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Validity of the NLS approximation for periodic quantum graphs

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Abstract. 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.

Mathematics Subject Classification. 35Q55, 35R02.

Contents

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 [31]. Quantum graphs are used in

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mesoscopic physics to obtain a theoretical understanding of nanotechnological objects such as nanotubes or graphen, cf. [13,15,16]. A recent monograph [6] 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 [18] 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 [2–5].

It is the purpose of this paper 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,

$$i\partial_t u + \partial_x^2 u + |u|^2 u = 0, \quad t \in \mathbb{R}, \quad x \in \Gamma, \tag{1}$$

where Γ is the quantum graph and $u : \mathbb{R} \times \Gamma \to \mathbb{C}$. The Kirchhoff boundary conditions at the vertices are defined below in (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 Fig. 1. However, our approach can be extended to other quantum graphs, as discussed in Sect. 7.

The spectral problems associated with the linear Schrödinger operator on the periodic quantum graph of Fig. 1 and its modifications have been recently studied in the literature [15–17]. 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 [24], we have studied the stationary NLS equation on the periodic quantum

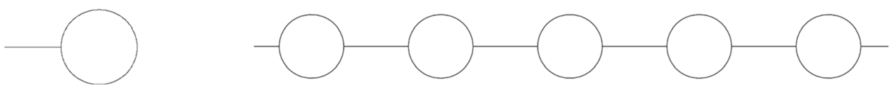

FIGURE 1. The basic cell Γ_0 (*left*) of the periodic quantum graph Γ (*right*)

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 [20]. In particular, tight-binding approximation [1,23,25] and coupled-mode approximation [9,22,29] 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 [14]. The envelope approximation provides a homogenization of the NLS equation (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 [7]. A modified analytical approach with a similar result was developed in Section 2.3.1 in [20] 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 [7,20] can be made applicable to the NLS equation (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 paper is organized as follows. The main results are described in Sect. 2, after introducing the spectral problem associated with the periodic quantum graph on Fig. 1. Local existence and uniqueness of solutions of the Cauchy problem for the NLS equation (1) is discussed in Sect. 3. The Bloch transform is introduced and studied in Sect. 4. In Sect. 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 Sect. 6. Discussion of other periodic quantum graphs is given in the concluding Sect. 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 paper, many different constants are denoted by C if they can be chosen independently of the small parameter $0<\varepsilon \ll 1$.

2. Main result

2.1. The periodic quantum graph

The periodic quantum graph Γ shown on Fig. 1 can be expressed as

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

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 $u : \Gamma \to \mathbb{C}$, 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 (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

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

and the continuity of the fluxes at the vertices

$$\begin{cases} \partial_x u_{n,0}(t, 2\pi n + \pi) = \partial_x u_{n,+}(t, 2\pi n + \pi) + \partial_x u_{n,-}(t, 2\pi n + \pi), \\ \partial_x u_{n+1,0}(t, 2\pi(n + 1)) = \partial_x u_{n,+}(t, 2\pi(n + 1)) + \partial_x u_{n,-}(t, 2\pi(n + 1)). \end{cases} \tag{3}$$

Remark 2.1. The symmetry constraint $u_{n,+}(t, x) = u_{n,-}(t, x)$ is an invariant reduction of the NLS equation (1) provided the initial data of the corresponding Cauchy problem satisfies the same reduction. In the case of symmetry reduction, the boundary conditions (2) and (3) can be simplified as follows:

$$\begin{cases} u_{n,0}(t, 2\pi n + \pi) = u_{n,+}(t, 2\pi n + \pi), \\ u_{n+1,0}(t, 2\pi(n + 1)) = u_{n,+}(t, 2\pi(n + 1)) \end{cases} \tag{4}$$

and

$$\begin{cases} \partial_x u_{n,0}(t, 2\pi n + \pi) = 2\partial_x u_{n,+}(t, 2\pi n + \pi), \\ \partial_x u_{n+1,0}(t, 2\pi(n + 1)) = 2\partial_x u_{n,+}(t, 2\pi(n + 1)). \end{cases} \tag{5}$$

In this way, the NLS equation (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

$$u_0(x) = \begin{cases} u_{n,0}(x), & x \in I_{n,0}, \\ 0, & x \in I_{n,\pm}, \end{cases} \quad n \in \mathbb{Z}, \tag{6}$$

and

$$u_\pm(x) = \begin{cases} u_{n,\pm}(x), & x \in I_{n,\pm}, \\ 0, & x \in I_{n,0}, \end{cases} \quad n \in \mathbb{Z}. \tag{7}$$

We introduce sets I_0 and $I_\pm$ by

$$I_0 = \bigcup_{n\in\mathbb{Z}} I_{n,0} = \mathrm{supp}(u_0) \quad \text{and} \quad I_\pm = \bigcup_{n\in\mathbb{Z}} I_{n,\pm} = \mathrm{supp}(u_\pm). \tag{8}$$

We collect the functions u_0 and $u_\pm$ in the vector $U = (u_0, u_+, u_-)$ and rewrite the evolutionary problem (1) as

$$i\partial_t U + \partial_x^2 U + |U|^2 U = 0, \quad t \in \mathbb{R}, \quad x \in \mathbb{R}\backslash\{k\pi : k \in \mathbb{Z}\}, \tag{9}$$

subject to the conditions (2)–(3) at the vertex points $x \in \{k\pi : k \in \mathbb{Z}\}$, where the cubic nonlinear term stands for the vector $|U|^2U = (|u_0|^2u_0, |u_+|^2u_+, |u_-|^2u_-)$.

2.2. The Floquet–Bloch spectrum

The spectral problem

$$\omega W = -\partial_x^2 W, \quad x \in \mathbb{R}\backslash\{k\pi : k \in \mathbb{Z}\}, \tag{10}$$

is obtained by inserting $U(t, x) = W(x)e^{i\omega t}$ into the linearization associated to the NLS equation (9). The components of $W = (w_0, w_+, w_-)$ satisfy the conditions (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

$$W(x) = e^{i\ell x} f(\ell, x), \quad \ell,\ x \in \mathbb{R}, \tag{11}$$

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

$$f(\ell, x) = f(\ell, x + 2\pi), \quad f(\ell, x) = f(\ell + 1, x)e^{ix}, \quad \ell,\ x \in \mathbb{R}, \tag{12}$$

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

$$-(\partial_x + i\ell)^2 f = \omega(\ell) f, \quad x \in \mathbb{T}_{2\pi}, \tag{13}$$

subject to the boundary conditions

$$\begin{cases} f_0(\ell, \pi) = f_+(\ell, \pi) = f_-(\ell, \pi), \\ f_0(\ell, 0) = f_+(\ell, 2\pi) = f_-(\ell, 2\pi) \end{cases} \tag{14}$$

and

$$\begin{cases} (\partial_x + i\ell) f_0(\ell, \pi) = (\partial_x + i\ell) f_+(\ell, \pi) + (\partial_x + i\ell) f_-(\ell, \pi), \\ (\partial_x + i\ell) f_0(\ell, 0) = (\partial_x + i\ell) f_+(\ell, 2\pi) + (\partial_x + i\ell) f_-(\ell, 2\pi). \end{cases} \tag{15}$$

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 (14)–(15) are derived from (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 (10) consists of two parts [15,16, 24]. 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

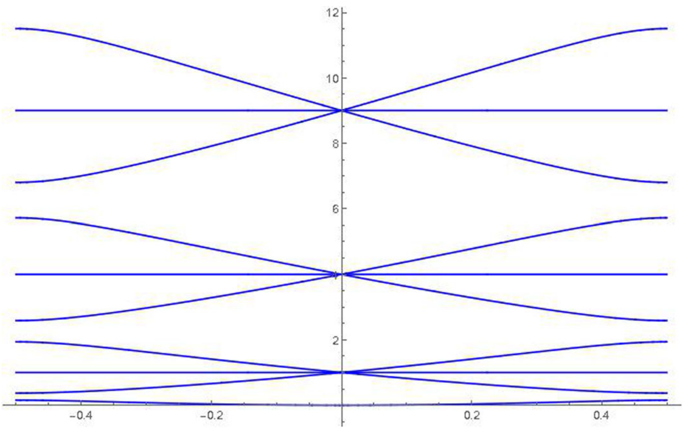

FIGURE 2. The spectral bands ω of the spectral problem (13) plotted versus the Bloch wave number ℓ for the periodic quantum graph Γ

$(W^{m,k})_{k\in\mathbb{Z}}$ of the spectral problem (10) exists and is supported compactly in each circle with the explicit representation:

$$w_{n,0}^{m,k}(x) = 0, \quad w_{n,+}^{m,k}(x) = -w_{n,-}^{m,k}(x) = \delta_{nk} \sin(m(x - 2\pi k)), \quad n \in \mathbb{Z}. \quad (16)$$

The second part in the spectrum of the spectral problem (10) 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 $\rho^2 - \mathrm{tr}(M)(\omega) + 1 = 0$. Here

$$\mathrm{tr}(M)(\omega) := \frac{1}{4}\left[9\cos(2\pi\sqrt{\omega}) - 1\right] \quad (17)$$

is the trace of the monodromy matrix M associated with the linear difference equation obtained after solving the differential equation (10) subject to the conditions (2)–(3), cf. [10,24]. Real roots are obtained when $\mathrm{tr}(M)(\omega) \in [-2, 2]$.

The corresponding eigenfunctions of the spectral problem (10) 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 (4)–(5).

The spectral bands of the periodic eigenvalue problem (13) are shown on Fig. 2. The flat bands at $\omega = m^2$, $m \in \mathbb{N}$ correspond to the eigenvalues of the spectral problem (10) of infinite algebraic multiplicity. It is clear from the explicit representation (16) that the corresponding eigenfunctions can also be written in the Bloch wave form (11) associated with the Bloch wave number $\ell \in \mathbb{T}_1$.

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

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

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 $\mathrm{tr}(M)(\omega) = -2$ do not overlap and the spectral band has a nonzero length because $\mathrm{tr}(M)(\omega)$ has a minimum at $\omega = \frac{m^2}{4}$ with $m \in \mathbb{N}_{\mathrm{odd}}$ and $\mathrm{tr}(M)(\frac{m^2}{4}) = -\frac{5}{2} < -2$.

Let us now define the L^2-based spaces, where the eigenfunctions of the periodic eigenvalue problem (13) are properly defined. For fixed $\ell \in \mathbb{T}_1$, we define

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

and

$$H^2_\Gamma(\ell) := \{\widetilde{U} \in L^2_\Gamma : \quad \widetilde{u}_j \in H^2(I_{0,j}), \quad j \in \{0,+,-\}, \quad (14)-(15) \text{ are satisfied}\},$$

equipped with the norm

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

The parameter ℓ is defined in $H^2_\Gamma(\ell)$ by means of the boundary conditions (14)–(15). We obtain the following elementary result.

Lemma 2.2. *For fixed $\ell \in \mathbb{T}_1$, the operator $\widetilde{L}(\ell) := -(\partial_x + i\ell)^2$ is a self-adjoint, positive semi-definite operator in L^2_Γ.*

Proof. Using the conditions (14)–(15), we find for every $f(\ell,\cdot), g(\ell,\cdot) \in H^2_\Gamma(\ell)$ and every $\ell \in \mathbb{T}_1$:

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

Using another integration by parts with the conditions (14)–(15), we confirm that

$$\langle \widetilde{L}(\ell) f, g\rangle_{L^2_\Gamma} = \langle f, \widetilde{L}(\ell) g\rangle_{L^2_\Gamma},$$

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

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

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

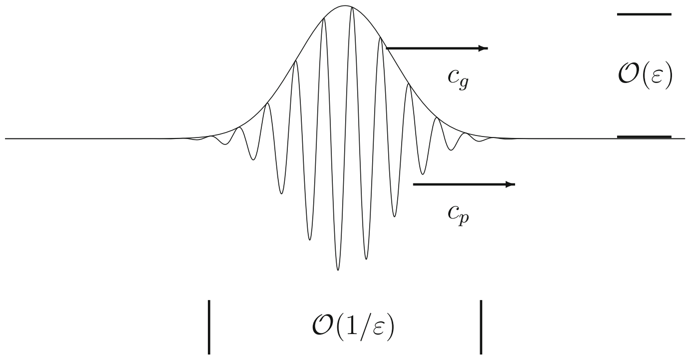

FIGURE 3. A schematic representation of the asymptotic solution (19)–(20) to the NLS equation (1) on the periodic quantum graph Γ. The envelope advances with the group velocity c_{g} and the underlying carrier wave advances with the phase velocity c_{p}

By Lemma 2.2 and the spectral theorem for self-adjoint operators, cf. [26], 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 $\widetilde{L}(\ell)$ 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 (12). They also satisfy the orthogonality and normalization relations:

$$\langle f^{(m)}(\ell,\cdot), f^{(m')}(\ell,\cdot)\rangle_{L^2_\Gamma} = \delta_{m,m'}, \quad \ell \in \mathbb{T}_1. \tag{18}$$

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 $x \in I_{0,j}$.

2.3. The effective amplitude equation

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

$$U(t,x) = \varepsilon\Psi_{\mathrm{nls}}(t,x) + \text{higher-order terms}, \tag{19}$$

with

$$\varepsilon\Psi_{\mathrm{nls}}(t,x) = \varepsilon A(T,X) f^{(m_0)}(\ell_0,x) e^{i\ell_0 x} e^{-i\omega^{(m_0)}(\ell_0)t}, \tag{20}$$

where $0 < \varepsilon \ll 1$ is a small perturbation parameter, $T = \varepsilon^2 t$, $X = \varepsilon(x - c_{\mathrm{g}}t)$, and $A(T,X) \in \mathbb{C}$ is the wave amplitude. The parameter $c_{\mathrm{g}} := \partial_\ell \omega^{(m_0)}(\ell_0)$ 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 $c_{\mathrm{p}} := \omega^{(m_0)}(\ell_0)/\ell_0$, which characterizes movement of the carrier wave inside the wave packet. Figure 3 shows the characteristic scales of the wave packet given by the asymptotic expansion (19) with (20).

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:

$$i\partial_T A + \frac{1}{2}\partial_\ell^2 \omega^{(m_0)}(\ell_0)\partial_X^2 A + \nu |A|^2 A = 0, \tag{21}$$

where the cubic coefficient is given by

$$\nu = \frac{\|f^{(m_0)}(\ell_0,\cdot)\|_{L^4_\Gamma}^4}{\|f^{(m_0)}(\ell_0,\cdot)\|_{L^2_\Gamma}^2}. \tag{22}$$

Mathematical justification of the effective amplitude equation (21) by means of the error estimates for the original system (9) is the main purpose of this work. The approximation result is given by the following theorem.

Theorem 2.3. *Pick $m_0 \in \mathbb{N}$ and $\ell_0 \in \mathbb{T}_1$ such that the following non-resonance condition is satisfied:*

$$\omega^{(m)}(\ell_0) \neq \omega^{(m_0)}(\ell_0), \quad \textit{for every } m \neq m_0. \tag{23}$$

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 (21) 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 (9) satisfying the bound

$$\sup_{t\in[0,T_0/\varepsilon^2]} \sup_{x\in\mathbb{R}} |U(t,x) - \varepsilon\Psi_{\mathrm{nls}}(t,x)| \leq C\varepsilon^{3/2}, \tag{24}$$

where $\varepsilon\Psi_{\mathrm{nls}}$ is given by (20).

Remark 2.4. Thanks to the global well-posedness and integrability of the cubic NLS equation (21) in one space dimension [8,30], 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 2.5. As it follows from the spectral bands shown on Fig. 2, it is clear that the non-resonance assumption (23) 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 2.6. The approximation result of Theorem 2.3 should not be taken for granted. There exists a number of counterexamples [27,28], where a formally correctly derived amplitude equation makes wrong predictions about the dynamics of the original system.

Remark 2.7. The new difficulty in the proof of Theorem 2.3 on the periodic quantum graph Γ comes from the vertex conditions (2)–(3), which have to be incorporated into the functional analytic set-up from [7,20] used for the derivation of the amplitude equation (21). Since the NLS equation (1) only contains cubic nonlinearities, the proof of Theorem 2.3 does not require near-identity transformations and is based on a simple application of Gronwall's inequality.

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 Fig. 2 with the exception of the lowest spectral band, see Remark 2.5, the cubic NLS equation (21) 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 [20]). Eigenvalues of infinite multiplicities appearing as the flat bands in Fig. 2 represent an obstacle in the standard justification analysis.

To overcome the obstacle, we can consider solutions of the original system (9) which satisfy the symmetry constraint $u_{n,+}(t,x) = u_{n,-}(t,x)$, see Remark 2.1. In this way, all flat bands shown on Fig. 2 disappear as they violate the symmetry constraint.

Figure 4 shows the spectral bands of the spectral problem (13) 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 2.3.

To be specific, we consider an intersection point of the two spectral bands at $\ell = 0$, as per Figure 4, such that $\omega^{(2m_0)}(0) = \omega^{(2m_0+1)}(0)$ for some fixed

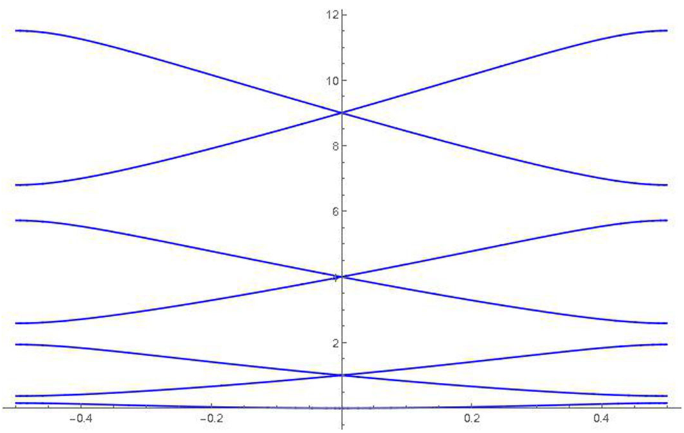

FIGURE 4. The spectral bands ω of the spectral problem (13) plotted versus the Bloch wave number ℓ for the periodic quantum graph Γ under the symmetry constraint $u_{n,+} = u_{n,-}$. The intersection points of the spectral curves at $\ell = 0$ are called Dirac points

$m_0 \in \mathbb{N}$. We relabel these two bands, and introduce

$$\omega_+(\ell) = \begin{cases} \omega^{(2m_0)}(\ell), & \text{for } \ell \le 0, \\ \omega^{(2m_0+1)}(\ell), & \text{for } \ell > 0, \end{cases} \tag{25}$$

and

$$\omega_-(\ell) = \begin{cases} \omega^{(2m_0+1)}(\ell), & \text{for } \ell \le 0, \\ \omega^{(2m_0)}(\ell), & \text{for } \ell > 0. \end{cases} \tag{26}$$

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

$$\varepsilon\Psi_{\text{dirac}}(t,x) = \varepsilon A_+(T,X) f^+(0,x) e^{-i\omega^+(0)t} + \varepsilon A_-(T,X) f^-(0,x) e^{-i\omega^-(0)t}, \tag{27}$$

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:

$$i\partial_T A_+ + i\partial_\ell \omega^+(0)\partial_X A_+ + \sum_{j_1,j_2,j_3 \in \{+,-\}} \nu^+_{j_1 j_2 j_3} A_{j_1} A_{j_2} \overline{A_{j_3}} = 0, \tag{28}$$

$$i\partial_T A_- + i\partial_\ell \omega^-(0)\partial_X A_- + \sum_{j_1,j_2,j_3 \in \{+,-\}} \nu^-_{j_1 j_2 j_3} A_{j_1} A_{j_2} \overline{A_{j_3}} = 0, \tag{29}$$

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

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

The system (28)–(29) 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 [21]. Assuming existence of a global solution to the cubic Dirac system (28)–(29), the approximation result is given by the following theorem.

Theorem 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 (28)–(29) with*

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

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 (9) satisfying the bound

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

where $\varepsilon\Psi_{\text{dirac}}$ is given by (27).

The proof of Theorem 2.8 is a straightforward modification of the proof of Theorem 2.3, cf. Remark 6.1.

3. Local existence and uniqueness

Here we prove the local existence and uniqueness of solutions to the original system (9). We consider the operator $L = -\partial_x^2$ in the space

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

with the domain of definition

$$\mathcal{H}^2 := \{U \in \mathcal{L}^2 : \;\; u_{n,j} \in H^2(I_{n,j}), \quad n \in \mathbb{Z}, \;\; j \in \{0, +, -\}, \;\; (2) - (3) \text{ is satisfied}\},$$

equipped with the norm

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

For the local existence and uniqueness of solutions to system (9), we need the following results.

Lemma 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 (3), then by the product rule for continuous functions U and V, the product UV also satisfies the flux continuity conditions (3). The support for U, V, and UV is identical. Finally, by the Cauchy-Schwarz inequality, we have

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

The statement of the lemma is proved.

Lemma 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)–(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 [6]). Positivity and semi-definiteness of L follows from the integration by parts

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

where the Kirchhoff boundary conditions (2)–(3) have been used again. □

As a consequence of classical semigroup theory, cf. [19], we have

Corollary 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 3.3, we obtain another ingredient of the existence and uniqueness theory.

Lemma 3.4. *There exists a positive constant C_L such that*

$$\|e^{-iLt}U\|_{\mathcal{H}^2} \leq C_L\|U\|_{\mathcal{H}^2} \tag{30}$$

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 3.3. □

We are now ready to prove the local existence and uniqueness of solutions of the Cauchy problem associated with the original system (9) in $\mathcal{H}^2$.

Theorem 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 (9) with the initial data $U|_{t=0} = U_0$.*

Proof. The estimates from Lemmas 3.1 and 3.4 allow us to proceed with the general theory for semilinear dynamical systems [19]. Namely, by Duhamel's principle, we rewrite the Cauchy problem associated with the original system (9) as the integral equation

$$U(t,\cdot) = e^{-iLt}U(0,\cdot) + i\int_0^t e^{-iL(t-\tau)}|U(\tau,\cdot)|^2U(\tau,\cdot)d\tau, \tag{31}$$

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 (30) in Lemma 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 (31) 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. □

4. Bloch transform

The justification of the NLS approximation in the context of nonlinear Klein–Gordon equations with smooth spatially periodic coefficients in [7] or in the context of the Gross–Pitaevskii equation with a smooth periodic potential in [20] heavily relies on the use of the Bloch transform. In order to transfer the evolution problem (9) 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 Sect. 7, we explain how to generalize our approach developed for the periodic graph sketched in Fig. 1 to other periodic graphs.

General Floquet–Bloch theory for spectral problems posed on periodic quantum graphs is reviewed in [6, Chapter 4]. However, as far as we can see, the approach of [6, Chapter 4] does not allow us to transfer the proof of [7] and [20] to the periodic quantum graphs. In what follows, we explain the necessary modifications of the Bloch transform for the periodic quantum graphs.

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 [12] and it appears for instance in the handling of the Schrödinger operator with a spatially periodic potential [26]. Bloch transform is (formally) defined by

$$\widetilde{u}(\ell,x) = (\mathcal{T}u)(\ell,x) = \sum_{n\in\mathbb{Z}} u(x+2\pi n)e^{-i\ell x-2\pi in\ell}. \tag{32}$$

The inverse of Bloch transform is given by

$$u(x) = (\mathcal{T}^{-1}\widetilde{u})(x) = \int_{-1/2}^{1/2} e^{i\ell x}\widetilde{u}(\ell,x)d\ell. \tag{33}$$

By construction, $\widetilde{u}(\ell,x)$ 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:

$$\widetilde{u}(\ell,x) = \widetilde{u}(\ell,x+2\pi) \quad \text{and} \quad \widetilde{u}(\ell,x) = \widetilde{u}(\ell+1,x)e^{ix}. \tag{34}$$

The following lemma specifies the well-known property of Bloch transform acting on Sobolev function spaces, cf. [11,20].

Lemma 4.1. *Bloch transform $\mathcal{T}$ is an isomorphism between*

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

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

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

Bloch transform $\mathcal{T}$ defined by (32) is related to the Fourier transform $\mathcal{F}$ by the following formula, cf. [11,20],

$$\widetilde{u}(\ell,x)=\sum_{j\in\mathbb{Z}}e^{ijx}\widehat{u}(\ell+j), \tag{35}$$

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:

$$(\tilde{u}\star\tilde{v})(\ell,x)=\int_{-1/2}^{1/2}\tilde{u}(\ell-m,x)\tilde{v}(m,x)dm, \tag{36}$$

where the continuation conditions (34) have to be used for $|\ell-m|>1/2$.

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

$$\mathcal{T}(\chi u)(\ell,x)=\chi(x)(\mathcal{T}u)(\ell,x). \tag{37}$$

The relations (36) and (37) are well-known [7,11] and can be proved from (32) and (35).

4.2. The system in Bloch space

Thanks to the definitions (6), (7), and (8), it is obvious how to transfer the evolution problem (9) into Bloch space. We apply the Bloch transform $\mathcal{T}$ to all components of $U=(u_0,u_+,u_-)$ and obtain

$$i\partial_t\widetilde{U}(t,\ell,x)=\widetilde{L}(\ell)\widetilde{U}(t,\ell,x)-(\widetilde{U}\star\widetilde{U}\star\overline{\widetilde{U}})(t,\ell,x), \tag{38}$$

where the operator $\widetilde{L}(\ell):=-(\partial_x+i\ell)^2$ appears in the periodic spectral problem (13), the function $\widetilde{U}(t,\ell,x)=(\widetilde{u}_0,\widetilde{u}_+,\widetilde{u}_-)(t,\ell,x)$ satisfies the continuation conditions

$$\widetilde{U}(t,\ell,x)=\widetilde{U}(t,\ell,x+2\pi)\quad\text{and}\quad\widetilde{U}(t,\ell,x)=\widetilde{U}(t,\ell+1,x)e^{ix}, \tag{39}$$

and the convolution integrals are applied componentwise as in

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

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

$$\chi_j(x)=\begin{cases}1, & x\in I_j,\\ 0, & \text{elsewhere,}\end{cases}\qquad j\in\{0,+,-\}. \tag{40}$$

With the help of property (37), 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 $j\in\{0,+,-\}$.

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 with its counterpart $\widetilde{\mathcal{H}}^2$, the domain of definition of the operator $\widetilde{L}(\ell) := -(\partial_x + i\ell)^2$ in the space $L^2(\mathbb{T}_1, L^2_\Gamma)$. We define

$$\begin{aligned}\widetilde{\mathcal{H}}^2 = \{&\widetilde{U} \in L^2(\mathbb{T}_1, L^2_\Gamma): \quad \widetilde{u}_j \in L^2(\mathbb{T}_1, H^2(I_{0,j})), \quad j \in \{0,+,-\},\\ &(14)-(15) \text{ is satisfied}\},\end{aligned}$$

equipped with the norm

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

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

Lemma 4.2. *The Bloch transform $\mathcal{T}$ is an isomorphism between the spaces $\mathcal{H}^2$ and $\widetilde{\mathcal{H}}^2$.*

Proof. We start with the function u_0 defined in (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 $u_{0,ext}$. According to Lemma 4.1, we have $\mathcal{T}(u_{0,ext}) \in L^2(\mathbb{T}_1, H^2(\mathbb{T}_{2\pi}))$. With the cut-off function χ_0 defined in (40), we find by using (37) that

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

Therefore, for fixed $\ell \in \mathbb{T}_1$, we have $\operatorname{supp}(\widetilde{u}_0) = I_{0,0}$. From the properties of $\mathcal{T}(u_{0,ext})$, we conclude that $\widetilde{u}_0 \in L^2(\mathbb{T}_1, H^2(I_{0,0}))$. The components $u_\pm$ are handled with the same technique. The boundary conditions (2)–(3) transfer in Bloch space into the boundary conditions (14)–(15). □

5. Estimates for the residual terms

Here we decompose the evolution problem (38) into two parts. The first part reduces to the effective amplitude equation of the type (21) but written in Fourier space. The other part satisfies the evolution problem where the residual terms can be estimated in the space $\widetilde{\mathcal{H}}^2$. Since the residual term after a standard decomposition similar to (19) and (20) 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 (19) and (20) used for the derivation of the effective amplitude equation (21) in Bloch space, we split the solution to the evolution problem (38) into two parts. We write

$$\widetilde{U}(t,\ell,x) = \widetilde{V}(t,\ell) f^{(m_0)}(\ell,x) + \widetilde{U}^\perp(t,\ell,x), \tag{41}$$

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

$$i\partial_t \widetilde{V}(t,\ell) = \omega^{(m_0)}(\ell)\widetilde{V}(t,\ell) - N_V(\widetilde{V},\widetilde{U}^{\perp})(t,\ell) \tag{42}$$

and

$$i\partial_t \widetilde{U}^{\perp}(t,\ell,x) = \widetilde{L}(\ell)\widetilde{U}^{\perp}(t,\ell,x) - N^{\perp}(\widetilde{V},\widetilde{U}^{\perp})(t,\ell,x), \tag{43}$$

where

$$N_V(\widetilde{V},\widetilde{U}^{\perp})(t,\ell) = \langle f^{(m_0)}(\ell,\cdot), (\widetilde{U}\star\widetilde{U}\star\overline{\widetilde{\widetilde{U}}})(t,\ell,\cdot)\rangle_{L^2_\Gamma}$$

and

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

Next, we estimate each part of the evolution problem.

5.1. Derivation of the effective amplitude equation

The effective amplitude equation (21) can be derived from equation (42) by evaluating it at $\widetilde{U}^{\perp} = 0$. To be precise, we write

$$\begin{aligned} N_V(\widetilde{V},\widetilde{U}^{\perp})(t,\ell) = \int_{\mathbb{T}_1}\int_{\mathbb{T}_1} \beta(\ell,\ell_1,\ell_2,\ell_1+\ell_2-\ell) \\ \times \widetilde{V}(t,\ell_1)\widetilde{V}(t,\ell_2)\overline{\widetilde{\widetilde{V}}}(t,\ell_1+\ell_2-\ell)d\ell_1 d\ell_2 + N_{V,rest}(\widetilde{V},\widetilde{U}^{\perp})(t,\ell) \end{aligned} \tag{44}$$

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

$$\begin{aligned} &\beta(\ell,\ell_1,\ell_2,\ell_1+\ell_2-\ell) \\ &\quad := \left\langle f^{(m_0)}(\ell,\cdot), f^{(m_0)}(\ell_1,\cdot) f^{(m_0)}(\ell_2,\cdot)\overline{f^{(m_0)}}(\ell_1+\ell_2-\ell,\cdot)\right\rangle_{L^2_\Gamma}. \end{aligned} \tag{45}$$

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

$$\widetilde{V}_{\rm app}(t,\ell) = \widetilde{A}\left(\varepsilon^2 t, \frac{\ell-\ell_0}{\varepsilon}\right)\mathbf{E}(t,\ell), \tag{46}$$

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 (46) into the evolution problem (42), and set the coefficients of $\varepsilon^2\mathbf{E}$ to zero. As a result, we obtain the leading-order equation in the form

$$\begin{aligned} i\partial_T \widetilde{A}(T,\xi) = \frac{1}{2}\partial_\ell^2\omega^{(m_0)}(\ell_0)\xi^2\widetilde{A}(T,\xi) \\ -\nu\int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}}\int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} \widetilde{A}(T,\xi_1)\widetilde{A}(T,\xi_2)\overline{\widetilde{A}}(T,\xi_1+\xi_2-\xi)d\xi_1 d\xi_2, \end{aligned} \tag{47}$$

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 (21).

By letting $\varepsilon \to 0$, in particular $\int_{-\frac{1}{2\varepsilon}}^{\frac{1}{2\varepsilon}} d\xi \to \int_{-\infty}^{\infty} d\xi$, and $\widetilde{A}(T,\xi) \to \widehat{A}(T,\xi)$ as $\varepsilon \to 0$, equation (47) yields formally the NLS equation in Fourier space, namely

$$i\partial_T \widehat{A}(T,\xi) - \frac{1}{2}\partial_\ell^2 \omega^{(m_0)}(\ell_0)\xi^2 \widehat{A}(T,\xi) + \nu(\widehat{A} * \widehat{A} * \widehat{\overline{A}})(T,\xi) = 0. \tag{48}$$

Equation (48) corresponds to the amplitude equation (21) in physical space. The formal calculations will be made rigorous in Sect. 5.3.

Remark 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 $\varepsilon^{-1}\widehat{A}(\varepsilon^{-1}\cdot)$. 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 (46) compared to the standard approximation (19).

5.2. The improved approximation

The simple approximation (46) produces a number of terms in the second equation (43) which are of the formal order $\mathcal{O}(\varepsilon^2)$ in Bloch space and which do not cancel 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 Sect. 6, we need the residual to be of the formal order $\mathcal{O}(\varepsilon^3)$ in Bloch space.

As in [14], the $\mathcal{O}(\varepsilon^2)$ terms can be canceled by adding higher order terms to the approximation (46) in (41). Therefore, we set

$$\widetilde{U}_{\text{app}}^{\perp}(t,\ell,x) = \varepsilon^2 \widetilde{B}\left(\varepsilon^2 t, \frac{\ell-\ell_0}{\varepsilon}, x\right) \mathbf{E}(t,\ell). \tag{49}$$

Inserting (49) into the evolution problem (43) and equating the coefficients of $\varepsilon^2\mathbf{E}$ to zero gives the following equation in the lowest order in ε:

$$\begin{aligned}\omega^{(m_0)}(\ell_0)\widetilde{B}\left(\varepsilon^2 t, \xi, x\right) = \widetilde{L}(\ell_0)\widetilde{B}\left(\varepsilon^2 t, \xi, x\right)\\ -\varepsilon^{-2}\mathbf{E}^{-1}(t,\ell)N^{\perp}(\widetilde{V}_{\text{app}}, 0)(t,\ell,x),\end{aligned} \tag{50}$$

where $\ell = \ell_0 + \varepsilon\xi$. Note that all $\mathbf{E}$ factors cancel each other 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 (50) can be solved with respect to $\widetilde{B}$ if $\widetilde{L}(\ell_0) - \omega^{(m_0)}(\ell_0)I$ is invertible. The invertibility condition

$$\inf_{m\in\mathbb{N}\backslash\{m_0\}} \left|\omega^{(m)}(\ell_0) - \omega^{(m_0)}(\ell_0)\right| > 0 \tag{51}$$

is satisfies for the spectral problem (10) under the condition (23) of Theorem 2.3. Substituting $\widetilde{A}$ and $\widetilde{B}$ obtained from (47) and (50) into (46) and (49), and inserting the approximation $(\widetilde{V}_{\text{app}}, \widetilde{U}_{\text{app}}^{\perp})$ into the evolution problem (42) and (43) cancel out all terms of the formal order $\mathcal{O}(\varepsilon^2)$. According to Remark 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.

5.3. From Fourier space to Bloch space

As in Theorem 2.3, let $A \in C(\mathbb{R}, H^3(\mathbb{R}))$ be a solution of the effective amplitude equation (21). Here we show that the residual of the evolution problem (38) given by

$$\widetilde{\mathrm{Res}}(\widetilde{U})(t,\ell,x) = -i\partial_t \widetilde{U}(t,\ell,x) + \widetilde{L}(\ell)\widetilde{U}(t,\ell,x) - (\widetilde{U} \star \widetilde{U} \star \overline{\widetilde{U}})(t,\ell,x), \tag{52}$$

can be estimated in $\widetilde{\mathcal{H}}^2$ to be of order $\mathcal{O}(\varepsilon^{7/2})$ if the improved approximations is constructed by using the decomposition (41) with $(\widetilde{V}_{\mathrm{app}}, \widetilde{U}^{\perp}_{\mathrm{app}})$ given by (46) and (49).

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 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 5.4.

As a consequence of the assumptions on $A \in C(\mathbb{R}, H^3(\mathbb{R}))$, the Fourier transform $\widehat{A}$ is a solution of the NLS equation in Fourier space (48) and satisfies $\widehat{A}\rho_{0,1,3} \in L^2(\mathbb{R})$. By the Cauchy–Schwarz inequality, we have

$$\|\widehat{A}\rho_{0,1,2}\|_{L^1} \leq \|\widehat{A}\rho_{0,1,3}\|_{L^2} \|\rho_{0,1,-1}\|_{L^2} \leq C\|\widehat{A}\rho_{0,1,3}\|_{L^2}, \tag{53}$$

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

$$\widetilde{A}(T, \varepsilon^{-1}(\ell - \ell_0)) = \widetilde{\chi}_{\ell_0}(\ell)\widehat{A}(T, \varepsilon^{-1}(\ell - \ell_0)), \tag{54}$$

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

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

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

$$\widetilde{A}\left(T, \varepsilon^{-1}(\ell + 1 - \ell_0)\right) = \widetilde{A}\left(T, \varepsilon^{-1}(\ell - \ell_0)\right), \quad \ell \in \mathbb{R}, \tag{55}$$

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

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

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 $\widetilde{\mathcal{H}}^2$. In order to avoid losing $\varepsilon^{1/2}$, let us consider estimates in the following L^1-based space

$$\widetilde{\mathcal{C}}^2 = \{\widetilde{U} \in L^1(\mathbb{T}_1, L^2_\Gamma) : \quad \widetilde{u}_j \in L^1(\mathbb{T}_1, H^2(I_{0,j})), \quad j \in \{0,+,-\}, \\ (14) - (15) \text{ is satisfied}\},$$

equipped with the norm

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

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

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

is of the order $\mathcal{O}(\varepsilon)$. Due to Young's inequality and (53) we have

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

respectively with weights

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

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

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

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

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

Hence, we drop (50) and define

$$\widetilde{B}\left(\varepsilon^2 t, \xi, x\right) = (\widetilde{L}(\ell) - \omega^{(m_0)}(\ell_0)I)^{-1} \varepsilon^{-2} \mathbf{E}^{-1}(t,\ell) N^\perp(\widetilde{V}_{\text{app}}, 0)(t,\ell,x), \tag{56}$$

where again $\ell = \ell_0 + \varepsilon\xi$. The inverse $(\widetilde{L}(\ell) - \omega^{(m_0)}(\ell_0)I)^{-1}$ exists due to the non-resonance condition (23) for $\delta > 0$ sufficiently small, but independent of the small parameter $\varepsilon > 0$. The change from $\widetilde{L}(\ell_0)$ in equation (50) to $\widetilde{L}(\ell)$ here allows us to avoid an expansion of $\widetilde{L}(\ell)$ at $\ell = \ell_0$, which would correspond to a loss of regularity.

By construction in (49), we have that $\widetilde{U}^\perp_{\text{app}}\rho_{\ell_0,\varepsilon,2} \in \widetilde{\mathcal{H}}^2$ is of the order $\mathcal{O}(\varepsilon^{5/2})$ and $\widetilde{U}^\perp_{\text{app}}\rho_{\ell_0,\varepsilon,1} \in \widetilde{\mathcal{C}}^2$ is of the order $\mathcal{O}(\varepsilon^3)$. Thus, we set

$$\varepsilon\widetilde{\Psi}(t,\ell,x) = \widetilde{V}_{\text{app}}(t,\ell) f^{(m_0)}(\ell,x) + \widetilde{U}^\perp_{\text{app}}(t,\ell,x), \tag{57}$$

with $\widetilde{V}_{\text{app}}$ and $\widetilde{U}^\perp_{\text{app}}$ defined in (46) and (49).

Remark 5.3. In contrast to the approximation $\varepsilon\Psi_{\text{nls}}$, the approximation $\varepsilon\Psi = \mathcal{T}^{-1}(\varepsilon\widetilde{\Psi})$ satisfies the Kirchhoff boundary conditions (2)–(3).

5.4. Estimates in Bloch space

By construction of $\varepsilon\widetilde{\Psi}$, the lower order terms are canceled out so that $\widetilde{\mathrm{Res}}(\varepsilon\widetilde{\Psi})$ 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 5.4. *Let $m, s \geq 0$ and let $g : \mathbb{T}_1 \to \mathbb{R}$ satisfy*

$$|g(\ell)| \leq C|\ell - \ell_0|^s, \quad \ell \in \mathbb{T}_1, \tag{58}$$

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

$$\|\rho_{0,1,m}(\cdot)g(\cdot)\widetilde{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2(\mathbb{T}_1)} \leq C\varepsilon^{s+1/2}\|\rho_{0,1,m+s}\widehat{A}\|_{L^2(\mathbb{R})}. \tag{59}$$

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

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

where the last inequality follows from the scaling transformation for the squared L^2-norm, cf. also the subsequent Remark 5.6. □

By using Lemma 5.4, we obtain the estimate on $\widetilde{\mathrm{Res}}(\varepsilon\widetilde{\Psi})$ given by (57).

Lemma 5.5. *Let $A \in C([0, T_0], H^3)$ be a solution of the amplitude equation (21) 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*

$$\sup_{t\in[0,T_0/\varepsilon^2]} \|\widetilde{\mathrm{Res}}(\varepsilon\widetilde{\Psi})\|_{\widetilde{\mathcal{H}}^2} \leq C_{\mathrm{Res}}\varepsilon^{7/2}. \tag{60}$$

or equivalently,

$$\sup_{t\in[0,T_0/\varepsilon^2]} \|\mathrm{Res}(\varepsilon\Psi)\|_{\mathcal{H}^2} \leq C_{\mathrm{Res}}\varepsilon^{7/2}. \tag{61}$$

Proof. We define

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

By construction we have

$$\widetilde{\mathrm{Res}}^\perp(\widetilde{V}_{\mathrm{app}}, \widetilde{U}^\perp_{\mathrm{app}})(t,\ell,x) = s_1 + s_2, \tag{62}$$

where

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

and

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

again with $\ell = \ell_0 + \varepsilon\xi$. Via (56) the term $\partial_T \widetilde{B}$ in s_1 can be expressed in terms of $\partial_T \widetilde{V}_{\mathrm{app}}$, respectively in terms of $\partial_T A$, where $\partial_T A$ can be expressed by the right-hand side of the amplitude equation (21). Similarly, the term $\xi \widetilde{B}\,(T, \xi, x)$ can be estimated in terms of $\xi \widehat{A}(T, \xi)$. Since $\widetilde{U}^{\perp}_{\mathrm{app}}$ obviously is in $\widetilde{\mathcal{H}}^2$, we eventually have the estimate

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

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

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

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

Next we have

$$\widetilde{\mathrm{Res}}_V(\widetilde{V}_{\mathrm{app}}, \widetilde{U}^{\perp}_{\mathrm{app}})(t, \ell) = r_1 + r_2, \tag{63}$$

where

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

and

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

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 (21). 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 $\widetilde{\chi}_{\ell_0}$ is needed to bring (21) from Fourier space to Bloch space.

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

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

the difference between the nonlinear coefficient $\beta = \beta(\ell, \ell_1, \ell_2, \ell_1 + \ell_2 - \ell)$ defined in (45) and the coefficient $\nu = \beta(\ell_0, \ell_0, \ell_0, \ell_0)$, and the difference between $\widehat{A}$ and $\widetilde{A}$.

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 5.4 with $m = 0$ and $s = 3$ to find

$$\|(\omega^{(m_0)}(\cdot) - T_2(\cdot; \ell_0))\widetilde{A}(\varepsilon^{-1}(\cdot - \ell_0))\|_{L^2(\mathbb{T}_1)} \leq C\varepsilon^{7/2} \|\rho_{0,1,3}\widehat{A}\|_{L^2(\mathbb{R})}. \tag{64}$$

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

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

and apply an obvious generalization of Lemma 5.4 to multilinear terms. It remains to estimate the difference between $\widehat{A}$ and $\widetilde{A}$. Since $|\widetilde{\chi}_{\ell_0}(\ell)-1|\le C|\ell-\ell_0|^m$ for every $m\ge 0$, we have for $m=3$,

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

By using these expansions, we derive the bound (60). Bound (61) holds thanks to the isomorphism of Bloch transform $\mathcal{T}$ between $\mathcal{H}^2$ and $\widetilde{\mathcal{H}}^2$. □

Remark 5.6. Compared to Remark 5.1 on the formal order in physical and Bloch space, we note that bounds (60) and (61) are identical in physical and Bloch space. This is because we gain $\varepsilon^{1/2}$ in the $\tilde{\mathcal{H}}^2$-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 $\varepsilon\Psi_{\mathrm{nls}}$ given by (20) that leads to the effective amplitude equation (21) is different from the improved approximation $\varepsilon\Psi$, which is given by (57) in Bloch space. The next result compares the two approximations. It is obtained by an elementary application of the Lemmas 3.1, 4.2 and 5.4.

Lemma 5.7. *Let $A\in C([0,T_0],H^3)$ be a solution of the amplitude equation (21) 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*

$$\sup_{t\in[0,T_0/\varepsilon^2]}\|\varepsilon\widetilde{\Psi}\|_{\widetilde{\mathcal{C}}^2}\le C_\Psi\varepsilon \tag{65}$$

and

$$\sup_{t\in[0,T_0/\varepsilon^2]}\|\varepsilon\Psi-\varepsilon\Psi_{\mathrm{nls}}\|_{L^\infty}\le C\varepsilon^{3/2}. \tag{66}$$

Proof. The first estimate (65) immediately follows by the previous estimates on each component of $\widetilde{\Psi}$. The second estimate (66) follows by applying a slight generalization of Lemma 5.4 to the difference $f^{(m_0)}(\ell,\cdot)-f^{(m_0)}(\ell_0,\cdot)$ and using the triangle inequality, since the term $\widetilde{U}^{\perp}_{\mathrm{app}}$ is much smaller compared to the term $\widetilde{V}_{\mathrm{app}}f^{(m_0)}$ in (57). 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

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

With the obvious generalization of Lemma 5.4 we obtain

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

Lemma 4.1 with $s=1$ and Sobolev's embedding theorem yield estimate (66). □

6. Estimates for the error term

Here we complete the proof of Theorem 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 (9) constructed in Theorem 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 $t \to \infty$. We do not worry about the possible growth of the global solution U because the approximation result of Theorem 2.3 is obtained on finite but long time intervals with a precise control of the error terms, cf. bound (24).

We write the solution U to the evolution problem (9) as a sum of the approximation term $\varepsilon\Psi$ controlled by Lemma 5.7 and the error term $\varepsilon^{3/2}R$, i.e.,

$$U = \varepsilon\Psi + \varepsilon^{3/2}R. \tag{67}$$

Inserting this decomposition into the evolution problem (9) gives

$$\partial_t R = -iLR + iG(\Psi, R) \tag{68}$$

where the linear operator $L = -\partial_x^2$ is studied in Lemma 3.2 and the nonlinear terms are expanded as

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

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

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

where C_Ψ appears in (65) of Lemma 5.7, we estimate each term of G with the help of Lemmas 3.1 and 5.5:

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

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

$$\begin{aligned}
\|G(\Psi, R)\|_{\mathcal{H}^2} \leq\ & C_{\mathrm{Res}}\varepsilon^2 + 3C_1\varepsilon^2\|R\|_{\mathcal{H}^2} + 3C_1\varepsilon^{5/2}\|R\|_{\mathcal{H}^2}^2 \\
& + C_1\varepsilon^3\|R\|_{\mathcal{H}^2}^3.
\end{aligned} \tag{69}$$

For simplicity, we assume $R(0) = 0$. Then, the variation of constant formula for the evolution system (68) yields the integral formula

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

By Lemma 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

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

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 (66), and the decomposition (67) complete the proof of the approximation result (24) of Theorem 2.3. □

Remark 6.1. We explain how the proof of Theorem 2.3 has to be modified in order to prove Theorem 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 $\omega_\pm$ given by (25) and (26) have to be expanded in ℓ up to quadratic order for estimating the residual terms. The decomposition formula (41) is replaced by

$$\widetilde{U}(t, \ell, x) = \widetilde{V}_+(t, \ell) f^+(\ell, x) + \widetilde{V}_-(t, \ell) f^-(\ell, x) + \widetilde{U}^\perp(t, \ell, x), \tag{70}$$

subject to the orthogonality constraints

$$\langle f^+(\ell, \cdot), \widetilde{U}^\perp(t, \ell, \cdot)\rangle_{L^2_\Gamma} = \langle f^-(\ell, \cdot), \widetilde{U}^\perp(t, \ell, \cdot)\rangle_{L^2_\Gamma} = 0.$$

For the derivation of the coupled-mode system (28)–(29) we then make the ansatz

$$\widetilde{V}_{\mathrm{app},\pm}(t, \ell) = \varepsilon^{-1} \widetilde{A}_\pm \left(\varepsilon^2 t, \varepsilon^{-2} \ell\right) e^{-i\omega_\pm(0)t}. \tag{71}$$

Straightforward modifications of this kind can be performed at each step in the proof of Theorem 2.3. This procedure yields the proof of Theorem 2.8.

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. Fig. 5, which are slightly more complicated than the periodic graph plotted in Fig. 1.

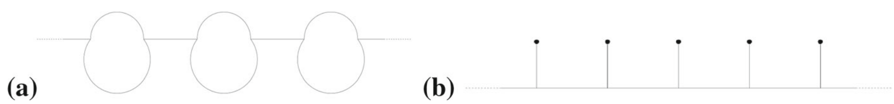

FIGURE 5. **a** Generalization of the periodic quantum graph sketched in Fig. 1. The central segment $\Gamma_{n,0}$ has length L_0 and the circular segments $\Gamma_{n,\pm}$ have lengths L_+ and L_-. **b** A periodic quantum graph with a vertical pendant and a horizontal bond, each of length π, with Dirichlet boundary conditions at the dead end

In order to bring the quantum graph plotted in Fig. 5a 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:

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

and

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

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 Fig. 5a depend on parameter L_0, L_+, and L_-.

In the case $L_0 \neq L_+ = L_-$ (left panel on Fig. 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 (21) can still be developed for the NLS equation on the periodic quantum graph but the non-resonance condition (23) 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.

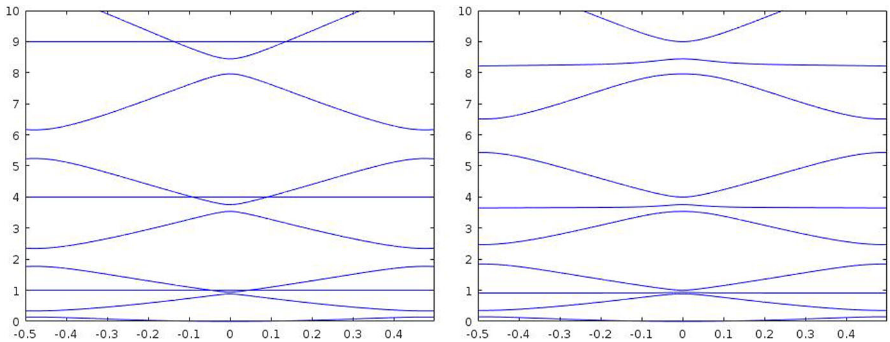

FIGURE 6. The Floquet–Bloch spectrum of the linear operator $L = -\partial_x^2$ for the periodic quantum graph plotted on Fig. 5a with $L_0 = \pi + 0.3$ and $L_+ = L_- = \pi$ (*left*) and $L_0 = \pi$, $L_+ = \pi$, and $L_- = \pi + 0.3$ (*right*)

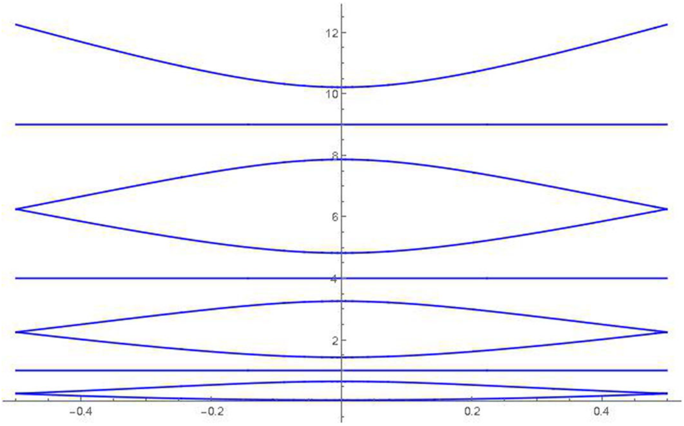

Figure 7. The Floquet–Bloch spectrum of the linear operator $L = -\partial_x^2$ for the periodic quantum graph plotted in Fig. 5b

In the case $L_0 = L_+ \neq L_-$ (right panel on Fig. 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 (23) is now satisfied for every $m_0 \in \mathbb{N}$ and $\ell_0 \in \mathbb{T}_1$ without any reservations.

In a similar way, the quantum graph plotted in Fig. 5b can be handled. We refrain here from details and only show the spectral picture in Fig. 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.

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 [7]. 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 (1). Thus, it will be a purpose of subsequent works to extend the justification analysis to other nonlinear evolution equations.

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