure 2.2. First, eigenvalues of infinite multiplicity at $\omega = m^2$, $m \in \mathbb{N}$, are at the end points of the spectral bands, because $\text{tr}(M)(m^2) = 2$. Second, since

$$\frac{d}{d\omega} \text{tr}(M)(\omega)|_{\omega=m^2} = -\frac{9\pi}{4\sqrt{\omega}} \sin(2\pi\sqrt{\omega})|_{\omega=m^2} = 0,$$

the two adjacent spectral bands of $\sigma(-\partial_x^2)$ overlap at $\omega = m^2$ without a spectral gap. Coincidentally, these so-called Dirac points of the dispersion relation happen to occur at the eigenvalues of infinite multiplicities. Finally, the two adjacent spectral bands at $\text{tr}(M)(\omega) = -2$ do not overlap and the spectral band has a nonzero length because $\text{tr}(M)(\omega)$ has a minimum at $\omega = \frac{m^2}{4}$ with $m \in \mathbb{N}_{\text{odd}}$ and $\text{tr}(M)\left(\frac{m^2}{4}\right) = -\frac{5}{2} < -2$.

Let us now define the L^2 -based spaces, where the eigenfunctions of the periodic eigenvalue problem (2.12) are properly defined. For fixed $\ell \in \mathbb{T}_1$, we define

$$L_{\Gamma}^2 := \{ \tilde{U} = (\tilde{u}_0, \tilde{u}_+, \tilde{u}_-) \in (L^2(\mathbb{T}_{2\pi}))^3 : \text{supp}(\tilde{u}_j) = I_{0,j}, \quad j \in \{0, +, -\} \} \quad (2.16)$$

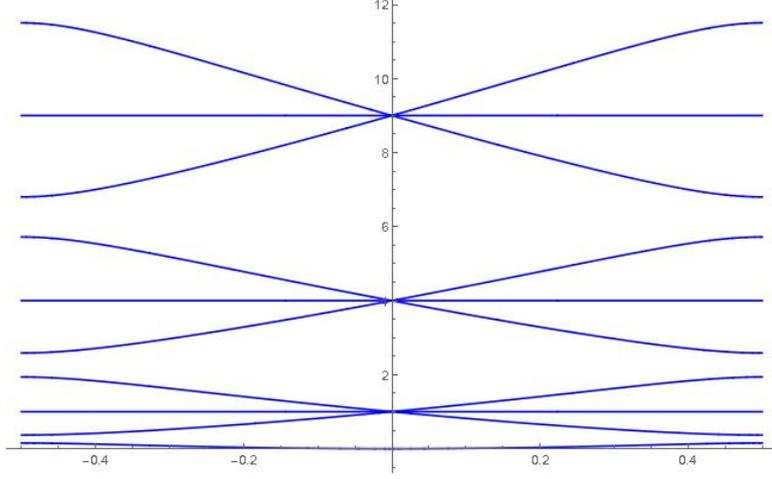


Figure 2.2.: The spectral bands ω of the spectral problem (2.12) plotted versus the Bloch wave number ℓ for the periodic quantum graph Γ .

and

$$H_{\Gamma}^2(\ell) := \{\tilde{U} \in L_{\Gamma}^2 : \tilde{u}_j \in H^2(I_{0,j}), \quad j \in \{0, +, -\}, \quad (2.13) - (2.14) \text{ are satisfied}\},$$

equipped with the norm

$$\|\tilde{U}\|_{H_{\Gamma}^2(\ell)} = \left(\|\tilde{u}_0\|_{H^2(I_{0,0})}^2 + \|\tilde{u}_+\|_{H^2(I_{0,+})}^2 + \|\tilde{u}_-\|_{H^2(I_{0,-})}^2 \right)^{1/2}.$$

The parameter ℓ is defined in $H_{\Gamma}^2(\ell)$ by means of the boundary conditions (2.13)-(2.14). We obtain the following elementary result.

Lemma 2.2.2. *For fixed $\ell \in \mathbb{T}_1$, the operator $\tilde{L}(\ell) := -(\partial_x + i\ell)^2$ is a self-adjoint, positive semi-definite operator in L_{Γ}^2 .*

Proof. Using the conditions (2.13)-(2.14), we find for every $f(\ell, \cdot), g(\ell, \cdot) \in H_{\Gamma}^2(\ell)$ and every $\ell \in \mathbb{T}_1$:

$$\begin{aligned} \langle \tilde{L}(\ell)f, g \rangle_{L_{\Gamma}^2} &= \int_0^{2\pi} (\partial_x + i\ell)f(\ell, x) \cdot \overline{(\partial_x + i\ell)g(\ell, x)} dx \\ &\quad - [\partial_x f_0(\ell, \pi) + i\ell f_0(\ell, \pi)] \overline{g_0(\ell, \pi)} + [\partial_x f_0(\ell, 0) + i\ell f_0(\ell, 0)] \overline{g_0(\ell, 0)} \\ &\quad - [\partial_x f_+(\ell, 2\pi) + i\ell f_+(\ell, 2\pi)] \overline{g_+(\ell, 2\pi)} + [\partial_x f_+(\ell, \pi) + i\ell f_+(\ell, \pi)] \overline{g_+(\ell, \pi)} \\ &\quad - [\partial_x f_-(\ell, 2\pi) + i\ell f_-(\ell, 2\pi)] \overline{g_-(\ell, 2\pi)} + [\partial_x f_-(\ell, \pi) + i\ell f_-(\ell, \pi)] \overline{g_-(\ell, \pi)} \\ &= \int_0^{2\pi} (\partial_x + i\ell)f(\ell, x) \cdot \overline{(\partial_x + i\ell)g(\ell, x)} dx. \end{aligned}$$

Using another integration by parts with the conditions (2.13)-(2.14), we confirm that

$$\langle \tilde{L}(\ell)f, g \rangle_{L_{\Gamma}^2} = \langle f, \tilde{L}(\ell)g \rangle_{L_{\Gamma}^2}.$$

Hence, $\tilde{L}(\ell)$ is self-adjoint for every $\ell \in \mathbb{T}_1$. Since

$$\langle \tilde{L}(\ell)f, f \rangle_{L_{\Gamma}^2} = \int_0^{2\pi} (\partial_x + i\ell)f \cdot \overline{(\partial_x + i\ell)f} dx \geq 0,$$

the operator $\tilde{L}(\ell)$ is positive semi-definite. \square

By Lemma 2.2.2 and the spectral theorem for self-adjoint operators with compact resolvent, cf. [36], for each $\ell \in \mathbb{T}_1$ there exists a Schauder base $\{f^{(m)}(\ell, \cdot)\}_{m \in \mathbb{N}}$ of L^2_Γ consisting of eigenfunctions of $\tilde{L}(\ell)$ with positive eigenvalues $\{\omega^{(m)}(\ell)\}_{m \in \mathbb{N}}$ ordered as $\omega^{(m)}(\ell) \leq \omega^{(m+1)}(\ell)$. By construction, the Bloch wave functions satisfy the continuation properties (2.11). They also satisfy the orthogonality and normalization relations:

$$\langle f^{(m)}(\ell, \cdot), f^{(m')}(\ell, \cdot) \rangle_{L^2_\Gamma} = \delta_{m,m'}, \quad \ell \in \mathbb{T}_1.$$

Note that we use superscripts for the count of the spectral bands, because the subscripts in $f_j^{(m)}(\ell, x)$, $j \in \{0, +, -\}$ are reserved to indicate the component of $f^{(m)}(\ell, x)$ for $x \in I_{0,j}$.

2.2.3. The effective amplitude equation

Slow modulations in time and space of a small-amplitude modulated Bloch mode are described by the formal asymptotic expansion

$$U(t, x) = \varepsilon \Psi_{\text{nl}s}(t, x) + \text{higher-order terms}, \quad (2.17)$$

with

$$\varepsilon \Psi_{\text{nl}s}(t, x) = \varepsilon A(T, X) f^{(m_0)}(\ell_0, x) e^{i\ell_0 x} e^{-i\omega^{(m_0)}(\ell_0) t}, \quad (2.18)$$

where $0 < \varepsilon \ll 1$ is a small perturbation parameter, $T = \varepsilon^2 t$, $X = \varepsilon(x - c_g t)$, and $A(T, X) \in \mathbb{C}$ is the wave amplitude. The parameter $c_g := \partial_\ell \omega^{(m_0)}(\ell_0)$ is referred to as the group velocity associated with the Bloch wave and it corresponds to the velocity of the wave packet propagation. The group velocity is different from the phase velocity $c_p := \omega^{(m_0)}(\ell_0)/\ell_0$, which characterizes movement of the carrier wave inside the wave packet. Figure 2.3 shows the characteristic scales of the wave packet given by the asymptotic expansion (2.17) with (2.18).

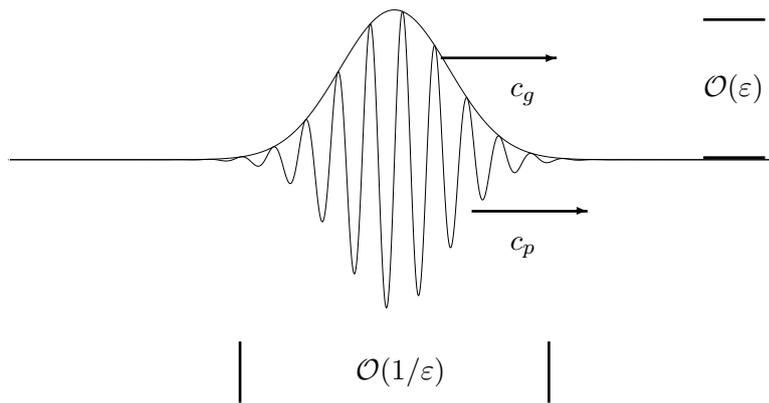


Figure 2.3.: A schematic representation of the asymptotic solution (2.17)-(2.18) to the NLS equation (2.1) on the periodic quantum graph Γ . The envelope advances with the group velocity c_g and the underlying carrier wave advances with the phase velocity c_p .

Formal asymptotic expansions show that at the lowest order in ε , the wave amplitude A satisfies the following cubic NLS equation on the homogeneous space:

$$i\partial_T A - \frac{1}{2}\partial_\ell^2 \omega^{(m_0)}(\ell_0)\partial_X^2 A + \nu|A|^2 A = 0, \quad (2.19)$$

where the cubic coefficient is given by

$$\nu = \frac{\|f^{(m_0)}(\ell_0, \cdot)\|_{L_\Gamma^4}^4}{\|f^{(m_0)}(\ell_0, \cdot)\|_{L_\Gamma^2}^2}.$$

Mathematical justification of the effective amplitude equation (2.19) by means of the error estimates for the original system (2.8) is the main purpose of this work. The approximation result is given by the following theorem.

Theorem 2.2.3. *Pick $m_0 \in \mathbb{N}$ and $\ell_0 \in \mathbb{T}_1$ such that the following non-resonance condition is satisfied:*

$$\omega^{(m)}(\ell_0) \neq \omega^{(m_0)}(\ell_0), \quad \text{for every } m \neq m_0. \quad (2.20)$$

Then, for every $C_0 > 0$ and $T_0 > 0$, there exist $\varepsilon_0 > 0$ and $C > 0$ such that for all solutions $A \in C(\mathbb{R}, H^3(\mathbb{R}))$ of the effective amplitude equation (2.19) with

$$\sup_{T \in [0, T_0]} \|A(T, \cdot)\|_{H^3} \leq C_0$$

and for all $\varepsilon \in (0, \varepsilon_0)$, there are solutions $U \in C([0, T_0/\varepsilon^2], L^\infty(\mathbb{R}))$ of the original system (2.8) satisfying the bound

$$\sup_{t \in [0, T_0/\varepsilon^2]} \sup_{x \in \mathbb{R}} |U(t, x) - \varepsilon \Psi_{\text{nls}}(t, x)| \leq C\varepsilon^{3/2}, \quad (2.21)$$

where $\varepsilon \Psi_{\text{nls}}$ is given by (2.18).

Remark 2.2.4. Thanks to the global well-posedness and integrability of the cubic NLS equation (2.19) in one space dimension [11, 40], a global solution $A \in C(\mathbb{R}, H^s(\mathbb{R}))$ for every integer $s \geq 0$ exists and satisfies the bound

$$\sup_{T \in [0, T_0]} \|A(T, \cdot)\|_{H^s} \leq C$$

for every $T_0 > 0$, where C is T_0 -independent.

Remark 2.2.5. As it follows from the spectral bands shown on Figure 2.2, it is clear that the non-resonance assumption (2.20) is satisfied for every $m_0 \in \mathbb{N}$ and $\ell_0 \neq 0$ and it fails for every $m_0 \in \mathbb{N}$ and $\ell_0 = 0$ with the exception of the lowest spectral band.

Remark 2.2.6. The approximation result of Theorem 2.2.3 should not be taken for granted. There exists a number of counterexamples [37, 38], where a formally correctly derived amplitude equation makes wrong predictions about the dynamics of the original system.

Remark 2.2.7. The new difficulty in the proof of Theorem 2.2.3 on the periodic quantum graph Γ comes from the vertex conditions (2.2)-(2.3), which have to be incorporated into the functional analytic set-up from [10, 29] used for the derivation of the amplitude equation (2.19). Since the NLS equation (2.1) only contains cubic nonlinearities, the proof of Theorem 2.2.3 does not require near-identity transformations and is based on a simple application of Gronwall's inequality.

2.2.4. The amplitude equations at the Dirac points

Near Dirac points, which correspond to $m_0 \in \mathbb{N}$ and $\ell_0 = 0$ on Figure 2.2 with the exception of the lowest spectral band, see Remark 2.2.5, the cubic NLS equation (2.19) cannot be justified. However, we can find a coupled-mode (Dirac) system, as it is done for smooth periodic potentials (see Section 2.2.1 in [29]). Eigenvalues of infinite multiplicities appearing as the flat bands in Figure 2.2 represent an obstacle in the standard justification analysis.

To overcome the obstacle, we can consider solutions of the original system (2.8) which satisfy the symmetry constraint $u_{n,+}(t, x) = u_{n,-}(t, x)$, see Remark 2.2.1. In this way, all flat bands shown on Figure 2.2 disappear as they violate the symmetry constraint.

Figure 2.4 shows the spectral bands of the spectral problem (2.12) under the symmetry constraint $u_{n,+} = u_{n,-}$. The flat bands are removed due to the symmetry constraints. Near the Dirac points, we can now justify the coupled-mode (Dirac) system by using the analysis developed in the proof of Theorem 2.2.3.

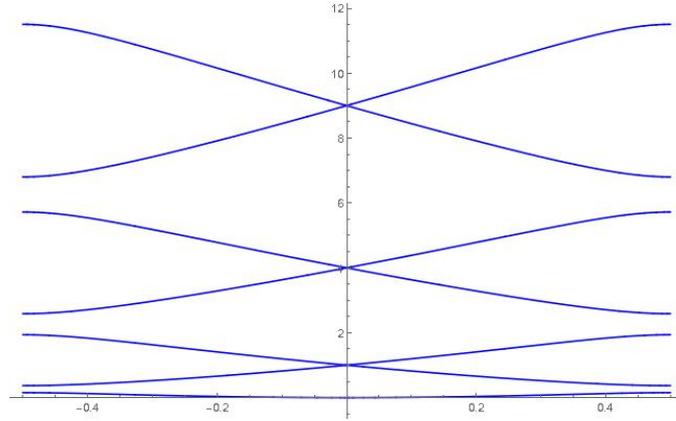


Figure 2.4.: The spectral bands ω of the spectral problem (2.12) plotted versus the Bloch wave number ℓ for the periodic quantum graph Γ under the symmetry constraint $u_{n,+} = u_{n,-}$. The intersection points of the spectral curves at $\ell = 0$ are called Dirac points.

To be specific, we consider an intersection point of the two spectral bands at $\ell = 0$, as per Figure 2.4, such that $\omega^{(2m_0)}(0) = \omega^{(2m_0+1)}(0)$ for some fixed $m_0 \in \mathbb{N}$. We relabel these two bands, and introduce

$$\omega_+(\ell) = \begin{cases} \omega^{(2m_0)}(\ell), & \ell \leq 0, \\ \omega^{(2m_0+1)}(\ell), & \ell > 0, \end{cases} \quad (2.22)$$

and

$$\omega_-(\ell) = \begin{cases} \omega^{(2m_0+1)}(\ell), & \ell \leq 0, \\ \omega^{(2m_0)}(\ell), & \ell > 0. \end{cases} \quad (2.23)$$

We denote the associated eigenfunctions with $f^+(\ell, x)$ and $f^-(\ell, x)$. In order to derive the Dirac system we make the ansatz

$$\varepsilon \Psi_{\text{dirac}}(t, x) = \varepsilon A_+(T, X) f^+(0, x) e^{-i\omega^+(0)t} + \varepsilon A_-(T, X) f^-(0, x) e^{-i\omega^-(0)t}, \quad (2.24)$$

where $T = \varepsilon^2 t$, $X = \varepsilon^2 x$, and $A_{\pm}(T, X) \in \mathbb{C}$. Formal asymptotic expansions show that at the lowest order in ε , the wave amplitudes A_{\pm} satisfy the cubic Dirac system on the homogeneous space:

$$i\partial_T A_+ + i\partial_\ell \omega^+(0)\partial_X A_+ + \sum_{j_1, j_2, j_3 \in \{+, -\}} \nu_{j_1 j_2 j_3}^+ A_{j_1} A_{j_2} \overline{A_{j_3}} = 0, \quad (2.25)$$

$$i\partial_T A_- + i\partial_\ell \omega^-(0)\partial_X A_- + \sum_{j_1, j_2, j_3 \in \{+, -\}} \nu_{j_1 j_2 j_3}^- A_{j_1} A_{j_2} \overline{A_{j_3}} = 0, \quad (2.26)$$

where the coefficients $\nu_{j_1 j_2 j_3}^{\pm} \in \mathbb{C}$ are given by

$$\nu_{j_1, j_2, j_3}^j = \frac{\langle f^{j_1}(0, \cdot) f^{j_2}(0, \cdot) \overline{f^{j_3}(0, \cdot)}, f^j(0, \cdot) \rangle_{L^2_{\mathbb{R}}}}{\|f^j(0, \cdot)\|_{L^2_{\mathbb{R}}}^2}, \quad j, j_1, j_2, j_3 \in \{+, -\}.$$

The system (2.25)-(2.26) is invariant under the transformation $(X, A_+, A_-) \mapsto (-X, A_-, A_+)$. The Cauchy problem is locally well-posed in Sobolev spaces. Depending on the nonlinear terms, it is also globally well-posed in Sobolev spaces [30]. Assuming existence of a global solution to the cubic Dirac system (2.25)-(2.26), the approximation result is given by the following theorem.

Theorem 2.2.8. *For every $C_0 > 0$ and $T_0 > 0$, there exist $\varepsilon_0 > 0$ and $C > 0$ such that for all solutions $A_{\pm} \in C(\mathbb{R}, H^2(\mathbb{R}))$ of the Dirac-system (2.25)-(2.26) with*

$$\sup_{T \in [0, T_0]} \|A_{\pm}(T, \cdot)\|_{H^2} \leq C_0$$

and for all $\varepsilon \in (0, \varepsilon_0)$, there are solutions $U \in C([0, T_0/\varepsilon^2], L^\infty(\mathbb{R}))$ of the original system (2.8) satisfying the bound

$$\sup_{t \in [0, T_0/\varepsilon^2]} \sup_{x \in \mathbb{R}} |U(t, x) - \varepsilon \Psi_{\text{dirac}}(t, x)| \leq C\varepsilon^{3/2}.$$

where $\varepsilon \Psi_{\text{dirac}}$ is given by (2.24).

The proof of Theorem 2.2.8 is a straightforward modification of the proof of Theorem 2.2.3, cf. Remark 2.6.1.

2.3. Local existence and uniqueness

Here we prove the local existence and uniqueness of solutions to the original system (2.8). We consider the operator $L = -\partial_x^2$ in the space

$$\mathcal{L}^2 = \{U = (u_0, u_+, u_-) \in (L^2(\mathbb{R}))^3 : \text{supp}(u_{n,j}) = I_{n,j}, \quad n \in \mathbb{Z}, \quad j \in \{0, +, -\}\}$$

with the domain of definition

$$\mathcal{H}^2 := \{U \in \mathcal{L}^2 : u_{n,j} \in H^2(I_{n,j}), \quad n \in \mathbb{Z}, \quad j \in \{0, +, -\}, \quad (2.2) - (2.3) \text{ are satisfied}\},$$

equipped with the norm

$$\|U\|_{\mathcal{H}^2} := \left(\sum_{n \in \mathbb{Z}} \|u_{n,0}\|_{H^2(I_{n,0})}^2 + \|u_{n,+}\|_{H^2(I_{n,+})}^2 + \|u_{n,-}\|_{H^2(I_{n,-})}^2 \right)^{1/2}.$$

For the local existence and uniqueness of solutions to system (2.8), we need the following results.

Lemma 2.3.1. *The space \mathcal{H}^2 is closed under pointwise multiplication.*

Proof. For each open interval $I_{n,j}$ for $n \in \mathbb{Z}$, $j \in \{0, +, -\}$, the Sobolev space $H^2(I_{n,j})$ is closed under pointwise multiplication. Therefore, there is a positive constant C such that for every $u, v \in \mathcal{H}^2$, we have

$$\|u_{n,j}v_{n,j}\|_{H^2(I_{n,j})} \leq C\|u_{n,j}\|_{H^2(I_{n,j})}\|v_{n,j}\|_{H^2(I_{n,j})}.$$

If U and V are continuous at the vertices, then UV is also continuous at the vertices. If U and V satisfy the flux continuity conditions (2.3), then by the product rule for continuous functions U and V , the product UV also satisfies the flux continuity conditions (2.3). The support for U , V , and UV is identical. Finally, by the Cauchy-Schwarz inequality, we have

$$\begin{aligned} \|UV\|_{\mathcal{H}^2}^2 &= \sum_{n \in \mathbb{Z}, j \in \{0, +, -\}} \|u_{n,j}v_{n,j}\|_{H^2(I_{n,j})}^2 \\ &\leq C^2 \sum_{n \in \mathbb{Z}, j \in \{0, +, -\}} \|u_{n,j}\|_{H^2(I_{n,j})}^2 \|v_{n,j}\|_{H^2(I_{n,j})}^2 \\ &\leq C^2 \|U\|_{\mathcal{H}^2}^2 \|V\|_{\mathcal{H}^2}^2. \end{aligned}$$

The statement of the lemma is proved. \square

Lemma 2.3.2. *The operator L with the domain \mathcal{H}^2 is self-adjoint and positive semi-definite in \mathcal{L}^2 .*

Proof. Using the Kirchhoff boundary conditions (2.2)-(2.3), it is an easy exercise to show that

$$\langle U, LV \rangle_{\mathcal{L}^2} = \langle LU, V \rangle_{\mathcal{L}^2}$$

is true for every $U, V \in \mathcal{H}^2$. Then, the operator L with the domain \mathcal{H}^2 is self-adjoint (similar to Theorem 1.4.4 in [9]). Positivity and semi-definiteness of L follows from the integration by parts

$$\langle U, LU \rangle_{\mathcal{L}^2} = \sum_{n \in \mathbb{Z}, j \in \{0, \pm\}} \|\partial_x u_{n,j}\|_{L^2(I_{n,j})}^2 \geq 0,$$

where the Kirchhoff boundary conditions (2.2)-(2.3) have been used again. \square

As a consequence of classical semigroup theory, cf. [28], we have

Corollary 2.3.3. *The skew symmetric operator $-iL$ with the domain \mathcal{H}^2 defines a unitary group $(e^{-iLt})_{t \in \mathbb{R}}$ in \mathcal{L}^2 such that $\|e^{-iLt}U\|_{\mathcal{L}^2} = \|U\|_{\mathcal{L}^2}$ for every $t \in \mathbb{R}$.*

By Corollary 2.3.3, we obtain another ingredient of the existence and uniqueness theory.

Lemma 2.3.4. *There exists a positive constant C_L such that*

$$\|e^{-iLt}U\|_{\mathcal{H}^2} \leq C_L \|U\|_{\mathcal{H}^2} \tag{2.27}$$

for every $U \in \mathcal{H}^2$ and every $t \in \mathbb{R}$.

Proof. We obtain the following chain of inequalities:

$$\begin{aligned}
\|e^{-iLt}U\|_{\mathcal{H}^2} &\leq C\|(1+L)e^{-iLt}U\|_{\mathcal{L}^2} \\
&\leq C\|e^{-iLt}(1+L)U\|_{\mathcal{L}^2} \\
&\leq C\|(1+L)U\|_{\mathcal{L}^2} \\
&\leq C\|U\|_{\mathcal{H}^2},
\end{aligned}$$

where we have used the equivalence between $\|U\|_{\mathcal{H}^2}$ and $\|(1+L)U\|_{\mathcal{L}^2}$, the commutativity of L and e^{-iLt} , and the existence of the unitary group in Corollary 2.3.3. \square

We are now ready to prove the local existence and uniqueness of solutions of the Cauchy problem associated with the original system (2.8) in \mathcal{H}^2 .

Theorem 2.3.5. *For every $U_0 \in \mathcal{H}^2$, there exists a $T_0 = T_0(\|U_0\|_{\mathcal{H}^2}) > 0$ and a unique solution $U \in C([-T_0, T_0], \mathcal{H}^2)$ of the original system (2.8) with the initial data $U|_{t=0} = U_0$.*

Proof. The estimates from Lemma 2.3.1 and Lemma 2.3.4 allow us to proceed with the general theory for semilinear dynamical systems [28]. Namely, by Duhamel's principle, we rewrite the Cauchy problem associated with the original system (2.8) as the integral equation

$$U(t, \cdot) = e^{-iLt}U(0, \cdot) + i \int_0^t e^{-iL(t-\tau)}|U(\tau, \cdot)|^2U(\tau, \cdot)d\tau, \quad (2.28)$$

where the solution is considered in the space

$$\mathcal{M} := \{U \in C([-T_0, T_0], \mathcal{H}^2) : \sup_{t \in [-T_0, T_0]} \|U(t, \cdot)\|_{\mathcal{H}^2} \leq 2C_L\|U(0, \cdot)\|_{\mathcal{H}^2}\},$$

and the constant C_L is defined by the bound (2.27) in Lemma 2.3.4. For every $U_0 \in \mathcal{H}^2$, there is a sufficiently small $T_0 = T_0(\|U_0\|_{\mathcal{H}^2}) > 0$ such that the right-hand side of the integral equation (2.28) is a contraction in the space \mathcal{M} . Therefore, the existence of a unique solution $U \in C([-T_0, T_0], \mathcal{H}^2)$ follows from Banach's fixed-point theorem. \square

2.4. Bloch transform

The justification of the NLS approximation in the context of nonlinear Klein-Gordon equations with smooth spatially periodic coefficients in [10] or in the context of the Gross-Pitaevskii equation with a smooth periodic potential in [29] heavily relies on the use of the Bloch transform. In order to transfer the evolution problem (2.8) to Bloch space, we first recall the fundamental properties of Bloch transform on the real line. Next, we generalize Bloch transform to periodic quantum graphs, first in L^2 and then for smooth functions. In Section 2.7, we explain how to generalize our approach developed for the periodic graph sketched in Figure 2.1 to other periodic graphs. General Floquet-Bloch theory for spectral problems posed on periodic quantum graphs is reviewed in [9, Chapter 4]. However, as far as we can see, the approach of [9, Chapter 4] does not allow us to transfer the proof of [10] and [29] to the periodic quantum graphs. In what follows, we explain the necessary modifications of the Bloch transform for the periodic quantum graphs.

2.4.1. Bloch transform on the real line

Bloch transform \mathcal{T} generalizes Fourier transform \mathcal{F} from spatially homogeneous problems to spatially periodic problems. It was introduced by Gelfand [16] and it appears for instance in the handling of the Schrödinger operator with a spatially periodic potential [36]. Bloch transform is (formally) defined by

$$\tilde{u}(\ell, x) = (\mathcal{T}u)(\ell, x) = \sum_{n \in \mathbb{Z}} u(x + 2\pi n) e^{-i\ell x - 2\pi i n \ell}. \quad (2.29)$$

The inverse of Bloch transform is given by

$$u(x) = (\mathcal{T}^{-1}\tilde{u})(x) = \int_{-1/2}^{1/2} e^{i\ell x} \tilde{u}(\ell, x) d\ell.$$

By construction, $\tilde{u}(\ell, x)$ is extended from $(\ell, x) \in \mathbb{T}_1 \times \mathbb{T}_{2\pi}$ to $(\ell, x) \in \mathbb{R} \times \mathbb{R}$ according to the continuation conditions:

$$\tilde{u}(\ell, x) = \tilde{u}(\ell, x + 2\pi) \quad \text{and} \quad \tilde{u}(\ell, x) = \tilde{u}(\ell + 1, x) e^{ix}. \quad (2.30)$$

The following lemma specifies the well-known property of Bloch transform acting on Sobolev function spaces, cf. [15, 29].

Lemma 2.4.1. *Bloch transform \mathcal{T} is an isomorphism between*

$$H^s(\mathbb{R}) \quad \text{and} \quad L^2(\mathbb{T}_1, H^s(\mathbb{T}_{2\pi})),$$

where $L^2(\mathbb{T}_1, H^s(\mathbb{T}_{2\pi}))$ is equipped with the norm

$$\|\tilde{u}\|_{L^2(\mathbb{T}_1, H^s(\mathbb{T}_{2\pi}))} = \left(\int_{-1/2}^{1/2} \|\tilde{u}(\ell, \cdot)\|_{H^s(\mathbb{T}_{2\pi})}^2 d\ell \right)^{1/2}.$$

Bloch transform \mathcal{T} defined by (2.29) is related to the Fourier transform \mathcal{F} by the following formula, cf. [15, 29],

$$\tilde{u}(\ell, x) = \sum_{j \in \mathbb{Z}} e^{ijx} \widehat{u}(\ell + j), \quad (2.31)$$

where $\widehat{u}(\xi) = (\mathcal{F}u)(\xi)$, $\xi \in \mathbb{R}$, is the Fourier transform of u on the real axis.

Multiplication of two functions $u(x)$ and $v(x)$ in x -space corresponds to the convolution integral in Bloch space:

$$(\tilde{u} \star \tilde{v})(\ell, x) = \int_{-1/2}^{1/2} \tilde{u}(\ell - m, x) \tilde{v}(m, x) dm, \quad (2.32)$$

where the continuation conditions (2.30) have to be used for $|\ell - m| > 1/2$.

If $\chi : \mathbb{R} \rightarrow \mathbb{R}$ is 2π -periodic, then

$$\mathcal{T}(\chi u)(\ell, x) = \chi(x) (\mathcal{T}u)(\ell, x). \quad (2.33)$$

The relations (2.32) and (2.33) are well-known [10, 15] and can be proved from (2.29) and (2.31).

2.4.2. The system in Bloch space

Thanks to the definitions (2.6), (2.7), and (2.8), it is obvious how to transfer the evolution problem (2.8) into Bloch space. We apply the Bloch transform \mathcal{T} to all components of $U = (u_0, u_+, u_-)$ and obtain

$$i\partial_t \tilde{U}(t, \ell, x) = \tilde{L}(\ell) \tilde{U}(t, \ell, x) - (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, x), \quad (2.34)$$

where the operator $\tilde{L}(\ell) := -(\partial_x + i\ell)^2$ appears in the periodic spectral problem (2.12), the function $\tilde{U}(t, \ell, x) = (\tilde{u}_0, \tilde{u}_+, \tilde{u}_-)(t, \ell, x)$ satisfies the continuation conditions

$$\tilde{U}(t, \ell, x) = \tilde{U}(t, \ell, x + 2\pi) \quad \text{and} \quad \tilde{U}(t, \ell, x) = \tilde{U}(t, \ell + 1, x) e^{ix},$$

and the convolution integrals are applied componentwise as in

$$\tilde{U} \star \tilde{U} \star \tilde{U} = \left(\tilde{u}_0 \star \tilde{u}_0 \star \tilde{u}_0, \tilde{u}_+ \star \tilde{u}_+ \star \tilde{u}_+, \tilde{u}_- \star \tilde{u}_- \star \tilde{u}_- \right).$$

In order to guarantee that $\tilde{u}_j(t, \ell, \cdot)$ has support in $I_{0,j}$ for $j \in \{0, +, -\}$, we define periodic cut-off functions

$$\chi_j(x) = \begin{cases} 1, & x \in I_j, \\ 0, & \text{elsewhere,} \end{cases} \quad j \in \{0, +, -\}. \quad (2.35)$$

With the help of property (2.33), we obtain

$$\mathcal{T}(u_j)(\ell, x) = \mathcal{T}(\chi_j u_j)(\ell, x) = \chi_j(x) (\mathcal{T}u_j)(\ell, x), \quad j \in \{0, +, -\}.$$

Therefore, the support of $\mathcal{T}(u_j)(\ell, x)$ with respect to x is contained in I_j for any $j \in \{0, +, -\}$.

2.4.3. Bloch transform for smooth functions

Since we proved the local existence and uniqueness of solutions in \mathcal{H}^2 , the domain of definition of the operator $L := -\partial_x^2$ in \mathcal{L}^2 , we have to work in Bloch space in its counterpart $\tilde{\mathcal{H}}^2$, the domain of definition of the operator $\tilde{L}(\ell) := -(\partial_x + i\ell)^2$ in the space $L^2(\mathbb{T}_1, L^2_\Gamma)$, where L^2_Γ is defined by (2.16). We define

$\tilde{\mathcal{H}}^2 = \{ \tilde{U} \in L^2(\mathbb{T}_1, L^2_\Gamma) : \tilde{u}_j \in L^2(\mathbb{T}_1, H^2(I_{0,j})), \quad j \in \{0, +, -\}, \quad (2.13) - (2.14) \text{ are satisfied} \}$,
equipped with the norm

$$\|\tilde{U}\|_{\tilde{\mathcal{H}}^2} = \left(\int_{-1/2}^{1/2} \left(\|\tilde{u}_0(\ell, \cdot)\|_{H^2(I_{0,0})}^2 + \|\tilde{u}_+(\ell, \cdot)\|_{H^2(I_{0,+})}^2 + \|\tilde{u}_-(\ell, \cdot)\|_{H^2(I_{0,-})}^2 \right) d\ell \right)^{1/2}.$$

The following lemma presents an important result for the justification analysis in Bloch space.

Lemma 2.4.2. *The Bloch transform \mathcal{T} is an isomorphism between the spaces \mathcal{H}^2 and $\tilde{\mathcal{H}}^2$.*

Proof. We start with the function u_0 defined in (2.6). The L^2 -function u_0 which is in H^2 on the intervals $[2n\pi, 2n\pi + \pi]$ for $n \in \mathbb{Z}$ is extended smoothly to a global H^2 function $u_{0,\text{ext}}$. According to Lemma 2.4.1, we have $\mathcal{T}(u_{0,\text{ext}}) \in L^2(\mathbb{T}_1, H^2(\mathbb{T}_{2\pi}))$. With the cut-off function χ_0 defined in (2.35), we find by using (2.33) that

$$\tilde{u}_0 = \mathcal{T}(u_0) = \mathcal{T}(\chi_0 u_{0,\text{ext}}) = \chi_0 \mathcal{T}(u_{0,\text{ext}}).$$

Therefore, for fixed $\ell \in \mathbb{T}_1$, we have $\text{supp}(\tilde{u}_0) = I_{0,0}$. From the properties of $\mathcal{T}(u_{0,\text{ext}})$, we conclude that $\tilde{u}_0 \in L^2(\mathbb{T}_1, H^2(I_{0,0}))$. The components u_\pm are handled with the same technique. The boundary conditions (2.2)-(2.3) transfer in Bloch space into the boundary conditions (2.13)-(2.14). \square

2.5. Estimates for the residual terms

Here we decompose the evolution problem (2.34) into two parts. The first part reduces to the effective amplitude equation of the type (2.19) but written in Fourier space. The other part satisfies the evolution problem where the residual terms can be estimated in the space $\tilde{\mathcal{H}}^2$. Since the residual term after a standard decomposition similar to (2.17) and (2.18) is still large for estimates, we will also introduce an improved approximation by singling out some terms in the second part of the decomposition. Although the estimates are performed in Fourier and Bloch space, they can be easily transferred back to physical space.

In order to recover the ansatz (2.17) and (2.18) used for the derivation of the effective amplitude equation (2.19) in Bloch space, we split the solution to the evolution problem (2.34) into two parts. We write

$$\tilde{U}(t, \ell, x) = \tilde{V}(t, \ell) f^{(m_0)}(\ell, x) + \tilde{U}^\perp(t, \ell, x), \quad (2.36)$$

where the orthogonality condition $\langle \tilde{U}^\perp(t, \ell, \cdot), f^{(m_0)}(\ell, \cdot) \rangle_{L^2_{\mathbb{T}^d}} = 0$ is used for uniqueness of the decomposition. We find two parts of the evolution problem:

$$i\partial_t \tilde{V}(t, \ell) = \omega^{(m_0)}(\ell) \tilde{V}(t, \ell) - N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell) \quad (2.37)$$

and

$$i\partial_t \tilde{U}^\perp(t, \ell, x) = \tilde{L}(\ell) \tilde{U}^\perp(t, \ell, x) - N^\perp(\tilde{V}, \tilde{U}^\perp)(t, \ell, x), \quad (2.38)$$

where

$$N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell) = \langle (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, \cdot), f^{(m_0)}(\ell, \cdot) \rangle_{L^2_{\mathbb{T}^d}}$$

and

$$N^\perp(\tilde{V}, \tilde{U}^\perp)(t, \ell, x) = (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, x) - N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell) f^{(m_0)}(\ell, x).$$

Next, we estimate each part of the evolution problem.

2.5.1. Derivation of the effective amplitude equation

The effective amplitude equation (2.19) can be derived from equation (2.37) by evaluating it at $\tilde{U}^\perp = 0$. To be precise, we write

$$\begin{aligned} N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell) &= \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \beta(\ell, \ell_1, \ell_2, \ell_1 + \ell_2 - \ell) \\ &\quad \times \tilde{V}(t, \ell_1) \tilde{V}(t, \ell_2) \overline{\tilde{V}(t, \ell_1 + \ell_2 - \ell)} d\ell_1 d\ell_2 + N_{V, \text{rest}}(\tilde{V}, \tilde{U}^\perp)(t, \ell) \end{aligned}$$

where we used $\overline{\tilde{V}(t, \ell)} = \overline{\tilde{V}(t, -\ell)}$, and introduced the kernel β by

$$\beta(\ell, \ell_1, \ell_2, \ell_1 + \ell_2 - \ell) := \langle f^{(m_0)}(\ell_1, \cdot) f^{(m_0)}(\ell_2, \cdot) \overline{f^{(m_0)}(\ell_1 + \ell_2 - \ell, \cdot)}, f^{(m_0)}(\ell, \cdot) \rangle_{L^2_{\mathbb{T}^d}}.$$

We note that $N_{V, \text{rest}}(\tilde{V}, 0) = 0$. Let us now make the ansatz

$$\tilde{V}_{\text{app}}(t, \ell) = \tilde{A} \left(\varepsilon^2 t, \frac{\ell - \ell_0}{\varepsilon} \right) \mathbf{E}(t, \ell), \quad (2.39)$$

with

$$\mathbf{E}(t, \ell) := e^{-i\omega^{(m_0)}(\ell_0)t} e^{-i\partial_\ell \omega^{(m_0)}(\ell_0)(\ell - \ell_0)t},$$

insert (2.39) into the evolution problem (2.37), and set the coefficients of $\varepsilon^2 \mathbf{E}$ to zero. As a result, we obtain the leading-order equation in the form

$$\begin{aligned} i\partial_T \tilde{A}(T, \xi) &= \frac{1}{2} \partial_\ell^2 \omega^{(m_0)}(\ell_0) \xi^2 \tilde{A}(T, \xi) \\ &\quad - \nu \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \tilde{A}(T, \xi_1) \tilde{A}(T, \xi_2) \overline{\tilde{A}(T, \xi_1 + \xi_2 - \xi)} d\xi_1 d\xi_2, \end{aligned} \quad (2.40)$$

where $\ell = \ell_0 + \varepsilon\xi$, $T = \varepsilon^2 t$, and $\nu = \beta(\ell_0, \ell_0, \ell_0, \ell_0)$ coincides with the definition of ν in the amplitude equation (2.19).

By letting $\varepsilon \rightarrow 0$, in particular $\int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} d\xi \rightarrow \int_{-\infty}^{\infty} d\xi$, and $\tilde{A}(T, \xi) \rightarrow \hat{A}(T, \xi)$ as $\varepsilon \rightarrow 0$, equation (2.40) yields formally the NLS equation in Fourier space, namely

$$i\partial_T \hat{A}(T, \xi) - \frac{1}{2} \partial_\ell^2 \omega^{(m_0)}(\ell_0) \xi^2 \hat{A}(T, \xi) + \nu (\hat{A} * \hat{A} * \overline{\hat{A}})(T, \xi) = 0. \quad (2.41)$$

Equation (2.41) corresponds to the amplitude equation (2.19) in physical space. The formal calculations will be made rigorous in Section 2.5.3.

Remark 2.5.1. If $A(\cdot)$ is defined on \mathbb{R} and if it is scaled with the small parameter ε , then the Fourier transform of $A(\varepsilon \cdot)$ is $\varepsilon^{-1} \hat{A}(\varepsilon^{-1} \cdot)$. Therefore, a small term of the formal order $\mathcal{O}(\varepsilon^r)$ in physical space corresponds to a small term of the formal order $\mathcal{O}(\varepsilon^{r-1})$ in Fourier space. Since Bloch space is very similar to Fourier space, we have implemented the corresponding orders in the representation (2.39) compared to the standard approximation (2.17).

2.5.2. The improved approximation

The simple approximation (2.39) produces a number of terms in the second equation (2.38) which are of the formal order $\mathcal{O}(\varepsilon^2)$ in Bloch space and which do not cancel out each other. These terms are collected together in the so called residual. However, in order to bound the error with a simple application of Gronwall's inequality, as we do in Section 2.6, we need the residual to be of the formal order $\mathcal{O}(\varepsilon^3)$ in Bloch space.

As in [19], the $\mathcal{O}(\varepsilon^2)$ terms can be canceled out by adding higher order terms to the approximation (2.39) in (2.36). Therefore, we set

$$\tilde{U}_{\text{app}}^\perp(t, \ell, x) = \varepsilon^2 \tilde{B} \left(\varepsilon^2 t, \frac{\ell - \ell_0}{\varepsilon}, x \right) \mathbf{E}(t, \ell). \quad (2.42)$$

Inserting (2.42) into the evolution problem (2.38) and equating the coefficients of $\varepsilon^2 \mathbf{E}$ to zero gives the following equation in the lowest order in ε :

$$\begin{aligned} \omega^{(m_0)}(\ell_0) \tilde{B}(\varepsilon^2 t, \xi, x) &= \tilde{L}(\ell_0) \tilde{B}(\varepsilon^2 t, \xi, x) \\ &\quad - \varepsilon^{-2} \mathbf{E}^{-1}(t, \ell) N^\perp(\tilde{V}_{\text{app}}, 0)(t, \ell, x), \end{aligned} \quad (2.43)$$

where $\ell = \ell_0 + \varepsilon\xi$. Note that all \mathbf{E} -factors cancel each other out in the nonlinear terms. Moreover, the pre-factor ε^{-2} cancels with the factor ε^2 coming from the two times convolution of the scaled

ansatz functions. The equation (2.43) can be solved with respect to \tilde{B} if $\tilde{L}(\ell_0) - \omega^{(m_0)}(\ell_0)I$ is invertible. The invertibility condition

$$\inf_{m \in \mathbb{N} \setminus \{m_0\}} \left| \omega^{(m)}(\ell_0) - \omega^{(m_0)}(\ell_0) \right| > 0$$

is satisfied for the spectral problem (2.9) under the condition (2.20) of Theorem 2.2.3. Substituting \tilde{A} and \tilde{B} obtained from (2.40) and (2.43) into (2.39) and (2.42), and inserting the approximation $(\tilde{V}_{\text{app}}, \tilde{U}_{\text{app}}^\perp)$ into the evolution problem (2.37) and (2.38) cancel out all terms of the formal order $\mathcal{O}(\varepsilon^2)$. According to Remark 2.5.1, this corresponds to the cancelation of all terms of the formal order $\mathcal{O}(\varepsilon^3)$ in physical space. Hence the residual is formally of the order $\mathcal{O}(\varepsilon^3)$ in Bloch space and of the order $\mathcal{O}(\varepsilon^4)$ in physical space.

2.5.3. From Fourier space to Bloch space

As in Theorem 2.2.3, let $A \in C(\mathbb{R}, H^3(\mathbb{R}))$ be a solution of the effective amplitude equation (2.19). Here we show that the residual of the evolution problem (2.34) given by

$$\widetilde{\text{Res}}(\tilde{U})(t, \ell, x) = -i\partial_t \tilde{U}(t, \ell, x) + \tilde{L}(\ell)\tilde{U}(t, \ell, x) - (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, x),$$

can be estimated in $\tilde{\mathcal{H}}^2$ to be of order $\mathcal{O}(\varepsilon^{7/2})$ if the improved approximation is constructed by using the decomposition (2.36) with $(\tilde{V}_{\text{app}}, \tilde{U}_{\text{app}}^\perp)$ given by (2.39) and (2.42).

Before we start, we introduce some weights with respect to the ℓ -variable, namely

$$\rho_{\ell_0, \varepsilon, s}(\ell) = \left[1 + \left(\frac{\ell - \ell_0}{\varepsilon} \right)^2 \right]^{s/2}.$$

Remark 2.5.2. Regularity of functions in physical space corresponds to decay rates of their Fourier transforms at infinity. Due to Parseval's identity, Fourier transform is an isomorphism between H^s and L^2 equipped with a weight $\rho_{0,1,s}$. Furthermore, weights $\rho_{*,1,*}$ appear with functions which are not scaled with respect to ε , whereas weights $\rho_{*,\varepsilon,*}$ appear with functions which are scaled with respect to ε . The scaled weights $\rho_{*,\varepsilon,*}$ are necessary to transfer the smallness property $\partial_x A(\varepsilon x) = \varepsilon \partial_X A(X) = \mathcal{O}(\varepsilon)$ from physical space into Fourier space, cf. Lemma 2.5.4.

As a consequence of the assumptions on $A \in C(\mathbb{R}, H^3(\mathbb{R}))$, the Fourier transform \hat{A} is a solution of the NLS equation in Fourier space (2.41) and satisfies $\hat{A}\rho_{0,1,3} \in L^2(\mathbb{R})$. By the Cauchy-Schwarz inequality, we have

$$\|\hat{A}\rho_{0,1,2}\|_{L^1} \leq \|\hat{A}\rho_{0,1,3}\|_{L^2} \|\rho_{0,1,-1}\|_{L^2} \leq C \|\hat{A}\rho_{0,1,3}\|_{L^2}, \quad (2.44)$$

hence, $\hat{A}\rho_{0,1,2} \in L^1(\mathbb{R})$. For such a function \hat{A} in Fourier space, we define a function \tilde{A} in Bloch space by

$$\tilde{A}(T, \varepsilon^{-1}(\ell - \ell_0)) = \tilde{\chi}_{\ell_0}(\ell) \hat{A}(T, \varepsilon^{-1}(\ell - \ell_0)),$$

where $\tilde{\chi}_{\ell_0}$ is defined as the cutoff function

$$\tilde{\chi}_{\ell_0}(\ell) = \begin{cases} 1, & \ell - \ell_0 \in [-\delta, \delta], \\ 0, & \text{otherwise,} \end{cases}$$

with $\delta > 0$ being sufficiently small but independent of the small parameter ε . Using the periodicity condition

$$\tilde{A}(T, \varepsilon^{-1}(\ell + 1 - \ell_0)) = \tilde{A}(T, \varepsilon^{-1}(\ell - \ell_0)), \quad \ell \in \mathbb{R},$$

we extend $\tilde{A}(T, \varepsilon^{-1}(\ell - \ell_0))$ periodically in ℓ over \mathbb{R} . By construction, the leading-order approximation

$$\tilde{V}_{\text{app}} f^{(m_0)} \rho_{\ell_0, \varepsilon, 3} \in \tilde{\mathcal{H}}^2$$

is of the order $\mathcal{O}(\varepsilon^{1/2})$ due to the scaling properties of the L^2 -norm. Therefore, we are losing $\varepsilon^{1/2}$ when we perform estimates in $\tilde{\mathcal{H}}^2$. In order to avoid losing $\varepsilon^{1/2}$, let us consider estimates in the following L^1 -based space

$$\tilde{\mathcal{C}}^2 = \{\tilde{U} \in L^1(\mathbb{T}_1, L^2_\Gamma) : \tilde{u}_j \in L^1(\mathbb{T}_1, H^2(I_{0,j})), \quad j \in \{0, +, -\}, \quad (2.13) - (2.14) \text{ is satisfied}\},$$

equipped with the norm

$$\|\tilde{U}\|_{\tilde{\mathcal{C}}^2} = \int_{-1/2}^{1/2} \left(\|\tilde{u}_0(\ell, \cdot)\|_{H^2(I_{0,0})} + \|\tilde{u}_+(\ell, \cdot)\|_{H^2(I_{0,+})} + \|\tilde{u}_-(\ell, \cdot)\|_{H^2(I_{0,-})} \right) d\ell.$$

Compared to the estimates in $\tilde{\mathcal{H}}^2$, the leading-order approximation

$$\tilde{V}_{\text{app}} f^{(m_0)} \rho_{\ell_0, \varepsilon, 2} \in \tilde{\mathcal{C}}^2$$

is of the order $\mathcal{O}(\varepsilon)$. Due to Young's inequality and (2.44) we have

$$\|\tilde{V} \star \tilde{W}\|_{\tilde{\mathcal{H}}^2} \leq \|\tilde{V}\|_{\tilde{\mathcal{C}}^2} \|\tilde{W}\|_{\tilde{\mathcal{H}}^2},$$

respectively with weights

$$\|(\tilde{V} \star \tilde{W}) \rho_{\ell_0, \varepsilon, 2}\|_{\tilde{\mathcal{H}}^2} \leq C \|\tilde{V} \rho_{\ell_0, \varepsilon, 2}\|_{\tilde{\mathcal{C}}^2} \|\tilde{W} \rho_{\ell_0, \varepsilon, 2}\|_{\tilde{\mathcal{H}}^2},$$

with a constant C independent of the small parameter ε . Using these estimates shows that

$$\mathbf{E}^{-1}(t, \cdot) N^\perp(\tilde{V}_{\text{app}}, 0)(t, \cdot, \cdot) \rho_{\ell_0, \varepsilon, 2}(\cdot) \in \tilde{\mathcal{H}}^2$$

is of the order $\mathcal{O}(\varepsilon^{5/2})$ in $\tilde{\mathcal{H}}^2$ and of the order $\mathcal{O}(\varepsilon^3)$ in $\tilde{\mathcal{C}}^2$. Moreover, we have

$$\text{supp} \left(\mathbf{E}^{-1}(t, \cdot) N^\perp(\tilde{V}_{\text{app}}, 0)(t, \cdot, \cdot) \right) \subset [\ell_0 - 3\delta, \ell_0 + 3\delta].$$

Hence, we drop (2.43) and define

$$\tilde{B}(\varepsilon^2 t, \xi, x) = (\tilde{L}(\ell) - \omega^{(m_0)}(\ell_0)I)^{-1} \varepsilon^{-2} \mathbf{E}^{-1}(t, \ell) N^\perp(\tilde{V}_{\text{app}}, 0)(t, \ell, x), \quad (2.45)$$

where again $\ell = \ell_0 + \varepsilon\xi$. The inverse $(\tilde{L}(\ell) - \omega^{(m_0)}(\ell_0)I)^{-1}$ exists due to the non-resonance condition (2.20) for $\delta > 0$ sufficiently small, but independent of the small parameter $\varepsilon > 0$. The change from $\tilde{L}(\ell_0)$ in equation (2.43) to $\tilde{L}(\ell)$ here allows us to avoid an expansion of $\tilde{L}(\ell)$ at $\ell = \ell_0$, which would correspond to a loss of regularity.

By construction in (2.42), we have that $\tilde{U}_{\text{app}}^\perp \rho_{\ell_0, \varepsilon, 2} \in \tilde{\mathcal{H}}^2$ is of the order $\mathcal{O}(\varepsilon^{5/2})$ and $\tilde{U}_{\text{app}}^\perp \rho_{\ell_0, \varepsilon, 1} \in \tilde{\mathcal{C}}^2$ is of the order $\mathcal{O}(\varepsilon^3)$. Thus, we set

$$\varepsilon \tilde{\Psi}(t, \ell, x) = \tilde{V}_{\text{app}}(t, \ell) f^{(m_0)}(\ell, x) + \tilde{U}_{\text{app}}^\perp(t, \ell, x), \quad (2.46)$$

with \tilde{V}_{app} and $\tilde{U}_{\text{app}}^\perp$ defined in (2.39) and (2.42).

Remark 2.5.3. In contrast to the approximation $\varepsilon \Psi_{\text{nls}}$ the approximation $\varepsilon \Psi = \mathcal{T}^{-1}(\varepsilon \tilde{\Psi})$ satisfies the Kirchhoff boundary conditions (2.2)-(2.3).

2.5.4. Estimates in Bloch space

By construction of $\varepsilon\widetilde{\Psi}$, the lower order terms are canceled out so that $\widetilde{\text{Res}}(\varepsilon\widetilde{\Psi})$ is formally of the order $\mathcal{O}(\varepsilon^4)$ in physical space and of the order of $\mathcal{O}(\varepsilon^3)$ in Bloch space. In order to put this formal count on a rigorous footing, we use the following elementary result.

Lemma 2.5.4. *Let $m, s \geq 0$ and let $g : \mathbb{T}_1 \rightarrow \mathbb{R}$ satisfy*

$$|g(\ell)| \leq C|\ell - \ell_0|^s, \quad \ell \in \mathbb{T}_1,$$

for some $C > 0$. Then, we have

$$\|\rho_{0,1,m}(\cdot)g(\cdot)\widetilde{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2(\mathbb{T}_1)} \leq C\varepsilon^{s+1/2}\|\rho_{0,1,m+s}\widehat{A}\|_{L^2(\mathbb{R})}.$$

Proof. We estimate the left-hand side as follows:

$$\begin{aligned} \|\rho_{0,1,m}(\cdot)g(\cdot)\widetilde{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2(\mathbb{T}_1)}^2 &= \int_{\mathbb{T}_1} |g(\ell)|^2 (1 + \ell^2)^m \left| \widetilde{A}\left(\frac{\ell - \ell_0}{\varepsilon}\right) \right|^2 d\ell \\ &\leq \sup_{\ell \in \mathbb{T}_1} |g(\ell)|^2 (1 + \varepsilon^{-2}|\ell - \ell_0|^2)^{-s-m} (1 + \ell^2)^m \int_{\mathbb{T}_1} (1 + \varepsilon^{-2}(\ell - \ell_0)^2)^{m+s} \left| \widetilde{A}\left(\frac{\ell - \ell_0}{\varepsilon}\right) \right|^2 d\ell \\ &\leq C^2 \varepsilon^{2s} \varepsilon \|\rho_{0,1,m+s}\widehat{A}\|_{L^2(\mathbb{R})}^2 \end{aligned}$$

where the last inequality follows from the scaling transformation for the squared L^2 -norm, cf. also the subsequent Remark 2.5.6. \square

By using Lemma 2.5.4, we obtain the estimate on $\widetilde{\text{Res}}(\varepsilon\widetilde{\Psi})$ given by (2.46).

Lemma 2.5.5. *Let $A \in C([0, T_0], H^3)$ be a solution of the amplitude equation (2.19) for some $T_0 > 0$. Then, there is a positive ε -independent constant C_{Res} that only depends on the norm of the solution A such that*

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\widetilde{\text{Res}}(\varepsilon\widetilde{\Psi})\|_{\widetilde{\mathcal{H}}^2} \leq C_{\text{Res}}\varepsilon^{7/2}, \quad (2.47)$$

or equivalently,

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\text{Res}(\varepsilon\Psi)\|_{\mathcal{H}^2} \leq C_{\text{Res}}\varepsilon^{7/2}. \quad (2.48)$$

Proof. We define

$$\begin{aligned} \widetilde{\text{Res}}_V(\widetilde{V}, \widetilde{U}^\perp)(t, \ell) &= -i\partial_t \widetilde{V}(t, \ell) + \omega^{(m_0)}(\ell)\widetilde{V}(t, \ell) - N_V(\widetilde{V}, \widetilde{U}^\perp)(t, \ell), \\ \widetilde{\text{Res}}^\perp(\widetilde{V}, \widetilde{U}^\perp)(t, \ell, x) &= -i\partial_t \widetilde{U}^\perp(t, \ell, x) + \widetilde{L}(\ell)\widetilde{U}^\perp(t, \ell, x) - N^\perp(\widetilde{V}, \widetilde{U}^\perp)(t, \ell, x). \end{aligned}$$

By construction we have

$$\widetilde{\text{Res}}^\perp(\widetilde{V}_{\text{app}}, \widetilde{U}_{\text{app}}^\perp)(t, \ell, x) = s_1 + s_2,$$

where

$$\begin{aligned} s_1 &= (-i\partial_t + \omega^{(m_0)}(\ell_0))\widetilde{U}_{\text{app}}^\perp(t, \ell, x) \\ &= (-\varepsilon^2\partial_\ell\omega^{(m_0)}(\ell_0)(\ell - \ell_0) + \varepsilon^4\partial_T)\widetilde{B}(T, \xi, x)\mathbf{E}(t, \ell) \\ &= (-\varepsilon^3\partial_\ell\omega^{(m_0)}(\ell_0)\xi + \varepsilon^4\partial_T)\widetilde{B}(T, \xi, x)\mathbf{E}(t, \ell) \end{aligned}$$

and

$$s_2 = N^\perp(\tilde{V}, 0)(t, \ell, x) - N^\perp(\tilde{V}, \tilde{U}^\perp)(t, \ell, x),$$

again with $\ell = \ell_0 + \varepsilon\xi$. Via (2.45) the term $\partial_T \tilde{B}$ in s_1 can be expressed in terms of $\partial_T \tilde{V}_{\text{app}}$, respectively in terms of $\partial_T A$, where $\partial_T A$ can be expressed by the right-hand side of the amplitude equation (2.19). Similarly, the term $\xi \tilde{B}(T, \xi, x)$ can be estimated in terms of $\xi \hat{A}(T, \xi)$. Since $\tilde{U}_{\text{app}}^\perp$ obviously is in $\tilde{\mathcal{H}}^2$, we eventually have the estimate

$$\begin{aligned} \|s_1\|_{\tilde{\mathcal{H}}^2} &\leq C\varepsilon^{7/2} \|\hat{A}\|_{L^1}^2 \|\hat{A}\rho_{0,1,1}\|_{L^2} \\ &\quad + C\varepsilon^{9/2} \|\hat{A}\|_{L^1}^2 (\|\hat{A}\rho_{0,1,2}\|_{L^2} + \|\hat{A}\|_{L^1}^2 \|\hat{A}\|_{L^2}). \end{aligned}$$

In s_2 by pure counting of powers of ε we find the formal order $\mathcal{O}(\varepsilon^3)$ in Bloch space and due to the scaling properties of the L^2 -norm, we have

$$\|s_2\|_{\tilde{\mathcal{H}}^2} \leq C_A \varepsilon^{7/2},$$

where the constant C_A depend on $\|\hat{A}\rho_{0,1,3}\|_{L^2}$.

Next we have

$$\widetilde{\text{Res}}_V(\tilde{V}_{\text{app}}, \tilde{U}_{\text{app}}^\perp)(t, \ell) = r_1 + r_2,$$

where

$$\begin{aligned} r_1 &= -i\partial_t \tilde{V}_{\text{app}}(t, \ell) + \omega^{(m_0)}(\ell) \tilde{V}_{\text{app}}(t, \ell) - N_V(\tilde{V}_{\text{app}}, 0)(t, \ell) \\ &\quad + \mathbf{E} \tilde{\chi}_{\ell_0}(\ell) (i\partial_T \hat{A}(T, \xi) - \frac{1}{2} \partial_\ell^2 \omega^{(m_0)}(\ell_0) \xi^2 \hat{A}(T, \xi) + \nu(\hat{A} * \hat{A} * \hat{A})(T, \xi)) \end{aligned}$$

and

$$r_2 = N_V(\tilde{V}_{\text{app}}, 0)(t, \ell) - N_V(\tilde{V}_{\text{app}}, \tilde{U}_{\text{app}}^\perp)(t, \ell).$$

The term r_2 is of the formal order $\mathcal{O}(\varepsilon^3)$ in Bloch space and due to the scaling properties of the L^2 -norm, it is of the order $\mathcal{O}(\varepsilon^{7/2})$ in L^2 . The second line in r_1 vanishes identically since it is a multiple of the effective amplitude equation (2.19). The prefactor \mathbf{E} is necessary to compare the second line in r_1 with the first line in r_1 . The cut-off function $\tilde{\chi}_{\ell_0}$ is needed to bring (2.19) from Fourier space to Bloch space.

The comparison of the terms of the first and of the second line in r_1 condense in estimates for the difference between $\omega^{(m_0)}(\ell)$ and its second Taylor polynomial at ℓ_0 ,

$$T_2(\ell; \ell_0) = \omega^{(m_0)}(\ell_0) + \partial_\ell \omega^{(m_0)}(\ell_0)(\ell - \ell_0) + \frac{1}{2} \partial_\ell^2 \omega^{(m_0)}(\ell_0)(\ell - \ell_0)^2,$$

the difference between the nonlinear coefficient $\beta = \beta(\ell, \ell_1, \ell_2, \ell_1 + \ell_2 - \ell)$ defined in (2.39) and the coefficient $\nu = \beta(\ell_0, \ell_0, \ell_0, \ell_0)$, and the difference between \hat{A} and \tilde{A} .

In detail, we use the estimate

$$\left| \omega^{(m_0)}(\ell) - T_2(\ell; \ell_0) \right| \leq C |\ell - \ell_0|^3$$

and apply Lemma 2.5.4 with $m = 0$ and $s = 3$ to find

$$\|(\omega^{(m_0)}(\cdot) - T_2(\cdot; \ell_0)) \tilde{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2(\mathbb{T}_1)} \leq C \varepsilon^{7/2} \|\rho_{0,1,3} \hat{A}\|_{L^2(\mathbb{R})}.$$

For the difference between the nonlinear coefficients, we use the estimate

$$\begin{aligned} & |\beta(\ell, \ell_1, \ell_2, \ell_1 + \ell_2 - \ell) - \beta(\ell_0, \ell_0, \ell_0, \ell_0)| \\ & \leq C(|\ell - \ell_0| + |\ell_1 - \ell_0| + |\ell_2 - \ell_0| + |\ell_1 + \ell_2 - \ell - \ell_0|) \end{aligned}$$

and apply an obvious generalization of Lemma 2.5.4 to multilinear terms. It remains to estimate the difference between \widehat{A} and \widetilde{A} . Since $|\widetilde{\chi}_{\ell_0}(\ell) - 1| \leq C|\ell - \ell_0|^m$ for every $m \geq 0$, we have for $m = 3$,

$$\begin{aligned} \|\widehat{A}(\varepsilon^{-1}(\cdot - \ell_0)) - \widetilde{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2} &= \|(1 - \widetilde{\chi}_{\ell_0})\widehat{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2} \\ &\leq \varepsilon^{1/2} \sup_{\ell \in \mathbb{R}} |(1 - \widetilde{\chi}_0(\varepsilon\ell))(1 + |\ell|)^{-3}| \|\widehat{A}\rho_{0,1,3}\|_{L^2} \\ &\leq C\varepsilon^{7/2} \|\widehat{A}\rho_{0,1,3}\|_{L^2}. \end{aligned}$$

By using these expansions, we derive the bound (2.47). Bound (2.48) holds thanks to the isomorphism of Bloch transform \mathcal{T} between \mathcal{H}^2 and $\widetilde{\mathcal{H}}^2$. \square

Remark 2.5.6. Compared to Remark 2.5.1 on the formal order in physical and Bloch space, we note that bounds (2.47) and (2.48) are identical in physical and Bloch space. This is because we gain $\varepsilon^{1/2}$ in the $\widetilde{\mathcal{H}}^2$ -norm due to the concentration and lose $\varepsilon^{-1/2}$ in the \mathcal{H}^2 -norm due to the long wave scaling.

Let us now recall that the approximation $\varepsilon\Psi_{\text{nl}s}$ given by (2.18) that leads to the effective amplitude equation (2.19) is different from the improved approximation $\varepsilon\Psi$, which is given by (2.46) in Bloch space. The next result compares the two approximations. It is obtained by an elementary application of the Lemmas 2.3.1, 2.4.2 and 2.5.4.

Lemma 2.5.7. *Let $A \in C([0, T_0], H^3)$ be a solution of the amplitude equation (2.19) for some $T_0 > 0$. Then, there exist positive ε -independent constants C and C_ψ that only depend on the norm of the solution A such that*

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\varepsilon\widetilde{\Psi}\|_{\widetilde{\mathcal{C}}^2} \leq C_\Psi \varepsilon \quad (2.49)$$

and

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\varepsilon\Psi - \varepsilon\Psi_{\text{nl}s}\|_{L^\infty} \leq C\varepsilon^{3/2}. \quad (2.50)$$

Proof. The first estimate (2.49) immediately follows by the previous estimates on each component of $\widetilde{\Psi}$. The second estimate (2.50) follows by applying a slight generalization of Lemma 2.5.4 to the difference $f^{(m_0)}(\ell, \cdot) - f^{(m_0)}(\ell_0, \cdot)$ and using the triangle inequality, since the term $\widetilde{U}_{\text{app}}^\perp$ is very small compared to the term $\widetilde{V}_{\text{app}} f^{(m_0)}$ in (2.46). Since the boundary conditions for the derivatives of the eigenfunctions depend on ℓ they can only be compared in $H^1(\mathbb{T}_{2\pi})$. We have

$$\|f^{(m_0)}(\ell, \cdot) - f^{(m_0)}(\ell_0, \cdot)\|_{H^1(\mathbb{T}_{2\pi})} \leq C|\ell - \ell_0|.$$

With the obvious generalization of Lemma 2.5.4 we obtain

$$\|(f^{(m_0)}(\ell, \cdot) - f^{(m_0)}(\ell_0, \cdot))\widetilde{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2(\mathbb{T}_1, H^1(\mathbb{T}_{2\pi}))} \leq C\varepsilon^{3/2} \|\rho_{0,1,1}\widehat{A}\|_{L^2(\mathbb{R})}.$$

Lemma 2.4.1 and Sobolev's embedding theorem yield estimate (2.50). \square

2.6. Estimates for the error term

Here we complete the proof of Theorem 2.2.3. The proof of the approximation result is based on a simple application of Gronwall's inequality.

First we note that, by the standard energy estimates, the local solution U to the evolution problem (2.8) constructed in Theorem 2.3.5 can be continued to the global solution U in \mathcal{H}^2 with a possible growth of the \mathcal{H}^2 -norm as $t \rightarrow \infty$. We do not worry about the possible growth of the global solution U because the approximation result of Theorem 2.2.3 is obtained on finite but long time intervals with a precise control of the error terms, cf. bound (2.21).

We write the solution U to the evolution problem (2.8) as a sum of the approximation term $\varepsilon\Psi$ controlled by Lemma 2.5.7 and the error term $\varepsilon^{3/2}R$, i.e.,

$$U = \varepsilon\Psi + \varepsilon^{3/2}R. \quad (2.51)$$

Inserting this decomposition into the evolution problem (2.8) gives

$$\partial_t R = -iLR + iG(\Psi, R) \quad (2.52)$$

where the linear operator $L = -\partial_x^2$ is studied in Lemma 2.3.2 and the nonlinear terms are expanded as

$$G(\Psi, R) = \varepsilon^{-3/2}\text{Res}(\varepsilon\Psi) + \varepsilon^2\Psi^2\bar{R} + 2\varepsilon^2\Psi R\bar{\Psi} + 2\varepsilon^{5/2}\Psi R\bar{R} + \varepsilon^{5/2}R^2\bar{\Psi} + \varepsilon^3R^2\bar{R}.$$

The product terms in the definition of $G(\Psi, R)$ are understood componentwise with $R = (r_0, r_+, r_-)$ and $\Psi = (\psi_0, \psi_+, \psi_-)$. Using the bounds

$$\|\Psi R\|_{\mathcal{H}^2} \leq C\|\tilde{\Psi}\tilde{R}\|_{\tilde{\mathcal{H}}^2} \leq C\|\tilde{\Psi}\|_{\tilde{\mathcal{C}}^2}\|\tilde{R}\|_{\tilde{\mathcal{H}}^2} \leq CC_\Psi\|\tilde{R}\|_{\tilde{\mathcal{H}}^2} \leq C^2C_\Psi\|R\|_{\mathcal{H}^2},$$

where C_Ψ appears in (2.49) of Lemma 2.5.7, we estimate each term of G with the help of Lemmas 2.3.1 and 2.5.5:

$$\begin{aligned} \|\varepsilon^{-3/2}\text{Res}(\varepsilon\Psi)\|_{\mathcal{H}^2} &\leq C_{\text{Res}}\varepsilon^2, \\ \|2\varepsilon^2\Psi R\bar{\Psi}\|_{\mathcal{H}^2} &\leq 2C_1\varepsilon^2\|R\|_{\mathcal{H}^2}, \\ \|\varepsilon^2\Psi^2\bar{R}\|_{\mathcal{H}^2} &\leq C_1\varepsilon^2\|R\|_{\mathcal{H}^2}, \\ \|\varepsilon^{5/2}R^2\bar{\Psi}\|_{\mathcal{H}^2} &\leq C_1\varepsilon^{5/2}\|R\|_{\mathcal{H}^2}^2, \\ \|2\varepsilon^{5/2}\Psi R\bar{R}\|_{\mathcal{H}^2} &\leq 2C_1\varepsilon^{5/2}\|R\|_{\mathcal{H}^2}^2, \\ \|\varepsilon^3R^2\bar{R}\|_{\mathcal{H}^2} &\leq C_1\varepsilon^3\|R\|_{\mathcal{H}^2}^3, \end{aligned}$$

where C_1 is a constant independent of $\|R\|_{\mathcal{H}^2}$ and the small parameter $\varepsilon > 0$. Therefore, we find

$$\|G(\Psi, R)\|_{\mathcal{H}^2} \leq C_{\text{Res}}\varepsilon^2 + 3C_1\varepsilon^2\|R\|_{\mathcal{H}^2} + 3C_1\varepsilon^{5/2}\|R\|_{\mathcal{H}^2}^2 + C_1\varepsilon^3\|R\|_{\mathcal{H}^2}^3.$$

For simplicity, we assume $R(0) = 0$. Then, the variation of constant formula for the evolution system (2.52) yields the integral formula

$$R(t) = \int_0^t e^{-iL(t-\tau)} iG(\Psi, R)(\tau) d\tau.$$

By Lemma 2.3.4, the operator e^{-iLt} forms a group in \mathcal{H}^2 which is uniformly bounded with respect to t . Using Gronwall's inequality finally allows us to estimate the error term on the time scale $T = \varepsilon^2 t$ for $T \in [0, T_0]$ by

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|R(t)\|_{\mathcal{H}^2} \leq C_{\text{Res}} T_0 e^{4C_1 T_0} =: M$$

for all $\varepsilon \in (0, \varepsilon_0)$, if $\varepsilon_0 > 0$ is chosen so small that $3\varepsilon_0^{1/2} M + \varepsilon_0 M^2 \leq 1$. Sobolev's embedding theorem, bound (2.50), and the decomposition (2.51) complete the proof of the approximation result (2.21) of Theorem 2.2.3. \square

Remark 2.6.1. We explain how the proof of Theorem 2.2.3 has to be modified in order to prove Theorem 2.2.8. We only need H^2 for the Dirac case instead of H^3 in the NLS case due to the fact that the functions ω_{\pm} given by (2.22) and (2.23) have to be expanded in ℓ up to quadratic order for estimating the residual terms. The decomposition formula (2.36) is replaced by

$$\tilde{U}(t, \ell, x) = \tilde{V}_+(t, \ell) f^+(\ell, x) + \tilde{V}_-(t, \ell) f^-(\ell, x) + \tilde{U}^\perp(t, \ell, x),$$

subject to the orthogonality constraints $\langle \tilde{U}^\perp(t, \ell, \cdot), f^+(\ell, \cdot) \rangle_{L^2_{\mathbb{F}}} = \langle \tilde{U}^\perp(t, \ell, \cdot), f^-(\ell, \cdot) \rangle_{L^2_{\mathbb{F}}} = 0$. For the derivation of the coupled-mode system (2.25)-(2.26) we then make the ansatz

$$\tilde{V}_{\text{app}, \pm}(t, \ell) = \varepsilon^{-1} \tilde{A}_{\pm}(\varepsilon^2 t, \varepsilon^{-2} \ell) e^{-i\omega_{\pm}(0)t}.$$

Straightforward modifications of this kind can be performed at each step in the proof of Theorem 2.2.3. This procedure yields the proof of Theorem 2.2.8.

2.7. Discussion

Here we discuss why the previously presented theory applies to other periodic quantum graphs. The general strategy is as follows. Rescale the length of the bonds in such a way that the basic cell of the periodic graph has a length of 2π . The differential operators and the Kirchhoff boundary conditions at the vertices have to be rescaled, too. We refrain from greatest generality and explain this approach for two periodic quantum graphs, cf. Figure 2.5, which are slightly more complicated than the periodic graph plotted in Figure 2.1.

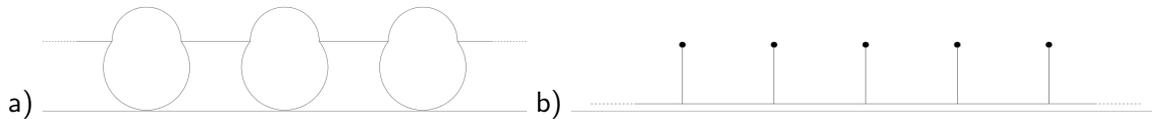


Figure 2.5.: a) Generalization of the periodic quantum graph sketched in Figure 2.1. The central segment $\Gamma_{n,0}$ has length L_0 and the circular segments $\Gamma_{n,\pm}$ have lengths L_+ and L_- . b) A periodic quantum graph with a vertical pendant and a horizontal bond, each of length π , with Dirichlet boundary conditions at the dead end.

In order to bring the quantum graph plotted in Figure 2.5(a) into a form for which our previous theory applies, we first identify $\Gamma_{0,0}$ with $[0, L_0]$, $\Gamma_{0,+}$ with $[0, L_+]$, and $\Gamma_{0,-}$ with $[0, L_-]$. The coordinates in these bonds are denoted with y . Then on $\Gamma_{0,0}$ we introduce $\pi y = L_0 x$ and on

$\Gamma_{0,\pm}$ we introduce $\pi y = L_{\pm}(x - \pi)$. Hence we are back on our original quantum graph, but with different equations and different vertex conditions, namely:

$$i\partial_t U + \frac{L_0^2}{\pi^2} \partial_x^2 U + |U|^2 U = 0, \quad \text{for } x \in (2\pi n, 2\pi n + \pi)$$

and

$$i\partial_t U + \frac{L_{\pm}^2}{\pi^2} \partial_x^2 U + |U|^2 U = 0, \quad \text{for } x \in (2\pi n + \pi, 2\pi(n+1)),$$

subject to

$$\begin{cases} u_{n,0}(t, 2\pi n + \pi) = u_{n,+}(t, 2\pi n + \pi) = u_{n,-}(t, 2\pi n + \pi), \\ u_{n+1,0}(t, 2\pi(n+1)) = u_{n,+}(t, 2\pi(n+1)) = u_{n,-}(t, 2\pi(n+1)), \end{cases}$$

and

$$\begin{cases} L_0 \partial_x u_{n,0}(t, 2\pi n + \pi) = L_+ \partial_x u_{n,+}(t, 2\pi n + \pi) + L_- \partial_x u_{n,-}(t, 2\pi n + \pi), \\ L_0 \partial_x u_{n+1,0}(t, 2\pi(n+1)) = L_+ \partial_x u_{n,+}(t, 2\pi(n+1)) + L_- \partial_x u_{n,-}(t, 2\pi(n+1)). \end{cases}$$

The spectral bands of the linear operator for the periodic graph on Figure 2.5(a) depend on parameter L_0 , L_+ , and L_- .

In the case $L_0 \neq L_+ = L_-$ (left panel on Fig. 2.6), the Dirac points disappear and all spectral bands but the flat bands are disjoint. The flat bands still intersect with the interior points of the spectral bands of L . As a result, the justification of the amplitude equation (2.19) can still be developed for the NLS equation on the periodic quantum graph but the non-resonance condition (2.20) is satisfied for every $m_0 \in \mathbb{N}$ and $\ell_0 \in \mathbb{T}_1$, for which $\omega^{(m_0)}(\ell_0)$ is different from the eigenvalue corresponding to the flat spectral bands.

In the case $L_0 = L_+ \neq L_-$ (right panel on Fig. 2.6), the degeneracy of all flat bands is broken and all spectral bands have nonzero curvature and are disjoint from each other. As a result, the non-resonance condition (2.20) is now satisfied for every $m_0 \in \mathbb{N}$ and $\ell_0 \in \mathbb{T}_1$ without any reservations.

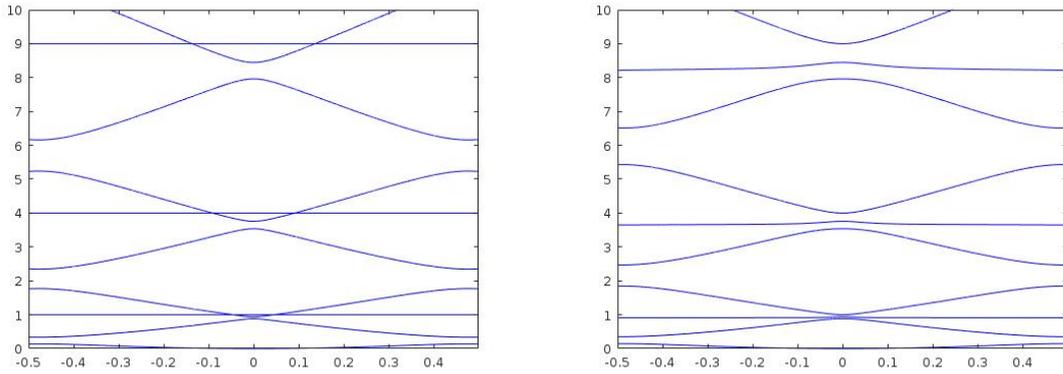


Figure 2.6.: The Floquet-Bloch spectrum of the linear operator $L = -\partial_x^2$ for the periodic quantum graph plotted on Figure 2.5(a) with $L_0 = \pi + 0.3$ and $L_+ = L_- = \pi$ (left) and $L_0 = \pi$, $L_+ = \pi$, and $L_- = \pi + 0.3$ (right).

In a similar way, the quantum graph plotted in Figure 2.5(b) can be handled. We refrain here from details and only show the spectral picture in Figure 2.7. Dirac points appear now at $\ell = \pm \frac{1}{2}$ and the flat bands are now disjoint from the other bands. Correspondingly, both the NLS amplitude equation and the coupled-mode (Dirac) equations can be justified for the periodic quantum graph at the corresponding points in the spectral bands.

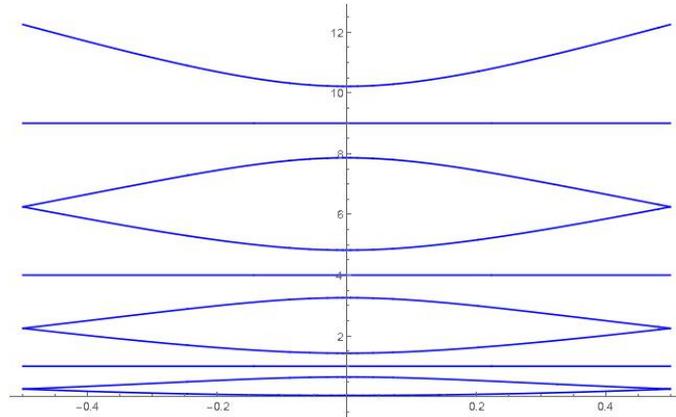


Figure 2.7.: The Floquet-Bloch spectrum of the linear operator $L = -\partial_x^2$ for the periodic quantum graph plotted in Figure 2.5(b).

Finally, we can think of transferring the ideas of the justification analysis to other nonlinear evolution equations, which would include the nonlinear wave equations and systems with quadratic nonlinearities. Since the eigenfunctions are not smooth at the graph vertices due to the Kirchhoff boundary conditions, we may face difficulties with analysis of convolution terms and near-identity transformations, in comparison with a similar analysis for smooth periodic potentials [10]. Additionally, more complicated non-resonance conditions may appear in the analysis of the nonlinear wave equation without the gauge covariance compared to the case of the cubic NLS equation (2.1). Thus, it will be a purpose of subsequent works to extend the justification analysis to other nonlinear evolution equations.

3. Approximation of a cubic Klein-Gordon equation on periodic quantum graphs

After proving an approximation result for the NLS equation on a spatially extended periodic quantum graph, we now consider a cubic Klein-Gordon (cKG) equation as original system in the same setting. In Chapter 2, a multiple scaling expansion yields a NLS equation as effective amplitude equation describing slow modulations in time and space of an oscillating wave packet. It is the goal of this chapter to transfer the analysis from [17] to this situation. A similar result for the spatially homogeneous case is given in [10].

Here we have to deal with two major differences compared to the problem described in Chapter 2. First of all, the cKG equation is a second order differential equation with respect to time in contrast to the NLS equation, and is also not invariant under the transformation $u(t, x) \mapsto u(t, x)e^{i\phi_0}$ for every $\phi_0 \in \mathbb{R}$. Both points force us to modify the arguments for the construction of the solutions and the higher order approximations which are necessary to get rid of some regularity problems associated with the Kirchoff boundary conditions at the vertices.

Our strategy to obtain an approximation theorem for the cKG equation is the same as in [17] and Chapter 2, respectively. We describe the model in Section 3.1 and the main result is stated in Section 3.2 after introducing the spectral situation on the periodic quantum graph. The local existence and uniqueness of solutions of the original system is discussed in Section 3.3. Then, in Section 3.4, we transfer the system into Bloch space and derive an effective amplitude equation. We also construct an improved approximation and estimate the corresponding residual. Finally, the amplitude equation is justified by estimating the error terms in Section 3.6.

Notation: According to Chapter 2, we use the standard notations for the Sobolev space $H^s(\mathbb{R})$ and the Lebesgue space $L^p(\mathbb{R})$ for $s \geq 0$ and $p \geq 1$.

3.1. The model

We consider the cKG equation

$$\partial_t^2 u - \partial_x^2 u + u + u^3 = 0, \quad t \in \mathbb{R}, \quad x \in \Gamma, \quad (3.1)$$

as original system on the periodic quantum graph

$$\Gamma = \bigoplus_{n \in \mathbb{Z}} \Gamma_n, \quad \text{with} \quad \Gamma_n = \Gamma_{n,0} \oplus \Gamma_{n,+} \oplus \Gamma_{n,-},$$

which was already introduced in Section 2.2. At the vertex points $x \in \{k\pi : k \in \mathbb{Z}\}$ of the quantum graph Γ , we again use the Kirchoff boundary conditions

$$\begin{cases} u_{n,0}(t, 2\pi n + \pi) = u_{n,+}(t, 2\pi n + \pi) = u_{n,-}(t, 2\pi n + \pi), \\ u_{n+1,0}(t, 2\pi(n+1)) = u_{n,+}(t, 2\pi(n+1)) = u_{n,-}(t, 2\pi(n+1)), \end{cases} \quad (3.2)$$

and

$$\begin{cases} \partial_x u_{n,0}(t, 2\pi n + \pi) = \partial_x u_{n,+}(t, 2\pi n + \pi) + \partial_x u_{n,-}(t, 2\pi n + \pi), \\ \partial_x u_{n+1,0}(t, 2\pi(n+1)) = \partial_x u_{n,+}(t, 2\pi(n+1)) + \partial_x u_{n,-}(t, 2\pi(n+1)). \end{cases} \quad (3.3)$$

Remark 3.1.1. Similar to the discussion in Section 2.7, we can extend the subsequent approach to other one-dimensional quantum graphs by rescaling the length of the bonds, the differential operators and the boundary conditions.

Studying the NLS equation on the periodic quantum graph Γ , it turned out to be advantageous to transfer the scalar partial differential equation on Γ to a vector-valued PDE on the real axis by introducing the functions

$$u_0(x) = \begin{cases} u_{n,0}(x), & x \in I_{n,0}, \\ 0, & x \in I_{n,\pm}, \end{cases} \quad n \in \mathbb{Z},$$

and

$$u_{\pm}(x) = \begin{cases} u_{n,\pm}(x), & x \in I_{n,\pm}, \\ 0, & x \in I_{n,0}, \end{cases} \quad n \in \mathbb{Z}.$$

Hence, we get $I_0 = \text{supp}(u_0)$ and $I_{\pm} = \text{supp}(u_{\pm})$. We collect the functions u_0 and u_{\pm} in the vector $U = (u_0, u_+, u_-)$ and rewrite the evolution problem (3.1) as

$$\partial_t^2 U - \partial_x^2 U + U + U^3 = 0, \quad t \in \mathbb{R}, \quad x \in \mathbb{R} \setminus \{k\pi : k \in \mathbb{Z}\}, \quad (3.4)$$

subject to the conditions (2.2)-(2.3) at the vertex points $x \in \{k\pi : k \in \mathbb{Z}\}$. Here, the cubic nonlinear term U^3 stands for the vector (u_0^3, u_+^3, u_-^3) .

3.2. Main result

The first part of this section is devoted to the analysis of the spectral situation of the linearized problem associated to the cKG equation (3.4), namely

$$\partial_t^2 U = \partial_x^2 U - U. \quad (3.5)$$

In the second part, we introduce the multiscale ansatz $\varepsilon \Psi_{\text{nls}}$ and state the resulting amplitude equation on the homogenous space. We finish the section with the formulation of the approximation theorem.

3.2.1. The Floquet-Bloch spectrum

The linear partial differential equation (3.5) is solved by the Bloch modes

$$U(t, x) = e^{i\omega t} e^{i\ell x} f(\ell, x), \quad \ell, x \in \mathbb{R},$$

where $f(\ell, \cdot) = (f_0, f_+, f_-)(\ell, \cdot)$ is a 2π -periodic function for every $\ell \in \mathbb{R}$ and satisfies the continuation conditions

$$f(\ell, x) = f(\ell, x + 2\pi), \quad f(\ell, x) = f(\ell + 1, x) e^{ix}, \quad \ell, x \in \mathbb{R}.$$

Therefore, we can restrict the definition of $f(\ell, x)$ to $x \in \mathbb{T}_{2\pi}$ and $\ell \in \mathbb{T}_1$ as in Section 2.2.2 and the Bloch function $f(\ell, x)$ is a solution of the eigenvalue problem

$$-(\partial_x + i\ell)^2 f(\ell, x) + f(\ell, x) = \omega^2(\ell) f(\ell, x), \quad x \in \mathbb{T}_{2\pi}, \quad (3.6)$$

subject to the boundary conditions

$$\begin{cases} f_0(\ell, \pi) = f_+(\ell, \pi) = f_-(\ell, \pi), \\ f_0(\ell, 0) = f_+(\ell, 2\pi) = f_-(\ell, 2\pi) \end{cases} \quad (3.7)$$

and

$$\begin{cases} (\partial_x + i\ell)f_0(\ell, \pi) = (\partial_x + i\ell)f_+(\ell, \pi) + (\partial_x + i\ell)f_-(\ell, \pi), \\ (\partial_x + i\ell)f_0(\ell, 0) = (\partial_x + i\ell)f_+(\ell, 2\pi) + (\partial_x + i\ell)f_-(\ell, 2\pi). \end{cases} \quad (3.8)$$

The functions $f_0(\ell, \cdot)$ and $f_{\pm}(\ell, \cdot)$ have their supports in $I_{0,0} = [0, \pi] \subset \mathbb{T}_{2\pi}$ and $I_{0,\pm} = [\pi, 2\pi] \subset \mathbb{T}_{2\pi}$, respectively.

As in Section 2.2.2, we define for the periodic eigenvalue problem (3.6) the L^2 -based spaces

$$L_{\Gamma}^2 := \{ \tilde{U} = (\tilde{u}_0, \tilde{u}_+, \tilde{u}_-) \in (L^2(\mathbb{T}_{2\pi}))^3 : \text{supp}(\tilde{u}_j) = I_{0,j}, \quad j \in \{0, +, -\} \}$$

and

$$H_{\Gamma}^2(\ell) := \{ \tilde{U} \in L_{\Gamma}^2 : \tilde{u}_j \in H^2(I_{0,j}), \quad j \in \{0, +, -\}, \quad (3.7) - (3.8) \text{ are satisfied} \},$$

equipped with the norm

$$\|\tilde{U}\|_{H_{\Gamma}^2(\ell)} = \left(\|\tilde{u}_0\|_{H^2(I_{0,0})}^2 + \|\tilde{u}_+\|_{H^2(I_{0,+})}^2 + \|\tilde{u}_-\|_{H^2(I_{0,-})}^2 \right)^{1/2},$$

where $\ell \in \mathbb{T}_1$ is fixed and defined in $H_{\Gamma}^2(\ell)$ by means of the boundary conditions (3.7)-(3.8).

Next, we present an elementary result for the linear operator $\tilde{L}(\ell) := -(\partial_x + i\ell)^2 + 1$ similar to the one of Lemma 2.2.2.

Lemma 3.2.1. *For fixed $\ell \in \mathbb{T}_1$, the operator $\tilde{L}(\ell)$ is a self-adjoint, positive semi-definite operator in L_{Γ}^2 .*

Proof. We find for every $f(\ell, \cdot), g(\ell, \cdot) \in H_{\Gamma}^2(\ell)$ and every $\ell \in \mathbb{T}_1$ the following representation of the operator $\tilde{L}(\ell)$:

$$\begin{aligned} \langle \tilde{L}(\ell)f, g \rangle_{L_{\Gamma}^2} &= \langle -(\partial_x + i\ell)^2 + 1 \rangle f, g \rangle_{L_{\Gamma}^2} \\ &= \langle -(\partial_x + i\ell)^2 f, g \rangle_{L_{\Gamma}^2} + \langle f, g \rangle_{L_{\Gamma}^2}. \end{aligned}$$

Using Lemma 2.2.2, we conclude that

$$\langle -(\partial_x + i\ell)^2 f, g \rangle_{L_{\Gamma}^2} = \langle f, -(\partial_x + i\ell)^2 g \rangle_{L_{\Gamma}^2}$$

and with

$$\langle f, -(\partial_x + i\ell)^2 g \rangle_{L_{\Gamma}^2} + \langle f, g \rangle_{L_{\Gamma}^2} = \langle f, \tilde{L}(\ell)g \rangle_{L_{\Gamma}^2}.$$

the operator $\tilde{L}(\ell)$ is self-adjoint for every $\ell \in \mathbb{T}_1$ due to the conditions (3.7)-(3.8), see [9, Theorem 1.4.4]. Since

$$\langle \tilde{L}(\ell)f, f \rangle_{L_{\Gamma}^2} = \int_0^{2\pi} (\partial_x + i\ell)f \cdot \overline{(\partial_x + i\ell)f} dx + \int_0^{2\pi} f \bar{f} dx \geq 0,$$

the operator $\tilde{L}(\ell)$ is positive semi-definite. □

As in the argumentation for the linear problem of the NLS equation on the periodic quantum graph Γ , we conclude that by Lemma 3.2.1 and the spectral theorem for self-adjoint operators with compact resolvent, cf. [36], for each $\ell \in \mathbb{T}_1$ there exists a Schauder base $\{f^{(m)}(\ell, \cdot)\}_{m \in \mathbb{N}}$ of L^2_Γ consisting of eigenfunctions of $\tilde{L}(\ell)$ with positive eigenvalues $\{\lambda^{(m)}(\ell)\}_{m \in \mathbb{N}}$ ordered as $\lambda^{(m)}(\ell) \leq \lambda^{(m+1)}(\ell)$. By construction, the Bloch wave functions satisfy the continuation properties (3.6) and the orthogonality and normalization relations

$$\langle f^{(m)}(\ell, \cdot), f^{(m')}(\ell, \cdot) \rangle_{L^2_\Gamma} = \delta_{m,m'}, \quad \ell \in \mathbb{T}_1.$$

Here we use again superscripts to count the spectral curves. The subscripts in $f_j^{(m)}(\ell, x)$, $j \in \{0, +, -\}$ are once more reserved to indicate the component of $f^{(m)}(\ell, x)$ for $x \in I_{0,j}$. Via the $\lambda^{(m)}$ we find $\omega = \omega^{(\pm m)}$ with $\omega^{(m)} = \sqrt{\lambda^{(m)}}$ and $\omega^{(-m)} = -\omega^{(m)}$.

The spectral bands of the periodic eigenvalue problem (3.6) are shown on Figure 3.1. The flat spectral curves correspond to the eigenvalues of infinite algebraic multiplicity $\{\pm\sqrt{m^2 + 1}\}_{m \in \mathbb{N}}$. For these eigenvalues, we again obtain eigenfunctions localized in the circles of the graph. A detailed calculation of the spectral curves can be found in Appendix A.1.

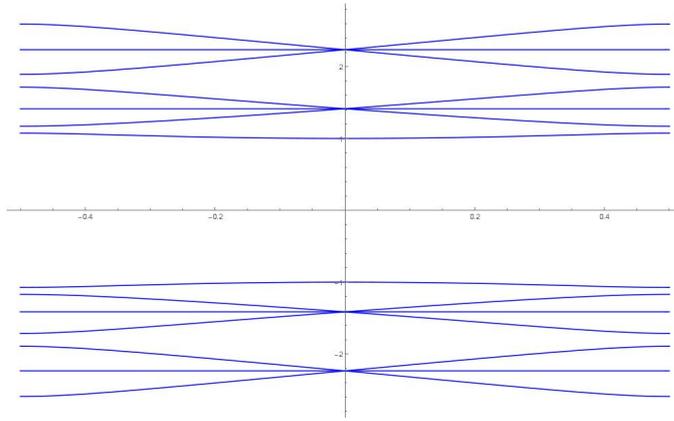


Figure 3.1.: The spectral curves ω of the spectral problem (3.6) plotted versus the Bloch wave number ℓ for the periodic quantum graph Γ .

3.2.2. The effective amplitude equation

We represent slow modulations in time and space of a small-amplitude modulated Bloch mode by the formal asymptotic expansion

$$U(t, x) = \varepsilon \Psi_{\text{nl}s}(t, x) + \text{higher-order terms}, \quad (3.9)$$

with

$$\varepsilon \Psi_{\text{nl}s}(t, x) = \varepsilon A(T, X) f^{(m_0)}(\ell_0, x) e^{i\ell_0 x} e^{i\omega^{(m_0)}(\ell_0) t} + \text{c.c.}, \quad (3.10)$$

where $0 < \varepsilon \ll 1$ is a small perturbation parameter, $T = \varepsilon^2 t$ is the slow time variable, $X = \varepsilon(x - c_g t)$ is the large space variable and $A(T, X) \in \mathbb{C}$ describes the amplitude function. The parameter $c_g := \partial_\ell \omega^{(m_0)}(\ell_0)$ is defined as the group velocity associated with the Bloch wave number ℓ_0 .

We again take use of formal asymptotic expansions to show that, at the lowest order in ε , the amplitude function A satisfies the NLS equation

$$i\partial_T A + \frac{1}{2}\partial_\ell^2 \omega^{(m_0)}(\ell_0) \partial_X^2 A + \nu |A|^2 A = 0, \quad (3.11)$$

where the cubic coefficient is given by

$$\nu = \frac{3\langle f^{(m_0)}(\ell_0, \cdot) f^{(m_0)}(\ell_0, \cdot) f^{(m_0)}(-\ell_0, \cdot), f^{(m_0)}(\ell_0, \cdot) \rangle_{L^2_{\mathbb{T}}}}{2\omega^{(m_0)}(\ell_0)}.$$

Our main goal is the mathematical justification of the effective amplitude equation (3.11) by means of error estimates. The approximation result is similar to Theorem 2.2.3. The main difference lies in the given non-resonance conditions.

Theorem 3.2.2. *Pick $m_0 \in \mathbb{Z}$ and $\ell_0 \in \mathbb{T}_1$ such that the following non-resonance conditions are satisfied:*

$$\omega^{(m)}(\ell_0) \neq \omega^{(m_0)}(\ell_0) \quad \text{for every } m \neq m_0 \quad (3.12)$$

and

$$\omega^{(m)}(3\ell_0) \neq 3\omega^{(m_0)}(\ell_0) \quad \text{for every } m. \quad (3.13)$$

Then, for every $C_0 > 0$ and $T_0 > 0$, there exist $\varepsilon_0 > 0$ and $C > 0$ such that for all solutions $A \in C(\mathbb{R}, H^3(\mathbb{R}))$ of the effective amplitude equation (3.11) with

$$\sup_{T \in [0, T_0]} \|A(T, \cdot)\|_{H^3} \leq C_0$$

and for all $\varepsilon \in (0, \varepsilon_0)$, there are solutions $U \in C([0, T_0/\varepsilon^2], L^\infty(\mathbb{R}))$ of the original system (3.4) satisfying the bound

$$\sup_{t \in [0, T_0/\varepsilon^2]} \sup_{x \in \mathbb{R}} |U(t, x) - \varepsilon \Psi_{\text{nls}}(t, x)| \leq C\varepsilon^{3/2}, \quad (3.14)$$

where $\varepsilon \Psi_{\text{nls}}$ is given by (3.10).

Remark 3.2.3. The justification of the NLS approximation for the spatially homogeneous cKG equation is rather trivial and follows by a simple application of Gronwall's inequality, cf. [19]. In the context with smooth spatially periodic coefficients, the justification of the NLS approximation was carried out in [10]. This analysis has to be adjusted to the present non-smooth situation by using the methods introduced in Chapter 2.

3.3. Local existence and uniqueness

In order to prove the local existence and uniqueness of solutions of the original system (3.4), we first show that $L = -\partial_x^2 + 1$ with the domain \mathcal{H}^2 is self-adjoint and positive semi-definite in \mathcal{L}^2 by adapting the proof of Lemma 2.3.2 to the linear differential operator L used in this problem. Therefore, we define the function spaces

$$\mathcal{L}^2 = \{U = (u_0, u_+, u_-) \in (L^2(\mathbb{R}))^3 : \text{supp}(u_{n,j}) = I_{n,j}, \quad n \in \mathbb{Z}, \quad j \in \{0, +, -\}\}$$

and

$$\mathcal{H}^2 = \{U \in \mathcal{L}^2 : u_{n,j} \in H^2(I_{n,j}), \quad n \in \mathbb{Z}, \quad j \in \{0, +, -\}, \quad (3.2) - (3.3) \text{ is satisfied}\},$$

identically to the ones in Section 2.3. Hence, there exists a self-adjoint and positive semi-definite root Ω in \mathcal{L}^2 with $L = \Omega^2$ and we can rewrite (3.4) as

$$\partial_t W = \Lambda W + N(W) \quad (3.15)$$

with

$$W = \begin{pmatrix} U \\ V \end{pmatrix}, \quad \Lambda = \begin{pmatrix} 0 & -\Omega \\ \Omega & 0 \end{pmatrix} \quad \text{and} \quad N(W) = \begin{pmatrix} 0 \\ \Omega^{-1}U^3 \end{pmatrix}.$$

Now we show that the initial-value problem for the first-order system (3.15) is locally well-posed in the space $\mathcal{Y}^2 := \mathcal{H}^2 \times \mathcal{H}^2$.

Theorem 3.3.1. *For every $W_0 \in \mathcal{Y}^2$, there exists a $T_0 = T_0(\|W_0\|_{\mathcal{Y}^2}) > 0$ and a unique solution $W \in C([-T_0, T_0], \mathcal{Y}^2)$ of the first-order system (3.15) with the initial data $W|_{t=0} = W_0$.*

Proof. The skew symmetric operator Λ with domain $D(\Lambda)$ defines a unitary group $(e^{\Lambda t})_{t \in \mathbb{R}}$ in $\mathcal{X}^2 := \mathcal{L}^2 \times \mathcal{L}^2$ such that $\|e^{\Lambda t}W\|_{\mathcal{X}^2} = \|W\|_{\mathcal{X}^2}$ for every $t \in \mathbb{R}$. This is a consequence of classical semigroup theory, see Stone's theorem in [28]. Moreover, there exists a positive constant C_L such that

$$\|e^{\Lambda t}W\|_{\mathcal{Y}^2} \leq C_L \|W\|_{\mathcal{Y}^2} \quad (3.16)$$

for every $W \in \mathcal{Y}^2$ and every $t \in \mathbb{R}$ because the following chain of inequalities holds:

$$\begin{aligned} \|e^{\Lambda t}W\|_{\mathcal{Y}^2} &\leq C \| \Lambda^2 e^{\Lambda t}W \|_{\mathcal{X}^2} \\ &\leq C \| e^{\Lambda t} \Lambda^2 W \|_{\mathcal{X}^2} \\ &\leq C \| \Lambda^2 W \|_{\mathcal{X}^2} \\ &\leq C \| W \|_{\mathcal{Y}^2}. \end{aligned} \quad (3.17)$$

Alongside the existence of the unitary group $(e^{\Lambda t})_{t \in \mathbb{R}}$, we used the commutativity of Λ and $e^{\Lambda t}$ and the equivalence between $\|W\|_{\mathcal{Y}^2}$ and $\|\Lambda^2 W\|_{\mathcal{X}^2}$ to obtain (3.17).

Using the fact from Lemma 2.3.1 that the function space \mathcal{H}^2 is closed under pointwise multiplication, we have $U^3 \in \mathcal{H}^2$ for every $U \in \mathcal{H}^2$ and therefore we estimate

$$\|\Omega^{-1}U^3\|_{\mathcal{H}^2} = \|\Omega U^3\|_{\mathcal{L}^2} \leq C \|\Omega^2 U^3\|_{\mathcal{L}^2} \leq C \|U^3\|_{\mathcal{H}^2} \quad (3.18)$$

such that the nonlinearity is locally Lipschitz continuous from \mathcal{H}^2 to \mathcal{H}^2 .

By Duhamel's principle, we now rewrite the Cauchy problem associated with the first-order system (3.15) as the integral equation

$$W(t, \cdot) = e^{\Lambda t}W(0, \cdot) + i \int_0^t e^{\Lambda(t-\tau)} N(W)(\tau) d\tau, \quad (3.19)$$

where the solution is considered in the space

$$\mathcal{M} := \{W \in C([-T_0, T_0], \mathcal{Y}^2) : \sup_{t \in [-T_0, T_0]} \|W(t, \cdot) - e^{\Lambda t}W(0, \cdot)\|_{\mathcal{Y}^2} \leq C_W\},$$

and the constant $C_W > 0$ is fixed. For every $W_0 \in \mathcal{Y}^2$, there is a sufficiently small $T_0 = T_0(\|W_0\|_{\mathcal{Y}^2}) > 0$ such that the right-hand side of the integral equation (3.19) is a contraction in the space \mathcal{M} , where we used (3.17) and (3.18). The existence of a unique solution $W \in C([-T_0, T_0], \mathcal{Y}^2)$ then follows from Banach's fixed-point theorem. \square

Remark 3.3.2. Using Theorem 3.3.1, it is easy to see that there exists a unique solution $U \in C([-T_0, T_0], \mathcal{H}^2)$ of the original system (3.4) with the initial conditions $W_0 = (U_0, -\Omega^{-1}\partial_t U_0)$.

3.4. Derivation of the NLS approximation

The Bloch transform is the main tool to justify the NLS approximation on a periodic quantum graph. Here, we will transfer the approach from Chapter 2 to the cKG equation (3.4), write the system in Bloch space and use this representation to derive the amplitude equation for this problem.

For an overview on the basic properties of the Bloch transform on periodic quantum graphs, we refer to Section 2.4.

3.4.1. The system in Bloch space

First, we apply the Bloch transform \mathcal{T} to (3.4) and get

$$\partial_t^2 \tilde{U}(t, \ell, x) = -\tilde{L}(\ell)\tilde{U}(t, \ell, x) - (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, x), \quad (3.20)$$

with the linear operator $\tilde{L}(\ell) = -(\partial_x + i\ell)^2 + 1$ defined in Section 3.2.1 and the function $\tilde{U}(t, \ell, x) = (\tilde{u}_0, \tilde{u}_+, \tilde{u}_-)(t, \ell, x)$ satisfying the continuation conditions

$$\tilde{U}(t, \ell, x) = \tilde{U}(t, \ell, x + 2\pi) \quad \text{and} \quad \tilde{U}(t, \ell, x) = \tilde{U}(t, \ell + 1, x)e^{ix}.$$

The convolution integrals in (3.20) are defined componentwise:

$$\tilde{U} \star \tilde{U} \star \tilde{U} = (\tilde{u}_0 \star \tilde{u}_0 \star \tilde{u}_0, \tilde{u}_+ \star \tilde{u}_+ \star \tilde{u}_+, \tilde{u}_- \star \tilde{u}_- \star \tilde{u}_-).$$

As in Section 2.4.2, every function $\tilde{u}_j(t, \ell, \cdot)$ with $j \in \{0, +, -\}$ has support in $I_{0,j}$ due to the fact that the equality

$$\mathcal{T}(u_j)(\ell, x) = \mathcal{T}(\chi_j u_j)(\ell, x) = \chi_j(x)(\mathcal{T}u_j)(\ell, x), \quad j \in \{0, +, -\}$$

holds for the periodic cut-off functions χ_j stated in (2.35).

Next, we consider the underlying function space for (3.20) and recall the definition of the Bloch space

$$\tilde{\mathcal{H}}^2 = \{\tilde{U} \in L^2(\mathbb{T}_1, L^2_{\Gamma}) : \tilde{u}_j \in L^2(\mathbb{T}_1, H^2(I_{0,j})), \quad j \in \{0, +, -\}, \quad (3.7) - (3.8) \text{ is satisfied}\},$$

which is equipped with the norm

$$\|\tilde{U}\|_{\tilde{\mathcal{H}}^2} = \left(\int_{-1/2}^{1/2} \left(\|\tilde{u}_0(\ell, \cdot)\|_{H^2(I_{0,0})}^2 + \|\tilde{u}_+(\ell, \cdot)\|_{H^2(I_{0,+})}^2 + \|\tilde{u}_-(\ell, \cdot)\|_{H^2(I_{0,-})}^2 \right) d\ell \right)^{1/2}.$$

With the same arguments as in the previous chapter, the space $\tilde{\mathcal{H}}^2$ is the domain of definition of the operator $\tilde{L}(\ell)$ in $L^2(\mathbb{T}_1, L^2_{\Gamma})$ and Lemma 2.4.2 guarantees that the Bloch transform \mathcal{T} is an isomorphism between the spaces $\tilde{\mathcal{H}}^2$ and \mathcal{H}^2 , in which the initial value problem for the system (3.4) is locally well-posed.

3.4.2. Derivation of the effective amplitude equation

We recover the ansatz (3.9) and (3.10) and derive an effective amplitude equation of the type (3.11) in Bloch space. Therefore, we first decompose the solution of the problem (3.20) into two parts and write

$$\tilde{U}(t, \ell, x) = \tilde{V}(t, \ell) f^{(m_0)}(\ell, x) + \tilde{U}^\perp(t, \ell, x), \quad (3.21)$$

where the orthogonality condition $\langle f^{(m_0)}(\ell, \cdot), \tilde{U}^\perp(t, \ell, \cdot) \rangle_{L^2_{\mathbb{T}^d}} = 0$ is again used for uniqueness of the decomposition. We find

$$\partial_t^2 \tilde{V}(t, \ell) = -(\omega^{(m_0)}(\ell))^2 \tilde{V}(t, \ell) - N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell), \quad (3.22)$$

$$\partial_t^2 \tilde{U}^\perp(t, \ell, x) = -\tilde{L}(\ell) \tilde{U}^\perp(t, \ell, x) - N^\perp(\tilde{V}, \tilde{U}^\perp)(t, \ell, x), \quad (3.23)$$

where

$$N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell) = \langle (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, \cdot), f^{(m_0)}(\ell, \cdot) \rangle_{L^2_{\mathbb{T}^d}},$$

and

$$N^\perp(\tilde{V}, \tilde{U}^\perp)(t, \ell, x) = (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, x) - N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell) f^{(m_0)}(\ell, x).$$

Since the original system has no quadratic terms in the nonlinearity, it is sufficient to evaluate equation (3.22) at $\tilde{U}^\perp = 0$ as in Section 2.5.1. In the case of quadratic nonlinearities, the terms of this order have to be first eliminated by near identity transformations, cf. [10]. For a cubic nonlinearity, we directly get

$$\begin{aligned} N_V(\tilde{V}, \tilde{U}^\perp)(t, \ell) &= \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \beta(\ell, \ell_1, \ell_2, \ell - \ell_1 - \ell_2) \\ &\quad \times \tilde{V}(t, \ell_1) \tilde{V}(t, \ell_2) \tilde{V}(t, \ell - \ell_1 - \ell_2) d\ell_1 d\ell_2 + N_{V, \text{rest}}(\tilde{V}, \tilde{U}^\perp)(t, \ell) \end{aligned} \quad (3.24)$$

where $N_{V, \text{rest}}(\tilde{V}, 0) = 0$ and the kernel β is given by

$$\beta(\ell, \ell_1, \ell_2, \ell_1 + \ell_2 - \ell) := \langle f^{(m_0)}(\ell_1, \cdot) f^{(m_0)}(\ell_2, \cdot) f^{(m_0)}(\ell - \ell_1 - \ell_2, \cdot), f^{(m_0)}(\ell, \cdot) \rangle_{L^2_{\mathbb{T}^d}}. \quad (3.25)$$

In order to derive a NLS equation as effective amplitude equation, we now insert the ansatz

$$\tilde{V}_{\text{app}}(t, \ell) = \tilde{A}_1 \left(\varepsilon^2 t, \frac{\ell - \ell_0}{\varepsilon} \right) \mathbf{E}^1(t, \ell) + \tilde{A}_{-1} \left(\varepsilon^2 t, \frac{\ell + \ell_0}{\varepsilon} \right) \mathbf{E}^{-1}(t, \ell), \quad (3.26)$$

with

$$\mathbf{E}^{\pm 1}(t, \ell) := e^{\pm i \omega^{(m_0)}(\ell_0) t} e^{\pm i \partial_\ell \omega^{(m_0)}(\ell_0) (\ell \mp \ell_0) t}$$

into (3.22) and obtain in the leading order $\varepsilon^2 \mathbf{E}^1$ the equation

$$\begin{aligned} i \partial_T \tilde{A}_1(T, \xi) &= -\frac{1}{2} \partial_\ell^2 \omega^{(m_0)}(\ell_0) \xi^2 \tilde{A}_1(T, \xi) \\ &\quad - \nu \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \tilde{A}_1(T, \xi_1) \tilde{A}_1(T, \xi_2) \tilde{A}_{-1}(T, \xi - \xi_1 - \xi_2) d\xi_1 d\xi_2, \end{aligned} \quad (3.27)$$

where $\ell = \ell_0 + \varepsilon\xi$, $T = \varepsilon^2 t$ and $\nu = 3\beta(\ell_0, \ell_0, \ell_0, -\ell_0)/2\omega^{(m_0)}(\ell_0)$. We also find additional terms of the formal order $\mathcal{O}(\varepsilon^2)$ which do not cancel each other. A detailed calculation of these terms is given in Appendix A.2.

By taking the limit $\varepsilon \rightarrow 0$, the amplitude equation (3.27) yields to the equation

$$i\partial_T \widehat{A}_1(T, \xi) + \frac{1}{2}\partial_\ell^2 \omega^{(m_0)}(\ell_0) \xi^2 \widehat{A}_1(T, \xi) + \nu(\widehat{A}_1 * \widehat{A}_1 * \widehat{A}_{-1})(T, \xi) = 0 \quad (3.28)$$

in Fourier space which corresponds to the amplitude equation (3.11) in physical space. This will be made rigorous in Section 3.5.2.

3.5. The improved approximation and estimates for the residual terms

As we mentioned above, the ansatz (3.26) yields to remaining terms in the equation (3.22) which are of the formal order $\mathcal{O}(\varepsilon^2)$ in Bloch space and furthermore produces terms of this order in the second equation (3.23), too. Since we want to bound the error with a Gronwall argument as in Chapter 2, we again need the residual to be of the formal order $\mathcal{O}(\varepsilon^3)$ in Bloch space. Therefore, we add higher order terms to the approximation to cancel out the terms of the formal order $\mathcal{O}(\varepsilon^2)$ in (3.22)-(3.23) and then estimate the residual of this improved ansatz.

3.5.1. The improved approximation

In order to improve the ansatz (3.26), we define the terms of the decomposition (3.21) in the following way:

$$\begin{aligned} \widetilde{V}_{\text{app}}(t, \ell) &= \widetilde{V}_{\text{app},1}(t, \ell) + \widetilde{V}_{\text{app},-1}(t, \ell) + \widetilde{V}_{\text{app},3}(t, \ell) + \widetilde{V}_{\text{app},-3}(t, \ell) \\ &= \widetilde{A}_1 \left(\varepsilon^2 t, \frac{\ell - \ell_0}{\varepsilon} \right) \mathbf{E}^1(t, \ell) + \widetilde{A}_{-1} \left(\varepsilon^2 t, \frac{\ell + \ell_0}{\varepsilon} \right) \mathbf{E}^{-1}(t, \ell) \\ &\quad + \varepsilon^2 \widetilde{A}_3 \left(\varepsilon^2 t, \frac{\ell - 3\ell_0}{\varepsilon} \right) \mathbf{E}^3(t, \ell) + \varepsilon^2 \widetilde{A}_{-3} \left(\varepsilon^2 t, \frac{\ell + 3\ell_0}{\varepsilon} \right) \mathbf{E}^{-3}(t, \ell) \end{aligned} \quad (3.29)$$

and

$$\begin{aligned} \widetilde{U}_{\text{app}}^\perp(t, \ell, x) &= \widetilde{U}_{\text{app},1}^\perp(t, \ell, x) + \widetilde{U}_{\text{app},-1}^\perp(t, \ell, x) + \widetilde{U}_{\text{app},3}^\perp(t, \ell, x) + \widetilde{U}_{\text{app},-3}^\perp(t, \ell, x) \\ &= \varepsilon^2 \widetilde{B}_1 \left(\varepsilon^2 t, \frac{\ell - \ell_0}{\varepsilon}, x \right) \mathbf{E}^1(t, \ell) + \varepsilon^2 \widetilde{B}_{-1} \left(\varepsilon^2 t, \frac{\ell + \ell_0}{\varepsilon}, x \right) \mathbf{E}^{-1}(t, \ell) \\ &\quad + \varepsilon^2 \widetilde{B}_3 \left(\varepsilon^2 t, \frac{\ell - 3\ell_0}{\varepsilon}, x \right) \mathbf{E}^3(t, \ell) + \varepsilon^2 \widetilde{B}_{-3} \left(\varepsilon^2 t, \frac{\ell + 3\ell_0}{\varepsilon}, x \right) \mathbf{E}^{-3}(t, \ell). \end{aligned} \quad (3.30)$$

Remark 3.5.1. In contrast to the analysis in Section 2.5.2, we need to improve the ansatz $\widetilde{V}_{\text{app}}(t, \ell)$ as well. This is necessary because we have to eliminate the terms concentrated in neighborhoods of the Bloch numbers $-\ell_0$ and $\pm 3\ell_0$ which also appear in (3.22) for the simple approximation (3.26), cf. Appendix A.2.

Inserting (3.29) and (3.30) into the system (3.22)-(3.23), we set the coefficients in the leading order $\varepsilon^2 \mathbf{E}^j$ with

$$\mathbf{E}^j(t, \ell) := e^{j i \omega^{(m_0)}(\ell_0) t} e^{j i \partial_\ell \omega^{(m_0)}(\ell_0) (\ell - j \ell_0) t}$$

for $j = \pm 1, \pm 3$ to zero and thus obtain the following equalities:

$$\begin{aligned}
-9(\omega^{(m_0)}(\ell_0))^2 \tilde{A}_3(\varepsilon^2 t, \xi_3) &= -(\omega^{(m_0)}(3\ell_0))^2 \tilde{A}_3(\varepsilon^2 t, \xi_3) \\
&\quad - \beta(\ell_0, \ell_0, \ell_0, \ell_0)(\tilde{A}_1 \star \tilde{A}_1 \star \tilde{A}_1)(\varepsilon^2 t, \xi_3), \\
-(\omega^{(m_0)}(\ell_0))^2 \tilde{B}_1(\varepsilon^2 t, \xi_1, x) &= -\tilde{L}(\ell_0) \tilde{B}_1(\varepsilon^2 t, \xi_1, x) \\
&\quad - \varepsilon^{-2} (\mathbf{E}^1(t, \ell))^{-1} N_1^\perp(\tilde{V}_{\text{app}}, 0)(t, \ell, x), \\
-9(\omega^{(m_0)}(\ell_0))^2 \tilde{B}_3(\varepsilon^2 t, \xi_3, x) &= -\tilde{L}(3\ell_0) \tilde{B}_3(\varepsilon^2 t, \xi_3, x) \\
&\quad - \varepsilon^{-2} (\mathbf{E}^3(t, \ell))^{-1} N_3^\perp(\tilde{V}_{\text{app}}, 0)(t, \ell, x),
\end{aligned} \tag{3.31}$$

where $\xi_3 = \varepsilon^{-1}(\ell - 3\ell_0)$, $\xi_1 = \varepsilon^{-1}(\ell - \ell_0)$ and the nonlinear terms are given by

$$\begin{aligned}
N_1^\perp(\tilde{V}_{\text{app}}, 0)(t, \ell, x) &= 3(\tilde{V}_{\text{app},1} \star \tilde{V}_{\text{app},1} \star \tilde{V}_{\text{app},-1})(t, \ell, x) \\
&\quad - 3\varepsilon^2 \beta(\ell_0, \ell_0, \ell_0, -\ell_0)(\tilde{A}_1 \star \tilde{A}_1 \star \tilde{A}_{-1})(\varepsilon^2 t, \xi_1) f^{(m_0)}(\ell, x) \mathbf{E}^1(t, \ell)
\end{aligned}$$

and

$$\begin{aligned}
N_3^\perp(\tilde{V}_{\text{app}}, 0)(t, \ell, x) &= (\tilde{V}_{\text{app},1} \star \tilde{V}_{\text{app},1} \star \tilde{V}_{\text{app},1})(t, \ell, x) \\
&\quad - \varepsilon^2 \beta(\ell_0, \ell_0, \ell_0, \ell_0)(\tilde{A}_1 \star \tilde{A}_1 \star \tilde{A}_1)(\varepsilon^2 t, \xi_3) f^{(m_0)}(\ell, x) \mathbf{E}^3(t, \ell).
\end{aligned}$$

For the functions \tilde{A}_{-3} , \tilde{B}_{-1} and \tilde{B}_{-3} we find the associated complex conjugated equations to the ones in (3.31).

Note that the prefactor ε^{-2} of the terms N_1^\perp and N_3^\perp cancels with the factor ε^2 coming from the two-times convolution and therefore all terms in the respective equations (3.31) are of the same formal order. These equations can be solved by using the implicit function theorem, if the invertibility conditions

$$\begin{aligned}
9(\omega^{(m_0)}(\ell_0))^2 &\neq (\omega^{(m_0)}(3\ell_0))^2, \\
-(\omega^{(m_0)}(\ell_0))^2 &\notin \sigma(-\tilde{L}(\ell_0))|_{\{f^{(m_0)}(\ell_0, \cdot)\}^\perp}, \\
-9(\omega^{(m_0)}(\ell_0))^2 &\notin \sigma(-\tilde{L}(3\ell_0))|_{\{f^{(m_0)}(3\ell_0, \cdot)\}^\perp}.
\end{aligned}$$

hold. These conditions are satisfied due to the non-resonance conditions (3.12) and (3.13) of Theorem 3.2.2. With the same arguments we solve the complex conjugate equations for \tilde{A}_{-3} , \tilde{B}_{-1} and \tilde{B}_{-3} .

Hence, by inserting the approximation $(\tilde{V}_{\text{app}}, \tilde{U}_{\text{app}}^\perp)$ defined by the improved ansatz (3.29) and (3.30) into the system (3.22)-(3.23), we get rid of all the remaining terms of the formal order $\mathcal{O}(\varepsilon^2)$ in the residual.

3.5.2. From Fourier space to Bloch space

Using the arguments from Section 2.5.3 to link Fourier analysis and Bloch wave analysis, we define for every $j = \pm 1, \pm 3$ the amplitude function in Bloch space by

$$\tilde{A}_j(T, \varepsilon^{-1}(\ell - j\ell_0)) = \tilde{\chi}_{j\ell_0}(\ell) \hat{A}_j(T, \varepsilon^{-1}(\ell - j\ell_0)), \tag{3.32}$$

where we write the cutoff functions $\tilde{\chi}_{j\ell_0}$ as

$$\tilde{\chi}_{j\ell_0}(\ell) = \begin{cases} 1, & \ell - j\ell_0 \in [-\delta, \delta], \\ 0, & \text{otherwise,} \end{cases}$$

with $\delta > 0$ being sufficiently small but independent of the small parameter ε . The condition

$$\tilde{A}_j(T, \varepsilon^{-1}(\ell + 1 - j\ell_0)) = \tilde{A}_j(T, \varepsilon^{-1}(\ell - j\ell_0)), \quad \ell \in \mathbb{R},$$

then extends $\tilde{A}_j(T, \varepsilon^{-1}(\ell - j\ell_0))$ periodically in ℓ over \mathbb{R} .

As mentioned already in the last chapter, the assumption $A_j \in C(\mathbb{R}, H^3(\mathbb{R}))$ yields to the fact that the corresponding Fourier transform \hat{A}_j satisfies $\hat{A}_j \rho_{0,1,3} \in L^2(\mathbb{R})$ and therefore $\hat{A}_j \rho_{0,1,2} \in L^1(\mathbb{R})$. By the construction of the Bloch functions in (3.32) and using the scaled weights $\rho_{*,\varepsilon,*}$, we thus get for the leading order terms in \tilde{V}_{app} that

$$\tilde{V}_{\text{app},1} f^{(m_0)} \rho_{\ell_0,\varepsilon,3} \in \tilde{\mathcal{H}}^2 \quad \text{and} \quad \tilde{V}_{\text{app},-1} f^{(m_0)} \rho_{-\ell_0,\varepsilon,3} \in \tilde{\mathcal{H}}^2$$

and that these weighted terms are of the formal order $\mathcal{O}(\varepsilon^{1/2})$ in $\tilde{\mathcal{H}}^2$ due to the scaling properties of the L^2 -norm. In order to avoid losing the factor $\varepsilon^{1/2}$, we recall the L^1 -based space

$$\tilde{\mathcal{C}}^2 = \{\tilde{U} \in L^1(\mathbb{T}_1, L^2_\Gamma) : \tilde{u}_j \in L^1(\mathbb{T}_1, H^2(I_{0,j})), \quad j \in \{0, +, -\}, \quad (3.7) - (3.8) \text{ is satisfied}\},$$

equipped with the norm

$$\|\tilde{U}\|_{\tilde{\mathcal{C}}^2} = \int_{-1/2}^{1/2} \left(\|\tilde{u}_0(\ell, \cdot)\|_{H^2(I_{0,0})} + \|\tilde{u}_+(\ell, \cdot)\|_{H^2(I_{0,+})} + \|\tilde{u}_-(\ell, \cdot)\|_{H^2(I_{0,-})} \right) d\ell$$

from Section 2.5.3 and obtain that the weighted functions

$$\tilde{V}_{\text{app},1} f^{(m_0)} \rho_{\ell_0,\varepsilon,2} \in \tilde{\mathcal{C}}^2 \quad \text{and} \quad \tilde{V}_{\text{app},-1} f^{(m_0)} \rho_{-\ell_0,\varepsilon,2} \in \tilde{\mathcal{C}}^2$$

are of the formal order $\mathcal{O}(\varepsilon)$ in $\tilde{\mathcal{C}}^2$. With the same idea we get that the higher-order terms $\tilde{V}_{\text{app},\pm 3} f^{(m_0)} \rho_{\pm 3\ell_0,\varepsilon,3} \in \tilde{\mathcal{H}}^2$ are of the formal order $\mathcal{O}(\varepsilon^{5/2})$ in $\tilde{\mathcal{H}}^2$ and $\tilde{V}_{\text{app},\pm 3} f^{(m_0)} \rho_{\pm 3\ell_0,\varepsilon,2} \in \tilde{\mathcal{C}}^2$ are of the formal order $\mathcal{O}(\varepsilon^3)$ in $\tilde{\mathcal{C}}^2$.

Next, we study the second part $\tilde{U}_{\text{app}}^\perp$ of the decomposition (3.21) and see that the terms

$$(\mathbf{E}^j(t, \cdot))^{-1} N_j^\perp(\tilde{V}_{\text{app}}, 0)(t, \cdot, \cdot) \rho_{j\ell_0,\varepsilon,2}(\cdot) \in \tilde{\mathcal{H}}^2$$

are of the formal order $\mathcal{O}(\varepsilon^{5/2})$ in $\tilde{\mathcal{H}}^2$ and of the formal order $\mathcal{O}(\varepsilon^3)$ in $\tilde{\mathcal{C}}^2$ due to Young's inequality

$$\|(\tilde{V} \star \tilde{W}) \rho_{j\ell_0,\varepsilon,2}\|_{\tilde{\mathcal{H}}^2} \leq C \|\tilde{V} \rho_{j\ell_0,\varepsilon,2}\|_{\tilde{\mathcal{C}}^2} \|\tilde{W} \rho_{j\ell_0,\varepsilon,2}\|_{\tilde{\mathcal{H}}^2}$$

for weighted functions. The supports of the nonlinear terms in (3.31) and in the respective complex conjugate system are given by

$$\text{supp} \left((\mathbf{E}^j(t, \cdot))^{-1} N_j^\perp(\tilde{V}_{\text{app}}, 0)(t, \cdot, \cdot) \right) \subset [j\ell_0 - 3\delta, j\ell_0 + 3\delta].$$

and similar to (2.45), we define

$$\tilde{B}_j(\varepsilon^2 t, \xi_j, x) = (-\tilde{L}(\ell) + (j\omega^{(m_0)}(\ell_0))^2 I)^{-1} \varepsilon^{-2} (\mathbf{E}^j(t, \ell))^{-1} N_j^\perp(\tilde{V}_{\text{app}}, 0)(t, \ell, x), \quad (3.33)$$

where $\xi_j = \varepsilon^{-1}(\ell - j\ell_0)$ for every $j = \pm 1, \pm 3$. The inverse operators on the right hand side of (3.33) exist due to the non-resonance conditions (3.12) and (3.13) for $\delta > 0$ sufficiently small. Therefore, we obtain that the weighted functions $\tilde{U}_{\text{app},j}^\perp \rho_{j\ell_0,\varepsilon,2} \in \tilde{\mathcal{H}}^2$ are of the formal order $\mathcal{O}(\varepsilon^{5/2})$ in $\tilde{\mathcal{H}}^2$ and $\tilde{U}_{\text{app},j}^\perp \rho_{j\ell_0,\varepsilon,1} \in \tilde{\mathcal{C}}^2$ are of the formal order $\mathcal{O}(\varepsilon^3)$ in $\tilde{\mathcal{C}}^2$.

The estimates for the terms $\tilde{V}_{\text{app},j}$ and $\tilde{U}_{\text{app},j}^\perp$ now yield formally to the improved ansatz

$$\varepsilon \tilde{\Psi}(t, \ell, x) = \tilde{V}_{\text{app}}(t, \ell) f^{(m_0)}(\ell, x) + \tilde{U}_{\text{app}}^\perp(t, \ell, x), \quad (3.34)$$

with \tilde{V}_{app} and $\tilde{U}_{\text{app}}^\perp$ defined in (3.29) and (3.30), where the amplitude function \hat{A}_1 fulfills the NLS equation (3.28) in Fourier space and \hat{A}_{-1} the complex conjugate equation respectively. Moreover, the improved approximation $\varepsilon \Psi = \mathcal{T}^{-1}(\varepsilon \tilde{\Psi})$ in physical space satisfies by construction the Kirchhoff boundary conditions (3.2) - (3.3).

3.5.3. Estimates in Bloch space

Here we show that residual

$$\widetilde{\text{Res}}(\tilde{U})(t, \ell, x) = -\partial_t^2 \tilde{U}(t, \ell, x) - \tilde{L}(\ell) \tilde{U}(t, \ell, x) - (\tilde{U} \star \tilde{U} \star \tilde{U})(t, \ell, x)$$

of the evolution problem (3.20) can be estimated in $\tilde{\mathcal{H}}^2$ to be of the formal order $\mathcal{O}(\varepsilon^{7/2})$ if we approximate $\tilde{U}(t, \ell, x)$ with the ansatz (3.34). We also get the same result in physical space.

Lemma 3.5.2. *Let $A \in C([0, T_0], H^3)$ be a solution of the amplitude equation (3.11) for some $T_0 > 0$. Then, there is a positive ε -independent constant C_{Res} that only depends on the norm of the solution A such that*

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\widetilde{\text{Res}}(\varepsilon \tilde{\Psi})\|_{\tilde{\mathcal{H}}^2} \leq C_{\text{Res}} \varepsilon^{7/2}. \quad (3.35)$$

or equivalently,

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\text{Res}(\varepsilon \Psi)\|_{\mathcal{H}^2} \leq C_{\text{Res}} \varepsilon^{7/2}. \quad (3.36)$$

Proof. The proof is straightforward and follows almost line for line the one for Lemma 2.5.5 in Chapter 2 using the decompositions

$$\tilde{V}_{\text{app}}(t, \ell) = \tilde{V}_{\text{app},1}(t, \ell) + \tilde{V}_{\text{app},-1}(t, \ell) + \tilde{V}_{\text{app},3}(t, \ell) + \tilde{V}_{\text{app},-3}(t, \ell)$$

and

$$\tilde{U}_{\text{app}}^\perp(t, \ell, x) = \tilde{U}_{\text{app},1}^\perp(t, \ell, x) + \tilde{U}_{\text{app},-1}^\perp(t, \ell, x) + \tilde{U}_{\text{app},3}^\perp(t, \ell, x) + \tilde{U}_{\text{app},-3}^\perp(t, \ell, x).$$

□

Moreover, we obtain a similar result as Lemma 2.5.7 for the difference between the two approximations $\varepsilon \Psi_{\text{nls}}$, given by (3.10), and $\varepsilon \Psi$ given by (3.34) in Bloch space.

Lemma 3.5.3. *Let $A \in C([0, T_0], H^3)$ be a solution of the amplitude equation (3.11) for some $T_0 > 0$. Then, there exist positive ε -independent constants C and C_ψ that only depend on the norm of the solution A such that*

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\varepsilon \tilde{\Psi}\|_{\tilde{\mathcal{C}}^2} \leq C_\psi \varepsilon \quad (3.37)$$

and

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|\varepsilon \Psi - \varepsilon \Psi_{\text{nls}}\|_{L^\infty} \leq C \varepsilon^{3/2}. \quad (3.38)$$

Proof. Here we refer to the proof of Lemma 2.5.7 in Chapter 2. □

3.6. Estimates for the error term

In this section we want to complete the proof of Theorem 3.2.2 which is based on an energy estimate and a simple approximation of Gronwall's inequality.

Therefore, we write again the solution U of the equation as a sum of the approximation term $\varepsilon\Psi$ and the error term $\varepsilon^{3/2}R$, i.e.,

$$U = \varepsilon\Psi + \varepsilon^{3/2}R.$$

Inserting this decomposition into (3.4) we obtain the equation

$$\partial_t^2 R = -LR + G(\Psi, R) \quad (3.39)$$

with the linear operator $L = -\partial_x^2 + 1$ and the nonlinear terms

$$G(\Psi, R) = \varepsilon^{-3/2}\text{Res}(\varepsilon\Psi) + 3\varepsilon^2\Psi^2R + 3\varepsilon^{5/2}\Psi R^2 + \varepsilon^3R^3. \quad (3.40)$$

As in Section 2.7, the product terms in the definition of $G(\Psi, R)$ are understood componentwise with $R = (r_0, r_+, r_-)$ and $\Psi = (\psi_0, \psi_+, \psi_-)$. We recall Young's inequality

$$\|\tilde{V} \star \tilde{W}\|_{\tilde{\mathcal{H}}^2} \leq \|\tilde{V}\|_{\tilde{\mathcal{C}}^2} \|\tilde{W}\|_{\tilde{\mathcal{H}}^2}$$

as it is defined in Section 2.5.3 and thus get the bound

$$\|\Psi R\|_{\mathcal{H}^2} \leq C\|\tilde{\Psi}\tilde{R}\|_{\tilde{\mathcal{H}}^2} \leq C\|\tilde{\Psi}\|_{\tilde{\mathcal{C}}^2}\|\tilde{R}\|_{\tilde{\mathcal{H}}^2} \leq CC_\Psi\|\tilde{R}\|_{\tilde{\mathcal{H}}^2} \leq C^2C_\Psi\|R\|_{\mathcal{H}^2},$$

where the constant C_Ψ is defined in Lemma 3.5.3. Hence, for each term of (3.40) we find

$$\begin{aligned} \|\varepsilon^{-3/2}\text{Res}(\varepsilon\Psi)\|_{\mathcal{H}^2} &\leq C_{\text{Res}}\varepsilon^2, \\ \|3\varepsilon^2\Psi^2R\|_{\mathcal{H}^2} &\leq 3C_1\varepsilon^2\|R\|_{\mathcal{H}^2}, \\ \|3\varepsilon^{5/2}\Psi R^2\|_{\mathcal{H}^2} &\leq 3C_1\varepsilon^{5/2}\|R\|_{\mathcal{H}^2}^2, \\ \|\varepsilon^3R^3\|_{\mathcal{H}^2} &\leq C_1\varepsilon^3\|R\|_{\mathcal{H}^2}^3, \end{aligned}$$

where we used (3.36) and Lemma 2.3.1. Here C_1 is a constant independent of $\|R\|_{\mathcal{H}^2}$ and the small parameter $\varepsilon > 0$. Therefore, we get

$$\|G(\Psi, R)\|_{\mathcal{H}^2} \leq C_{\text{Res}}\varepsilon^2 + 3C_1\varepsilon^2\|R\|_{\mathcal{H}^2} + 3C_1\varepsilon^{5/2}\|R\|_{\mathcal{H}^2}^2 + C_1\varepsilon^3\|R\|_{\mathcal{H}^2}^3.$$

In order to obtain an energy estimate, we multiply (3.39) with $\partial_t LR$, take the scalar product in \mathcal{L}^2 and obtain

$$\langle \partial_t LR, \partial_t^2 R \rangle_{\mathcal{L}^2} = -\langle \partial_t LR, LR \rangle_{\mathcal{L}^2} + \langle \partial_t LR, G(\Psi, R) \rangle_{\mathcal{L}^2} \quad (3.41)$$

We rewrite the left-hand side of (3.41) to

$$\langle \partial_t LR, \partial_t^2 R \rangle_{\mathcal{L}^2} = \partial_t \langle \partial_t LR, \partial_t R \rangle_{\mathcal{L}^2} - \langle \partial_t^2 LR, \partial_t R \rangle_{\mathcal{L}^2}$$

and with

$$\begin{aligned} -\langle \partial_t^2 LR, \partial_t R \rangle_{\mathcal{L}^2} &= -\langle L\partial_t^2 R, \partial_t R \rangle_{\mathcal{L}^2} \\ &= -\langle L(-LR + G(\Psi, R)), \partial_t R \rangle_{\mathcal{L}^2} \\ &= \langle LR, \partial_t LR \rangle_{\mathcal{L}^2} - \langle G(\Psi, R), \partial_t LR \rangle_{\mathcal{L}^2}, \end{aligned}$$

the equation (3.41) changes to

$$\partial_t \langle \partial_t LR, \partial_t R \rangle_{\mathcal{L}^2} + \partial_t \langle LR, LR \rangle_{\mathcal{L}^2} = \langle G(\Psi, R), \partial_t LR \rangle_{\mathcal{L}^2} + \langle \partial_t LR, G(\Psi, R) \rangle_{\mathcal{L}^2}.$$

By introducing the representation $L = \Omega^2$, we have

$$\partial_t \langle \partial_t \Omega R, \partial_t \Omega R \rangle_{\mathcal{L}^2} + \partial_t \langle LR, LR \rangle_{\mathcal{L}^2} = 2 |\langle \partial_t \Omega R, \Omega G(\Psi, R) \rangle_{\mathcal{L}^2}|. \quad (3.42)$$

Since $\langle LR, LR \rangle_{\mathcal{L}^2} = \|LR\|_{\mathcal{L}^2}^2 = \|R\|_{\mathcal{H}^2}^2$ and with the estimate

$$|\langle \partial_t \Omega R, \Omega G(\Psi, R) \rangle_{\mathcal{L}^2}| \leq \|\partial_t \Omega R\|_{\mathcal{L}^2} \|G(\Psi, R)\|_{\mathcal{H}^2},$$

equation (3.42) is given by

$$\partial_t (\|\partial_t \Omega R\|_{\mathcal{L}^2}^2 + \|R\|_{\mathcal{H}^2}^2) \leq 2 \|\partial_t \Omega R\|_{\mathcal{L}^2} \|G(\Psi, R)\|_{\mathcal{H}^2}. \quad (3.43)$$

Now we define the energy $E_R = \|\partial_t \Omega R\|_{\mathcal{L}^2}^2 + \|R\|_{\mathcal{H}^2}^2$, insert (3.41) into (3.43) and thus find

$$\begin{aligned} \partial_t E_R &\leq 2 \|\partial_t \Omega R\|_{\mathcal{L}^2} \left(C_{\text{Res}} \varepsilon^2 + 3C_1 \varepsilon^2 \|R\|_{\mathcal{H}^2} + 3C_1 \varepsilon^{5/2} \|R\|_{\mathcal{H}^2}^2 + C_1 \varepsilon^3 \|R\|_{\mathcal{H}^2}^3 \right) \\ &\leq 2E_R^{1/2} \left(C_{\text{Res}} \varepsilon^2 + 3C_1 \varepsilon^2 E_R^{1/2} + 3C_1 \varepsilon^{5/2} E_R + C_1 \varepsilon^3 E_R^{3/2} \right). \end{aligned}$$

Using the estimate $E_R^{1/2} \leq 1 + E_R$, we finally get

$$\partial_t E_R \leq 2C_{\text{Res}} \varepsilon^2 + 2(3C_1 + C_{\text{Res}}) \varepsilon^2 E_R + 6C_1 \varepsilon^{5/2} E_R^{3/2} + 2C_1 \varepsilon^3 E_R^2. \quad (3.44)$$

For simplicity, we assume $R(0) = \partial_t R(0) = 0$ and therefore $E_R(0) = 0$. Using Gronwall's inequality for (3.44) allows us to estimate the energy E_R on the time scale $T = \varepsilon^2 t$ for $T \in [0, T_0]$ by

$$\sup_{t \in [0, T_0/\varepsilon^2]} E_R \leq 2C_{\text{Res}} e^{(6C_1 + 2C_{\text{Res}} + 1)T_0} =: M$$

for all $\varepsilon \in (0, \varepsilon_0)$, if $\varepsilon_0 > 0$ is chosen so small that $6C_1 \varepsilon^{1/2} E_R^{1/2} + 2C_1 \varepsilon E_R \leq 1$. This energy estimate yields to the bound

$$\sup_{t \in [0, T_0/\varepsilon^2]} \|R\|_{\mathcal{H}^2} \leq M^{1/2},$$

and by using Sobolev's embedding theorem, bound (3.38) and the decomposition (3.39), we complete the proof of Theorem 3.2.2.

4. Approximation of a two-dimensional Gross-Pitaevskii equation with a periodic potential

In this chapter, we change the topic from quantum graphs to a different kind of approximation problem for a NLS equation. Here we consider the two-dimensional Gross-Pitaevskii (GP) equation with a periodic potential of the formal order $\mathcal{O}(\varepsilon^{-2})$ in one space direction on the homogenous space and justify the validity of the discrete nonlinear Schrödinger (dNLS) equation as an effective amplitude equation in the asymptotic limit $\varepsilon \rightarrow 0$.

We start with a short introduction into the model and define the function space we need to prove our approximation result in Section 4.1. In Section 4.2, we give a short recap on the spectral theory of the one-dimensional Schrödinger operator with a periodic potential and the theory of Wannier function decomposition. This part is based on the more detailed introductions to this topic in Section 2.1. of [29] and [34]. We also shortly discuss the spectral properties of the harmonic oscillator problem in one space dimension. The main theorem is formulated in Section 4.3. This result can be interpreted as an extension of [32] to the two-dimensional case. In Section 4.4, we use a multiple scaling expansion to derive the effective amplitude equation. With an improved approximation we compute the residual and estimate the nonlinear terms. Local existence and uniqueness results for the error equation and the derived dNLS equation are stated in Section 4.5. An energy estimate using Gronwall's inequality, similar to the one in the updated version of [32], completes the proof in Section 4.6.

Notation: According to Chapters 2 and 3, we use the standard notations for the Sobolev space $H^s(\mathbb{R}^2)$ and the Lebesgue space $L^p(\mathbb{R}^2)$ for $s \geq 0$ and $p \geq 1$. We also denote with $l^1(\mathbb{Z})$ and $l^2(\mathbb{Z})$ the complex-valued sequence spaces equipped with the norms $\|\vec{a}\|_{l^1} = \sum_{m \in \mathbb{Z}} |a_m|$ and $\|\vec{a}\|_{l^2} = (\sum_{m \in \mathbb{Z}} |a_m|^2)^{1/2}$.

4.1. The model

The GP equation is well-known in physics literature [35] as a mean-field model of the Bose-Einstein condensation. Looking at a condensate in an optical gap, a periodic structure is very common in experimental and in theoretical research, see for example [23] and [24]. From a mathematical point of view, we have to deal with a nonlinear Schrödinger equation with an external periodic potential. The book [29] gives a good overview on the analysis of such systems.

Here, we consider the GP equation in two space dimensions,

$$i\partial_t u = -\Delta u + V(r)u + \sigma|u|^2 u, \quad t \in \mathbb{R}_+, \quad r \in \mathbb{R}^2, \quad (4.1)$$

where $u(t, r) : \mathbb{R}_+ \times \mathbb{R}^2 \rightarrow \mathbb{C}$ decays to zero sufficiently fast as $|r| \rightarrow \infty$ and the potential $V(r) = V_x(x) + V_y(y)$ is given by a piecewise-constant periodic potential $V_x(x)$ in the x -direction

and a harmonic oscillator potential of the form

$$V_y(y) = y^2 \quad (4.2)$$

in the y -direction. In particular, the potential V_x is bounded, real-valued, 2π -periodic and defined by

$$V_x(x) = \begin{cases} \varepsilon^{-2} & x \in (0, a) \pmod{2\pi}, \\ 0 & x \in (a, 2\pi) \pmod{2\pi}, \end{cases} \quad (4.3)$$

where $a \in (0, 2\pi)$ is fixed and $0 < \varepsilon \ll 1$. Both potentials are shown in Figure 4.1. The parameter $\sigma = \pm 1$ is normalized by convenience.

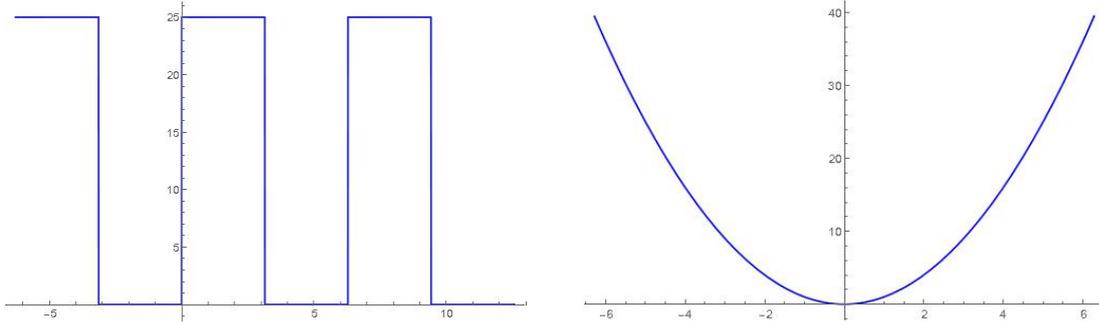


Figure 4.1.: The potential function $V_x(x)$ with $a = \pi$ and $\varepsilon = 0.2$ (left) and the potential function $V_y(y) = y^2$ (right).

Our goal in this chapter is to derive an effective equation in the tight-binding limit for the description of the dynamics of the wave function u , in detail we reduce the continuous equation (4.1) to a nonlinear lattice problem, cf. [7, 41]. In the one-dimensional case, this has recently been done by Pelinovsky and Schneider in [32], where a GP equation with the periodic potential (4.3) is approximated by a dNLS equation in the asymptotic limit $\varepsilon \rightarrow 0$. More results on the reduction of a one-dimensional GP equation to a dNLS equation can be found in [6, 8, 34].

In our two-dimensional problem, the periodicity of the potential is restricted to one space dimension and with the unbounded harmonic potential (4.2) in y -direction, we obtain in the slow time scale $T = \mu t$ with $\mu = \varepsilon e^{-\frac{a}{\varepsilon}}$ an effective equation of the form

$$i\partial_T a_m = \alpha(a_{m-1} + a_{m+1}) + \sigma\beta |a_m|^2 a_m, \quad (4.4)$$

where the sequence $\{a_m(T)\}_{m \in \mathbb{Z}} = \vec{a}(T)$ represents a small-amplitude solution of (4.1) with amplitude functions $a_m(T)$ located in the m -th potential well. The numerical coefficients α and β are ε -independent and will be explained later on.

In order to justify the effective equation (4.4) with the methods from [32], we need a suitable Banach space for our error estimates. As in the one-dimensional case, we have $\|V_x\|_{C_b^0} \rightarrow \infty$ in the limit $\varepsilon \rightarrow 0$ and since $V_x \geq 0$ for all $x \in \mathbb{R}$, it is convenient to work in the function space $\mathcal{H}^{1,2}(\mathbb{R}^2)$ equipped with the norm

$$\|u\|_{\mathcal{H}^{1,2}}^2 = \langle (L_x + I)u, u \rangle_{L^2} + \langle (L_y + I)^2 u, u \rangle_{L^2} + \langle u, u \rangle_{L^2}, \quad (4.5)$$

where the occurring scalar products are defined by the linear Schrödinger operators $L_x = -\partial_x^2 + V_x$ and $L_y = -\partial_y^2 + V_y$. This space also helps us to control the nonlinearity of the original problem

(4.1) in two space dimensions. The norm representation (4.5) makes it reasonable to use an approximation ansatz which decomposes the original solutions $u(t, x)$ of the GP equation (4.1) by the eigenfunctions of the linear problems corresponding to the one-dimensional operators L_x and L_y . Therefore, we first study the spectrum of these operators.

Remark 4.1.1. Note that it is not possible to use the space $\mathcal{H}^1(\mathbb{R}^2)$ with $\|u\|_{\mathcal{H}^1}^2 = \langle (L+I)u, u \rangle_{L^2}$ in our analysis due to Sobolev's embedding theorem in two space dimensions among other reasons. Also the function space $\mathcal{H}^2(\mathbb{R}^2)$ with $\|u\|_{\mathcal{H}^2}^2 = \langle (L+I)^2u, u \rangle_{L^2}$ is inappropriate for this problem because we cannot prove that this space is closed under pointwise multiplication with an ε -independent constant for a potential $V(r)$ of the formal order $\mathcal{O}(\varepsilon^{-2})$. Here the linear operator L is defined by $L = L_x + L_y = -\Delta + V(r)$.

4.2. The spectral situation

Let us consider the spectral problem

$$Lu = \lambda u \tag{4.6}$$

of the two-dimensional linear Schrödinger operator with the potential $V = V_x + V_y$ defined in (4.3) and (4.2). By using the product ansatz $u(r) = \varphi(x)\psi(y)$, the equation (4.6) can be separated as follows:

$$L_x\varphi = E\varphi \tag{4.7}$$

and

$$L_y\psi = \omega\psi. \tag{4.8}$$

Now we look at the spectral properties of the linear operators $L_x = -\partial_x^2 + V_x$ and $L_y = -\partial_y^2 + V_y$ separately.

4.2.1. Wannier function decomposition in one dimension

First, we focus on the one-dimensional eigenvalue problem (4.7). According to the Bloch wave ansatz (2.10) in Section 2.2.2, we set

$$\varphi(x) = e^{i\ell x} \phi(\ell, x), \quad \ell, x \in \mathbb{R},$$

where $\phi(\ell, \cdot)$ is a 2π -periodic function for every $\ell \in \mathbb{R}$. These functions also satisfy the continuation conditions (2.11) and therefore we can restrict the definition of $\phi(\ell, x)$ to $x \in \mathbb{T}_{2\pi}$ and $\ell \in \mathbb{T}_1$. With this ansatz, $\phi(\ell, \cdot)$ is a solution to the eigenvalue problem

$$-(\partial_x + i\ell)^2 \phi(\ell, x) + V(x)\phi(\ell, x) = E(\ell)\phi(\ell, x)$$

with the linear operator $\tilde{L}_x(\ell, x) := -(\partial_x + i\ell)^2 + V(x)$.

Now we obtain an elementary result on the Schrödinger operator \tilde{L}_x similar to Lemma 2.2.2.

Lemma 4.2.1. *For fixed $\ell \in \mathbb{T}_1$, the operator $\tilde{L}_x(\ell, x)$ is a self-adjoint, positive semi-definite operator in $L^2(\mathbb{T}_{2\pi})$.*

Proof. For every $\phi(\ell, \cdot), \psi(\ell, \cdot) \in H^2(\mathbb{T}_{2\pi})$ and every $\ell \in \mathbb{T}_1$, the relation

$$\begin{aligned} \langle -(\partial_x + i\ell)^2 \phi, \psi \rangle_{L^2(\mathbb{T}_{2\pi})} &= \int_0^{2\pi} (\partial_x + i\ell)\phi(\ell, x) \cdot \overline{(\partial_x + i\ell)\psi(\ell, x)} dx \\ &\quad - [\partial_x \phi(\ell, 2\pi) + i\ell\phi(\ell, 2\pi)] \overline{\psi(\ell, 2\pi)} \\ &\quad + [\partial_x \phi(\ell, 0) + i\ell\phi(\ell, 0)] \overline{\psi(\ell, 0)} \\ &= \int_0^{2\pi} (\partial_x + i\ell)\phi(\ell, x) \cdot \overline{(\partial_x + i\ell)\psi(\ell, x)} dx \end{aligned}$$

holds by using the continuation conditions $\phi(\ell, 0) = \phi(\ell, 2\pi)$ and $\psi(\ell, 0) = \psi(\ell, 2\pi)$. As it is shown in Lemma 2.2.2, we apply the integration by parts a second time and this leads to

$$\langle -(\partial_x + i\ell)^2 \phi, \psi \rangle_{L^2(\mathbb{T}_{2\pi})} = \langle \phi, -(\partial_x + i\ell)^2 \psi \rangle_{L^2(\mathbb{T}_{2\pi})}.$$

Because the potential function $V(x)$ is real-valued, we directly obtain

$$\langle \tilde{L}_x(\ell, x)\phi, \psi \rangle_{L^2(\mathbb{T}_{2\pi})} = \langle \phi, \tilde{L}_x(\ell, x)\psi \rangle_{L^2(\mathbb{T}_{2\pi})},$$

and thus the operator $\tilde{L}_x(\ell, x)$ is self-adjoint.

With the same conclusion as in the proof of Lemma 2.2.2, the operator $\tilde{L}_x(\ell, x)$ is positive semi-definite. \square

Referring to the argumentation in Section 2.2.2 and Section 3.2.1, by Lemma 4.2.1 and the spectral theorem for self-adjoint operators with compact resolvent, cf. [36], for each $\ell \in \mathbb{T}_1$ there exists a Schauder base $\{\phi_n(\ell, \cdot)\}_{n \in \mathbb{N}}$ of $L^2(\mathbb{T}_{2\pi})$ consisting of eigenfunctions of $\tilde{L}_x(\ell, x)$ with positive eigenvalues $\{E_n(\ell)\}_{n \in \mathbb{N}}$ ordered as $E_n(\ell) \leq E_{n+1}(\ell)$. Hence, we define the corresponding Bloch wave function in $L^2(\mathbb{R})$ to the eigenvalue $E_n(\ell)$ by $\tilde{\phi}_n(\ell, x) := e^{i\ell x} \phi_n(\ell, x)$ and each of these pairs solves the spectral problem

$$L_x \tilde{\phi}_n(\ell, x) = E_n(\ell) \tilde{\phi}_n(\ell, x) \quad (4.9)$$

for every $n \in \mathbb{N}$. By (2.11), the condition $\tilde{\phi}_n(\ell, x + 2\pi) = \tilde{\phi}_n(\ell, x) e^{i2\pi\ell}$ holds for all $x \in \mathbb{R}$, and also all Bloch wave functions $\tilde{\phi}_n(\ell, \cdot)$ satisfy the following orthogonality and normalization relation:

$$\langle \tilde{\phi}_n(\ell, \cdot), \tilde{\phi}_{n'}(\ell', \cdot) \rangle_{L^2(\mathbb{R})} = \delta_{n,n'} \delta(\ell - \ell'), \quad n, n' \in \mathbb{N}, \quad \ell, \ell' \in \mathbb{T}_1. \quad (4.10)$$

In order to normalize the phase factors of the Bloch wave functions as in [34], we set $\tilde{\tilde{\phi}}_n(\ell, x) = \tilde{\phi}_n(-\ell, x)$ as eigenfunctions for the eigenvalues $E_n(\ell) = \overline{E_n(\ell)} = E_n(-\ell)$. Note that in contrast to Section 2.2.2 and Section 3.2.1, we use subscripts for the count of the spectral bands \mathcal{E}_n . In our problem, it is more useful to use the Wannier function decomposition to approximate the continuous PDE (4.1) with the lattice equation (4.4). We follow very closely the well-written introduction to this topic in [32] and for a more detailed approach we again refer to [29] and [34]. The band function $E_n(\ell)$ and the Bloch wave function $\phi_n(\ell, x)$ introduced above are 1-periodic with respect to $\ell \in \mathbb{T}_1$ for any $n \in \mathbb{N}$. Therefore, we can represent them by the Fourier series

$$E_n(\ell) = \sum_{m \in \mathbb{Z}} \hat{E}_{n,m} e^{i2\pi m \ell}, \quad \ell \in \mathbb{T}_1, \quad (4.11)$$

and

$$\tilde{\phi}_n(\ell, x) = \sum_{m \in \mathbb{Z}} \hat{\phi}_{n,m}(x) e^{i2\pi m \ell}, \quad \ell \in \mathbb{T}_1, \quad x \in \mathbb{R}. \quad (4.12)$$

The Fourier coefficients in (4.11) and (4.12) are defined by the integrals

$$\hat{E}_{n,m} = \int_{\mathbb{T}_1} E_n(\ell) e^{-i2\pi m \ell} d\ell, \quad m \in \mathbb{Z},$$

and

$$\hat{\phi}_{n,m}(x) = \int_{\mathbb{T}_1} \tilde{\phi}_n(\ell, x) e^{-i2\pi m \ell} d\ell, \quad m \in \mathbb{Z}, \quad x \in \mathbb{R},$$

and satisfy the constraints

$$\hat{E}_{n,m} = \overline{\hat{E}_{n,-m}} = \hat{E}_{n,-m}, \quad \hat{\phi}_{n,m}(x) = \overline{\hat{\phi}_{n,m}(x)}, \quad \forall m \in \mathbb{Z}, \forall n \in \mathbb{N}, \forall x \in \mathbb{R}.$$

Because of the quasi-periodicity $\tilde{\phi}_n(\ell, x + 2\pi) = \tilde{\phi}_n(\ell, x) e^{i2\pi \ell}$ for any $x \in \mathbb{R}$ and $\ell \in \mathbb{T}_1$, we obtain the property

$$\hat{\phi}_{n,m}(x) = \hat{\phi}_{n,m-1}(x - 2\pi) = \hat{\phi}_{n,0}(x - 2\pi m), \quad \forall m \in \mathbb{Z}, \forall n \in \mathbb{N}, \forall x \in \mathbb{R}.$$

and the so-defined real-valued functions $\hat{\phi}_{n,m}$ are called Wannier functions.

Although the Wannier functions are no eigenfunctions of the Schrödinger operator L_x , we can substitute the Fourier series representations (4.11) and (4.12) into the one-dimensional linear problem (4.9) for a fixed $n \in \mathbb{N}$. Thereby, in every spectral band \mathcal{E}_n the set of functions $\{\hat{\phi}_{n,m}\}_{m \in \mathbb{Z}}$ satisfies the system

$$L_x \hat{\phi}_{n,m} = \sum_{m' \in \mathbb{Z}} \hat{E}_{n,m-m'} \hat{\phi}_{n,m'}, \quad \forall m \in \mathbb{Z}, \quad (4.13)$$

with the corresponding coefficients $\{\hat{E}_{n,m}\}_{m \in \mathbb{Z}}$. Orthogonality and normalization of Wannier functions, given by

$$\langle \hat{\phi}_{n,m}(\cdot), \hat{\phi}_{n',m'}(\cdot) \rangle_{L^2(\mathbb{R})} = \delta_{n,n'} \delta_{m,m'}, \quad n, n' \in \mathbb{N}, \quad m, m' \in \mathbb{Z}, \quad (4.14)$$

directly follows from the relation (4.10) for Bloch functions.

We complete this part with the following two lemmas from [34], which state important properties of the band functions $\hat{E}_n(\ell)$ and the Wannier functions $\hat{\phi}_{n,m}(x)$ of the linear one-dimensional spectral problem (4.7).

Lemma 4.2.2. *Let V_x be given by (4.3) and $\mu = \varepsilon e^{-a/\varepsilon}$. For any fixed $n_0 \in \mathbb{N}$, there exist $\varepsilon_0, C_s, E_0, C_1^\pm, C_2, C_0, C_m > 0$, such that, for any $\varepsilon \in [0, \varepsilon_0)$, the band functions and the Wannier functions of the operator $L_x = -\partial_x^2 + V_x$ satisfy the properties.*

(i) (band separation)

$$\min_{n \in \mathbb{N} \setminus \{n_0\}} \inf_{\ell \in \mathbb{T}_1} |E_n(\ell) - \hat{E}_{n_0,0}| \geq C_s \quad (4.15)$$

(ii) (band boundedness)

$$|\hat{E}_{n_0,0}| \leq E_0 \quad (4.16)$$

(iii) (tight-binding approximation)

$$\begin{aligned} C_1^- \mu &\leq |\hat{E}_{n_0,1}| \leq C_1^+ \mu, \\ |\hat{E}_{n_0,m}| &\leq C_2 \mu^2 \quad \text{for } m \geq 2 \end{aligned} \quad (4.17)$$

(iv) (compact support)

$$|\hat{\phi}_{n_0,0}(x) - \hat{\phi}_0| \leq C_0 \varepsilon, \quad \forall x \in [0, 2\pi], \quad (4.18)$$

where

$$\hat{\phi}_0(x) = \begin{cases} 0, & \forall x \in [0, a], \\ \frac{\sqrt{2}}{\sqrt{2\pi-a}} \sin\left(\frac{\pi n_0(2\pi-x)}{2\pi-a}\right), & \forall x \in [a, 2\pi]. \end{cases}$$

(v) (exponential decay)

$$|\hat{\phi}_{n_0,0}(x)| \leq C_m \mu^m, \quad \forall x \in [-2\pi m, -2\pi(m-1)] \cup [2\pi m, 2\pi(m+1)], m \in \mathbb{N} \quad (4.19)$$

Proof. The proof of (i)-(iii) is given in Appendix B and (iv)-(v) are shown in Appendix C of [34]. \square

Lemma 4.2.3. *Let \mathcal{E}_n be the invariant closed subspace of $L^2(\mathbb{R})$ associated with the n -th spectral band and assume that $\mathcal{E}_n \cap \mathcal{E}_{n'}$ for a fixed $n \in \mathbb{N}$ and all $n' \neq n$. Then, $\langle \hat{\phi}_{n,m}, \hat{\phi}_{n,m'} \rangle_{L^2(\mathbb{R})} = \delta_{m,m'}$ for any $m, m' \in \mathbb{Z}$ and there exists constants $\eta_n > 0$ and $C_n > 0$, such that*

$$|\hat{\phi}_{n,m}(x)| \leq C_n e^{-\eta_n |x-2\pi m|} \quad (4.20)$$

Proof. The orthogonality relation for the Wannier functions is already mentioned in (4.14). The exponential decay bound (4.20) follows from complex integration. For a detailed calculation we refer to the proof of Proposition 2 in [34]. \square

Remark 4.2.4. The exponential decay (4.20) is proven in [34] for the spectrum of an operator $L = -\partial_x^2 + V(x)$ consisting of the union of disjoint spectral bands. However, for the proof of Lemma 4.2.3 we do not need the assumption that all spectral bands are disjoint. It is sufficient that the particular n -th spectral band is disjoint from the other spectral bands of the linear operator. According to property (4.15), this condition is satisfied for the spectrum of the operator L_x in the asymptotic limit $\varepsilon \rightarrow 0$, cf. [32].

4.2.2. Properties of the harmonic oscillator

Here we give a short recap on the well-known spectral problem (4.8). The eigenvalue problem

$$-\partial_y^2 \psi + V_y \psi = \omega \psi$$

has an infinite set of isolated simple eigenvalues $\omega_j = 1 + 2j$ with $j \in \mathbb{N}_0$ and the L^2 -normalized orthogonal eigenfunctions of this system are given by

$$\psi_j(y) = \frac{1}{(\pi)^{1/4} (2^j j!)^{1/2}} H_j(y) e^{-y^2/2},$$

where the functions H_j represent the Hermite polynomials. For a more detailed derivation and calculation of the spectrum of the one-dimensional harmonic oscillator, we refer to classical textbooks in quantum mechanics like [12] and [27].

4.3. Main result

We represent an approximate solution of the given GP equation (4.1) by the formal asymptotic expansion

$$u(t, r) = \mu^{1/2} \Psi_0(t, r) + \text{higher-order terms},$$

with

$$\begin{aligned} \mu^{1/2} \Psi_0(t, r) &= \mu^{1/2} \sum_{m \in \mathbb{Z}} a_m(T) \widehat{\phi}_{n,m}(x) \psi_j(y) e^{-i(\widehat{E}_{n,0} + \omega_j)t} \\ &= \mu^{1/2} \varphi_0(T, r) e^{-i(\widehat{E}_{n,0} + \omega_j)t} \\ &= \mu^{1/2} \varphi_0(T, r) \mathbf{E}(t), \end{aligned} \quad (4.21)$$

where $T = \mu t$ with $\mu = \varepsilon e^{-a/\varepsilon} \ll 1$ is the slow time variable and $r = (x, y) \in \mathbb{R}^2$. The set of Wannier functions $\{\widehat{\phi}_{n,m}\}_{m \in \mathbb{Z}}$ belongs to the subspace of $L^2(\mathbb{R})$ associated with the n -th spectral band of the one-dimensional Schrödinger operator L_x . The function ψ_j represents the eigenfunction of the operator L_y with the corresponding energy ω_j .

Substituting the ansatz (4.21) into the original equation (4.1) shows that the amplitudes $\{a_m(T)\}_{m \in \mathbb{Z}}$ satisfy the dNLS equation (4.4) where the parameters are given by

$$\alpha = \frac{\widehat{E}_{n,1}}{\mu} \quad \text{and} \quad \beta = \|\widehat{\phi}_{n,0} \psi_j\|_{L^4}^4. \quad (4.22)$$

The values of both constants α and β are uniformly bounded and nonzero as $\mu \rightarrow 0$. For a bound on the constant α we refer to (4.17). Using the embedding result from Remark B.1.4,

$$\|\widehat{\phi}_{n,0} \psi_j\|_{L^4} \leq C \|\widehat{\phi}_{n,0} \psi_j\|_{H^1} \leq C \|\widehat{\phi}_{n,0} \psi_j\|_{H^{1,2}} \leq C \|\widehat{\phi}_{n,0} \psi_j\|_{\mathcal{H}^{1,2}},$$

and with (B.15), we immediately get that $\beta = \|\widehat{\phi}_{n,0} \psi_j\|_{L^4}^4 < \infty$. Properties (4.17) and (4.18) guarantee that $\alpha, \beta \neq 0$ for $0 < \mu \ll 1$.

The mathematical justification of the effective amplitude equation (4.4) by means of error estimates is the main purpose of this chapter. The approximation result is given by the following theorem.

Theorem 4.3.1. *Pick $n \in \mathbb{N}, j \in \mathbb{N}_0$ such that the following non-resonance condition is satisfied for all $\ell \in \mathbb{T}_1$:*

$$(E_{n'}(\ell) - \widehat{E}_{n,0}) + 2(j' - j) \neq 0, \quad \text{for every } n' \in \mathbb{N} \setminus \{n\} \quad \text{and} \quad j' \in \mathbb{N}_0 \setminus \{j\}. \quad (4.23)$$

Let $\vec{a}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ be a solution of the dNLS equation (4.4) with initial data $\vec{a}(0) = \vec{a}_0$ satisfying the bound

$$\left\| u_0 - \mu^{1/2} \sum_{m \in \mathbb{Z}} a_m(0) \widehat{\phi}_{n,m}(x) \psi_j(y) \right\|_{\mathcal{H}^{1,2}} \leq C_0 \mu^{3/2}$$

for some $C_0 > 0$. Then, for any $\mu \in (0, \mu_0)$ with sufficiently small $\mu_0 > 0$, there exists a μ -independent constant $C > 0$ such that the GP equation (4.1) admits a solution $u(t) \in C^1([0, T_0/\mu], \mathcal{H}^{1,2}(\mathbb{R}^2))$ satisfying the bound

$$\left\| u(\cdot, t) - \mu^{1/2} \sum_{m \in \mathbb{Z}} a_m(\mu t) \widehat{\phi}_{n,m}(x) \psi_j(y) e^{-i(\widehat{E}_{n,0} + \omega_j)t} \right\|_{\mathcal{H}^{1,2}} \leq C \mu^{3/2} \quad (4.24)$$

for all $t \in [0, T_0/\mu]$.

Remark 4.3.2. Since $\mu = \varepsilon e^{-a/\varepsilon}$, the finite time interval $[0, T_0/\mu]$ is exponentially large with respect to ε , c.f. [8, 32].

Remark 4.3.3. Such an approximation result was shown for the GP equation in one space dimension in [29] and [32]. Similar to the approach in the updated version of [32], we compute the residual of the approximation ansatz and use a simple application of Gronwall's inequality to estimate the error bound. The main difficulty in the proof of Theorem 4.3.1 lies in the definition of the associated function space $\mathcal{H}^{1,2}$ in two space dimensions, which has to satisfy certain conditions that are summarized in Appendix B.1.

Remark 4.3.4. The appearance of the non-resonance condition (4.23) in Theorem 4.3.1 is another main difference to the one-dimensional result in [29] and [32]. This additional condition is needed due to the orthogonal projection on the spectral bands which is introduced in Lemma 4.4.2.

4.4. Computation of the residual

Here we use the multi-scale expansion ansatz (4.21) and compute the corresponding residual. In order to control the remaining terms of $\text{Res}(\mu^{1/2}\Psi_0)$, we will also introduce an improved approximation by adding higher-order terms to our ansatz (4.21). With a projection on the subspace $\mathcal{E}_{n,j}$ and on its complement $\mathcal{E}_{n,j}^\perp$, we can decompose and simplify the problematic terms. By estimating the difference between the solution of the evolution problem (4.1) and the approximation Ψ_0 , we get a time evolution problem for this error and obtain bounds for the respective terms.

4.4.1. Residual of the approximate solution

Our goal is to compute the remaining terms of (4.25), which do not cancel after inserting the approximate solution $\mu^{1/2}\Psi_0$ into the GP equation (4.1). These terms are collected in the residual

$$\text{Res}(\mu^{1/2}\Psi_0) = -i\partial_t\mu^{1/2}\Psi_0 - \Delta\mu^{1/2}\Psi_0 + V(r)\Psi_0 + \sigma|\mu^{1/2}\Psi_0|^2\mu^{1/2}\Psi_0. \quad (4.25)$$

Substitution of the ansatz (4.21) into (4.25) leads to the relation

$$\begin{aligned} \text{Res}(\mu^{1/2}\Psi_0) &= -i\mu^{3/2} \sum_{m \in \mathbb{Z}} \partial_T a_m(T) \widehat{\phi}_{n,m}(x) \psi_j(y) \mathbf{E}(t) \\ &\quad - \mu^{1/2} \sum_{m \in \mathbb{Z}} a_m(T) \left(-\partial_x^2 + V_x(x) - \widehat{E}_{n,0} \right) \widehat{\phi}_{n,m}(x) \psi_j(y) \mathbf{E}(t) \\ &\quad - \mu^{1/2} \sum_{m \in \mathbb{Z}} a_m(T) \widehat{\phi}_{n,m}(x) \left(-\partial_y^2 + V_y(y) - \omega_j \right) \psi_j(y) \mathbf{E}(t) \\ &\quad + \sigma\mu^{3/2} |\varphi_0(T, r)|^2 \varphi_0(T, r) \mathbf{E}(t), \end{aligned} \quad (4.26)$$

where the time derivation is given by $\partial_t a_m(T) = \mu \partial_T a_m(T)$. Now we rewrite the Wannier condition (4.13) as follows:

$$\left(-\partial_x^2 + V_x(x) - \widehat{E}_{n,0} \right) \widehat{\phi}_{n,m}(x) = \sum_{\substack{m' \in \mathbb{Z} \\ m \neq m'}} \widehat{E}_{n,m-m'} \widehat{\phi}_{n,m'}(x). \quad (4.27)$$

Using (4.27) and the one-dimensional harmonic oscillator equation

$$(-\partial_y^2 + V_y(y) - \omega_j) \psi_j(y) = 0,$$

we simplify the residual (4.26) to

$$\begin{aligned} \text{Res}(\mu^{1/2}\Psi_0) &= -i\mu^{3/2} \sum_{m \in \mathbb{Z}} \partial_T a_m(T) \widehat{\phi}_{n,m}(x) \psi_j(y) \mathbf{E}(t) \\ &\quad - \mu^{1/2} \sum_{m \in \mathbb{Z}} a_m(T) \sum_{\substack{m' \in \mathbb{Z} \\ m \neq m'}} \widehat{E}_{n,m-m'} \widehat{\phi}_{n,m'}(x) \psi_j(y) \mathbf{E}(t) \\ &\quad + \sigma\mu^{3/2} |\varphi_0(T, r)|^2 \varphi_0(T, r) \mathbf{E}(t). \end{aligned}$$

Since the amplitude functions $\{a_m(T)\}_{m \in \mathbb{Z}}$ satisfy the dNLS equation (4.4) with the coefficients α and β stated in (4.22) and with an additional change of variables in the $\mathcal{O}(\mu^{1/2})$ -term, we obtain

$$\begin{aligned} \text{Res}(\mu^{1/2}\Psi_0) &= \mu^{1/2} \sum_{m \in \mathbb{Z}} \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} \widehat{E}_{n,m'-m} a_{m'}(T) \widehat{\phi}_{n,m}(x) \psi_j(y) \mathbf{E}(t) \\ &\quad + \sigma\mu^{3/2} \left(|\varphi_0(T, r)|^2 \varphi_0(T, r) - \sum_{m \in \mathbb{Z}} \beta |a_m(T)|^2 a_m(T) \widehat{\phi}_{n,m}(x) \psi_j(y) \right) \mathbf{E}(t). \end{aligned} \tag{4.28}$$

In order to get the residual sufficiently small, we extend the ansatz (4.21) by adding higher-order terms to the approximation.

4.4.2. The improved approximation

The residual of the simple approximation (4.21) contains remaining terms, which are of the formal order $\mathcal{O}(\mu^{1/2})$. However, we need the residual (4.28) to be of the formal order $\mathcal{O}(\mu^{3/2})$ and therefore we want to control the nonlinear $\mathcal{O}(\mu^{3/2})$ -term by adding higher-order terms $\mu^{3/2}\Psi_\mu$ to the ansatz (4.21). We set

$$\mu^{3/2}\Psi_\mu(t, r) = \mu^{3/2}\varphi_\mu(T, r) \mathbf{E}(t)$$

and thus define the improved approximation as follows:

$$\begin{aligned} \mu^{1/2}\Psi(t, r) &= \mu^{1/2}\Psi_0(t, r) + \mu^{3/2}\Psi_\mu(t, r) \\ &= \mu^{1/2}\varphi_0(T, r) \mathbf{E}(t) + \mu^{3/2}\varphi_\mu(T, r) \mathbf{E}(t). \end{aligned} \tag{4.29}$$

Computing the residual of the improved ansatz, we insert (4.29) into the GP equation (4.1) and get

$$\begin{aligned}
\text{Res}(\mu^{1/2}\Psi) &= \text{Res}(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu) \\
&= -i\partial_t \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) - \Delta \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) \\
&\quad + V(r) \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) \\
&\quad + \sigma \left| \mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right|^2 \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) \\
&= -i\partial_t \mu^{1/2}\Psi_0 - i\partial_t \mu^{3/2}\Psi_\mu - \Delta \mu^{1/2}\Psi_0 - \Delta \mu^{3/2}\Psi_\mu \\
&\quad + V(r)\mu^{1/2}\Psi_0 + V(r)\mu^{3/2}\Psi_\mu \\
&\quad + \sigma \mu^{3/2}\bar{\Psi}_0\Psi_0\Psi_0 + \sigma \mu^{5/2}\bar{\Psi}_0\Psi_\mu\Psi_0 + \sigma \mu^{5/2}\bar{\Psi}_\mu\Psi_0\Psi_0 + \sigma \mu^{7/2}\bar{\Psi}_\mu\Psi_\mu\Psi_0 \\
&\quad + \sigma \mu^{5/2}\bar{\Psi}_0\Psi_0\Psi_\mu + \sigma \mu^{7/2}\bar{\Psi}_0\Psi_\mu\Psi_\mu + \sigma \mu^{7/2}\bar{\Psi}_\mu\Psi_0\Psi_\mu + \sigma \mu^{9/2}\bar{\Psi}_\mu\Psi_\mu\Psi_\mu.
\end{aligned} \tag{4.30}$$

We recall the definition (4.25) for the residual $\text{Res}(\mu^{1/2}\Psi)$ and with

$$\text{Res}(\mu^{3/2}\Psi_\mu) = -i\partial_t \mu^{3/2}\Psi_\mu - \Delta \mu^{3/2}\Psi_\mu + V(r)\mu^{3/2}\Psi_\mu + \sigma \left| \mu^{3/2}\Psi_\mu \right|^2 \mu^{3/2}\Psi_\mu,$$

we rewrite (4.30) to

$$\begin{aligned}
\text{Res}(\mu^{1/2}\Psi) &= \text{Res}(\mu^{1/2}\Psi_0) + \text{Res}(\mu^{3/2}\Psi_\mu) \\
&\quad + 2\sigma \mu^{5/2} |\Psi_0|^2 \Psi_\mu + 2\sigma \mu^{7/2} |\Psi_\mu|^2 \Psi_0 + \sigma \mu^{5/2} \bar{\Psi}_\mu \Psi_0^2 + \sigma \mu^{7/2} \bar{\Psi}_0 \Psi_\mu^2.
\end{aligned} \tag{4.31}$$

In order to sort the nonlinear terms by the power of μ , we use the decompositions $\mu^{1/2}\Psi_0(t, r) = \mu^{1/2}\varphi_0(T, r)\mathbf{E}(t)$ and $\mu^{3/2}\Psi_\mu(t, r) = \mu^{3/2}\varphi_\mu(T, r)\mathbf{E}(t)$ to obtain the following result:

$$\begin{aligned}
\text{Res}(\mu^{1/2}\Psi) &= \text{Res}(\mu^{1/2}\Psi_0) + \text{Res}(\mu^{3/2}\Psi_\mu) \\
&\quad + 2\sigma \mu^{5/2} |\varphi_0(T, r)|^2 \varphi_\mu(T, r)\mathbf{E}(t) + 2\sigma \mu^{7/2} |\varphi_\mu(T, r)|^2 \varphi_0(T, r)\mathbf{E}(t) \\
&\quad + \sigma \mu^{5/2} \bar{\varphi}_\mu(T, r) \varphi_0^2(T, r)\mathbf{E}(t) + \sigma \mu^{7/2} \bar{\varphi}_0(T, r) \varphi_\mu^2(T, r)\mathbf{E}(t).
\end{aligned} \tag{4.32}$$

Next, we see that the residual of the additional term $\mu^{3/2}\Psi_\mu$ is given by

$$\begin{aligned}
\text{Res}(\mu^{3/2}\Psi_\mu) &= -i\partial_t \mu^{3/2}\Psi_\mu - \Delta \mu^{3/2}\Psi_\mu + V(r)\mu^{3/2}\Psi_\mu + \sigma \left| \mu^{3/2}\Psi_\mu \right|^2 \mu^{3/2}\Psi_\mu \\
&= -i\mu^{3/2} \partial_t (\varphi_\mu(T, r)\mathbf{E}(t)) + \mu^{3/2} (L\varphi_\mu(T, r)) \mathbf{E}(t) \\
&\quad + \sigma \mu^{9/2} |\varphi_\mu(T, r)|^2 \varphi_\mu(T, r)\mathbf{E}(t) \\
&= -i\mu^{5/2} (\partial_T \varphi_\mu(T, r)) \mathbf{E}(t) + \mu^{3/2} \left(L - \left(\widehat{E}_{n,0} + \omega_j \right) \right) \varphi_\mu(T, r)\mathbf{E}(t) \\
&\quad + \sigma \mu^{9/2} |\varphi_\mu(T, r)|^2 \varphi_\mu(T, r)\mathbf{E}(t),
\end{aligned} \tag{4.33}$$

and by substituting (4.28) and (4.33) into (4.32), we conclude

$$\begin{aligned}
\text{Res}(\mu^{1/2}\Psi) &= \mu^{1/2} \sum_{m \in \mathbb{Z}} \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} \widehat{E}_{n, m'-m} a_{m'}(T) \widehat{\phi}_{n, m}(x) \psi_j(y) \mathbf{E}(t) \\
&\quad + \sigma \mu^{3/2} \left(\frac{1}{\sigma} \left(L - \left(\widehat{E}_{n, 0} + \omega_j \right) \right) \varphi_\mu(T, r) + |\varphi_0(T, r)|^2 \varphi_0(T, r) \right. \\
&\quad \quad \left. - \sum_{m \in \mathbb{Z}} \beta |a_m(T)|^2 a_m(T) \widehat{\phi}_{n, m}(x) \psi_j(y) \right) \mathbf{E}(t) \\
&\quad + \sigma \mu^{5/2} \left(-\frac{i}{\sigma} \partial_T \varphi_\mu(T, r) + 2 |\varphi_0(T, r)|^2 \varphi_\mu(T, r) + \overline{\varphi}_\mu(T, r) \varphi_0^2(T, r) \right) \mathbf{E}(t) \\
&\quad + \sigma \mu^{7/2} \left(2 |\varphi_\mu(T, r)|^2 \varphi_0(T, r) \mathbf{E}(t) + \overline{\varphi}_0(T, r) \varphi_\mu^2(T, r) \right) \mathbf{E}(t) \\
&\quad + \sigma \mu^{9/2} |\varphi_\mu(T, r)|^2 \varphi_\mu(T, r) \mathbf{E}(t).
\end{aligned} \tag{4.34}$$

As we can see in the equations above, we get additional $\mathcal{O}(\mu^{3/2})$ terms in the residual of the improved approximation $\mu^{1/2}\Psi$. Our next goal is to control the terms of the formal order $\mathcal{O}(\mu^{3/2})$ in (4.34) by using the orthogonal projection $\Pi_{n, j} : L^2(\mathbb{R}^2) \rightarrow \mathcal{E}_{n, j}$, where $\mathcal{E}_{n, j} \subset L^2(\mathbb{R}^2)$ is defined as the direct product of the n -th spectral band \mathcal{E}_n in x -direction and the eigenspace U_j corresponding to the eigenvalue ω_j of the harmonic oscillator problem (4.6). Therefore, we map the nonlinear term $|\varphi_0|^2 \varphi_0$ onto $\mathcal{E}_{n, j}$ and its complement $\mathcal{E}_{n, j}^\perp$, such that

$$|\varphi_0|^2 \varphi_0 = \Pi_{n, j} |\varphi_0|^2 \varphi_0 + (I - \Pi_{n, j}) |\varphi_0|^2 \varphi_0. \tag{4.35}$$

Note that this approach is similar to the decomposition used in the one dimensional case, c.f. [29] and [32]. The following two lemmas are useful to control the projection $(I - \Pi_{n, j}) |\varphi_0|^2 \varphi_0$.

Lemma 4.4.1. *Let $\vec{a}(T) \in l^1(\mathbb{Z})$ for a fixed $T \in \mathbb{R}$ and $\varphi_0(r) = \sum_{m \in \mathbb{Z}} a_m \widehat{\phi}_{n, m}(x) \psi_j(y)$ for a fixed $n \in \mathbb{N}$, then $\varphi_0(r) \in \mathcal{E}_{n, j} \subset L^2(\mathbb{R}^2)$ and also $\varphi_0(r) \in \mathcal{H}^{1, 2}(\mathbb{R}^2)$.*

Proof. Since $\|\vec{a}\|_{l^2} \leq \|\vec{a}\|_{l^1}$, we have $\vec{a} \in l^2(\mathbb{Z})$ and it follows directly from spectral theory for the operator $L = L_x + L_y$ in $L^2(\mathbb{R}^2)$ that $\varphi_0 \in \mathcal{E}_{n, j} = \mathcal{E}_n \times U_j$ for a fixed $n \in \mathbb{N}$. The second part of the theorem follows from the fact that $\widehat{\phi}_{n, m}(x) = \widehat{\phi}_{n, 0}(x - 2\pi m)$. Hence, we get

$$\begin{aligned}
\|\varphi_0\|_{\mathcal{H}^{1, 2}}^2 &= \left\| \sum_{m \in \mathbb{Z}} a_m \widehat{\phi}_{n, m} \psi_j \right\|_{\mathcal{H}^{1, 2}}^2 \\
&\leq \sum_{m \in \mathbb{Z}} \|a_m \widehat{\phi}_{n, m} \psi_j\|_{\mathcal{H}^{1, 2}}^2 \\
&\leq \sum_{m \in \mathbb{Z}} |a_m|^2 \|\widehat{\phi}_{n, m} \psi_j\|_{\mathcal{H}^{1, 2}}^2 \\
&= \|\vec{a}\|_{l^2}^2 \|\widehat{\phi}_{n, 0} \psi_j\|_{\mathcal{H}^{1, 2}}^2 \\
&\leq \|\vec{a}\|_{l^1}^2 \|\widehat{\phi}_{n, 0} \psi_j\|_{\mathcal{H}^{1, 2}}^2,
\end{aligned} \tag{4.36}$$

where we used the triangular inequality and the bound (B.15). □

Lemma 4.4.2. *There exists a unique solution $\varphi \in \mathcal{H}^{1,2}(\mathbb{R}^2)$ of the inhomogeneous equation*

$$\left(L - \left(\widehat{E}_{n,0} + \omega_j \right) \right) \varphi = (I - \Pi_{n,j}) f, \quad (4.37)$$

for any $f \in L^2(\mathbb{R}^2)$, such that $\langle \varphi, \vartheta \rangle_{L^2} = 0$ for every $\vartheta \in \mathcal{E}_{n,j}$ and

$$\|\varphi\|_{\mathcal{H}^{1,2}} \leq C \|f\|_{L^2} \quad (4.38)$$

for some $C > 0$ uniformly in $0 < \mu \ll 1$.

Proof. At first, we write $\mathcal{E}_{n,j} = \mathcal{E}_n \times U_j$ and by the band separation property (4.15) of Lemma 4.2.2, we get $\widehat{E}_{n,0} \notin \sigma(L_x)|_{\mathcal{E}_n^\perp}$. It is also clear that $\omega_j \notin \sigma(L_y)|_{U_j^\perp}$. With the same argument as in [29], if φ is a solution of

$$\left((L_x - \widehat{E}_{n,0}) + (L_y - \omega_j) \right) \varphi = (I - \Pi_{n,j}) f,$$

then $\varphi \in L^2(\mathbb{R}^2)$ for any $f \in L^2(\mathbb{R}^2)$ because of the decomposition

$$\varphi(r) = \int_{\mathbb{T}_1} \int_{y'=-\infty}^{\infty} \sum_{n' \in \mathbb{N} \setminus \{n\}} \sum_{j' \in \mathbb{N} \setminus \{j\}} \frac{\widetilde{f}_{n'}(\ell, y') \overline{\psi}_{j'}(y') \widetilde{\phi}_{n'}(\ell, x)}{(E_{n'}(\ell) - \widehat{E}_{n,0}) + (\omega_{j'} - \omega_j)} dy' d\ell \cdot \psi_j(y),$$

which implies that there is a constant $C_N > 0$ such that

$$\begin{aligned} \|\varphi\|_{L^2}^2 &\leq \int_{\mathbb{T}_1} \int_{y'=-\infty}^{\infty} \sum_{n' \in \mathbb{N} \setminus \{n\}} \sum_{j' \in \mathbb{N} \setminus \{j\}} \frac{\left| \widetilde{f}_{n'}(\ell, y') \psi_{j'}(y') \right|^2}{\left((E_{n'}(\ell) - \widehat{E}_{n,0}) + (\omega_{j'} - \omega_j) \right)^2} dy' d\ell \\ &\leq C_N \int_{\mathbb{T}_1} \int_{y'=-\infty}^{\infty} \sum_{n' \in \mathbb{N} \setminus \{n\}} \sum_{j' \in \mathbb{N} \setminus \{j\}} \left| \widetilde{f}_{n'}(\ell, y') \psi_{j'}(y') \right|^2 dy' d\ell \\ &\leq C_N \|f\|_{L^2}^2. \end{aligned} \quad (4.39)$$

This inequality holds under the non-resonance condition (4.23) stated in Theorem 4.3.1.

Next, we prove the bound (4.38) and initially get

$$\begin{aligned} \|\varphi\|_{\mathcal{H}^{1,2}}^2 &\leq |\langle (L_x + I)\varphi, \varphi \rangle_{L^2}| + |\langle (L_y + I)^2\varphi, \varphi \rangle_{L^2}| + |\langle \varphi, \varphi \rangle_{L^2}| \\ &\leq |\langle L_x\varphi, \varphi \rangle_{L^2}| + |\langle \varphi, \varphi \rangle_{L^2}| + |\langle L_y\varphi, L_y\varphi \rangle_{L^2}| \\ &\quad + 2|\langle L_y\varphi, \varphi \rangle_{L^2}| + |\langle \varphi, \varphi \rangle_{L^2}| + |\langle \varphi, \varphi \rangle_{L^2}| \\ &\leq |\langle L\varphi, L\varphi \rangle_{L^2}| + 3|\langle L\varphi, \varphi \rangle_{L^2}| + 3|\langle \varphi, \varphi \rangle_{L^2}|. \end{aligned} \quad (4.40)$$

The last line of (4.40) follows directly from the inequalities

$$|\langle L_x\varphi, \varphi \rangle_{L^2}| \leq |\langle (L_x + L_y)\varphi, \varphi \rangle_{L^2}|, \quad |\langle L_y\varphi, \varphi \rangle_{L^2}| \leq |\langle (L_x + L_y)\varphi, \varphi \rangle_{L^2}| \quad (4.41)$$

and

$$|\langle L_y\varphi, L_y\varphi \rangle_{L^2}| \leq |\langle (L_x + L_y)\varphi, (L_x + L_y)\varphi \rangle_{L^2}|, \quad (4.42)$$

which can be verified by adding the scalar products

$$|\langle L_x\varphi, \varphi \rangle_{L^2}| = \|\partial_x\varphi\|_{L^2}^2 + \|V_x^{1/2}\varphi\|_{L^2}^2, \quad |\langle L_y\varphi, \varphi \rangle_{L^2}| = \|\partial_y\varphi\|_{L^2}^2 + \|V_y^{1/2}\varphi\|_{L^2}^2$$

and

$$|\langle L_y \varphi, L_x \varphi \rangle_{L^2}| = \|\partial_x(\partial_y \varphi)\|_{L^2}^2 + \|V_x^{1/2}(\partial_y \varphi)\|_{L^2}^2 + \|\partial_x(V_y^{1/2} \varphi)\|_{L^2}^2 + \|V_x^{1/2}(V_y^{1/2} \varphi)\|_{L^2}^2$$

to the left hand side of (4.41) and (4.42) respectively. Since $\Pi_{n,j} f \in \mathcal{E}_{n,j}$, we obtain that $\langle \Pi_{n,j} f, \varphi \rangle_{L^2} = 0$ and with (4.39), we write

$$\begin{aligned} |\langle L \varphi, \varphi \rangle_{L^2}| &= |\langle (I - \Pi_{n,j}) f - (\widehat{E}_{n,0} + \omega_j) \varphi, \varphi \rangle_{L^2}| \\ &\leq |\langle f, \varphi \rangle_{L^2}| + |\widehat{E}_{n,0} + \omega_j| |\langle \varphi, \varphi \rangle_{L^2}| \\ &\leq \|f\|_{L^2} \|\varphi\|_{L^2} + (E_0 + \omega_j) \|\varphi\|_{L^2}^2 \\ &\leq C_1 \|f\|_{L^2}^2. \end{aligned} \tag{4.43}$$

Since $\|(I - \Pi_{n,j}) f\|_{L^2} \leq \|f\|_{L^2}$, we also conclude

$$\begin{aligned} |\langle L \varphi, L \varphi \rangle_{L^2}| &\leq |\langle (I - \Pi_{n,j}) f, (I - \Pi_{n,j}) f \rangle_{L^2}| + |\langle (\widehat{E}_{n,0} + \omega_j) \varphi, (I - \Pi_{n,j}) f \rangle_{L^2}| \\ &\quad + |\langle (I - \Pi_{n,j}) f, (\widehat{E}_{n,0} + \omega_j) \varphi \rangle_{L^2}| + |\langle (\widehat{E}_{n,0} + \omega_j) \varphi, (\widehat{E}_{n,0} + \omega_j) \varphi \rangle_{L^2}| \\ &\leq \|f\|_{L^2}^2 + 2(E_0 + \omega_j) \|\varphi\|_{L^2} \|f\|_{L^2} + (E_0 + \omega_j)^2 \|\varphi\|_{L^2}^2 \\ &\leq C_2 \|f\|_{L^2}^2. \end{aligned} \tag{4.44}$$

Inserting the estimates (4.43) and (4.44) into (4.40) yields to

$$\|\varphi\|_{\mathcal{H}^{1,2}}^2 \leq C_2 \|f\|_{L^2}^2 + 3C_1 \|f\|_{L^2}^2 + 3C_N \|f\|_{L^2}^2 = C^2 \|f\|_{L^2}^2$$

and thus the bound (4.38) holds. Uniqueness of φ follows from the fact that the inverse operator $(I - \Pi_{n,j})(L - (\widehat{E}_{n,0} + \omega_j))^{-1}(I - \Pi_{n,j})$ is a continuous map from $L^2(\mathbb{R}^2)$ to $\mathcal{H}^{1,2}(\mathbb{R}^2)$ uniformly in $0 < \mu \ll 1$. \square

Now we return to the computation of $\text{Res}(\mu^{1/2} \Psi)$ and use Lemma 4.4.2 to define $\varphi_\mu \in \mathcal{E}_{n,j}^\perp$ as a unique solution of the system

$$\left(L - \left(\widehat{E}_{n,0} + \omega_j \right) \right) \varphi_\mu = -\sigma (I - \Pi_{n,j}) |\varphi_0|^2 \varphi_0. \tag{4.45}$$

Using the decomposition (4.35) and the projection (4.45), the $\mathcal{O}(\mu^{3/2})$ terms in the residual (4.34) can be rewritten as

$$\begin{aligned} &\Pi_{n,j} |\varphi_0(T, r)|^2 \varphi_0(T, r) - \sum_{m \in \mathbb{Z}} \beta |a_m(T)|^2 a_m(T) \widehat{\phi}_{n,m}(x) \psi_j(y) \\ &= \sum_{m \in \mathbb{Z}} \sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1}(T) a_{m_2}(T) a_{m_3}(T) \widehat{\phi}_{n,m}(x) \psi_j(y), \end{aligned} \tag{4.46}$$

where we introduced the integral kernel

$$\kappa_j(m, m_1, m_2, m_3) = \langle \widehat{\phi}_{n,m_1} \psi_j \widehat{\phi}_{n,m_2} \psi_j \widehat{\phi}_{n,m_3} \psi_j, \widehat{\phi}_{n,m} \psi_j \rangle_{L^2}. \tag{4.47}$$

As a result, we obtain the residual (4.34) in the form

$$\begin{aligned}
\text{Res}(\mu^{1/2}\Psi) &= \mu^{1/2} \sum_{m \in \mathbb{Z}} \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} \widehat{E}_{n, m'-m} a_{m'}(T) \widehat{\phi}_{n, m}(x) \psi_j(y) \mathbf{E}(t) \\
&+ \sigma \mu^{3/2} \sum_{m \in \mathbb{Z}} \sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1}(T) a_{m_2}(T) a_{m_3}(T) \\
&\quad \times \widehat{\phi}_{n, m}(x) \psi_j(y) \mathbf{E}(t) \\
&+ \sigma \mu^{5/2} \left(-\frac{i}{\sigma} \partial_T \varphi_\mu(T, r) + 2 |\varphi_0(T, r)|^2 \varphi_\mu(T, r) + \bar{\varphi}_\mu(T, r) \varphi_0^2(T, r) \right) \mathbf{E}(t) \\
&+ \sigma \mu^{7/2} \left(2 |\varphi_\mu(T, r)|^2 \varphi_0(T, r) \mathbf{E}(t) + \bar{\varphi}_0(T, r) \varphi_\mu^2(T, r) \right) \mathbf{E}(t) \\
&+ \sigma \mu^{9/2} |\varphi_\mu(T, r)|^2 \varphi_\mu(T, r) \mathbf{E}(t).
\end{aligned} \tag{4.48}$$

The formal derivation of (4.46) and (4.47) can be found in the second part of Appendix B.2.

4.4.3. Estimates on the error term

The improved approximation leads to the term (4.46), which is of the formal order $\mathcal{O}(\mu^{3/2})$ and does not vanish. However, Lemma 4.4.2 simplified these terms to be an element of the subspace $\mathcal{E}_{n, j}$ and this projection is required to control the approximation error.

As in [32], we now want to obtain an evolution equation for the error. Therefore, we write the solution u of the evolution problem (4.1) as a sum of the improved approximation $\mu^{1/2}\Psi$ and the error term $\mu^{3/2}R$, i.e.,

$$\begin{aligned}
u(t, r) &= \mu^{1/2}\Psi(t, r) + \mu^{3/2}R(t, r) \\
&= \mu^{1/2}\Psi_0(t, r) + \mu^{3/2}\Psi_\mu(t, r) + \mu^{3/2}R(t, r) \\
&= \mu^{1/2}\varphi_0(T, r) \mathbf{E}(t) + \mu^{3/2}\varphi_\mu(T, r) \mathbf{E}(t) + \mu^{3/2}\rho(t, r) \mathbf{E}(t) \\
&= \mu^{1/2}\varphi_0(T, r) \mathbf{E}(t) + \mu^{3/2} (\varphi_\mu(T, r) + \rho(t, r)) \mathbf{E}(t).
\end{aligned} \tag{4.49}$$

Substituting this decomposition into (4.1) yields to

$$\begin{aligned}
i\partial_t u &= i\partial_t \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu + \mu^{3/2}R \right) \\
&= -\Delta \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu + \mu^{3/2}R \right) \\
&\quad + V(r) \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu + \mu^{3/2}R \right) \\
&\quad + \sigma \left| \mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu + \mu^{3/2}R \right|^2 \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu + \mu^{3/2}R \right)
\end{aligned} \tag{4.50}$$

and by rearranging (4.50), we get the evolution problem

$$\begin{aligned}
i\partial_t \mu^{3/2}R &= i\partial_t \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) - \Delta \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) + V(r) \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) \\
&\quad + \sigma \left| \mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right|^2 \left(\mu^{1/2}\Psi_0 + \mu^{3/2}\Psi_\mu \right) \\
&\quad - \Delta \mu^{3/2}R + V(r) \mu^{3/2}R + \sigma \mu^{5/2} \left(2|\Psi_0|^2 R + \bar{R}\Psi_0^2 \right) \\
&\quad + \sigma \mu^{7/2} \left(2\bar{\Psi}_0 \Psi_\mu R + 2\bar{\Psi}_\mu \Psi_0 R + 2|R|^2 \Psi_0 + 2\bar{R}\Psi_0 \Psi_\mu + \bar{\Psi}_0 R^2 \right) \\
&\quad + \sigma \mu^{9/2} \left(2|\Psi_\mu|^2 R + 2|R|^2 \Psi_\mu + \bar{R}\Psi_\mu^2 + \bar{\Psi}_\mu R^2 + |R|^2 R \right).
\end{aligned} \tag{4.51}$$

As in the derivation for the residual of the improved approximation in Section 4.4.2, we insert the decompositions $\Psi_0(t, r) = \mu^{1/2}\varphi_0(T, r)\mathbf{E}(t)$, $\Psi_\mu(t, r) = \mu^{3/2}\varphi_\mu(T, r)\mathbf{E}(t)$ and $R(t, r) = \mu^{3/2}\rho(t, r)\mathbf{E}(t)$ into (4.51) and get

$$\begin{aligned}
i\mu^{3/2}\partial_t(\rho(t, r)\mathbf{E}(t)) &= \text{Res}(\mu^{1/2}\Psi) + \mu^{3/2}(-\Delta + V(r))\rho(t, r)\mathbf{E}(t) \\
&\quad + \sigma\mu^{5/2}(2|\varphi_0(T, r)|^2\rho(t, r) + \bar{\rho}(t, r)\varphi_0^2(T, r))\mathbf{E}(t) \\
&\quad + \sigma\mu^{7/2}(2\bar{\varphi}_0(T, r)\varphi_\mu(T, r)\rho(t, r) + 2\bar{\varphi}_\mu(T, r)\varphi_0(T, r)\rho(t, r) \\
&\quad\quad + 2|\rho(t, r)|^2\varphi_0(T, r) + 2\bar{\rho}(t, r)\varphi_0(T, r)\varphi_\mu(T, r) \\
&\quad\quad + \bar{\varphi}_0(T, r)\rho^2(t, r))\mathbf{E}(t) \\
&\quad + \sigma\mu^{9/2}(2|\varphi_\mu(T, r)|^2\rho(t, r) + 2|\rho(t, r)|^2\varphi_\mu(T, r) \\
&\quad\quad + \bar{\rho}(t, r)\varphi_\mu^2(T, r) + \bar{\varphi}_\mu(T, r)\rho^2(t, r) \\
&\quad\quad + |\rho(t, r)|^2\rho(t, r))\mathbf{E}(t).
\end{aligned} \tag{4.52}$$

Using (4.48) and the time derivative $i\partial_t(\rho(t, r)\mathbf{E}(t)) = (i\partial_t\rho(t, r))\mathbf{E}(t) + (\widehat{E}_{n,0} - \omega_j)\rho(t, r)\mathbf{E}(t)$, we summarize the terms in (4.52) by their formal order $\mathcal{O}(\mu)$ and find

$$\begin{aligned}
i\partial_t\rho(t, r) &= \frac{1}{\mu} \sum_{m \in \mathbb{Z}} \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} \widehat{E}_{n, m'-m} a_{m'}(T) \widehat{\phi}_{n, m}(x) \psi_j(y) \\
&\quad + \left(-\Delta + V(r) - (\widehat{E}_{n,0} - \omega_j)\right) \rho(t, r) \\
&\quad + \sigma \sum_{m \in \mathbb{Z}} \sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1}(T) a_{m_2}(T) a_{m_3}(T) \\
&\quad\quad \times \widehat{\phi}_{n, m}(x) \psi_j(y) \\
&\quad + \sigma\mu \left(-\frac{i}{\sigma} \partial_T \varphi_\mu(T, r) + 2|\varphi_0(T, r)|^2(\varphi_\mu(T, r) + \rho(t, r)) \right. \\
&\quad\quad \left. + \varphi_0^2(T, r)(\bar{\varphi}_\mu(T, r) + \bar{\rho}(t, r)) \right) \\
&\quad + \sigma\mu^2 \left(2\varphi_0(T, r)|\varphi_\mu(T, r) + \rho(t, r)|^2 + \bar{\varphi}_0(T, r)(\varphi_\mu(T, r) + \rho(t, r))^2 \right) \\
&\quad + \sigma\mu^3 \left((\varphi_\mu(T, r) + \rho(t, r))|\varphi_\mu(T, r) + \rho(t, r)|^2 \right).
\end{aligned} \tag{4.53}$$

For simplicity, we introduce the sum $S(\vec{a}) = \sum_{m \in \mathbb{Z}} s_m(\vec{a}) \widehat{\phi}_{n, m}(x) \psi_j(y)$ with

$$\begin{aligned}
s_m(\vec{a}) &= \frac{1}{\mu^2} \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} \widehat{E}_{n, m'-m} a_{m'}(T) \\
&\quad + \sigma \sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1}(T) a_{m_2}(T) a_{m_3}(T)
\end{aligned} \tag{4.54}$$

and the nonlinear term given by

$$\begin{aligned}
N(\vec{a}, \rho) = & \sigma \left(-\frac{i}{\sigma} \partial_T \varphi_\mu(T, r) + 2|\varphi_0(T, r)|^2 (\varphi_\mu(T, r) + \rho(t, r)) \right. \\
& \left. + \varphi_0^2(T, r) (\bar{\varphi}_\mu(T, r) + \bar{\rho}(t, r)) \right) \\
& + \sigma \mu \left(2\varphi_0(T, r) |\varphi_\mu(T, r) + \rho(t, r)|^2 + \bar{\varphi}_0(T, r) (\varphi_\mu(T, r) + \rho(t, r))^2 \right) \\
& + \sigma \mu^2 \left((\varphi_\mu(T, r) + \rho(t, r)) |\varphi_\mu(T, r) + \rho(t, r)|^2 \right).
\end{aligned} \tag{4.55}$$

Thus, with (4.54) and (4.55) the function $\rho(t, r)$ satisfies the evolution equation (4.53) in the abstract form

$$i\partial_t \rho = \left(L - \left(\widehat{E}_{n,0} - \omega_j \right) \right) \rho + \mu S(\vec{a}) + \mu N(\vec{a}, \rho). \tag{4.56}$$

As in the one-dimensional case, we now prove that the terms $S(\vec{a})$ and $N(\vec{a}, \rho)$ of the evolution problem (4.56) are uniformly bounded in $\mathcal{H}^{1,2}(\mathbb{R}^2)$ for $0 < \mu \ll 1$. Since the result (4.3.1) is local in time, we consider a ball of finite radius $\delta_1 > 0$ in $l^1(\mathbb{Z})$ denoted by $B_{\delta_1}(l^1(\mathbb{Z}))$ and a ball of finite radius $\delta_2 > 0$ in $\mathcal{H}^{1,2}(\mathbb{R}^2)$ denoted by $B_{\delta_2}(\mathcal{H}^{1,2}(\mathbb{R}^2))$ to control these terms with the following lemma, cf. [29, 32].

Lemma 4.4.3. *Let $\vec{a}(T), \partial_T \vec{a}(T) \in B_{\delta_1}(l^1(\mathbb{Z}))$ and $\rho(t, \cdot), \tilde{\rho}(t, \cdot) \in B_{\delta_2}(\mathcal{H}^{1,2}(\mathbb{R}^2))$ for fixed $\delta_1, \delta_2 > 0$. Then, for any $0 < \mu \ll 1$, there exist μ -independent constants $C_S, C_N, K_N > 0$ such that*

$$\|S(\vec{a})\|_{\mathcal{H}^{1,2}} \leq C_S \|\vec{a}\|_{l^1}, \tag{4.57}$$

$$\|N(\vec{a}, \rho)\|_{\mathcal{H}^{1,2}} \leq C_N (\|\vec{a}\|_{l^1} + \|\rho\|_{\mathcal{H}^{1,2}}), \tag{4.58}$$

$$\|N(\vec{a}, \rho) - N(\vec{a}, \tilde{\rho})\|_{\mathcal{H}^{1,2}} \leq K_N \|\rho - \tilde{\rho}\|_{\mathcal{H}^{1,2}}. \tag{4.59}$$

Proof. At first, we want to prove the bound (4.57) and therefore, we remember the notation $S(\vec{a}) = \sum_{m \in \mathbb{Z}} s_m(\vec{a}) \widehat{\phi}_{n,m}(x) \psi_j(y)$, where the components $s_m(\vec{a})$ are defined by (4.54). Using the triangle inequality

$$\left\| \sum_{m \in \mathbb{Z}} s_m(\vec{a}) \widehat{\phi}_{n,m}(x) \psi_j(y) \right\|_{\mathcal{H}^{1,2}} \leq \|\vec{s}(\vec{a})\|_{l^1} \|\widehat{\phi}_{n,0}(x) \psi_j(y)\|_{\mathcal{H}^{1,2}}$$

and (B.15), it remains to show that $\|\vec{s}(\vec{a})\|_{l^1} \leq C_s \|\vec{a}\|_{l^1}$ with $\vec{s}(\vec{a}) = \{s_m(\vec{a})\}_{m \in \mathbb{Z}}$ holds for some $C_s > 0$. The first term in $\vec{s}(\vec{a})$ is estimated as follows:

$$\begin{aligned}
\left\| \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} \widehat{E}_{n, m'-m} a_{m'}(T) \right\|_{l^1} & \leq \sum_{m \in \mathbb{Z}} \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} |\widehat{E}_{n, m'-m}| |a_{m'}(T)| \\
& \leq K_1 \|\vec{a}\|_{l^1},
\end{aligned}$$

where

$$K_1 = \sup_{m \in \mathbb{Z}} \sum_{\substack{m' \in \mathbb{Z} \\ m' \neq \{m-1, m, m+1\}}} |\widehat{E}_{n, m'-m}| = \sum_{\substack{l \in \mathbb{Z} \\ l \neq \{-1, 0, 1\}}} |\widehat{E}_{n, l}|. \tag{4.60}$$

The sum on the right hand side of (4.61) is bounded, because the band function $E_n(\ell)$ is analytically continued along the Riemann surface on $\ell \in \mathbb{T}_1$ by Theorem XIII.95 in [36]. Hence, $E_n(\ell)$ is infinitely often differentiable for $\ell \in \mathbb{T}_1$ and we have $E_n(\ell) \in H^s(\mathbb{T}_1)$ for any $s > 0$, such that $\{\widehat{E}_{n,l}\}_{l \in \mathbb{Z}} \in l^1(\mathbb{Z})$ and $K_1 < \infty$. By property (4.17) of Lemma 4.2.2, $\widehat{E}_{n,l} = \mathcal{O}(\mu^2)$ for all $l \geq 2$, such that K_1/μ^2 is uniformly bounded in $0 < \mu \ll 1$. Estimating the second term in $\vec{s}(\vec{a})$, we get

$$\begin{aligned} & \left\| \sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1}(T) a_{m_2}(T) a_{m_3}(T) \right\|_{l^1} \\ & \leq \sum_{m \in \mathbb{Z}} \sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} |\kappa_j(m, m_1, m_2, m_3)| |a_{m_1}(T)| |a_{m_2}(T)| |a_{m_3}(T)| \\ & \leq K_2 \|\vec{a}\|_{l^1}^3, \end{aligned}$$

where

$$K_2 = \sup_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \sum_{m \in \mathbb{Z}} |\kappa_j(m, m_1, m_2, m_3)|. \quad (4.61)$$

Now we use the exponential decay (4.20) and the explicit representation (4.21) of ψ_j for a fixed $j \in \mathbb{N}$ to obtain

$$\begin{aligned} \sum_{m \in \mathbb{Z}} |\widehat{\phi}_{n,m}(x) \psi_j(y)| & \leq \sum_{m \in \mathbb{Z}} |\widehat{\phi}_{n,m}(x)| |\psi_j(y)| \\ & \leq C_n C_j \sum_{m \in \mathbb{Z}} e^{-\eta_n |x - 2\pi m|} \\ & \leq A_n \end{aligned}$$

for some $A_n > 0$ uniformly in $r \in \mathbb{R}^2$ and therefore,

$$\begin{aligned} \sum_{m \in \mathbb{Z}} |\kappa_j(m, m_1, m_2, m_3)| & \leq A_n \int_{\mathbb{R}^2} |\widehat{\phi}_{n,m_1}(x) \psi_j(y)| |\widehat{\phi}_{n,m_2}(x) \psi_j(y)| |\widehat{\phi}_{n,m_3}(x) \psi_j(y)| dr \\ & \leq A_n \|\widehat{\phi}_{n,m}(x) \psi_j(y)\|_{L^4}^2 \|\widehat{\phi}_{n,m}(x) \psi_j(y)\|_{L^2} \end{aligned} \quad (4.62)$$

uniformly in $(m_1, m_2, m_3) \in \mathbb{Z}^3$, where the last line of (4.62) follows with $\widehat{\phi}_{n,m}(x) = \widehat{\phi}_{n,0}(x - 2\pi m)$ and the Hölder inequality. Using the embeddings stated in Appendix B.1, we conclude

$$\|\widehat{\phi}_{n,0}(x) \psi_j(y)\|_{L^4} \leq \widetilde{C}_L \|\widehat{\phi}_{n,0}(x) \psi_j(y)\|_{H^1} \leq \widetilde{C}_L \|\widehat{\phi}_{n,0}(x) \psi_j(y)\|_{H^{1,2}} \leq \widetilde{C}_L \|\widehat{\phi}_{n,0}(x) \psi_j(y)\|_{\mathcal{H}^{1,2}}$$

and then the bound (B.15) yields to $K_2 < \infty$. By property (4.19) of Lemma 4.2.2 and with $\psi_j = \mathcal{O}(1)$, we get that the integral kernel

$$\kappa_j(m, m_1, m_2, m_3) = \mathcal{O}(\mu^{|m_1-m|+|m_2-m|+|m_3-m|+|m_2-m_1|+|m_3-m_1|+|m_3-m_2|}),$$

for every $(m_1, m_2, m_3) \in \mathbb{Z}^3$, and so K_2/μ is uniformly bounded in $0 < \mu \ll 1$. Thus, we get a μ -independent constant $C_S > 0$ and the inequality (4.57) is proved.

In order to obtain the second bound (4.58), we have to control the norms of the nonlinear term $|\varphi_0|^2 \varphi_0$ and of the additional term φ_μ in $\mathcal{H}^{1,2}(\mathbb{R}^2)$. Using the inequality (4.36) from the proof of Lemma 4.4.1 and the bound (B.15), for a fixed $n \in \mathbb{N}$ and $\|\vec{a}(T)\| \in l^1(\mathbb{Z})$, there exists a $C_a > 0$ uniformly in $0 < \mu \ll 1$ such that

$$\|\varphi_0(T, \cdot)\|_{\mathcal{H}^{1,2}} \leq C_a \|\vec{a}(T)\|_{l^1}.$$

Moreover, we have shown in Theorem B.1.5 that the space $\mathcal{H}^{1,2}(\mathbb{R}^2)$ is closed under pointwise multiplication and hence

$$\| |\varphi_0(T, \cdot)|^2 \varphi_0(T, \cdot) \|_{\mathcal{H}^{1,2}} \leq C_B^2 \|\varphi_0(T, \cdot)\|_{\mathcal{H}^{1,2}}^3 \leq C_B^2 C_a^3 \|\vec{a}(T)\|_{l^1}^3. \quad (4.63)$$

Next, we bound the function φ_μ by recalling

$$\varphi_\mu(T, \cdot) = -\sigma(I - \Pi_{n,j})(L - (\widehat{E}_{n,0} + \omega_j))^{-1}(I - \Pi_{n,j}) |\varphi_0(T, \cdot)|^2 \varphi_0(T, \cdot)$$

and $\sigma = \pm 1$. As mentioned in the proof of Lemma 4.4.2, the inverse operator $(I - \Pi_{n,j})(L - (\widehat{E}_{n,0} + \omega_j))^{-1}(I - \Pi_{n,j})$ is a continuous map from $L^2(\mathbb{R}^2)$ to $\mathcal{H}^{1,2}(\mathbb{R}^2)$ uniformly in $0 < \mu \ll 1$ and therefore, we get

$$\|\varphi_\mu(T, \cdot)\|_{\mathcal{H}^{1,2}} \leq C_\varphi \|\vec{a}(T)\|_{l^1}^3. \quad (4.64)$$

Now, the bounds (4.63), (4.64) and the fact that both $\mathcal{H}^{1,2}(\mathbb{R}^2)$ and $l^1(\mathbb{Z})$ form Banach algebras with respect to pointwise multiplication lead directly to the estimate (4.58). Since $\vec{a}(T), \partial_T \vec{a}(T) \in B_{\delta_1}(l^1(\mathbb{Z}))$, the functions $\varphi(T, \cdot), \varphi_\mu(T, \cdot), \partial_T \varphi_\mu(T, \cdot) \in B_{\delta_2}(\mathcal{H}^{1,2}(\mathbb{R}^2))$ and $N(\vec{a}, \rho)$ maps $\rho \in \mathcal{H}^{1,2}(\mathbb{R}^2)$ to an element of $\mathcal{H}^{1,2}(\mathbb{R}^2)$. Thus, $N(\vec{a}, \rho)$ is uniformly bounded in $0 < \mu \ll 1$ and the constant $K_N > 0$ is μ -independent.

The proof of the third bound (4.59) also follows from the explicit expression of $N(\vec{a}, \rho)$. \square

Remark 4.4.4. Note that in our argumentation above, we followed very closely the proof of Lemma 4 in [32] and Lemma 2.18 in [29], respectively. This makes sense because the sum $S(\vec{a})$ is defined in the same way as in the one-dimensional case. Also, the nonlinear term $N(\vec{a}, \rho)$ is identical with the one in [32] and can be estimated in two space dimensions with the same ideas used there.

4.5. Local Existence and uniqueness

In this section, we prove the local existence and uniqueness of solutions of the evolution equation (4.56). However, we first need to show that the initial-value problem for the dNLS equation (4.4) is locally well-posed in $C^1([0, T_0], l^1(\mathbb{Z}))$ for a $T_0 > 0$. One can also find the following lemma as Theorem 2 in the updated version of [32].

Lemma 4.5.1. *Let $\vec{a}_0 \in l^1(\mathbb{Z})$. Then, there exists a $T_0 > 0$ and a unique solution $\vec{a}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ of the dNLS equation (4.4) with the initial data $\vec{a}(0) = \vec{a}_0$.*

Proof. By the variation of constant formula, we have

$$\vec{a}(T) = \vec{a}_0 - i \int_0^T (\alpha \Delta_d \vec{a}(s) + \sigma \beta \Gamma(\vec{a}(s))) ds,$$

where $(\Delta_d \vec{a})_m = a_{m+1} + a_{m-1}$ and $(\Gamma(\vec{a}))_m = |a_m|^2 a_m$. Since $l^1(\mathbb{Z})$ forms a Banach algebra, the right-hand side of the integral equation maps an element of $l^1(\mathbb{Z})$ to an element of $l^1(\mathbb{Z})$. Therefore, there exists a unique solution $\vec{a}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ of the integral equation for sufficiently small $T_0 > 0$. \square

As a consequence of this result, we now obtain the existence of a unique solution of the Cauchy problem associated with the system (4.56) in $\mathcal{H}^{1,2}(\mathbb{R})$.

Lemma 4.5.2. *Let $\vec{a}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$ and $\rho(0, \cdot) = \rho_0 \in \mathcal{H}^{1,2}(\mathbb{R}^2)$. Then, there exists a $\mu_0 > 0$ such that, for any $\mu \in (0, \mu_0)$, the time evolution problem (4.56) admits a unique solution $\rho(t, \cdot) \in C^1([0, T_0/\mu], \mathcal{H}^{1,2}(\mathbb{R}^2))$.*

Proof. The operators $L_x = -\partial_x^2 + V_x(x)$ and $L_y = -\partial_y^2 + V_y(y)$ are self-adjoint in $L^2(\mathbb{R}^2)$ and thus, by classical semigroup theory, cf. [28], we get

$$\|e^{-i(L_x - \widehat{E}_{n,0})t} \rho\|_{L^2} = \|\rho\|_{L^2} \quad \text{and} \quad \|e^{-i(L_y - \omega_j)t} \rho\|_{L^2} = \|\rho\|_{L^2}$$

with $L_x L_y = L_y L_x$. Moreover, the commutativity of L_x and $e^{-i(L_x - \widehat{E}_{n,0})t}$ and of L_y and $e^{-i(L_y - \omega_j)t}$ holds. Hence, with

$$e^{-i(L - (\widehat{E}_{n,0} + \omega_j))t} = e^{-i(L_x - \widehat{E}_{n,0})t} e^{-i(L_y - \omega_j)t}$$

and the definition (4.5) of the norm of $\mathcal{H}^{1,2}(\mathbb{R}^2)$, we obtain the following equality:

$$\begin{aligned} \|e^{-i(L - (\widehat{E}_{n,0} + \omega_j))t} \rho\|_{\mathcal{H}^{1,2}}^2 &= \|(L_x + I)^{1/2} e^{-i(L_x - \widehat{E}_{n,0})t} e^{-i(L_y - \omega_j)t} \rho\|_{L^2}^2 \\ &\quad + \|(L_y + I) e^{-i(L_x - \widehat{E}_{n,0})t} e^{-i(L_y - \omega_j)t} \rho\|_{L^2}^2 \\ &\quad + \|e^{-i(L_x - \widehat{E}_{n,0})t} e^{-i(L_y - \omega_j)t} \rho\|_{L^2}^2 \\ &= \|e^{-i(L_x - \widehat{E}_{n,0})t} e^{-i(L_y - \omega_j)t} (L_x + I)^{1/2} \rho\|_{L^2}^2 \\ &\quad + \|e^{-i(L_x - \widehat{E}_{n,0})t} e^{-i(L_y - \omega_j)t} (L_y + I) \rho\|_{L^2}^2 \\ &\quad + \|e^{-i(L_x - \widehat{E}_{n,0})t} e^{-i(L_y - \omega_j)t} \rho\|_{L^2}^2 \\ &= \|(L_x + I)^{1/2} \rho\|_{L^2}^2 + \|(L_y + I) \rho\|_{L^2}^2 + \|\rho\|_{L^2}^2 \\ &= \|\rho\|_{\mathcal{H}^{1,2}}^2. \end{aligned}$$

Therefore, the operator $e^{-i(L - (\widehat{E}_{n,0} + \omega_j))t}$ forms a unitary group in $\mathcal{H}^{1,2}(\mathbb{R}^2)$ for every $\rho \in \mathcal{H}^{1,2}(\mathbb{R}^2)$ and every $t \in \mathbb{R}$. By Duhamel's principle, we now rewrite the Cauchy problem associated with the evolution equation (4.56) as the integral equation

$$\begin{aligned} \rho(t, \cdot) &= e^{-i(L - (\widehat{E}_{n,0} + \omega_j))t} \rho_0 \\ &\quad + \mu \int_0^t e^{-i(L - (\widehat{E}_{n,0} + \omega_j))(t-s)} (S(\vec{a}(\mu s)) + N(\vec{a}(\mu s), \rho(s, \cdot))) ds, \end{aligned}$$

where the solution is considered in the subspace $B_{\delta_2}(\mathcal{H}^{1,2}(\mathbb{R}^2))$. For every $\rho_0 \in \mathcal{H}^{1,2}(\mathbb{R}^2)$, there is a sufficiently small $T_0 > 0$ such that the right-hand side of the integral equation is a contraction in the ball $B_{\delta_2}(\mathcal{H}^{1,2}(\mathbb{R}^2))$, where we used the bounds (4.57) and (4.58). The existence of a unique solution $\rho(t, \cdot) \in C^1([0, T_0/\mu], \mathcal{H}^{1,2}(\mathbb{R}^2))$ follows from Banach's fixed point theorem and (4.59). \square

4.6. Control on the error bound

Here we complete the proof of Theorem 4.3.1. The proof of the approximation result is based on an energy estimate for the evolution problem (4.56) and a simple application of Gronwall's

inequality. Although the analysis of this section is similar to the one in the updated version of [32], we have to transfer the calculations to our two-dimensional setting.

As in the one-dimensional case, our goal is to control the error term $\mu^{3/2}R = \mu^{3/2}\rho(t, r)\mathbf{E}(t)$ for every $t \in [0, T_0/\mu]$. The following lemma gives us a bound on the time evolution of $\rho(t, r)$ in the function space $\mathcal{H}^{1,2}(\mathbb{R}^2)$.

Lemma 4.6.1. *Let $\rho(t, \cdot) \in C^1([0, T_0/\mu], B_{\delta_2}(\mathcal{H}^{1,2}(\mathbb{R}^2)))$ be a local solution of the time evolution problem (4.56) for some $T_0 > 0$ and $\vec{a}(T) \in C^1([0, T_0], l^1(\mathbb{Z}))$. Then, for any $\mu \in (0, \mu_0)$, there exists a μ -independent constant $C_E > 0$ such that*

$$\left| \frac{d}{dt} \|\rho(t, \cdot)\|_{\mathcal{H}^{1,2}}^2 \right| \leq \mu C_E (\|\vec{a}\|_{l^1}^2 + \|\rho(t, \cdot)\|_{\mathcal{H}^{1,2}}^2). \quad (4.65)$$

Proof. Using definition (4.5), we write

$$\begin{aligned} \frac{d}{dt} \|\rho\|_{\mathcal{H}^{1,2}}^2 &= \frac{d}{dt} \langle (L_x + I)^{1/2} \rho, (L_x + I)^{1/2} \rho \rangle_{L^2} + \frac{d}{dt} \langle (L_y + I) \rho, (L_y + I) \rho \rangle_{L^2} + \frac{d}{dt} \langle \rho, \rho \rangle_{L^2} \\ &= \langle (L_x + I)^{1/2} (\partial_t \rho), (L_x + I)^{1/2} \rho \rangle_{L^2} + \langle (L_y + I) (\partial_t \rho), (L_y + I) \rho \rangle_{L^2} + \langle (\partial_t \rho), \rho \rangle_{L^2} \\ &\quad + \langle (L_x + I)^{1/2} \rho, (L_x + I)^{1/2} (\partial_t \rho) \rangle_{L^2} + \langle (L_y + I) \rho, (L_y + I) (\partial_t \rho) \rangle_{L^2} + \langle \rho, (\partial_t \rho) \rangle_{L^2} \end{aligned}$$

and with

$$\partial_t \rho = -i \left(L - \left(\widehat{E}_{n,0} - \omega_j \right) \right) \rho - i\mu S(\vec{a}) - i\mu N(\vec{a}, \rho),$$

we obtain by direct calculation the following equation:

$$\begin{aligned} \frac{d}{dt} \|\rho\|_{\mathcal{H}^{1,2}}^2 &= -i\mu \langle \partial_x S(\vec{a}), \partial_x \rho \rangle_{L^2} + i\mu \langle \partial_x \rho, \partial_x S(\vec{a}) \rangle_{L^2} \\ &\quad - i\mu \sigma \langle \partial_x N(\vec{a}, \rho), \partial_x \rho \rangle_{L^2} + i\mu \sigma \langle \partial_x \rho, \partial_x N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad - i\mu \langle V_x S(\vec{a}), \rho \rangle_{L^2} + i\mu \langle \rho, V_x S(\vec{a}) \rangle_{L^2} \\ &\quad - i\mu \sigma \langle V_x N(\vec{a}, \rho), \rho \rangle_{L^2} + i\mu \sigma \langle \rho, V_x N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad - i\mu \langle \partial_y^2 S(\vec{a}), \partial_y^2 \rho \rangle_{L^2} + i\mu \langle \partial_y^2 \rho, \partial_y^2 S(\vec{a}) \rangle_{L^2} \\ &\quad - i\mu \sigma \langle \partial_y^2 N(\vec{a}, \rho), \partial_y^2 \rho \rangle_{L^2} + i\mu \sigma \langle \partial_y^2 \rho, \partial_y^2 N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad - i\mu \langle V_y^2 S(\vec{a}), \rho \rangle_{L^2} + i\mu \langle \rho, V_y^2 S(\vec{a}) \rangle_{L^2} \\ &\quad - i\mu \sigma \langle V_y^2 N(\vec{a}, \rho), \rho \rangle_{L^2} + i\mu \sigma \langle \rho, V_y^2 N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad + i\mu \langle \partial_y^2 S(\vec{a}), V_y \rho \rangle_{L^2} - i\mu \langle \partial_y^2 \rho, V_y S(\vec{a}) \rangle_{L^2} \\ &\quad + i\mu \sigma \langle \partial_y^2 N(\vec{a}, \rho), V_y \rho \rangle_{L^2} - i\mu \sigma \langle \partial_y^2 \rho, V_y N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad + i\mu \langle V_y S(\vec{a}), \partial_y^2 \rho \rangle_{L^2} - i\mu \langle V_y \rho, \partial_y^2 S(\vec{a}) \rangle_{L^2} \\ &\quad + i\mu \sigma \langle V_y N(\vec{a}, \rho), \partial_y^2 \rho \rangle_{L^2} - i\mu \sigma \langle V_y \rho, \partial_y^2 N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad - 2i\mu \langle \partial_y S(\vec{a}), \partial_y \rho \rangle_{L^2} + 2i\mu \langle \partial_y \rho, \partial_y S(\vec{a}) \rangle_{L^2} \\ &\quad - 2i\mu \sigma \langle \partial_y N(\vec{a}, \rho), \partial_y \rho \rangle_{L^2} + 2i\mu \sigma \langle \partial_y \rho, \partial_y N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad - 2i\mu \langle V_y S(\vec{a}), \rho \rangle_{L^2} + 2i\mu \langle \rho, V_y S(\vec{a}) \rangle_{L^2} \\ &\quad - 2i\mu \sigma \langle V_y N(\vec{a}, \rho), \rho \rangle_{L^2} + 2i\mu \sigma \langle \rho, V_y N(\vec{a}, \rho) \rangle_{L^2} \\ &\quad - 3i\mu \langle S(\vec{a}), \rho \rangle_{L^2} + 3i\mu \langle \rho, S(\vec{a}) \rangle_{L^2} \\ &\quad - 3i\mu \sigma \langle N(\vec{a}, \rho), \rho \rangle_{L^2} + 3i\mu \sigma \langle \rho, N(\vec{a}, \rho) \rangle_{L^2}. \end{aligned} \quad (4.66)$$

Next, we summarize the terms in (4.66) to

$$\begin{aligned}
\frac{d}{dt} \|\rho\|_{\mathcal{H}^{1,2}}^2 &= -i\mu \langle S(\vec{a}), (L_x + I)\rho + (L_y + I)^2\rho + \rho \rangle_{L^2} \\
&\quad - i\mu \langle (L_x + I)\rho + (L_y + I)^2\rho + \rho, S(\vec{a}) \rangle_{L^2} \\
&\quad - i\mu\sigma \langle N(\vec{a}, \rho), (L_x + I)\rho + (L_y + I)^2\rho + \rho \rangle_{L^2} \\
&\quad - i\mu\sigma \langle (L_x + I)\rho + (L_y + I)^2\rho + \rho, N(\vec{a}, \rho) \rangle_{L^2}
\end{aligned} \tag{4.67}$$

where we applied the operator representation

$$\begin{aligned}
&\langle -\partial_x^2\rho + V_x\rho + (\partial_y^2)^2\rho + V_y^2\rho - V_y(\partial_y^2\rho) - \partial_y^2(V_y\rho) - 2\partial_y^2\rho + 2V_y\rho + 3\rho, \cdot \rangle_{L^2} \\
&= \langle L_x\rho + L_y^2\rho + 2L_y\rho + 3\rho, \cdot \rangle_{L^2} \\
&= \langle (L_x + I)\rho + (L_y + I)^2\rho + \rho, \cdot \rangle_{L^2}.
\end{aligned}$$

Then, the Cauchy-Schwarz inequality yields to

$$\begin{aligned}
\frac{d}{dt} \|\rho\|_{\mathcal{H}^{1,2}}^2 &\leq -i\mu \|S(\vec{a})\|_{L^2} \|\rho\|_{\mathcal{H}^{1,2}} - i\mu \|\rho\|_{\mathcal{H}^{1,2}} \|S(\vec{a})\|_{L^2} \\
&\quad - i\mu\sigma \|N(\vec{a}, \rho)\|_{L^2} \|\rho\|_{\mathcal{H}^{1,2}} - i\mu\sigma \|\rho\|_{\mathcal{H}^{1,2}} \|N(\vec{a}, \rho)\|_{L^2} \\
&\leq -2i\mu \|S(\vec{a})\|_{\mathcal{H}^{1,2}} \|\rho\|_{\mathcal{H}^{1,2}} - 2i\mu\sigma \|N(\vec{a}, \rho)\|_{\mathcal{H}^{1,2}} \|\rho\|_{\mathcal{H}^{1,2}},
\end{aligned}$$

and by inserting the bounds (4.57) and (4.58), we have

$$\begin{aligned}
\left| \frac{d}{dt} \|\rho\|_{\mathcal{H}^{1,2}}^2 \right| &\leq 2\mu \|\rho\|_{\mathcal{H}^{1,2}} (\|S(\vec{a})\|_{\mathcal{H}^{1,2}} + \|N(\vec{a}, \rho)\|_{\mathcal{H}^{1,2}}) \\
&\leq 2\mu \|\rho\|_{\mathcal{H}^{1,2}} ((C_S + C_N) \|\vec{a}\|_{l^1} + C_N \|\rho\|_{\mathcal{H}^{1,2}}) \\
&\leq 2\mu (C_S + C_N) \|\vec{a}\|_{l^1}^2 + 2\mu ((C_S + C_N) + C_N) \|\rho\|_{\mathcal{H}^{1,2}}^2 \\
&\leq \mu C_E (\|\vec{a}\|_{l^1}^2 + \|\rho\|_{\mathcal{H}^{1,2}}^2),
\end{aligned}$$

where we used the estimate $\|\rho\|_{\mathcal{H}^{1,2}} \|\vec{a}\|_{l^1} \leq \|\rho\|_{\mathcal{H}^{1,2}}^2 + \|\vec{a}\|_{l^1}^2$. \square

By using the bound (4.65), we obtain for the evolution problem the following integral formula:

$$\|\rho(t, \cdot)\|_{\mathcal{H}^{1,2}}^2 \leq \|\rho(0, \cdot)\|_{\mathcal{H}^{1,2}}^2 + \mu C_E \int_0^t (\|\vec{a}(\mu s)\|_{l^1}^2 + \|\rho(s, \cdot)\|_{\mathcal{H}^{1,2}}^2) ds.$$

Now Gronwall's inequality finally allows us to estimate the function $\rho(t, r)$ on the time interval $t \in [0, T_0/\mu]$ by

$$\sup_{t \in [0, T_0/\mu]} \|\rho(t, \cdot)\|_{\mathcal{H}^{1,2}}^2 \leq \left(\|\rho(0, \cdot)\|_{\mathcal{H}^{1,2}}^2 + C_E T_0 \sup_{t \in [0, T_0/\mu]} \|\vec{a}(T)\|_{l^1}^2 \right) e^{C_E T_0} =: M,$$

where the constant $M > 0$ is uniformly bounded in $0 < \mu \ll 1$. Then, the decomposition $\mu^{3/2}R = \mu^{3/2}\rho(t, r)\mathbf{E}(t)$ yields to a bound on the error term and with the bound (4.64) on the function $\varphi_\mu(T, r)$, the proof of Theorem 4.3.1 is completed.

A. Appendices to Chapter 3

A.1. Computation of the spectral bands $\omega(\ell)$

Our goal is to get an explicit representation of the the spectral bands $\omega(\ell)$ of the linear problem (3.5). Therefore, we restrict our calculations to the eigenvalue problem

$$-(\partial_x + i\ell)^2 f(\ell, x) + f(\ell, x) = \omega^2(\ell) f(\ell, x), \quad x \in \mathbb{T}_{2\pi}, \quad (\text{A.1})$$

of the Bloch function $f(\ell, \cdot) = (f_0, f_+, f_-)(\ell, \cdot)$ with the corresponding boundary conditions

$$\begin{cases} f_0(\ell, \pi) = f_+(\ell, \pi) = f_-(\ell, \pi), \\ f_0(\ell, 0) = f_+(\ell, 2\pi) = f_-(\ell, 2\pi) \end{cases} \quad (\text{A.2})$$

and

$$\begin{cases} (\partial_x + i\ell)f_0(\ell, \pi) = (\partial_x + i\ell)f_+(\ell, \pi) + (\partial_x + i\ell)f_-(\ell, \pi), \\ (\partial_x + i\ell)f_0(\ell, 0) = (\partial_x + i\ell)f_+(\ell, 2\pi) + (\partial_x + i\ell)f_-(\ell, 2\pi), \end{cases} \quad (\text{A.3})$$

which were introduced before in Chapter 3.

First, we want to obtain a solution for the equation (A.1) by using the ansatz

$$f_j(\ell, x) = C_j e^{\mu(\ell)x}, \quad j \in \{0, +, -\}, \quad x \in \mathbb{T}_{2\pi},$$

where $C_j \in \mathbb{R}$. This ansatz yields to the following result on the spectral bands $\omega(\ell)$:

$$\begin{aligned} -(\partial_x + i\ell)^2 C_j e^{\mu(\ell)x} + C_j e^{\mu(\ell)x} &= \omega^2(\ell) C_j e^{\mu(\ell)x} \\ -((\mu(\ell) + i\ell)^2 - 1) C_j e^{\mu(\ell)x} &= \omega^2(\ell) C_j e^{\mu(\ell)x} \\ -((\mu(\ell) + i\ell)^2 - 1) &= \omega^2(\ell). \end{aligned}$$

Now we define $\mu(\ell) = \pm i\sqrt{\omega^2(\ell) - 1} - i\ell$ and write the solutions $f_j(\ell, \cdot)$ of (A.1) as

$$f_j(\ell, x) = C_{j,1} e^{i(\sqrt{\omega^2(\ell) - 1} - \ell)x} + C_{j,2} e^{-i(\sqrt{\omega^2(\ell) - 1} + \ell)x}, \quad j \in \{0, +, -\}, \quad x \in \mathbb{T}_{2\pi}. \quad (\text{A.4})$$

Inserting (A.4) into (A.2) and (A.3) changes the continuity conditions at the vertices to the system

$$\left\{ \begin{array}{l} C_{0,1} e^{i(\sqrt{\omega^2(\ell) - 1} - \ell)\pi} + C_{0,2} e^{-i(\sqrt{\omega^2(\ell) - 1} + \ell)\pi} \\ \quad = C_{+,1} e^{i(\sqrt{\omega^2(\ell) - 1} - \ell)\pi} + C_{+,2} e^{-i(\sqrt{\omega^2(\ell) - 1} + \ell)\pi}, \\ C_{0,1} e^{i(\sqrt{\omega^2(\ell) - 1} - \ell)\pi} + C_{0,2} e^{-i(\sqrt{\omega^2(\ell) - 1} + \ell)\pi} \\ \quad = C_{-,1} e^{i(\sqrt{\omega^2(\ell) - 1} - \ell)\pi} + C_{-,2} e^{-i(\sqrt{\omega^2(\ell) - 1} + \ell)\pi}, \\ C_{0,1} + C_{0,2} = C_{+,1} e^{i(\sqrt{\omega^2(\ell) - 1} - \ell)2\pi} + C_{+,2} e^{-i(\sqrt{\omega^2(\ell) - 1} + \ell)2\pi}, \\ C_{0,1} + C_{0,2} = C_{-,1} e^{i(\sqrt{\omega^2(\ell) - 1} - \ell)2\pi} + C_{-,2} e^{-i(\sqrt{\omega^2(\ell) - 1} + \ell)2\pi}. \end{array} \right. \quad (\text{A.5})$$

The conditions for the continuity of the fluxes at the vertices are thus given by

$$\left\{ \begin{array}{l} i\sqrt{\omega^2(\ell)-1} \cdot C_{0,1} e^{i(\sqrt{\omega^2(\ell)-1}-\ell)\pi} - i\sqrt{\omega^2(\ell)-1} \cdot C_{0,2} e^{-i(\sqrt{\omega^2(\ell)-1}+\ell)\pi} \\ = i\sqrt{\omega^2(\ell)-1} \cdot C_{+,1} e^{i(\sqrt{\omega^2(\ell)-1}-\ell)\pi} - i\sqrt{\omega^2(\ell)-1} \cdot C_{+,2} e^{-i(\sqrt{\omega^2(\ell)-1}+\ell)\pi} \\ + i\sqrt{\omega^2(\ell)-1} \cdot C_{-,1} e^{i(\sqrt{\omega^2(\ell)-1}-\ell)\pi} - i\sqrt{\omega^2(\ell)-1} \cdot C_{-,2} e^{-i(\sqrt{\omega^2(\ell)-1}+\ell)\pi} \\ i\sqrt{\omega^2(\ell)-1} \cdot C_{0,1} - i\sqrt{\omega^2(\ell)-1} \cdot C_{0,2} \\ = i\sqrt{\omega^2(\ell)-1} \cdot C_{+,1} e^{i(\sqrt{\omega^2(\ell)-1}-\ell)2\pi} - i\sqrt{\omega^2(\ell)-1} \cdot C_{+,2} e^{-i(\sqrt{\omega^2(\ell)-1}+\ell)2\pi} \\ + i\sqrt{\omega^2(\ell)-1} \cdot C_{-,1} e^{i(\sqrt{\omega^2(\ell)-1}-\ell)2\pi} - i\sqrt{\omega^2(\ell)-1} \cdot C_{-,2} e^{-i(\sqrt{\omega^2(\ell)-1}+\ell)2\pi} . \end{array} \right. \quad (\text{A.6})$$

The boundary conditions (A.5) and (A.6) lead to a homogeneous system of linear equations given by the matrix equation

$$M \cdot C = 0,$$

where $C = (C_{j,1}, C_{j,2})^T$ with $j \in \{0, +, -\}$ is the 6-dimensional solution vector of the matrix M . It is obvious that a homogeneous system has nontrivial solutions if $\det(M) = 0$. We obtain

$$\begin{aligned} \det(M) = & -e^{-3i\pi(3\ell+\sqrt{\omega^2(\ell)-1})} \cdot \left(9e^{2i\pi\ell} - 2e^{2i\pi(\ell+\sqrt{\omega^2(\ell)-1})} - 8e^{2i\pi(2\ell+\sqrt{\omega^2(\ell)-1})} \right. \\ & \left. + 9e^{2i\pi(\ell+2\sqrt{\omega^2(\ell)-1})} - 8e^{2i\pi\sqrt{\omega^2(\ell)-1}} \right) \cdot \left(e^{2i\pi\sqrt{\omega^2(\ell)-1}} - 1 \right) \cdot (\omega^2(\ell) - 1), \end{aligned} \quad (\text{A.7})$$

which leaves us to solve the equations for the factors of the product (A.7) separately. While $e^{-3i\pi(3\ell+\sqrt{\omega^2(\ell)-1})} \neq 0$ for every $\ell \in \mathbb{T}_1$, we get for the second term

$$\begin{aligned} & 9e^{2i\pi\ell} - 2e^{2i\pi(\ell+\sqrt{\omega^2(\ell)-1})} - 8e^{2i\pi(2\ell+\sqrt{\omega^2(\ell)-1})} + 9e^{2i\pi(\ell+2\sqrt{\omega^2(\ell)-1})} - 8e^{2i\pi\sqrt{\omega^2(\ell)-1}} \\ & = 9e^{2i\pi\ell} e^{2i\pi\sqrt{\omega^2(\ell)-1}} \left(e^{2i\pi\sqrt{\omega^2(\ell)-1}} + e^{-2i\pi\sqrt{\omega^2(\ell)-1}} \right) - 2e^{2i\pi\ell} e^{2i\pi\sqrt{\omega^2(\ell)-1}} \\ & \quad - 8e^{2i\pi\ell} e^{2i\pi\sqrt{\omega^2(\ell)-1}} \left(e^{2i\pi\ell} + e^{-2i\pi\ell} \right) \\ & = 2e^{2i\pi(\ell+\sqrt{\omega^2(\ell)-1})} \left(9 \cos \left(2\pi \sqrt{\omega^2(\ell)-1} \right) - 8 \cos(2\pi\ell) - 1 \right) \end{aligned}$$

and the solutions $\omega(\ell)$ of the equation

$$9 \cos \left(2\pi \sqrt{\omega^2(\ell)-1} \right) - 8 \cos(2\pi\ell) - 1 = 0$$

are given by

$$\omega(\ell) = \pm \sqrt{\left(\frac{1}{2\pi} \arccos \left(\frac{8}{9} \cos(2\pi\ell) + \frac{1}{9} \right) + m \right)^2 + 1} \quad (\text{A.8})$$

for every $m \in \mathbb{Z}$. The last two factors on the right hand side of (A.7) lead to the relation

$$\omega(\ell) = \pm \sqrt{m^2 + 1}, \quad \forall m \in \mathbb{Z}, \quad (\text{A.9})$$

which represents the spectral bands corresponding to the eigenvalues of infinite multiplicity mentioned in Section 3.2.1. Using (A.8) and (A.9), we obtain the spectral curves shown in Figure 3.1.

A.2. Calculations for the derivation of the effective amplitude equation

In this section, we will show a formal derivation of the amplitude equation (3.27) and its associated complex conjugate equation. Therefore, we insert the simple approximation ansatz (3.26) given by

$$\begin{aligned}\tilde{V}_{\text{app}}(t, \ell) &= \tilde{V}_{\text{app},1}(t, \ell) + \tilde{V}_{\text{app},-1}(t, \ell) \\ &= \tilde{A}_1 \left(\varepsilon^2 t, \frac{\ell - \ell_0}{\varepsilon} \right) \mathbf{E}^1(t, \ell) + \tilde{A}_{-1} \left(\varepsilon^2 t, \frac{\ell + \ell_0}{\varepsilon} \right) \mathbf{E}^{-1}(t, \ell),\end{aligned}\quad (\text{A.10})$$

with $\tilde{U}^\perp = 0$ into the system (3.22)-(3.23). By using this ansatz, we just have to evaluate the first equation

$$\partial_t^2 \tilde{V}_{\text{app},1}(t, \ell) = -(\omega^{(m_0)}(\ell))^2 \tilde{V}_{\text{app},1}(t, \ell) - N_V(\tilde{V}_{\text{app},1}, 0)(t, \ell). \quad (\text{A.11})$$

to obtain a NLS equation for the amplitude function \tilde{A}_1 . First, we look at the left-hand side of (A.11) and with $\partial_t = \varepsilon^2 \partial_T$ for the slow time $T = \varepsilon^2 T$, we have

$$\begin{aligned}\partial_t^2 \tilde{V}_{\text{app},1}(t, \ell) &= - \left(\omega^{(m_0)}(\ell_0) + \partial_\ell \omega^{(m_0)}(\ell_0)(\ell - \ell_0) \right)^2 \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) \\ &\quad + 2i\varepsilon^2 \left(\omega^{(m_0)}(\ell_0) + \partial_\ell \omega^{(m_0)}(\ell_0)(\ell - \ell_0) \right) \partial_T \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) \\ &\quad + \varepsilon^4 \partial_T^2 \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) \\ &= - \left(\omega^{(m_0)}(\ell_0) \right)^2 \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) \\ &\quad - 2\varepsilon \left(\partial_\ell \omega^{(m_0)}(\ell_0) \right) \omega^{(m_0)}(\ell_0) \xi \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) \\ &\quad + 2i\varepsilon^2 \omega^{(m_0)}(\ell_0) \partial_T \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) - \varepsilon^2 \left(\partial_\ell \omega^{(m_0)}(\ell_0) \right)^2 \xi^2 \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) \\ &\quad + 2i\varepsilon^3 \left(\partial_\ell \omega^{(m_0)}(\ell_0) \right) \xi \partial_T \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell) \\ &\quad + \varepsilon^4 \partial_T^2 \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell).\end{aligned}\quad (\text{A.12})$$

where $\ell = \ell_0 + \varepsilon \xi$. In order to calculate the right-hand side, we now evolve the parameter $\omega^{(m_0)}(\ell)$ in terms of ℓ_0 and get

$$\begin{aligned}\omega^{(m_0)}(\ell) &= \omega^{(m_0)}(\ell_0) + \partial_\ell \omega^{(m_0)}(\ell_0)(\ell - \ell_0) + \frac{1}{2} \partial_\ell^2 \omega^{(m_0)}(\ell_0)(\ell - \ell_0)^2 \\ &= \omega^{(m_0)}(\ell_0) + \varepsilon \partial_\ell \omega^{(m_0)}(\ell_0) \xi + \frac{1}{2} \varepsilon^2 \partial_\ell^2 \omega^{(m_0)}(\ell_0) \xi^2.\end{aligned}\quad (\text{A.13})$$

Substituting (A.13) into (A.11) yields to the term

$$\begin{aligned}- \left(\omega^{(m_0)}(\ell) \right)^2 \tilde{V}_{\text{app},1}(t, \ell) &= - \left[\left(\omega^{(m_0)}(\ell_0) \right)^2 + 2\varepsilon \left(\partial_\ell \omega^{(m_0)}(\ell_0) \right) \omega^{(m_0)}(\ell_0) \xi \right. \\ &\quad + \varepsilon^2 \left(\omega^{(m_0)}(\ell_0) \left(\partial_\ell^2 \omega^{(m_0)}(\ell_0) \right) + \left(\partial_\ell \omega^{(m_0)}(\ell_0) \right)^2 \right) \xi^2 \\ &\quad + \varepsilon^3 \left(\partial_\ell \omega^{(m_0)}(\ell_0) \right) \left(\partial_\ell^2 \omega^{(m_0)}(\ell_0) \right) \xi^3 \\ &\quad \left. + \frac{1}{4} \varepsilon^4 \left(\partial_\ell^2 \omega^{(m_0)}(\ell_0) \right)^2 \xi^4 \right] \tilde{A}_1(T, \xi) \mathbf{E}^1(t, \ell).\end{aligned}\quad (\text{A.14})$$

For the calculation of the nonlinear terms, we recall (3.24) and write

$$N_V(\tilde{V}_{\text{app},1}, 0)(t, \ell) = \int_{\mathbb{T}_1} \int_{\mathbb{T}_1} \beta(\ell, \ell_1, \ell_2, \ell - \ell_1 - \ell_2) \\ \times \tilde{V}_{\text{app},1}(t, \ell_1) \tilde{V}_{\text{app},1}(t, \ell_2) \tilde{V}_{\text{app},1}(t, \ell - \ell_1 - \ell_2) d\ell_1 d\ell_2.$$

With the simple approximation ansatz (A.10), we then have in the formal order $\mathcal{O}(\varepsilon^2)$ the convolution integrals

$$N_V(\tilde{V}_{\text{app},1}, 0)(t, \ell) \\ = 3\beta(\ell_0, \ell_0, \ell_0, -\ell_0) \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \tilde{A}_1(T, \xi_1) \tilde{A}_1(T, \xi_2) \tilde{A}_{-1}(T, \xi - \xi_1 - \xi_2) d\xi_1 d\xi_2 \mathbf{E}^1(t, \ell) \\ + 3\beta(-\ell_0, -\ell_0, \ell_0, -\ell_0) \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \tilde{A}_{-1}(T, \xi_1) \tilde{A}_1(T, \xi_2) \tilde{A}_{-1}(T, \xi - \xi_1 - \xi_2) d\xi_1 d\xi_2 \mathbf{E}^{-1}(t, \ell) \quad (\text{A.15}) \\ + \beta(3\ell_0, \ell_0, \ell_0, \ell_0) \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \tilde{A}_1(T, \xi_1) \tilde{A}_1(T, \xi_2) \tilde{A}_1(T, \xi - \xi_1 - \xi_2) d\xi_1 d\xi_2 \mathbf{E}^3(t, \ell) \\ + \beta(-3\ell_0, -\ell_0, -\ell_0, -\ell_0) \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \tilde{A}_{-1}(T, \xi_1) \tilde{A}_{-1}(T, \xi_2) \tilde{A}_{-1}(T, \xi - \xi_1 - \xi_2) d\xi_1 d\xi_2 \mathbf{E}^{-3}(t, \ell),$$

where the integral kernels $\beta((j_1 + j_2 + j_3)\ell_0, j_1\ell_0, j_2\ell_0, j_3\ell_0)$ with $j_{1,2,3} = \pm 1$ are given by the definition (3.25) in Section 3.4.2. Comparing the terms (A.12), (A.14) and (A.15), we obtain in the leading order $\varepsilon^2 \mathbf{E}^1$ the NLS equation

$$2\omega^{(m_0)}(\ell_0) i \partial_T \tilde{A}_1(T, \xi) = - \left(\partial_\ell^2 \omega^{(m_0)}(\ell_0) \right) \omega^{(m_0)}(\ell_0) \xi^2 \tilde{A}_1(T, \xi) \\ - \tilde{\nu} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \tilde{A}_1(T, \xi_1) \tilde{A}_1(T, \xi_2) \tilde{A}_{-1}(T, \xi - \xi_1 - \xi_2) d\xi_1 d\xi_2, \quad (\text{A.16})$$

where $\tilde{\nu} = 3\beta(\ell_0, \ell_0, \ell_0, -\ell_0)$. Note that the terms of the formal order $\varepsilon^2 \mathbf{E}^{-1}$ fulfill the complex conjugate NLS equation associated to (A.16). The remaining nonlinear $\mathcal{O}(\varepsilon^2)$ -terms do not vanish. In order to eliminate them, we need an improved approximation ansatz which is discussed in Section 3.5.

B. Appendices to Chapter 4

B.1. The function space $\mathcal{H}^{1,2}$

In this section we take a closer look on the function space $\mathcal{H}^{1,2}(\mathbb{R}^2)$ defined in Chapter 4. As mentioned before in (4.5), the space $\mathcal{H}^{1,2}(\mathbb{R}^2)$ is equipped with the norm

$$\|u\|_{\mathcal{H}^{1,2}}^2 = \langle (L_x + I)u, u \rangle_{L^2} + \langle (L_y + I)^2 u, u \rangle_{L^2} + \langle u, u \rangle_{L^2} \quad (\text{B.1})$$

For the justification of the DNLS equation in two dimensions, we need $\mathcal{H}^{1,2}(\mathbb{R}^2)$ to satisfy several properties. The results stated in this section are used in different parts of the proof of Theorem 4.3.1.

First, we will show that $\mathcal{H}^{1,2}(\mathbb{R}^2)$ forms a Banach algebra under pointwise multiplication. Therefore, we additionally define the space $H^{1,2}(\mathbb{R}^2)$ and equip it with the squared norm

$$\|u\|_{H^{1,2}}^2 = \|\partial_x u\|_{L^2}^2 + \|\partial_y^2 u\|_{L^2}^2 + \|\partial_y u\|_{L^2}^2 + \|u\|_{L^2}^2. \quad (\text{B.2})$$

It is clear that $\|u\|_{H^1} \leq \|u\|_{H^{1,2}}$. The following lemmas now allow us to control two more norms with (B.2), which we need in the proof for the Banach algebra.

Lemma B.1.1. *There exists a positive constant $C_C > 0$ such that*

$$\|u\|_{C_b^0} \leq C_C \|u\|_{H^{1,2}} \quad (\text{B.3})$$

for all $u \in H^{1,2}(\mathbb{R}^2)$.

Proof. In this proof we use the Fourier transform \mathcal{F} and its inverse denoted by \mathcal{F}^{-1} . The continuous mapping $\mathcal{F}^{-1} : L^1(\mathbb{R}^2) \rightarrow C_b^0(\mathbb{R}^2)$ leads to

$$\begin{aligned} \|u\|_{C_b^0} &\leq \|\widehat{u}\|_{L^1} \\ &= \|\widehat{u}\rho\rho^{-1}\|_{L^1} \\ &\leq \|\widehat{u}\rho\|_{L^2} \|\rho^{-1}\|_{L^2}, \end{aligned}$$

where $\rho(k, l) = 1 + |k| + |l|^2$ and $\widehat{u} = \mathcal{F}(u)$. In fact, the Fourier transform \mathcal{F} is an isometric isomorphism from $L^2(\mathbb{R}^2)$ to $L^2(\mathbb{R}^2)$ and by using the weight ρ we get

$$\|\widehat{u}\rho\|_{L^2} \leq \|u\|_{H^{1,2}}.$$

Hence, it remains to show that $\|\rho^{-1}\|_{L^2} < \infty$ to obtain the bound (B.3). We find

$$\begin{aligned}
\|\rho^{-1}\|_{L^2}^2 &= \int_{l=-\infty}^{\infty} \int_{k=-\infty}^{\infty} (1 + |k| + |l|^2)^{-2} dkdl \\
&\leq \int_{l=-1}^1 \int_{k=-\infty}^{\infty} (1 + |k| + |l|^2)^{-2} dkdl + \int_{l=-\infty}^{\infty} \int_{k=-1}^1 (1 + |k| + |l|^2)^{-2} dkdl \\
&\quad + 4 \int_{l=1}^{\infty} \int_{k=1}^{\infty} (1 + |k| + |l|^2)^{-2} dkdl \\
&\leq 2 \int_{k=-\infty}^{\infty} (1 + |k|)^{-2} dkdl + 2 \int_{l=-\infty}^{\infty} (1 + |l|^2)^{-2} dkdl + 16 \int_{l=1}^{\infty} \int_{k=1}^{\infty} (k + l^2)^{-2} dkdl \\
&\leq 2C_1 + 2C_2 - 16 \int_{l=1}^{\infty} \left[(k + l^2)^{-1} \right]_{k=1}^{\infty} dl \\
&= 2C_1 + 2C_2 + 16 [\arctan(l)]_{l=1}^{\infty} \\
&= 2C_1 + 2C_2 + 4\pi < \infty,
\end{aligned}$$

and with $C_C = \sqrt{2C_1 + 2C_2 + 4\pi}$ the inequality (B.3) is proven. \square

Remark B.1.2. Note that this embedding just holds in two space dimensions. In the three-dimensional case, the integral

$$\int_{l_y=1}^{\infty} \int_{l_z=1}^{\infty} \int_{k=1}^{\infty} (k + l_y^2 + l_z^2)^{-2} dkdl_zdl_y = \int_{k=1}^{\infty} \int_{r=1}^{\infty} (k + r^2)^{-2} r drdk$$

is divergent and we cannot bound the norm $\|\rho^{-1}\|_{L^2}$ of the weight function $\rho(k, l_y, l_z)$.

Using the same idea as in the proof of Lemma B.1.1, we can also estimate $\|\partial_y u\|_{L^4}$ with the norm of the Sobolev space $H^{1,2}$ in two space dimensions.

Lemma B.1.3. *There exists a positive constant $C_L > 0$ such that*

$$\|\partial_y u\|_{L^4} \leq C_L \|u\|_{H^{1,2}} \tag{B.4}$$

for all $u \in H^{1,2}(\mathbb{R}^2)$.

Proof. The inverse Fourier transform \mathcal{F}^{-1} is a continuous mapping from L^q to L^p with $1/p + 1/q = 1$ for $q \leq 2$ due to the Hausdorff-Young inequality. For $p = 4$ and $q = 4/3$, this leads to the inequality

$$\begin{aligned}
\|\partial_y u\|_{L^4} &\leq \|il\hat{u}\|_{L^{4/3}} \\
&= \|il\hat{u}\rho^{-1}\|_{L^{4/3}} \\
&\leq \|\hat{u}\rho\|_{L^2} \|il\rho^{-1}\|_{L^4},
\end{aligned} \tag{B.5}$$

where $\rho = 1 + |k| + |l|^2$ and $il\hat{u} = \mathcal{F}(\partial_y u)$. We also applied the generalized Hölder inequality $\|uv\|_{L^r} \leq \|u\|_{L^p} \|v\|_{L^q}$ with $1/p + 1/q = 1/r$ to obtain the last line of (B.5). The norm of the

weight function

$$\begin{aligned}
\|il\rho^{-1}\|_{L^4}^4 &= \int_{l=-\infty}^{\infty} \int_{k=-\infty}^{\infty} |l|^4 \cdot (1 + |k| + |l|^2)^{-4} dkdl \\
&\leq \int_{l=-1}^1 \int_{k=-\infty}^{\infty} |l|^4 \cdot (1 + |k| + |l|^2)^{-4} dkdl + \int_{l=-\infty}^{\infty} \int_{k=-1}^1 |l|^4 \cdot (1 + |k| + |l|^2)^{-4} dkdl \\
&\quad + 4 \int_{l=1}^{\infty} \int_{k=1}^{\infty} |l|^4 \cdot (1 + |k| + |l|^2)^{-4} dkdl \\
&\leq 2 \int_{k=-\infty}^{\infty} (2 + |k|)^{-4} dkdl + 2 \int_{l=-\infty}^{\infty} |l|^4 \cdot (1 + |l|^2)^{-4} dkdl \\
&\quad + 16 \int_{l=1}^{\infty} \int_{k=1}^{\infty} l^4 \cdot (k + l^2)^{-4} dkdl \\
&\leq 2C_1 + 2C_2 - \frac{16}{3} \int_{l=1}^{\infty} \left[l^4 \cdot (k + l^2)^{-3} \right]_{k=1}^{\infty} dl \\
&= 2C_1 + 2C_2 + \frac{16}{3} \int_{l=1}^{\infty} l^4 \cdot (1 + l^2)^{-3} dl < \infty
\end{aligned}$$

is bounded and with $\|\widehat{u}\rho\|_{L^2} \leq \|u\|_{H^{1,2}}$, we complete the proof. \square

Remark B.1.4. With the same strategy as in the Proof of Lemma B.1.3 using the weight function $\rho = (1 + k^2 + l^2)^{1/2}$, we get in addition the embedding result $\|u\|_{L^4} \leq \widetilde{C}_L \|u\|_{H^1}$ for all $u \in H^1(\mathbb{R}^2)$.

With these two embedding results, the following inequality holds.

Theorem B.1.5. *The space $\mathcal{H}^{1,2}(\mathbb{R}^2)$ forms a Banach algebra under pointwise multiplication, such that*

$$\|uv\|_{\mathcal{H}^{1,2}} \leq C_B \|u\|_{\mathcal{H}^{1,2}} \|v\|_{\mathcal{H}^{1,2}} \quad (\text{B.6})$$

for every $u, v \in \mathcal{H}^{1,2}(\mathbb{R}^2)$ and some positive constant $C_B > 0$.

Proof. In order to obtain the inequality above, we first show that $\|u\|_{H^{1,2}} \leq \|u\|_{\mathcal{H}^{1,2}}$. Expanding the norm defined in (B.1), we get

$$\|u\|_{\mathcal{H}^{1,2}}^2 = \langle L_x u, u \rangle_{L^2} + \langle L_y^2 u, u \rangle_{L^2} + 2 \langle L_y u, u \rangle_{L^2} + 3 \langle u, u \rangle_{L^2}.$$

Now we look at the occurent terms separately and we obtain for the quadratic term

$$\begin{aligned}
\langle L_y^2 u, u \rangle_{L^2} &= \langle -\partial_y^2 u + V_y u, -\partial_y^2 u + V_y u \rangle_{L^2} \\
&= \|\partial_y^2 u\|_{L^2}^2 + \|V_y u\|_{L^2}^2 + \langle -\partial_y^2 u, V_y u \rangle_{L^2} + \langle V_y u, -\partial_y^2 u \rangle_{L^2}
\end{aligned} \quad (\text{B.7})$$

and for the linear terms

$$\langle L_y u, u \rangle_{L^2} = \langle -\partial_y^2 u + V_y u, u \rangle_{L^2} = \|\partial_y u\|_{L^2}^2 + \|V_y^{1/2} u\|_{L^2}^2 \quad (\text{B.8})$$

and

$$\langle L_x u, u \rangle_{L^2} = \langle -\partial_x^2 u + V_x u, u \rangle_{L^2} = \|\partial_x u\|_{L^2}^2 + \|V_x^{1/2} u\|_{L^2}^2 \quad (\text{B.9})$$

respectively. Using (B.7),(B.8) and (B.9), we can rewrite the norm as follows:

$$\begin{aligned}
\|u\|_{\mathcal{H}^{1,2}}^2 &= \|\partial_y^2 u\|_{L^2}^2 + \|V_y u\|_{L^2}^2 + \langle -\partial_y^2 u, V_y u \rangle_{L^2} + \langle V_y u, -\partial_y^2 u \rangle_{L^2} \\
&\quad + 2\|\partial_y u\|_{L^2}^2 + 2\|V_y^{1/2} u\|_{L^2}^2 + \|\partial_x u\|_{L^2}^2 + \|V_x^{1/2} u\|_{L^2}^2 + 3\|u\|_{L^2}^2 \\
&= \|u\|_{H^{1,2}}^2 + \|V_y u\|_{L^2}^2 + \langle -\partial_y^2 u, V_y u \rangle_{L^2} + \langle V_y u, -\partial_y^2 u \rangle_{L^2} \\
&\quad + \|\partial_y u\|_{L^2}^2 + 2\|V_y^{1/2} u\|_{L^2}^2 + \|V_x^{1/2} u\|_{L^2}^2 + 2\|u\|_{L^2}^2.
\end{aligned} \tag{B.10}$$

Hence, we simplify the scalar products in (B.10) to

$$\begin{aligned}
\langle -\partial_y^2 u, V_y u \rangle + \langle V_y u, -\partial_y^2 u \rangle_{L^2} &= \langle \partial_y u, \partial_y (V_y u) \rangle_{L^2} + \langle \partial_y (V_y u), \partial_y u \rangle_{L^2} \\
&= \langle \partial_y u, (\partial_y V_y) u \rangle_{L^2} + \langle (\partial_y V_y) u, \partial_y u \rangle_{L^2} \\
&\quad + 2\langle \partial_y u, V_y (\partial_y u) \rangle_{L^2} \\
&= -\langle u, (\partial_y^2 V_y) u \rangle_{L^2} - \langle u, (\partial_y V_y) (\partial_y u) \rangle_{L^2} \\
&\quad + \langle (\partial_y V_y) u, \partial_y u \rangle_{L^2} + 2\|V_y^{1/2} (\partial_y u)\|_{L^2}^2 \\
&= -\langle u, (\partial_y^2 V_y) u \rangle_{L^2} + 2\|V_y^{1/2} (\partial_y u)\|_{L^2}^2 \\
&= -2\|u\|_{L^2}^2 + 2\|V_y^{1/2} (\partial_y u)\|_{L^2}^2,
\end{aligned} \tag{B.11}$$

where $V_y, \partial_y V_y, \partial_y^2 V_y \in \mathbb{R}$ and $\partial_y^2 V_y = 2$. Inserting (B.11) into (B.10), we directly get

$$\begin{aligned}
\|u\|_{\mathcal{H}^{1,2}}^2 &= \|u\|_{H^{1,2}}^2 + \|V_y u\|_{L^2}^2 + 2\|V_y^{1/2} (\partial_y u)\|_{L^2}^2 \\
&\quad + \|\partial_y u\|_{L^2}^2 + 2\|V_y^{1/2} u\|_{L^2}^2 + \|V_x^{1/2} u\|_{L^2}^2
\end{aligned} \tag{B.12}$$

and thus the bound

$$\|u\|_{H^{1,2}}^2 \leq \|u\|_{\mathcal{H}^{1,2}}^2 \tag{B.13}$$

holds.

Now we return to the proof of the Banach algebra and write

$$\begin{aligned}
\|uv\|_{\mathcal{H}^{1,2}}^2 &= \|\partial_y^2 (uv)\|_{L^2}^2 + \|V_y (uv)\|_{L^2}^2 + 2\|V_y^{1/2} (\partial_y (uv))\|_{L^2}^2 \\
&\quad + 2\|\partial_y (uv)\|_{L^2}^2 + 2\|V_y^{1/2} (uv)\|_{L^2}^2 + \|\partial_x (uv)\|_{L^2}^2 \\
&\quad + \|V_x^{1/2} (uv)\|_{L^2}^2 + \|uv\|_{L^2}^2.
\end{aligned} \tag{B.14}$$

We look at the particular terms on the right hand side of (B.14) separately:

- The triangle inequality yields to

$$\begin{aligned}
\|\partial_y^2 (uv)\|_{L^2} &\leq \|(\partial_y^2 u)v\|_{L^2} + 2\|(\partial_y u)(\partial_y v)\|_{L^2} + \|u(\partial_y^2 v)\|_{L^2} \\
&\leq \|\partial_y^2 u\|_{L^2} \|v\|_{C_b^0} + 2\|\partial_y u\|_{L^4} \|\partial_y v\|_{L^4} + \|u\|_{C_b^0} \|\partial_y^2 v\|_{L^2}
\end{aligned}$$

and with the bounds (B.3), (B.4) and (B.13), we obtain

$$\|\partial_y^2 (uv)\|_{L^2} \leq 2C_C \|u\|_{H^{1,2}} \|v\|_{H^{1,2}} + 2C_L^2 \|u\|_{H^{1,2}} \|v\|_{H^{1,2}} \leq C \|u\|_{\mathcal{H}^{1,2}} \|v\|_{\mathcal{H}^{1,2}}$$

- Using the representation (B.12) and the bound (B.3), we can estimate the term $\|V_y(uv)\|_{L^2}^2$ as follows:

$$\begin{aligned}\|V_y(uv)\|_{L^2} &\leq \|v\|_{C_b^0} \|V_y u\|_{L^2} \\ &\leq C_C \|v\|_{H^{1,2}} \|u\|_{\mathcal{H}^{1,2}} \\ &\leq C_C \|v\|_{\mathcal{H}^{1,2}} \|u\|_{\mathcal{H}^{1,2}}.\end{aligned}$$

- The estimates for the remaining terms follow with the same idea as in the calculations above.

In total, we get the inequality

$$\|uv\|_{\mathcal{H}^{1,2}}^2 \leq C_B^2 \|u\|_{\mathcal{H}^{1,2}}^2 \|v\|_{\mathcal{H}^{1,2}}^2$$

and the function space $\mathcal{H}^{1,2}(\mathbb{R}^2)$ is closed under pointwise multiplication. \square

In the second part of this section, we want to estimate the norm $\|\widehat{\phi}_{n,m}\psi_j\|_{\mathcal{H}^{1,2}}$. This bound will help us to control the parameter β and the terms of the nonlinear evolution problem (4.56).

Lemma B.1.6. *For every $n \in \mathbb{N}$, we get the bound*

$$\|\widehat{\phi}_{n,0}\psi_j\|_{\mathcal{H}^{1,2}} \leq (\omega_j + 1)^2 + (E_0 + 1) + 1, \quad (\text{B.15})$$

and therefore $\widehat{\phi}_{n,0}(x)\psi_j(y) \in \mathcal{H}^{1,2}(\mathbb{R}^2)$ uniformly in $\varepsilon > 0$.

Proof. The representation (B.1) directly leads to the equation

$$\begin{aligned}\|\widehat{\phi}_{n,0}\psi_j\|_{\mathcal{H}^{1,2}}^2 &= \langle (L_x + I)\widehat{\phi}_{n,0}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2} + \langle (L_y + I)^2\widehat{\phi}_{n,0}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2} \\ &\quad + \langle \widehat{\phi}_{n,0}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2},\end{aligned}$$

and since the orthogonality and normalization relation (4.14) holds, we have

$$\begin{aligned}\langle \widehat{\phi}_{n,0}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2} &= \int_{\mathbb{R}^2} \widehat{\phi}_{n,0}(x)\psi_j(y)\overline{\widehat{\phi}_{n,0}(x)\psi_j(y)} dx \\ &= \int_{x=-\infty}^{\infty} \widehat{\phi}_{n,0}(x)\overline{\widehat{\phi}_{n,0}(x)} dx \cdot \int_{y=-\infty}^{\infty} \psi_j(y)\overline{\psi_j(y)} dy \\ &= 1.\end{aligned}$$

Now it remains to calculate the scalar products associated with the one-dimensional differential operators L_x and L_y . By applying (4.13) and using the band boundedness (4.16), we obtain

$$\begin{aligned}\langle (L_x + I)\widehat{\phi}_{n,0}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2} &= \langle L_x\widehat{\phi}_{n,0}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2} + \langle \widehat{\phi}_{n,0}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2} \\ &= \left\langle \sum_{m' \in \mathbb{Z}} \widehat{E}_{n,-m'} \widehat{\phi}_{n,m'}\psi_j, \widehat{\phi}_{n,0}\psi_j \right\rangle_{L^2} + 1 \\ &= \sum_{m' \in \mathbb{Z}} \widehat{E}_{n,m'} \langle \widehat{\phi}_{n,m'}\psi_j, \widehat{\phi}_{n,0}\psi_j \rangle_{L^2} + 1 \\ &= \widehat{E}_{n,0} + 1 \\ &\leq E_0 + 1,\end{aligned}$$

while the scalar product associated with the quadratic term $(L_y + I)^2$ is estimated as follows:

$$\begin{aligned}
\langle (L_y + I)^2 \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} &= \langle L_y^2 \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + \langle L_y \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} \\
&\quad + \langle \widehat{\phi}_{n,0} \psi_j, L_y \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + \langle \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} \\
&= \langle L_y \widehat{\phi}_{n,0} \psi_j, L_y \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + 2 \langle L_y \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + 1 \\
&= \langle \omega_j \widehat{\phi}_{n,0} \psi_j, \omega_j \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + 2 \langle \omega_j \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + 1 \\
&= \omega_j^2 \langle \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + 2 \omega_j \langle \widehat{\phi}_{n,0} \psi_j, \widehat{\phi}_{n,0} \psi_j \rangle_{L^2} + 1 \\
&= \omega_j^2 + 2 \omega_j + 1 \\
&= (\omega_j + 1)^2,
\end{aligned}$$

where $L_y \psi_j = \omega_j \psi_j$. In total, we conclude

$$\|\widehat{\phi}_{n,0} \psi_j\|_{\mathcal{H}^{1,2}} \leq (\omega_j + 1)^2 + (E_0 + 1) + 1 < \infty.$$

□

B.2. Computation of the projection $\Pi_{n,j}$

In this section, we will focus on the explicit calculation of the $\mathcal{O}(\mu^{3/2})$ terms of the residual (4.34) by using the orthogonal projection $\Pi_{n,j}$ introduced in Lemma 4.4.2. First, we recall the decomposition (4.35) and the differential equation (4.45) to obtain

$$\begin{aligned}
&\frac{1}{\sigma} \left(L - \left(\widehat{E}_{n,0} + \omega_j \right) \right) \varphi_\mu + |\varphi_0|^2 \varphi_0 - \sum_{m \in \mathbb{Z}} \beta |a_m|^2 a_m \widehat{\phi}_{n,m} \psi_j \\
&= \Pi_{n,j} |\varphi_0|^2 \varphi_0 - \sum_{m \in \mathbb{Z}} \beta |a_m|^2 a_m \widehat{\phi}_{n,m} \psi_j.
\end{aligned} \tag{B.16}$$

In order to further simplify (B.16), we need $\Pi_{n,j} |\varphi_0|^2 \varphi_0$ to be represented by an expansion of the functions $\widehat{\phi}_{n,m}(x) \psi_j(y) \in \mathcal{E}_{n,j} \subset L^2(\mathbb{R}^2)$ and thus rewrite the projection as follows:

$$\Pi_{n,j} |\varphi_0|^2 \varphi_0 = \sum_{m \in \mathbb{Z}} \langle |\varphi_0|^2 \varphi_0, \widehat{\phi}_{n,m} \psi_j \rangle_{L^2} \cdot \widehat{\phi}_{n,m} \psi_j.$$

Using $\varphi_0(T, r) = \sum_{m \in \mathbb{Z}} a_m(T) \widehat{\phi}_{n,m}(x) \psi_j(y)$, the nonlinear term in the scalar product is given by

$$\begin{aligned}
|\varphi_0|^2 \varphi_0 &= \left(\sum_{m_1 \in \mathbb{Z}} \bar{a}_{m_1} \widehat{\phi}_{n,m_1} \psi_j \right) \cdot \left(\sum_{m_2 \in \mathbb{Z}} a_{m_2} \widehat{\phi}_{n,m_2} \psi_j \right) \cdot \left(\sum_{m_3 \in \mathbb{Z}} a_{m_3} \widehat{\phi}_{n,m_3} \psi_j \right) \\
&= \sum_{(m_1, m_2, m_3) \in \mathbb{Z}^3} \bar{a}_{m_1} a_{m_2} a_{m_3} \widehat{\phi}_{n,m_1} \psi_j \widehat{\phi}_{n,m_2} \psi_j \widehat{\phi}_{n,m_3} \psi_j
\end{aligned}$$

and therefore, we get

$$\begin{aligned}
\Pi_{n,j} |\varphi_0|^2 \varphi_0 &= \sum_{m \in \mathbb{Z}} \sum_{(m_1, m_2, m_3) \in \mathbb{Z}^3} \langle \widehat{\phi}_{n,m_1} \psi_j \widehat{\phi}_{n,m_2} \psi_j \widehat{\phi}_{n,m_3} \psi_j, \widehat{\phi}_{n,m} \psi_j \rangle_{L^2} \\
&\quad \times \bar{a}_{m_1} a_{m_2} a_{m_3} \widehat{\phi}_{n,m} \psi_j \\
&= \sum_{m \in \mathbb{Z}} \sum_{(m_1, m_2, m_3) \in \mathbb{Z}^3} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1} a_{m_2} a_{m_3} \widehat{\phi}_{n,m} \psi_j
\end{aligned} \tag{B.17}$$

where the integral kernel is defined as in (4.47). Inserting (B.17) into (B.16) yields to the equation

$$\begin{aligned}
& \Pi_{n,j} |\varphi_0|^2 \varphi_0 - \sum_{m \in \mathbb{Z}} \beta |a_m|^2 a_m \widehat{\phi}_{n,m} \psi_j \\
&= \sum_{m \in \mathbb{Z}} \sum_{(m_1, m_2, m_3) \in \mathbb{Z}^3} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1} a_{m_2} a_{m_3} \widehat{\phi}_{n,m} \psi_j \\
&\quad - \sum_{m \in \mathbb{Z}} \kappa_j(0, 0, 0, 0) \bar{a}_m a_m a_m \widehat{\phi}_{n,m} \psi_j,
\end{aligned} \tag{B.18}$$

with $\beta = \|\widehat{\phi}_{n,0} \psi_j\|_{L^4}^4 = \kappa_j(0, 0, 0, 0)$. Now, we want to summarize the two terms on the left hand side of (B.18) and thereby rearrange the sum to

$$\begin{aligned}
& \sum_{m \in \mathbb{Z}} \sum_{(m_1, m_2, m_3) \in \mathbb{Z}^3} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1} a_{m_2} a_{m_3} \widehat{\phi}_{n,m} \psi_j \\
&\quad - \sum_{m \in \mathbb{Z}} \kappa_j(0, 0, 0, 0) \bar{a}_m a_m a_m \widehat{\phi}_{n,m} \psi_j \\
&= \sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1} a_{m_2} a_{m_3} \widehat{\phi}_{n,m} \psi_j \\
&\quad + \sum_{m \in \mathbb{Z}} (\kappa_j(m, m, m, m) - \kappa_j(0, 0, 0, 0)) \bar{a}_m a_m a_m \widehat{\phi}_{n,m} \psi_j.
\end{aligned}$$

Since $\widehat{\phi}_{n,m}(x) = \widehat{\phi}_{n,0}(x - 2\pi m)$, the difference of the integral kernels $\kappa_j(m, m, m, m) - \kappa_j(0, 0, 0, 0) = 0$ and we obtain

$$\sum_{\substack{(m_1, m_2, m_3) \in \mathbb{Z}^3 / \\ \{(m, m, m)\}}} \kappa_j(m, m_1, m_2, m_3) \bar{a}_{m_1} a_{m_2} a_{m_3} \widehat{\phi}_{n,m} \psi_j$$

for the terms (B.16) of the formal order $\mathcal{O}(\mu^{3/2})$ of the residual $\text{Res}(\mu^{1/2} \Psi)$.

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