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ORIGINAL PAPER

# Nonlinear dynamics of modulated waves on graphene like quantum graphs

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**Abstract**
We consider cubic Klein–Gordon equations on infinite two-dimensional periodic metric graphs having for instance the form of graphene. At non-Dirac points of the spectrum, with a multiple scaling expansion Nonlinear Schrödinger (NLS) equations can be derived in order to describe slow modulations in time and space of traveling wave packets. Here we justify this reduction by proving error estimates between solutions of the cubic Klein–Gordon equations and the associated NLS approximations. Moreover, we discuss the validity of the modulation equations appearing by the same procedure at the Dirac points of the spectrum.

**KEYWORDS**
approximation, Dirac points, error estimates, NLS equation

**MSC (2020)**
35Q55, 35R02

## 1 | INTRODUCTION

In [20], with a multiple scaling expansion the NLS equation and the Dirac equations have been derived as effective equations for the description of slow modulations in time and space of traveling oscillating wave packets on infinite one-dimensional periodic metric graphs such as the necklace graph. The associated NLS approximation and Dirac approximation have been justified by error estimates.

It is the goal of this paper to transfer the results from [20] from one-dimensional (1D) to two-dimensional (2D) periodic metric graphs, where we concentrate on the most prominent 2D periodic metric graph, namely the honeycomb graph, which reminds of the hexagonal form of graphene. The approximation result for the NLS approximation is given in Theorem 7.1 and the approximation result for the counterpart to the Dirac approximation is given in Theorem 8.1. At a first view the transfer seems rather straightforward, but on a second view various new challenges occur.

First, in 1D the spectral curves at the Dirac points are smooth and a Taylor expansion of those is possible, whereas in 2D the spectral surfaces at the Dirac points form a cone and so no Taylor expansion of the spectral surfaces is possible. In Section 8 we get rid of this problem by extracting other smooth two-dimensional structures.

Secondly, for the derivation and justification of modulation equations, such as the NLS equation and the Dirac equations, in periodic media Bloch transform turned out to be a fundamental tool. For the 1D necklace graph it is straightforward how to Bloch transform the original nonlinear PDE posed on the 1D necklace graph. However, in order to apply

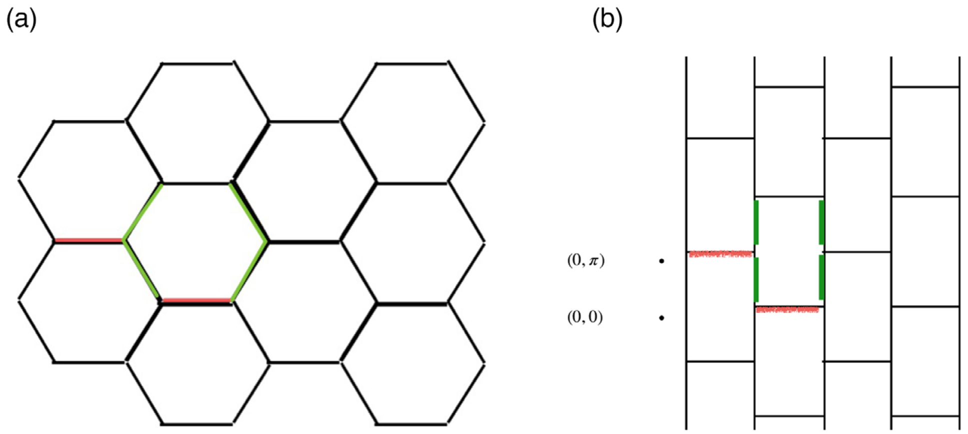


**FIGURE 1** (a) A graphene like metric graph, and (b) the associated equivalent metric "brick" graph with the indices of two vertex points. For both graphs we take the edge lengths $\pi$.

the existing theory for the derivation and justification of modulation equations in periodic media to the 2D honeycomb graph we have to Bloch transform the original nonlinear PDE over a Brillouin zone which is a torus. For the hexagonal graph the standard cell is trapezoidal. Since we work with metric graphs, we can use the fact that with this respect the honeycomb graph is equivalent to the brick graph which easily can be Bloch transformed over a 2D torus as Brillouin zone. See Section 2 and Section 6.

Thirdly, since our theory is $L^2$-based, due to the scaling property of the $L^2$-norm, in 1D we lose $\mathcal{O}(\varepsilon^{-1/2})$ in the residual estimates, but in 2D we lose $\mathcal{O}(\varepsilon^{-1})$, where $0 < \varepsilon \ll 1$ is the small perturbation parameter occurring in the derivation of the modulation equations. As a consequence of this loss, higher order terms have to be added to the approximation. One has to be careful in doing so for metric graphs due to the Kirchhoff boundary conditions at the vertices, cf. Section 2, in order to avoid an unwanted loss of regularity. See Section 7.3.

Finally, we consider a cubic Klein–Gordon (cKG) equation instead of a NLS equation as in [20] as original system on the metric graph and to our knowledge prove a first local existence and uniqueness result for the cKG equation posed on a periodic metric graph, see Section 5.

The plan of the paper is as follows. In Section 2 we define what is meant by posing the cKG equation on a honeycomb graph and explain that it is advantageous to consider the associated nonlinear initial value problem on the equivalent brick graph. In Section 3 we recall spectral properties of the Laplacian on the honeycomb/brick graph. We explain in Section 4 for two other 2D periodic metric graphs how they can be handled with our approach. In Section 5 we use semigroup theory and suitable function spaces for a local existence and uniqueness result. In Section 6 we derive a Bloch wave representation of the cKG equation on the periodic brick graph. This representation is the basis of the derivation of effective amplitude equations in Section 7 for non-Dirac points of the spectrum and in Section 8 for Dirac points of the spectrum.

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

## 2 | THE CKG EQUATION ON A HONEYCOMB/BRICK GRAPH

We are interested in the nonlinear dynamics of modulated waves on graphene like quantum graphs. We consider the cubic Klein–Gordon (cKG) equation

$$\partial_t^2 u = \Delta u - u - u^3, \quad t \in \mathbb{R}, \quad \xi \in \Gamma, \quad u : \mathbb{R} \times \Gamma \to \mathbb{R}, \tag{2.1}$$

on the periodic metric graph $\tilde{\Gamma}$ in Figure 1(a). Equation (2.1) can be seen a phenomenological model describing electromagnetic waves on graphene like wave guides.

A metric graph is a network of one-dimensional bonds (or edges) of certain lengths, connected at the vertices. As a metric graph, $\tilde{\Gamma}$ is equivalent to the brick graph $\Gamma$ plotted in Figure 1(b), because angles between bonds are irrelevant in this context. The hexagonal geometry of $\tilde{\Gamma}$ motivates coordinates that allow a simple analytical solution of spectral problems for typical Schrödinger operators on $\tilde{\Gamma}$, see [27] and below. Our representation $\Gamma$ makes such spectral problems somewhat more complicated, because we essentially have to choose a fundamental cell which is four times bigger than the one for $\tilde{\Gamma}$, but we believe that the nonlinear problems we consider are more transparent in the rectangular coordinates used in $\Gamma$. See Remark 3.3 for further comments.

The graph $\Gamma$ can be described as

$$\Gamma = \Gamma^x \oplus \Gamma^y, \qquad \text{with} \qquad \Gamma^x = \oplus_{n\in\mathbb{Z},m\in\mathbb{Z},m+n\in 2\mathbb{Z}+1}\Gamma^x_{m,n} \qquad \text{and} \qquad \Gamma^y = \oplus_{n\in\mathbb{Z},m\in\mathbb{Z}}\Gamma^y_{m,n},$$

where $\Gamma^x_{m,n}$ is the horizontal link of length $\pi$ between the points $\xi = (x,y) = (m\pi, n\pi)$ and $\xi = ((m+1)\pi, n\pi)$, and $\Gamma^y_{m,n}$ is the vertical link of length $\pi$ between the points $(m\pi, n\pi)$ and $(m\pi, (n+1)\pi)$. For a function $u : \Gamma \to \mathbb{C}$, we denote the part on $\Gamma^x_{m,n}$ with $u^x_{m,n}$ and the part on $\Gamma^y_{m,n}$ with $u^y_{m,n}$.

The second-order differential operator $L = -\Delta + 1$ is given by $-\partial_x^2 + 1$ on $\Gamma^x_{m,n}$, and by $-\partial_y^2 + 1$ on $\Gamma^y_{m,n}$. We use Kirchhoff conditions at the vertex points $\mathcal{V} = \{(x,y) = (m\pi, n\pi) : m,n \in \mathbb{Z}\}$, which are given by the continuity of the functions and of the fluxes at the vertices. For $m+n$ odd we have

$$u^x_{m,n}(m\pi, n\pi) = u^y_{m,n}(m\pi, n\pi) = u^y_{m,n-1}(m\pi, n\pi), \quad \text{and} \tag{2.2}$$

$$\partial_x u^x_{m,n}(m\pi, n\pi) + \partial_y u^y_{m,n}(m\pi, n\pi) - \partial_y u^y_{m,n-1}(m\pi, n\pi) = 0. \tag{2.3}$$

For $m+n$ even we have

$$u^x_{m-1,n}(m\pi, n\pi) = u^y_{m,n}(m\pi, n\pi) = u^y_{m,n-1}(m\pi, n\pi), \quad \text{and} \tag{2.4}$$

$$\partial_x u^x_{m-1,n}(m\pi, n\pi) - \partial_y u^y_{m,n}(m\pi, n\pi) + \partial_y u^y_{m,n-1}(m\pi, n\pi) = 0. \tag{2.5}$$

We introduce the functions

$$u^x(x,y) = \begin{cases} u^x_{m,n}(x,y), & (x,y) \in \Gamma^x_{m,n},\ m+n \text{ odd}, \\ 0, & \text{elsewhere}, \end{cases}$$

$$u^y(x,y) = \begin{cases} u^y_{m,n}(x,y), & (x,y) \in \Gamma^y_{m,n}, \\ 0, & \text{elsewhere}, \end{cases}$$

collect $u^x$ and $u^y$ in the vector $U = (u^x, u^y)$, and rewrite the evolutionary problem (2.1) as

$$\partial_t^2 U = \Delta U - U - U^3, \quad t \in \mathbb{R}, \quad \xi \in \Gamma \setminus \mathcal{V}, \tag{2.6}$$

with the conditions (2.2)–(2.5) at the vertex points. The cubic nonlinear term $U^3$ stands for the vector $((u^x)^3, (u^y)^3)$.

## 3 | THE SPECTRAL PROBLEM

We are interested in the dynamics of modulated waves of small amplitude. Thus in the derivation of effective equations the linearized problem plays a fundamental role. The linearization of (2.6) at $U = 0$ reads

$$\partial_t^2 U = -LU := \Delta U - U, \tag{3.1}$$

i.e., $LU = -\Delta U + U$ together with the vertex conditions (2.2)–(2.5). Linear Schrödinger operators on metric graphs, such as $L$ and more general versions, have been studied extensively, see, e.g., [4]. Here we consider $L$ in the space

$$\mathcal{L}^2 = \left\{ U = (u^x, u^y) \in \left(L^2(\Gamma)\right)^2 \right\},$$

with the domain of definition

$$\mathcal{H}^2 := \left\{ U \in \mathcal{L}^2 : u^{\zeta}_{n_1,n_2} \in H^2\left(\Gamma^{\zeta}_{n_1,n_2}\right), (2.2)-(2.5) \text{ are satisfied} \right\}.$$

We also need the intermediate space

$$\mathcal{H}^1 := \left\{ U \in \mathcal{L}^2 : u^{\zeta}_{n_1,n_2} \in H^1\left(\Gamma^{\zeta}_{n_1,n_2}\right), (2.2) \text{ and } (2.4) \text{ hold} \right\}.$$

The $H^s$ norms on these spaces are

$$\|U\|_{\mathcal{H}^s} := \left( \sum_{(\zeta,n_1,n_2)} \left\|u^{\zeta}_{n_1,n_2}\right\|^2_{H^s\left(\Gamma^{\zeta}_{n_1,n_2}\right)} \right)^{1/2}.$$

Problem (3.1) is solved by so-called Bloch modes

$$U(t,x,y) = e^{\mathrm{i}\omega t} e^{\mathrm{i}kx} e^{\mathrm{i}ly} f(k,l,x,y), \quad k,l \in \mathbb{R},\ (x,y) \in \Gamma, \tag{3.2}$$

where $f = (f^x, f^y)$ satisfies

$$f(k,l,x,y) = f(k,l,x+2\pi,y) = f(k,l,x,y+2\pi), \tag{3.3}$$

$$f(k,l,x,y) = f(k+1,l,x,y)e^{\mathrm{i}x} = f(k,l+1,x,y)e^{iy}. \tag{3.4}$$

Due to (3.3) and (3.4) we can restrict ourselves to the Brillouin zone $(k,l) \in \mathbb{T}_1^2$, and for $f^x$ to $x \in \mathbb{T}_{2\pi}$ and $y \in \{0,\pi\}$, and for $f^y$ to $y \in \mathbb{T}_{2\pi}$ and $x \in \{0,\pi\}$. The torus $\mathbb{T}_1$ is isometrically parameterized with $k$ or $l \in [-1/2, 1/2]$ and the torus $\mathbb{T}_{2\pi}$ with $x$ or $y \in [0, 2\pi]$, where the endpoints of the intervals are identified to be the same. Hence, $f$ can be found as a solution of the eigenvalue problem

$$-\left(\partial_x + \mathrm{i}k\right)^2 f^x(k,l,x,y) + f^x(k,l,x,y) = \omega^2(k,l) f^x(k,l,x,y), \qquad \text{for} \quad x \in \mathbb{T}_{2\pi}, \tag{3.5}$$

$$-\left(\partial_y + \mathrm{i}l\right)^2 f^y(k,l,x,y) + f^y(k,l,x,y) = \omega^2(k,l) f^y(k,l,x,y), \qquad \text{for} \quad y \in \mathbb{T}_{2\pi}, \tag{3.6}$$

subject to the following vertex conditions. For odd $m+n$ we have

$$f^x_{m,n}(k,l,m\pi,n\pi) = f^y_{m,n}(k,l,m\pi,n\pi) = f^y_{m,n-1}(k,l,m\pi,n\pi), \quad \text{and} \tag{3.7}$$

$$\left(\partial_x + \mathrm{i}k\right) f^x_{m,n}(k,l,m\pi,n\pi) + \left(\partial_y + \mathrm{i}l\right) f^y_{m,n}(k,l,m\pi,n\pi) - \left(\partial_y + \mathrm{i}l\right) f^y_{m,n-1}(k,l,m\pi,n\pi) = 0, \tag{3.8}$$

and for even $m+n$ we have

$$f^x_{m-1,n}(k,l,m\pi,n\pi) = f^y_{m,n}(k,l,m\pi,n\pi) = f^y_{m,n-1}(k,l,m\pi,n\pi), \quad \text{and} \tag{3.9}$$

$$\left(\partial_x + \mathrm{i}k\right) f^x_{m-1,n}(k,l,m\pi,n\pi) - \left(\partial_y + \mathrm{i}l\right) f^y_{m,n}(k,l,m\pi,n\pi) + \left(\partial_y + \mathrm{i}l\right) f^y_{m,n-1}(k,l,m\pi,n\pi) = 0. \tag{3.10}$$

Due to (3.3) and (3.4) we can restrict the function $f$ to the (fundamental) cell

$$\Gamma_b = \oplus_{(\zeta,n_1,n_2)\in I_b} \Gamma^{\zeta}_{n_1,n_2},$$

cf. Figure 1 and Figure 2(a), with the index set

$$I_b = \{(x,1,0),(x,0,1),(y,1,0),(y,1,1),(y,2,0),(y,2,1)\}. \tag{3.11}$$

Together, for fixed $k,l \in \mathbb{T}_1$, (3.5)–(3.10) define the eigenvalue problem

$$\widetilde{L}(k,l) f = \lambda(k,l) f, \tag{3.12}$$

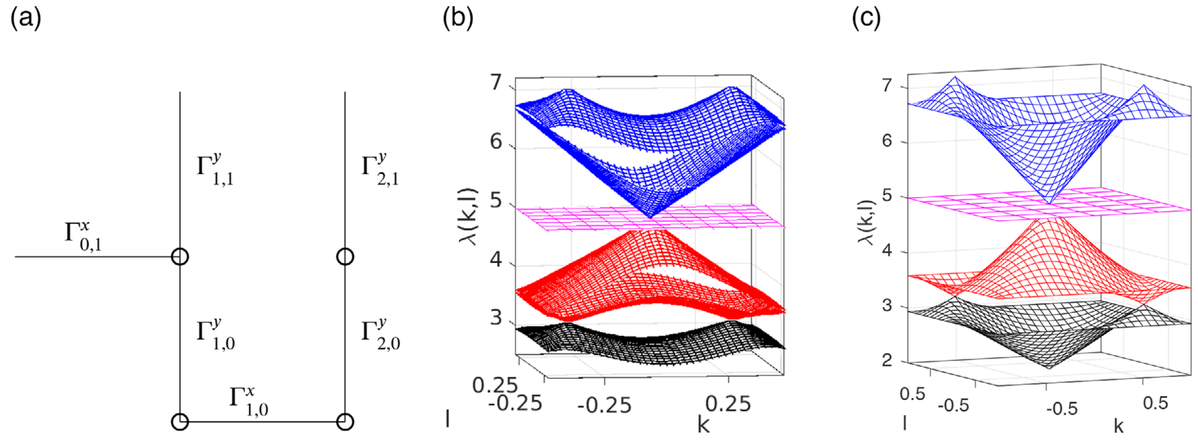


**FIGURE 2** (a) The basic cell. (b) A selection of spectral surfaces $\lambda_m$, and the flat band $\lambda \equiv 5$, showing in particular five Dirac points, two at $\lambda \approx 3.25$, one at $\lambda = 5$, and two at $\lambda \approx 7.25$. The colors of the bands are chosen to be consistent with those in (c), and the Brillouin zone $\mathbb{T}_1^2$ is slightly cut off in $l$ for graphical reasons. (c) The spectral surfaces $\tilde{\lambda}_m$, $m = 0$ (black), $m = 1$ (blue), and $m = -1$, associated to a minimal trapezoidal fundamental cell and associated Brillouin zone $\mathbb{T}_2^2$, cf. (3.15), again with the flat band $\lambda \equiv 5$, cf. Remark 3.3 for a more detailed explanation.

where $\lambda(k,l) = \omega^2(k,l)$. For fixed $k, l \in \mathbb{T}_1$, we define

$$L^2_\Gamma := \left\{ \widetilde{U} = \left(\widetilde{u}^\zeta_{n_1,n_2}\right)_{(\zeta,n_1,n_2)\in I_b} \in \left(L^2(\mathbb{T}_{2\pi})\right)^6 : \operatorname{supp}\left(\widetilde{u}^\zeta_{n_1,n_2}\right) \subset \Gamma^\zeta_{n_1,n_2} \right\} \tag{3.13}$$

and

$$H^2_\Gamma(k,l) := \left\{ \widetilde{U} \in L^2_\Gamma \ : \ \widetilde{u}_j \in H^2(\Gamma^\zeta_{n_1,n_2}),\ (\zeta,n_1,n_2) \in I_b,\ (3.7)\text{–}(3.10) \text{ are satisfied} \right\},$$

equipped with the norm

$$\|\widetilde{U}\|_{H^2_\Gamma(k,l)} = \left( \sum_{(\zeta,n_1,n_2)\in I_b} \|\widetilde{u}^\zeta_{n_1,n_2}\|^2_{H^2(\Gamma^\zeta_{n_1,n_2})} \right)^{1/2}.$$

Similar to [20, Lemma 2.2] we obtain the following result.

**Lemma 3.1.** *For fixed $k, l \in \mathbb{T}_1$, the operator $\widetilde{L}(k,l) : H^2_\Gamma(k,l) \to L^2_\Gamma$ is self-adjoint, positive definite, and has compact resolvents.*

By Lemma 3.1 and the spectral theorem for self-adjoint operators with compact resolvents, for each $k, l \in \mathbb{T}_1$ there exists a Schauder basis $\{f^{(m)}(k,l,\cdot,\cdot)\}_{m\in\mathbb{N}}$ of $L^2_\Gamma$ consisting of eigenfunctions of $\widetilde{L}(k,l)$ with positive eigenvalues $\{\lambda_m(k,l)\}_{m\in\mathbb{N}}$, ordered as $\lambda_m(k,l) \le \lambda_{m+1}(k,l)$. By construction, the $\lambda_m$ are periodic w.r.t. $k$ and $l$, and the Bloch wave functions satisfy (3.3) and (3.4), and the orthogonality and normalization relations

$$\left\langle f^{(m)}(k,l,\cdot,\cdot), f^{(m')}(k,l,\cdot,\cdot)\right\rangle_{L^2_\Gamma} = \delta_{m,m'}, \quad k,l \in \mathbb{T}_1. \tag{3.14}$$

Via the $\lambda_m$ we find $\omega = \omega^{(\pm m)}$ with $\omega^{(m)} = \sqrt{\lambda_m}$ and $\omega^{(-m)} = -\omega^{(m)}$.

Additionally, let $\Sigma^D = \{\lambda = k^2 + 1 : k \in \mathbb{N}\}$ denote the set of Dirichlet eigenvalues of $-\partial_x^2 + 1$ on $(0,\pi)$. Then each $\lambda \in \Sigma^D$ yields an eigenvalue $\lambda$ of $L$ of infinite multiplicity, with eigenspaces generated by so called simple loops which are localized in a single hexagon, see [27, Lemma 3.5]. By linear combinations of these localized eigenfunctions an associated Bloch mode representation can be constructed. Therefore, horizontal planes occur in the spectral picture plotted in Figure 2(b), which shows a selection of spectral surfaces $\lambda_m(k,l)$. For some $\lambda_m$ there appear conical singularities at certain so called Dirac points $(k,l) \in \mathbb{T}_1^2$. See Remark 3.3 for further comments. In summary, we have, cf. [27, Theorem 3.6].

**Theorem 3.2.** *The spectrum $\sigma(L)$ consists of the spectral surfaces $\mathbb{T}_1^2 \ni (k,l) \mapsto \lambda_m(k,l)$, $m \in \mathbb{N}$ (absolutely continous spectrum), and the eigenvalues $\Sigma^D$ of infinite multiplicity.*

*Remark* 3.3.

a) As already said above, the spectral problem can be analyzed more efficiently on the original hexagonal graph $\tilde{\Gamma}$ by choosing a minimal trapezoidal fundamental cell [27]. Transfering the analysis from [27] to our case (bond lengths $\pi$, potential $q_0 = 1$, cf. d)), we obtain that the spectral surfaces $\lambda \notin \Sigma^D$ are given by

$$\lambda_m(k,l) = 1 + \left(\frac{1}{\pi}\arccos(F(k,l)/3) + m\right)^2, \quad m \in \mathbb{Z}, \tag{3.15}$$

see Figure 2(c), where $F(k,l) = \left|1 + e^{i\pi k} + e^{i\pi l}\right|$, and $k,l$ are quasimomenta associated to non–orthogonal directions, e.g., $e_1 = \left(\sqrt{3}/2, 1/2\right)$ and $e_2 = (0,1)$. The function $F$ has range [0,3] with minima at $(k,l)_{\min} = \pm(2/3,-2/3)$ and a maximum at $(k,l)_{\max} = (0,0)$, yielding Dirac points. Similar fairly explicit results on dispersion relations for other periodic quantum graphs associated to tilings of the plane such as triangular graphs and trihexagonal (or Kagome) graphs are given in [30], again based on non-rectangular fundamental cells.

However, such non-orthogonal coordinates make the treatment of nonlinear terms (see below) in momentum space somewhat inconvenient, and we believe that our results on the nonlinear problems are easier interpreted in the orthogonal coordinates $x, y$. For these reasons we prefer to work on $\Gamma$. We remark that 'distorted' hexagonal graphs (of unequal side-length) also fit into this framework via rescaling of side-lengths, and that subsequently we comment on two other periodic quantum graphs which can be treated similarly, namely the rectangular graph (trivially), and the triangular graph, cf. Examples 4.1 and 4.2.

b) To (numerically) compute the dispersion relation in Figure 2(b) we proceed as follows. On $\Gamma^x_{0,1}$ and $\Gamma^x_{1,0}$ we have the ODE (3.5), while on the remaining bonds (3.6) applies. For (3.5) we choose a fundamental system $\phi_0, \phi_1$, and for (3.6) we choose $\psi_0, \psi_1$, which depend on $k$ and $l$, respectively. The solutions $f^x_{0,1}, f^y_{1,1}, \dots, f^y_{2,1}$ are then written as $f^x_{0,1} = \alpha_1\phi_0 + \beta_1\phi_1$, $f^y_{1,1} = \alpha_2\psi_0 + \beta_2\psi_1, \dots, f^y_{2,1} = \alpha_6\psi_0 + \beta_6\psi_1$, such that the vertex conditions (3.7)–(3.10) lead to a 12-dimensional system $M(k,l,\omega)\Phi = 0$ for the unknown coefficients $\Phi = \left(\alpha_1, \beta_1, \dots, \alpha_6, \beta_6\right)$ with nontrivial solutions if and only if

$$\det M(k,l,\omega) = 0. \tag{3.16}$$

This can be simplified considerably, starting with a smart choice of the fundamental system(s). For the different and simpler choice of the fundamental cell, this is done in [27], leading to the analytic solution in (3.15), and similarly in [30]. However, to obtain Figure 2(b) we simply solve (3.16) numerically, starting with different initial guesses for $\lambda(k,l)$ to obtain the given selection of surfaces.

c) Alternatively to (3.2) one can consider Bloch modes of the form $f(k,l,x,y)$ with cyclic boundary conditions

$$\begin{aligned} &f(k,l,x+2\pi,y) = e^{2\pi ikx} f(k,l,x,y) \quad \text{and} \quad f(k,l,x,y+2\pi) = e^{2\pi ily} f(k,l,x,y), \\ &f(k+1,l,x,y) = f(k,l+1,x,y) = f(k,l,x,y), \end{aligned} \tag{3.17}$$

in which case the associated linear problem is (3.5)–(3.10) with $\partial_x + ik$ and $\partial_y + il$ reset to $\partial_x$ and $\partial_y$, respectively. This for instance yields a slightly simpler calculus for the fundamental systems on the edges. One advantage of our ansatz (3.2) is a simpler isomorphism property of the associated Bloch transform stated in Lemma 6.1.

d) Instead of $-\partial_x^2 + 1$ on the edges we could also consider $-\partial_x^2 + q_0$ with a potential $q_0 \geq 0$, or even more generally $q_0 \in L^2((0,2\pi))$ nonnegative and even, i.e., $q_0(2\pi - x) = q_0(x)$, see [27]. The numerics as in b) work as long as we can find a fundamental system for the ODEs on the bonds. However, in order to not proliferate symbols we set $q_0 = 1$.

e) The flux vertex conditions (2.3) and (2.5) are often generalized to so called $\delta$ vertex conditions [4] of the form $\sum_{j=1}^N u_j' = \delta u$, assuming that $N$ edges meet in a vertex with suitable orientations of $x$ for incoming and outgoing edges. This can also be modified to so called $\delta'$ vertex conditions, and the only restriction is that $L$ stays self-adjoint. In many of these cases, a similar spectral analysis as above holds. However, here we are interested in the nonlinear problem (2.6), and for $\delta \neq 0$ the corresponding space $H^2_\Gamma$ is no longer closed under multiplication, and therefore we stick to (2.3), (2.5), i.e., $\delta = 0$.

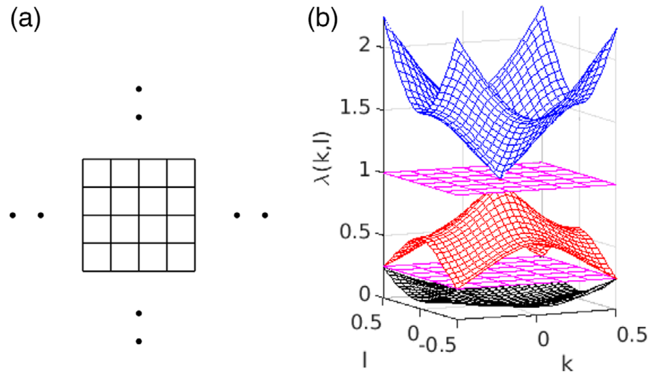


**FIGURE 3** A square periodic metric graph Γ (a), and exampe spectral surfaces (b), see (4.4).

## 4 | TWO OTHER EXAMPLES

We give two more examples of 2D periodic metric graphs for which the analysis of the present paper applies. For the first one this is trivial, but the second one shows that a treatment with rectangular fundamental cells is possible for, e.g., all the metric graphs treated in [30], i.e., for instance also for the trihexagonal (Kagome) graph. We emphazise that the procedure is useless for the linear problems, which can be treated more efficiently using non-rectangular fundamental cells, and that our transform to axis-parallel bonds is exclusively motivated by the nonlinear problems.

**Example 4.1** (The square graph). The periodic metric graph Γ from Figure 3(a) can be expressed as

$$\Gamma = \Gamma^x \oplus \Gamma^y, \qquad \text{with} \qquad \Gamma^x = \oplus_{n\in\mathbb{Z},m\in\mathbb{Z}}\Gamma^x_{m,n} \qquad \text{and} \qquad \Gamma^y = \oplus_{n\in\mathbb{Z},m\in\mathbb{Z}}\Gamma^y_{m,n},$$

where $\Gamma^x_{m,n}$ represents the horizontal link of length $2\pi$ between the points $(2\pi m, 2\pi n)$ and $(2\pi(m+1), 2\pi n)$ and where $\Gamma^y_{m,n}$ represents the vertical link of length $2\pi$ between the points $(2\pi m, 2\pi n)$ and $(2\pi m, 2\pi(n+1))$. For a function $u : \Gamma \to \mathbb{C}$, we denote the part on $\Gamma^x_{m,n}$ with $u^x_{m,n}$ and the parts on $\Gamma^y_{m,n}$ with $u^y_{m,n}$.

The second-order differential operator $-\Delta + q_0$, with $q_0 \geq 0$ a constant, is given by $-\partial_x^2 + q_0$ on $\Gamma^x_{m,n}$ and by $-\partial_y^2 + q_0$ on $\Gamma^y_{m,n}$. The Kirchhoff boundary conditions at the vertex points $\{(x,y)=(2\pi m, 2\pi n) : m,n\in\mathbb{Z}\}$ are now

$$u^x_{m,n}(2\pi m, 2\pi n) = u^x_{m-1,n}(2\pi m, 2\pi n) = u^y_{m,n}(2\pi m, 2\pi n) = u^y_{m,n-1}(2\pi m, 2\pi n), \tag{4.1}$$

$$\partial_x u^x_{m,n}(2\pi m, 2\pi n) - \partial_x u^x_{m-1,n}(2\pi m, 2\pi n) + \partial_y u^y_{m,n}(2\pi m, 2\pi n) - \partial_y u^y_{m,n-1}(2\pi m, 2\pi n) = 0. \tag{4.2}$$

Again we introduce the functions

$$u^x(x,y) = \begin{cases} u^x_{m,n}(x,y), & (x,y) \in \Gamma^x_{m,n}, \\ 0, & \text{elsewhere}, \end{cases} \qquad u^y(x,y) = \begin{cases} u^y_{m,n}(x,y), & (x,y) \in \Gamma^y_{m,n}, \\ 0, & \text{elsewhere}, \end{cases}$$

collect $u^x$ and $u^y$ in the vector $U = (u^x, u^y)$, and rewrite the evolutionary problem (2.1) as

$$\partial_t^2 U = \Delta U - q_0 U - U^3 = 0, \quad t \in \mathbb{R}, \quad (x,y) \in \Gamma \setminus (2\pi\mathbb{Z})^2, \tag{4.3}$$

subject to the conditions (4.1)–(4.2) at the vertex points $(x,y) \in (2\pi\mathbb{Z})^2$, and where the cubic nonlinear term stands for the vector $U^3 = \big((u^x)^3, (u^y)^3\big)$. Now we can proceed exactly as above. For instance, for $q_0 = 0$ (cf. Remark 3.3(d)), the spectral surfaces $\lambda_m = \omega_m^2$ are obtained from

$$\omega_m(k,l) = \frac{1}{2\pi} \arccos\left(\frac{1}{2}(\cos(2\pi k) + \cos(2\pi l))\right) + \frac{m}{2}, \quad m \in \mathbb{N}, \tag{4.4}$$

together with flat bands $\lambda = (m/2)^2, m \in \mathbb{N}$, see [11], and Figure 3(b) for a sketch. Obviously, rectangular graphs can be treated in the same way.

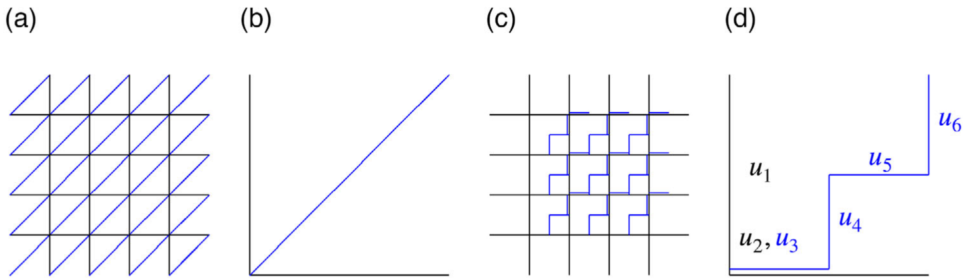


**FIGURE 4** (a),(b) The triangle graph and its fundamental cell. (c),(d) An equivalent metric triangle graph and its basic cell. Since we have metric graphs it does not matter which path we choose on the diagonal. However, since we changed the length from (b) to (d) we have to rescale the differential operator on the diagonal elements in (d). See the explanations above.

**Example 4.2** (The triangle graph). Figure 4 shows a triangle graph and a possible representation in rectangular coordinates, for which we choose as fundamental cell $\Gamma_1 \cup ... \cup \Gamma_6$ consisting of $\Gamma_1$ connecting $(0,0)$ with $(2\pi, 0)$, $\Gamma_2$ connecting $(0,0)$ with $(0, 2\pi)$, $\Gamma_3$ connecting $(0,0)$ with $(\pi, 0)$, $\Gamma_4$ connecting $(\pi, 0)$ with $(\pi,\pi)$, $\Gamma_5$ connecting $(\pi,\pi)$ with $(2\pi,\pi)$, and $\Gamma_6$ connecting $(2\pi,\pi)$ with $(2\pi, 2\pi)$. The parts $\Gamma_1$ and $\Gamma_2$ will be identified with the interval $[0, 2\pi]$, the parts $\Gamma_3$ and $\Gamma_4$ with the interval $[0,\pi]$, and the parts $\Gamma_5$ and $\Gamma_6$ with the interval $[\pi, 2\pi]$. The part of the solution living on $\Gamma_j$ is denoted by $u_j$. We obtain the following Bloch transformed eigenvalue problem

$$\begin{aligned}
(\partial_x + \mathrm{i}k)^2 u_1 - u_1 &= -\omega^2 u_1, && \text{on } \Gamma_1,\\
(\partial_y + \mathrm{i}l)^2 u_2 - u_2 &= -\omega^2 u_2, && \text{on } \Gamma_2,\\
\left(\sqrt{2}\partial_x + \mathrm{i}k\right)^2 u_{3,5} - u_{3,5} &= -\omega^2 u_{3,5}, && \text{on } \Gamma_{3,5},\\
\left(\sqrt{2}\partial_y + \mathrm{i}l\right)^2 u_{4,6} - u_{4,6} &= -\omega^2 u_{4,6}, && \text{on } \Gamma_{4,6},
\end{aligned}$$

where the scaling in the last two equations comes from the scaling of the diagonal to come from the original graph to the equivalent graph, i.e., $\tilde{x} = \sqrt{2}x$ implies $\partial_{\tilde{x}} = \sqrt{2}\partial_x$. The vertex conditions then are

$$\begin{aligned}
&u_1(0,0) = u_2(0,0) = u_3(0,0) = u_1(2\pi,0) = u_2(0,2\pi) = u_6(2\pi,2\pi),\\
&u_3(\pi,0) = u_4(\pi,0), \qquad u_4(\pi,\pi) = u_5(\pi,\pi), \qquad u_5(2\pi,\pi) = u_6(2\pi,\pi),\\
&\partial_x u_3(\pi,0) = \partial_y u_4(\pi,0), \qquad \partial_y u_4(\pi,\pi) = \partial_x u_5(\pi,\pi), \qquad \partial_x u_5(2\pi,\pi) = \partial_y u_6(2\pi,\pi), \text{ and}\\
&\partial_x u_1(0,0) + \partial_y u_2(0,0) + \sqrt{2}\partial_x u_3(0,0) - \partial_x u_1(2\pi,0) - \partial_y u_2(0,2\pi) - \sqrt{2}\partial_y u_6(2\pi,2\pi) = 0.
\end{aligned}$$

## 5 | LOCAL EXISTENCE AND UNIQUENESS

In this section we prove that the cKG equation (2.6) defines a well-posed initial value problem. The functional analytic frame which we use for the local existence and uniqueness of solutions of the cKG equation (2.6) will also be used as the basics for establishing the error estimates for the two approximations introduced in the subsequent sections.

From Theorem 3.2 we obtain the existence of a self-adjoint and positive definite root $\Omega$ of $L$. Thus, setting $V = -\Omega^{-1}\partial_t U$ we can rewrite (2.6) as

$$\partial_t W = \Lambda W + N(W), \tag{5.1}$$

with

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

As a consequence of classical semigroup theory [33], we have:

**Corollary 5.1.** *The skew symmetric operator* $\Lambda$ *with domain* $D(\Lambda) = D(\Omega) \times D(\Omega)$ *defines a unitary group* $\left(e^{\Lambda t}\right)_{t\in\mathbb{R}}$ *in* $\mathcal{L}^2$ *such that* $\left\|e^{\Lambda t} W\right\|_{\mathcal{L}^2} = \|W\|_{\mathcal{L}^2}$ *for every* $t \in \mathbb{R}$.

Another direct consequence of classical semigroup theory is

**Corollary 5.2.** *There exists a positive constant* $C_L$ *such that*

$$\left\|e^{\Lambda t} W\right\|_{(\mathcal{H}^2)^2} \leq C_L \|W\|_{(\mathcal{H}^2)^2} \tag{5.2}$$

*for every* $W \in \left(\mathcal{H}^2\right)^2$ *and every* $t \in \mathbb{R}$.

*Proof.* We find

$$\left\|e^{\Lambda t} W\right\|_{(\mathcal{H}^2)^2} \leq C\left\|\Lambda^2 e^{\Lambda t} W\right\|_{(\mathcal{L}^2)^2} \leq C\left\|e^{\Lambda t}\Lambda^2 W\right\|_{(\mathcal{L}^2)^2} = C\left\|\Lambda^2 W\right\|_{(\mathcal{L}^2)^2} \leq C\|W\|_{(\mathcal{H}^2)^2},$$

where we used the equivalence of the norms $\|\cdot\|_{(\mathcal{H}^2)^2}$ and $\left\|\Lambda^2 \cdot\right\|_{(\mathcal{L}^2)^2} = \|\mathrm{diag}(L, L)\cdot\|_{(\mathcal{L}^2)^2}$, that $\Lambda^2$ and $e^{\Lambda t}$ commute, and that $e^{\Lambda t}$ is a unitary group, cf. Corollary 5.1. □

Using additionally that the space $\mathcal{H}^2$ is closed under multiplication, cf. [20, Lemma 3.1], allows us to proceed with the general theory for semilinear dynamical systems [33] in proving the local existence and uniqueness of solutions of the initial value problem associated with the cKG equation (5.1) in the phase space $(\mathcal{H}^2)^2$.

**Theorem 5.3.** *For every* $W_0 \in \left(\mathcal{H}^2\right)^2$*, there exists a* $t_0 = t_0\left(\|W_0\|_{(\mathcal{H}^2)^2}\right) > 0$ *and a unique solution* $W \in C\left(\left[-t_0, t_0\right], \left(\mathcal{H}^2\right)^2\right)$ *of the cKG equation (5.1) with the initial data* $W|_{t=0} = W_0$.

*Proof.* From $U \in \mathcal{H}^2$ it follows that $U^3 \in \mathcal{H}^2$, cf. [20, Lemma 3.1]. Moreover, we have

$$\left\|\Omega^{-1} U^3\right\|_{\mathcal{H}^2} = \left\|\Omega U^3\right\|_{\mathcal{L}^2} \leq C\left\|\Omega^2 U^3\right\|_{\mathcal{L}^2} \leq \left\|U^3\right\|_{\mathcal{H}^2} \leq C\|W\|^3_{(\mathcal{H}^2)^2},$$

such that the nonlinearity is locally Lipschitz continuous from $\left(\mathcal{H}^2\right)^2$ to $\left(\mathcal{H}^2\right)^2$. Then we use the variation of constant formula to rewrite the initial value problem associated with (5.1) as

$$W(t, \cdot) = e^{\Lambda t} W_0 + \int_0^t e^{\Lambda(t-\tau)} N(W)(\tau)\, d\tau, \tag{5.3}$$

and seek the solution in the space

$$\mathcal{M} := \left\{ W \in C\left(\left[-t_0, t_0\right], \left(\mathcal{H}^2\right)^2\right) : \sup_{t\in[-t_0,t_0]} \left\|W(t,\cdot) - e^{\Lambda t} W_0\right\|_{(\mathcal{H}^2)^2} \leq C_3 \right\},$$

for a constant $C_3 > 0$ arbitrary, but fixed. For every $W_0 \in \left(\mathcal{H}^2\right)^2$, there is a sufficiently small $t_0 = t_0\left(\|W_0\|_{(\mathcal{H}^2)^2}\right) > 0$ such that the right-hand side of (5.3) is a contraction in the space $\mathcal{M}$. Therefore, Banach's fixed-point theorem implies the existence of a unique solution $W \in C\left(\left[-t_0, t_0\right], \left(\mathcal{H}^2\right)^2\right)$. □

*Remark* 5.4. Theorem 5.3 implies that there exists a unique solution $U \in C\left(\left[-t_0, t_0\right], \mathcal{H}^2\right) \cap C^1\left(\left[-t_0, t_0\right], \mathcal{H}^1\right)$ of the original system (2.6) with the initial conditions $W_0 = \left(U_0, \partial_t U_0\right) \in \mathcal{H}^2 \times \mathcal{H}^1 = D(L) \times D\left(L^{1/2}\right)$.

## 6 THE SYSTEM IN BLOCH SPACE

In order to apply the existing theory for the derivation and justification of modulation equations in periodic media to the 2D honeycomb graph, we have to Bloch transform the original nonlinear PDE over a Brillouin zone which is a torus. Since we work with metric graphs, we use the fact that the honeycomb graph is equivalent to the brick graph which easily can be Bloch transformed over a 2D torus as Brillouin zone. We briefly recall the main properties of Bloch transform $\mathcal{T}$ but refer to [20] and [36, §11.6.3] for further details. See also [26] for a very useful extensive summary and guide to the literature, based on a somewhat more general approach but also including many pointers to applications in the context of quantum graphs and otherwise.

Bloch transform $\mathcal{T}$ is the counterpart to Fourier transform $\mathcal{F}$ for spatially periodic problems. Bloch transform in $\mathbb{R}^d$ for media which is $2\pi$-periodic in every direction is defined by

$$\tilde{u}(\ell,\xi) = (\mathcal{T}u)(\ell,\xi) = \sum_{j\in\mathbb{Z}^d} e^{\mathrm{i}j\cdot\xi}\hat{u}(\ell+j), \tag{6.1}$$

where $\hat{u}(\kappa) = (\mathcal{F}u)(\kappa)$, $\kappa\in\mathbb{R}^d$, is the Fourier transform of $u$. The inverse Bloch transform is given by

$$u(\xi) = \left(\mathcal{T}^{-1}\tilde{u}\right)(\xi) = \int_{\mathbb{T}_1^d} e^{\mathrm{i}\ell\cdot\xi}\tilde{u}(\ell,\xi)\,d\ell. \tag{6.2}$$

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

$$\tilde{u}(\ell,\xi) = \tilde{u}\left(\ell,\xi+2\pi e_j\right) \quad\text{and}\quad \tilde{u}(\ell,\xi) = \tilde{u}\left(\ell+e_j,\xi\right)e^{\mathrm{i}\xi_j}, \tag{6.3}$$

where $e_j$ is the $j$-th unit vector in $\mathbb{R}^d$. The following lemma [5, 20] allows to transfer estimates from Bloch space into physical space and vice versa.

**Lemma 6.1.** *The Bloch transform $\mathcal{T}$ is an isomorphism between $H^s(\mathbb{R}^d)$ and $L^2\left(\mathbb{T}_1^d, H^s\left(\mathbb{T}_{2\pi}^d\right)\right)$, where $L^2\left(\mathbb{T}_1^d, H^s\left(\mathbb{T}_{2\pi}^d\right)\right)$ is equipped with the norm* $\|\tilde{u}\|_{L^2\left(\mathbb{T}_1^d,H^s\left(\mathbb{T}_{2\pi}^d\right)\right)} = \left(\int_{\mathbb{T}_1^d}\|\tilde{u}(\ell,\cdot)\|^2_{H^s\left(\mathbb{T}_{2\pi}^d\right)}\,d\ell\right)^{1/2}$.

Multiplication of two functions $u$ and $v$ in physical space corresponds to convolution in Bloch space, i.e.,

$$\mathcal{T}(uv)(\ell,\xi) = (\tilde{u}\star\tilde{v})(\ell,\xi) = \int_{\mathbb{T}_1^d}\tilde{u}(\ell-m,\xi)\tilde{v}(m,\xi)\,dm, \tag{6.4}$$

where the continuation conditions (6.3) have to be used for $\left|\ell_j-m_j\right|\geq 1$. If $\chi:\mathbb{R}^d\to\mathbb{R}^d$ is $2\pi$-periodic in every $e_j$-direction, then

$$\mathcal{T}(\chi u)(\ell,\xi) = \chi(\xi)(\mathcal{T}u)(\ell,\xi). \tag{6.5}$$

The relations (6.4) and (6.5) are well-known and can be proved directly from the definition (6.1).

We apply the Bloch transform $\mathcal{T}$ to (2.6) and obtain

$$\partial_t^2\tilde{U}(t,k,l,x,y) = -\tilde{L}(k,l)\tilde{U}(t,k,l,x,y) - \left(\tilde{U}\star\tilde{U}\star\tilde{U}\right)(t,k,l,x,y), \tag{6.6}$$

where the operator $\tilde{L}(k,l) := -\left(\partial_x+\mathrm{i}k\right)^2 - \left(\partial_y+\mathrm{i}l\right)^2 + 1$ is as in Lemma 3.1. The function $\tilde{U}(t,k,l,x,y) = \left(\tilde{u}^x,\tilde{u}^y\right)(t,k,l,x,y)$ satisfies

$$\tilde{U}(t,k,l,x,y) = \tilde{U}(t,k,l,x+2\pi,y) = \tilde{U}(t,k,l,x,y+2\pi) \text{ and} \tag{6.7}$$

$$\tilde{U}(t,k,l,x,y) = \tilde{U}(t,k+1,l,x,y)e^{\mathrm{i}x} = \tilde{U}(t,k,l+1,x,y)e^{\mathrm{i}y}, \tag{6.8}$$

and the convolution integrals $\tilde{U}\star\tilde{U}\star\tilde{U} = (\tilde{u}^x\star\tilde{u}^x\star\tilde{u}^x, \tilde{u}^y\star\tilde{u}^y\star\tilde{u}^y)$ are applied component-wise.

The Bloch transform $\widetilde{u}^x$ consists of $\widetilde{u}^x_{1,0}$ and $\widetilde{u}^x_{0,1}$ which for fixed $t, k, l$ have supports in $\Gamma^x_{1,0}$ and $\Gamma^x_{0,1}$, and similarly $\widetilde{u}^y$ consists of $\widetilde{u}^y_{1,0}, \widetilde{u}^y_{1,1}, \widetilde{u}^y_{2,0}$ and $\widetilde{u}^y_{2,1}$ which for fixed $t, k, l$ have supports in $\Gamma^y_{1,0}, \Gamma^y_{1,1}, \Gamma^y_{2,0}$ and $\Gamma^y_{2,1}$. This is a direct consequence of applying (6.5) to the function

$$u^{\zeta,\Sigma}_{m,n}(x,y) = \begin{cases} u^{\zeta}_{m,n}(x,y), (x,y) \in \Gamma^y_{\widetilde{m},\widetilde{n}}, & m - \widetilde{m} \in 2\mathbb{Z}, n - \widetilde{n} \in 2\mathbb{Z}, \\ 0, & \text{elsewhere}, \end{cases} \tag{6.9}$$

for $(\zeta, m, n) \in I_b$ (cf. 3.11) and with suitably chosen periodic cut-off functions $\chi$.

We proved the local existence and uniqueness of solutions of the cKG equation in $\mathcal{H}^2$, which is the domain of definition of the operator $L$ in $\mathcal{L}^2$. Its counterpart in Bloch space is given by

$$\widetilde{\mathcal{H}}^2 = \left\{ \widetilde{U} \in L^2\left(\mathbb{T}^2_1, L^2_\Gamma\right) : \widetilde{u}^{\zeta}_{m,n} \in L^2\left(\mathbb{T}^2_1, H^2\left(\Gamma^{\zeta}_{m,n}\right)\right), (\zeta, m, n) \in I_b, \text{(3.7)–(3.10) are satisfied} \right\},$$

which is the domain of definition of the operator $\widetilde{L}(k,l)$ from (3.12) in the space $L^2\left(\mathbb{T}_1, L^2_\Gamma\right)$, where $L^2_\Gamma$ is defined by (3.13). $\widetilde{\mathcal{H}}^2$ is equipped with the norm

$$\|\widetilde{U}\|_{\widetilde{\mathcal{H}}^2} = \left( \sum_{(\zeta,m,n)\in I_b} \int_{-1/2}^{1/2} \int_{-1/2}^{1/2} \left\| \widetilde{u}^{\zeta}_{m,n}(k,l,\cdot,\cdot) \right\|^2_{H^2(\Gamma^{\zeta}_{m,n})} dk\, dl \right)^{1/2},$$

and the Bloch transform $\mathcal{T}$ is an isomorphism between the spaces $\mathcal{H}^2$ and $\widetilde{\mathcal{H}}^2$, cf. [20, Lemma 4.2].

## 7 | EFFECTIVE DYNAMICS AT NON-DIRAC POINTS

At non-Dirac points of the spectrum with a multiple scaling expansion Nonlinear Schrödinger (NLS) equations can be derived in order to describe slow modulations in time and space of traveling wave packets. It is the purpose of this section to prove the validity of the NLS approximation for the cKG equation posed on the honeycomb graph.

### 7.1 | The result

We start by choosing a Bloch mode as underlying carrier wave with a Bloch wave vector $(k_0, l_0)$ which is not a Dirac point. Slow modulations in time and space of a small-amplitude modulated wave packet with this Bloch mode are described by the perturbation ansatz

$$U(t,x,y) = \varepsilon\Psi_{\text{nls}}(t,x,y) + \text{higher order terms}, \tag{7.1}$$

with

$$\varepsilon\Psi_{\text{nls}}(t,x,y) = \varepsilon A(T,X,Y) f^{(m_0)}\left(k_0, l_0, x, y\right) e^{\mathrm{i}k_0 x} e^{\mathrm{i}l_0 y} e^{\mathrm{i}\omega^{(m_0)}(k_0,l_0)t} + \text{c.c.}, \tag{7.2}$$

where $0 < \varepsilon \ll 1$ is a small perturbation parameter, $T = \varepsilon^2 t$ is the slow time variable, $X = \varepsilon(x - c_{g,x}t)$ and $Y = \varepsilon\left(y - c_{g,y}t\right)$ are long space variables, $A(T,X,Y) \in \mathbb{C}$ is the amplitude function, and c.c. stands for the complex conjugate of the preceding terms. The vector

$$\left(c_{g,x}, c_{g,y}\right) := \left(\partial_k \omega^{(m_0)}\left(k_0, l_0\right), \partial_l \omega^{(m_0)}\left(k_0, l_0\right)\right) \tag{7.3}$$

is the group velocity associated with the Bloch wave vector $(k_0, l_0)$. In particular, while $(x, y)$ are always coordinates on the graph $\Gamma$, and thus 'partially discrete', i.e., either $x = m\pi$ for some $m$, or $y = n\pi$ for some $n$, the large scale vector $(X, Y)$ runs continuously through all of $\mathbb{R}^2$. It turns out, cf. §3, that in the lowest order w.r.t. $\varepsilon$ the amplitude function $A$ satisfies the NLS equation

$$\mathrm{i}\partial_T A = -\left(\nu_{20}\partial_X^2 A + \nu_{11}\partial_X\partial_Y A + \nu_{02}\partial_Y^2 A\right) - \nu|A|^2 A, \tag{7.4}$$

with, due to our rectilinear coordinates $x, y$,

$$\nu_{20} = \frac{1}{2}\partial_k^2\omega^{(m_0)}(k_0, l_0), \quad \nu_{11} = \partial_k\partial_l\omega^{(m_0)}(k_0, l_0), \quad \nu_{02} = \frac{1}{2}\partial_l^2\omega^{(m_0)}(k_0, l_0), \tag{7.5}$$

and cubic coefficient

$$\nu = \frac{3\gamma}{2\mathrm{i}\omega^{(m_0)}(k_0, l_0)}, \text{ where } \gamma = \int_{\Gamma_b} \left| f^{(m_0)}(k_0, l_0, x, y)\right|^4 \mathrm{d}x\,\mathrm{d}y. \tag{7.6}$$

Our goal is the mathematical justification of the effective equation (7.4) by error estimates.

**Theorem 7.1.** *Choose $m_0 \in \mathbb{Z}$ and $k_0, l_0 \in \mathbb{T}_1$ such that the non-resonance conditions*

$$\omega^{(m)}(k_0, l_0) \neq \omega^{(m_0)}(k_0, l_0) \quad \textit{for all } m \neq m_0 \tag{7.7}$$

*and*

$$\omega^{(m)}(3k_0, 3l_0) \neq 3\omega^{(m_0)}(k_0, l_0) \quad \textit{for all } m \tag{7.8}$$

*are satisfied, where in (7.8) the periodicity of the $\omega^{(m)}$ has to be used. Then for every $\vartheta \in (1, 2]$, $C_0, C_1 > 0$ and $T_0 > 0$ there exist $\varepsilon_0 > 0$ and $C_2 > 0$ such that for all solutions $A \in C([0, T_0], H^4(\mathbb{R}^2))$ of the NLS equation (7.4) with*

$$\sup_{T\in[0,T_0]} \|A(T, \cdot)\|_{H^4} \leq C_0$$

*and all $\varepsilon \in (0, \varepsilon_0)$ the following holds. If*

$$\|U_0(\cdot,\cdot) - \varepsilon\Psi_{\mathrm{nls}}(0,\cdot,\cdot)\|_{\mathcal{H}^2} + \left\|U_1(\cdot,\cdot) - \varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\Psi_{\mathrm{nls}}(0,\cdot,\cdot)\right\|_{\mathcal{H}^1} \leq C_1\varepsilon^{\vartheta}, \tag{7.9}$$

*where $\varepsilon\Psi_{\mathrm{nls}}$ has been defined in (7.2), then there exists a unique solution $U \in C([-t_0, t_0], \mathcal{H}^2)$ of the cKG equation, $t_0 = T_0/\varepsilon^2$, with initial conditions $(U, \partial_t U)_{t=0} = (U_0, U_1)$, and this solution satisfies*

$$\sup_{t\in[0,T_0/\varepsilon^2]} \left( \|U(t,\cdot,\cdot) - \varepsilon\Psi_{\mathrm{nls}}(t,\cdot,\cdot)\|_{\mathcal{H}^2} + \left\|\partial_t U(t,\cdot,\cdot) - \varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\Psi_{\mathrm{nls}}(t,\cdot,\cdot)\right\|_{\mathcal{H}^1}\right) \leq C_2\varepsilon^{\vartheta}. \tag{7.10}$$

*Remark* 7.2.

a) (7.10) in particular implies

$$\sup_{t\in[0,T_0/\varepsilon^2]} \sup_{(x,y)\in\Gamma} |U(t,x,y) - \varepsilon\Psi_{\mathrm{nls}}(t,x,y)| \leq C\varepsilon^{\vartheta}. \tag{7.11}$$

b) It will be obvious that Theorem 7.1 remains valid if the rate $\varepsilon^{\vartheta}$ is replaced by a rate $o(\varepsilon)$ for $\varepsilon \to 0$.
c) The coefficients in (7.5) and (7.6) and the non-resonance conditions (7.7) and (7.8) are defined in terms of the eigenvalues and modes $\omega^{(m)}$ and $f^{(m)}$. Hence, the NLS equation (7.4) can be derived and justified whenever the spectral surfaces $\lambda_m$ can be computed and (7.7) and (7.8) hold. In this limit, the specifics of the problem condense in the coefficients $\nu_{ij}, \nu$. Adding higher order nonlinear terms such as $u^5$ to (2.1) does not change the effective equation (7.4) or the justification result Theorem 7.1 as they only produce higher order terms in the residual, which contains the terms that do not cancel on insertion of the approximation into the cKG equation. On the other hand, the case of quadratic nonlinearities is considerably more complicated already in the spatially homogeneous or smooth spatially periodic case, cf. [5], and is open for the case of graphs.
d) The non-resonance conditions (7.7) and (7.8) are used for defining an improved approximation which makes the residual sufficiently small. Although formally these are infinitely many conditions, for elliptic operators as above we only have finitely many 'dangerous' ones, which in practice can be checked. Additionally, (7.7) is already used in the derivation of $\nu$ in (7.6) to have a well defined $\gamma$, which requires some regularity of $(k, l) \mapsto f^{(m_0)}(k, l, \cdot, \cdot)$, cf. (7.20).

In particular, (7.7) excludes intersection points of the spectral surfaces, and thus here especially the Dirac points, cf. Figure 2.

e) This approximation has successfully been used as a universal envelope or modulation equation in many fields, such as in nonlinear optics [2], for the description of water waves [39], for waves in DNA [37], for Bose–Einstein condensates [34], or in plasma physics [8].
f) 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 [24]. See [36, Chapter 11] for an introduction into the mathematical validity theory of NLS approximations. In the context of smooth spatially periodic coefficients the justification of the NLS approximation has been carried out in [5]. In [20] the validity of the NLS approximation for the NLS equation posed on a 1D necklace graph has been proven.
g) We finally remark that in contrast to the 1D NLS equation there is the possibility of finite time blow up in the 2D NLS equation, cf. [29].

## 7.2 | Derivation of the NLS equation

In Bloch space we split the solution to the evolution problem (6.6) into two parts. We introduce

the Bloch wave vector $\ell = (k, l)$, and the coordinate vector $\xi = (x, y)$,

and write

$$\widetilde{U}(t, \ell, \xi) = \widetilde{V}(t, \ell) f^{(m_0)}(\ell, \xi) + \widetilde{U}^{\perp}(t, \ell, \xi), \tag{7.12}$$

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

$$\partial_t^2 \widetilde{V}(t, \ell) = -\left(\omega^{(m_0)}(\ell)\right)^2 \widetilde{V}(t, \ell) - N_V\left(\widetilde{V}, \widetilde{U}^{\perp}\right)(t, \ell), \tag{7.13}$$

$$\partial_t^2 \widetilde{U}^{\perp}(t, \ell, \xi) = -\widetilde{L}(k, \ell) \widetilde{U}^{\perp}(t, \ell, \xi) - N^{\perp}\left(\widetilde{V}, \widetilde{U}^{\perp}\right)(t, \ell, \xi), \tag{7.14}$$

where

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

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

Since we have an original system (2.1) without quadratic terms, for the derivation of the NLS equation it is sufficient to consider (7.13) and to set there $\widetilde{U}^{\perp} = 0$. The nonlinear terms in (7.13) are of the form

$$\begin{aligned} N_V\left(\widetilde{V}, \widetilde{U}^{\perp}\right)(t, \ell) = & \int_{\mathbb{T}_1^2} \int_{\mathbb{T}_1^2} \beta(\ell, \ell - \ell_1, \ell_1 - \ell_2, \ell_2) \widetilde{V}(t, \ell - \ell_1) \widetilde{V}(t, \ell_1 - \ell_2) \widetilde{V}(t, \ell_2)\, d\ell_2\, d\ell_1 \\ & + N_{V,rest}\left(\widetilde{V}, \widetilde{U}^{\perp}\right)(t, \ell), \end{aligned} \tag{7.15}$$

where the kernel $\beta$ is given by

$$\beta(\ell, \ell - \ell_1, \ell_1 - \ell_2, \ell_2) = \left\langle f^{(m_0)}(\ell, \cdot), f^{(m_0)}(\ell - \ell_1, \cdot) f^{(m_0)}(\ell_1 - \ell_2, \cdot) f^{(m_0)}(\ell_2, \cdot)\right\rangle_{L^2_\Gamma}, \tag{7.16}$$

and where $N_{V,rest}(\widetilde{V}, 0) = 0$.

For the formal derivation of the NLS equation in Bloch space we make the ansatz

$$\widetilde{V}_{\mathrm{app}}(t, \ell) = \varepsilon\varepsilon^{-2} \widetilde{A}_1\left(\varepsilon^2 t, \frac{\ell - \ell_0}{\varepsilon}\right) \mathbf{E}^1(t, \ell) + \varepsilon\varepsilon^{-2} \widetilde{A}_{-1}\left(\varepsilon^2 t, \frac{\ell + \ell_0}{\varepsilon}\right) \mathbf{E}^{-1}(t, \ell), \tag{7.17}$$

with

$$\mathbf{E}^j(t,\ell) = e^{-j\mathrm{i}\omega^{(m_0)}(\ell_0)t}e^{-\mathrm{i}\partial_\ell\omega^{(m_0)}(\ell_0)(\ell-j\ell_0)t}, \text{ where } \partial_\ell\omega^{(m_0)} := \left(\partial_k\omega^{(m_0)}, \partial_l\omega^{(m_0)}\right).$$

*Remark* 7.3. If $A(\cdot)$ is defined on $\mathbb{R}^d$ and if it is scaled with the small parameter $\varepsilon$, then the Fourier transform of $A(\varepsilon\cdot)$ is $\varepsilon^{-d}\widehat{A}(\varepsilon^{-1}\cdot)$. Therefore, a small term of the formal order $\mathcal{O}(\varepsilon^r)$ in physical space corresponds to a small term of the formal order $\mathcal{O}(\varepsilon^{r-d})$ in Fourier space. The same holds in Bloch space, which explains the scaling and somewhat unusual notation $\varepsilon\varepsilon^{-2}$ in (7.17) and henceforth.

However, there is a problem with (7.17), namely that the support of the scaled $\widetilde{A}_{\pm1}$ gets bigger with $\varepsilon > 0$ getting smaller, and becomes the whole infinite plane for $\varepsilon \to 0$. Moreover, since the $\widetilde{A}_{\pm1}$ should satisfy in physical space a NLS equation on the infinite plane, the $\widetilde{A}_{\pm1}$ will be taken in Fourier space and not in Bloch space. So let $\widehat{A}_1$ be the solution of the Fourier transformed NLS equation (7.4).

In order to bring together the Fourier space representation of the NLS equation with the Bloch wave representation (6.6) of the cKG equation we introduce a number of operators. We start with a cut-off operator $\chi \in C_0^\infty(\mathbb{R}^2, \mathbb{R})$ with $\chi(\ell) \in [0,1]$, $\chi(\ell) = 1$ for $|\ell| \le 1/5$, and $\chi(\ell) = 0$ for $|\ell| \ge 2/5$, and an extension operator $\mathcal{P}$ which extends a function with length of support less than 1 in the $k$- and the $l$-direction to a function on $\mathbb{R}^2$ with period 1 in the $k$- and the $l$-direction. With these operators we modify the previous ansatz (7.17) to

$$\widetilde{V}(\ell,t) = \varepsilon\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot-\ell_0)\widehat{A}_1\left(\varepsilon^2 t, \frac{\cdot-\ell_0}{\varepsilon}\right)\mathbf{E}^1(t,\cdot)\right)(\ell) + \varepsilon\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot+\ell_0)\widehat{A}_{-1}\left(\varepsilon^2 t, \frac{\cdot+\ell_0}{\varepsilon}\right)\mathbf{E}^{-1}(t,\cdot)\right)(\ell). \tag{7.18}$$

Plugging (7.18) into (7.13) we find that all terms at $\varepsilon\varepsilon^{-2}\mathbf{E}$ and $\varepsilon^2\varepsilon^{-2}\mathbf{E}$ cancel, and at $\varepsilon^3\varepsilon^{-2}\mathbf{E}$ we obtain the NLS equation

$$-2i\omega^{(m_0)}(\ell_0)\partial_T\widehat{A}_1 = \frac{1}{2}\left(\partial_\ell^2\lambda^{m_0}(\ell_0) - 2\left(\partial_\ell\omega^{(m_0)}(\ell_0)\right)\left(\partial_\ell\omega^{(m_0)}(\ell_0)\right)^T\right)|\kappa|^2\widehat{A}_1 - 3\gamma\widehat{A}_1 * \widehat{A}_1 * \widehat{A}_{-1}, \tag{7.19}$$

where $T = \varepsilon^2 t$, $\kappa = \varepsilon^{-1}(\ell - \ell_0)$ and $\gamma = \beta(\ell_0, \ell_0, \ell_0, -\ell_0) \in \mathbb{R}$, while $A_{-1} = \mathcal{F}^{-1}\widehat{A}_{-1}$ satisfies the complex conjugate NLS equation. In order to obtain (7.19) we used formal calculations such as

$$\begin{aligned}
&\partial_t^2\left(\varepsilon\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot-\ell_0)\widehat{A}_1\left(\varepsilon^2 t, \frac{\cdot-\ell_0}{\varepsilon}\right)\mathbf{E}^1(t,\cdot)\right)(\ell)\right)\\
&= \partial_t^2\left(\varepsilon\varepsilon^{-2}\mathcal{P}(\chi(\cdot-\ell_0)\widehat{A}_1\left(\varepsilon^2 t, \frac{\cdot-\ell_0}{\varepsilon}\right)e^{-\mathrm{i}\omega^{(m_0)}(\ell_0)t}e^{-\mathrm{i}\partial_\ell\omega^{(m_0)}(\ell_0)(\ell-\ell_0)t}\right)\\
&= \mathbf{E}^1(t,\cdot)(\ell)\left(-\mathrm{i}\omega^{(m_0)}(\ell_0) - \varepsilon\mathrm{i}\partial_\ell\omega^{(m_0)}(\ell_0)\kappa\right)^2\widehat{A}_1(T,\kappa)\\
&\quad + \mathbf{E}^1(t,\cdot)(\ell)2\varepsilon^2\left(-\mathrm{i}\omega^{(m_0)}(\ell_0) - \varepsilon\mathrm{i}\partial_\ell\omega^{(m_0)}(\ell_0)\kappa\right)\partial_T\widehat{A}_1(T,\kappa) + \mathcal{O}(\varepsilon^3)
\end{aligned}$$

and

$$\begin{aligned}
&-\left(\omega^{(m_0)}(\ell)\right)^2\left(\varepsilon\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot-\ell_0)\widehat{A}_1\left(\varepsilon^2 t, \frac{\cdot-\ell_0}{\varepsilon}\right)\mathbf{E}^1(t,\cdot)\right)(\ell)\right)\\
&= -\left(\omega^{(m_0)}(\ell_0+\varepsilon\kappa)\right)^2\left(\varepsilon\varepsilon^{-2}\mathcal{P}\left(\chi(\varepsilon\kappa)\widehat{A}_1(T,\kappa)\mathbf{E}^1(t,\cdot)\right)(\ell)\right)\\
&= -\left(\omega^{(m_0)}(\ell_0) + \varepsilon\partial_\ell\omega^{(m_0)}(\ell_0)\kappa + \frac{1}{2}\varepsilon^2\kappa^T\partial_\ell^2\omega^{(m_0)}(\ell_0)\kappa + \mathcal{O}(\varepsilon^3)\right)^2\widehat{A}_1(T,\kappa)\mathbf{E}^1(t,\cdot)(\ell) + \mathcal{O}(\varepsilon^3),
\end{aligned}$$

and that formally

$$\begin{aligned}
&\varepsilon^{-4}\int_{\mathbb{T}^2_{1/\varepsilon}}\int_{\mathbb{T}^2_{1/\varepsilon}}\beta(\ell_0+\varepsilon\kappa, \ell_0+\varepsilon(\kappa-\kappa_1), \ell_0+\varepsilon(\kappa_1-\kappa_2), -\ell_0+\varepsilon\kappa_2)\widetilde{A}_1(\kappa-\kappa_1)\widetilde{A}_1(\kappa_1-\kappa_2)\widetilde{A}_{-1}(\kappa_2)\,d\kappa_2\,d\kappa_1\\
&\longrightarrow \gamma\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\widehat{A}_1(\kappa-\kappa_1)\widehat{A}_1(\kappa_1-\kappa_2)\widehat{A}_{-1}(\kappa_2)\,d\kappa_2\,d\kappa_1
\end{aligned} \tag{7.20}$$

for $\varepsilon \to 0$, and the symmetry of the kernel. Division by $2i\omega^{(m_0)}(\ell_0)$ yields (7.4).

*Remark* 7.4. This derivation of (7.4) from (7.19) is consistent with the derivation from the associated first order system, cf. [9, Chapter 5], since for instance

$$
\begin{aligned}
&\big(\partial_\ell^2 \lambda^{m_0}(\ell_0) - 2\big(\partial_\ell \omega^{(m_0)}(\ell_0)\big)\big(\partial_\ell \omega^{(m_0)}(\ell_0)\big)^T\big)/\big(4i\omega^{(m_0)}(\ell_0)\big)\\
&\quad = -\big(\partial_\ell^2 \big(\omega^{(m_0)}(\ell_0)^2\big) - 2\big(\partial_\ell \omega^{(m_0)}(\ell_0)\big)\big(\partial_\ell \omega^{(m_0)}(\ell_0)\big)^T\big)/\big(4i\omega^{(m_0)}(\ell_0)\big)\\
&\quad = i\partial_\ell^2 \omega^{(m_0)}(\ell_0)/2.
\end{aligned}
$$

## 7.3 | The improved approximation and estimates for the residual terms

The approximation (7.17) produces a number of terms in (7.14) which are of the formal order $\mathcal{O}(\varepsilon^3)$ in physical space. These terms are collected together in the so called residual. However, in order to subsequently bound the error with a simple application of Gronwall's inequality, we need the residual to be of the formal order $\mathcal{O}(\varepsilon^{4+\delta})$ in physical space for a $\delta > 0$. This can be achieved by adding higher order terms to the approximation (7.17) such that all terms up to formal order $\mathcal{O}(\varepsilon^4)$ in physical space cancel.

In order to obtain a not too restrictive set of non-resonance conditions we modify our previous separation of the modes. Again we set

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

with $\big\langle f^{(m_0)}(\ell,\cdot), \widetilde{U}^{\perp}(\ell,\cdot,t)\big\rangle_{L^2_\Gamma} = 0$, but now the two functions $\widetilde{V}(\ell,t)$ and $\widetilde{U}^{\perp}(\ell,\xi,t)$ are defined to satisfy

$$
\begin{aligned}
\partial_t^2 \widetilde{V}(\ell,t) &= -\lambda_{m_0}(\ell)\widetilde{V}(\ell,t) + E_c(\ell)\big\langle f^{(m_0)}(\ell,\cdot),\, \widetilde{U}^{\star 3}(\ell,\cdot,t)\big\rangle_{L^2_\Gamma},\\
\partial_t^2 \widetilde{U}^{\perp}(\ell,\xi,t) &= -\widetilde{L}(\ell,\partial_\xi)\widetilde{U}^{\perp}(\ell,\xi,t) + \widetilde{U}^{\star 3}(\ell,\xi) - E_c(\ell)\big\langle f^{(m_0)}(\ell,\cdot),\, \widetilde{U}^{\star 3}(\ell,\cdot,t)\big\rangle_{L^2_\Gamma} f^{(m_0)}(\ell,\xi),
\end{aligned}
$$

where the so called mode-filter $E_c$ is in $C^\infty(\mathbb{T}_1^2,\mathbb{R})$ and fulfills $E_c(\ell) \in [0,1]$ with $E_c(\ell) = 1$ for $\ell \in U_\rho(-\ell_0) \cup U_\rho(\ell_0)$ for a small $\rho > 0$, $E_c(\ell) = 0$ elsewhere. Thus, the support of $\widetilde{V}(\ell,t)$ can and will be chosen to be contained in the support of $E_c$.

We add higher order terms to the ansatz to make the residual smaller, i.e., we consider

$$
\begin{aligned}
\widetilde{V}(\ell,t) = \sum_{j=0,1} \Bigg( &\varepsilon^{1+j}\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot-\ell_0)\widehat{A}_{1,j}\left(\frac{\cdot-\ell_0}{\varepsilon},\varepsilon^2 t\right)\mathbf{E}^1\right)(\ell)\\
&+\varepsilon^{1+j}\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot+\ell_0)\widehat{A}_{-1,j}\left(\frac{\cdot+\ell_0}{\varepsilon},\varepsilon^2 t\right)\mathbf{E}^{-1}\right)(\ell)\\
&+\varepsilon^{3+j}\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot-3\ell_0)\widehat{A}_{3,j}\left(\frac{\cdot-3\ell_0}{\varepsilon},\varepsilon^2 t\right)\mathbf{E}^3\right)(\ell)\\
&+\varepsilon^{3+j}\varepsilon^{-2}\mathcal{P}\left(\chi(\cdot+3\ell_0)\widehat{A}_{-3,j}\left(\frac{\cdot+3\ell_0}{\varepsilon},\varepsilon^2 t\right)\mathbf{E}^{-3}\right)(\ell)\Bigg),\\
\widetilde{U}^{\perp}(\ell,\xi) = {}&\varepsilon^3\varepsilon^{-2}\widetilde{U}_1^{\perp}\left(\frac{\ell-\ell_0}{\varepsilon},\xi,\varepsilon^2 t\right)\mathbf{E}^1 + \varepsilon^3\varepsilon^{-2}\widetilde{U}_{-1}^{\perp}\left(\frac{\ell+\ell_0}{\varepsilon},\xi,\varepsilon^2 t\right)\mathbf{E}^{-1}\\
&+\varepsilon^3\varepsilon^{-2}\widetilde{U}_3^{\perp}\left(\frac{\ell-3\ell_0}{\varepsilon},\xi,\varepsilon^2 t\right)\mathbf{E}^3 + \varepsilon^3\varepsilon^{-2}\widetilde{U}_{-3}^{\perp}\left(\frac{\ell+3\ell_0}{\varepsilon},\xi,\varepsilon^2 t\right)\mathbf{E}^{-3}.
\end{aligned}
$$

As before we find $\widehat{A}_{1,0}$ as a solution of the NLS equation (7.19) and $\widehat{A}_{-1,0}$ as a solution of the complex conjugate equation. The $\widehat{A}_{\pm 1,j}$, $j \neq 0$, satisfy linearized Schrödinger equations with an inhomogeneity which contains third derivatives of $\omega^{(m_0)}$

in $\ell_0$ and first derivatives of the kernel $\beta$. For instance $\widehat{A}_{1,1}$ satisfies

$$-2i\omega^{(m_0)}(\ell_0)\partial_T\widehat{A}_{1,1} = \frac{1}{2}\left(\partial_\ell^2\lambda^{m_0}(\ell_0) - 2\left(\partial_\ell\omega^{(m_0)}(\ell_0)\right)\left(\partial_\ell\omega^{(m_0)}(\ell_0)\right)^T\right)|\kappa|^2\widehat{A}_{1,1}$$
$$-6\gamma\widehat{A}_{1,1} * \widehat{A}_1 * \widehat{A}_{-1} - 3\gamma\widehat{A}_1 * \widehat{A}_1 * \widehat{A}_{-1,1} + g_{1,1},$$

where the inhomogeneity $g_{1,1}$ here only depend on the $\widehat{A}_{\pm1}$ and contains terms such as the linear term $\frac{1}{6}\left(\partial_k^3\lambda^{m_0}(\ell_0)\right)\kappa_{(1)}^3\widehat{A}_1$ or the nonlinear term

$$\int_{\mathbb{R}^2}\int_{\mathbb{R}^2}\left(\partial_1\beta(\ell_0,\ell_0,\ell_0,-\ell_0)\cdot\kappa\right)\widehat{A}_1(\kappa-\kappa_1)\widehat{A}_1(\kappa_1-\kappa_2)\widehat{A}_{-1}(\kappa_2)\,d\kappa_2\,d\kappa_1.$$

Using appropriate non–resonance conditions (see below), we choose $\widehat{A}_{3,0}$ as the solution of

$$0 = 9\left(\omega^{(m_0)}\right)^2(\ell_0)\widehat{A}_{3,0}(\kappa,T) - \lambda_{m_0}(3\ell_0)\widehat{A}_{3,0}(\kappa,T) + \left\langle f^{(m_0)}(3\ell_0,\cdot),\ \left(f^{(m_0)}(\ell_0,\cdot)\right)^3\right\rangle_{L^2_\Gamma}\widehat{A}_{1,0}^{*3}(\kappa,T),$$

and $\widehat{A}_{3,1}$ as the solution of the linearized equation with an inhomogeneity which contains first derivatives of $\omega^{(m_0)}$ in $3\ell_0$ and first order derivatives of the kernel $\beta$. We choose the $\widehat{A}_{-3,j}$ as the solutions of the associated complex conjugate equations. All this is well documented in the literature, cf. [9, Chapter 5]. Here we concentrate on new aspects having to do with non-smoothness w.r.t. $\xi$. We choose $\widetilde{U}_1^\perp$ and $\widetilde{U}_3^\perp$ as the solutions of

$$0 = \left(\omega^{(m_0)}\right)^2(\ell_0)\widetilde{U}_1^\perp(\ell,\xi,t) - \widetilde{L}(\ell_0+\varepsilon\kappa,\partial_\xi)\widetilde{U}_1^\perp(\kappa,\xi,T) + N_1^\perp(A_{\pm1,j}),$$
$$0 = 9\left(\omega^{(m_0)}\right)^2(\ell_0)\widetilde{U}_3^\perp(\ell,\xi,t) - \widetilde{L}(3\ell_0+\varepsilon\kappa,\partial_\xi)\widetilde{U}_3^\perp(\kappa,\xi,T) + N_3^\perp(A_{\pm1,j}),$$

respectively, where $N_1^\perp$ and $N_3^\perp$ contain all nonlinear terms concentrated at $\ell_0$ and $3\ell_0$ and which solely depend on $A_{\pm1,j}$. By this choice formally all terms of $\mathcal{O}(\varepsilon^3)$ and $\mathcal{O}(\varepsilon^4)$ cancel. This choice has the advantage that we do not have to expand the operator $\widetilde{L}(\ell_0+\varepsilon\kappa,\partial_\xi)$ w.r.t. $\kappa$ which would lead to a loss of regularity w.r.t. $\xi$. We choose $\widetilde{U}_{-1}^\perp$ and $\widetilde{U}_{-3}^\perp$ as the solutions of the associated complex conjugate equations.

In order to solve the equations for $\widehat{A}_3$, $\widetilde{U}_1^\perp$, and $\widetilde{U}_3^\perp$, a number of non-resonance conditions are needed. By making the support of $E_c$ smaller these condense in

$$\left(\omega^{(m_0)}\right)^2(\ell_0) \notin \operatorname{spec}\left(\widetilde{L}(\ell_0,\partial_\xi)\right)|_{\{f^{(m_0)}(\ell_0,\cdot)\}^\perp}, \tag{7.21}$$

which corresponds to (7.7), and

$$9\left(\omega^{(m_0)}\right)^2(\ell_0) \neq \lambda^{(m_0)}(3\ell_0),\ \text{and}\ 9\left(\omega^{(m_0)}\right)^2(\ell_0) \notin \operatorname{spec}\left(\widetilde{L}(3\ell_0,\partial_\xi)\right)|_{\{f^{(m_0)}(3\ell_0,\cdot)\}^\perp}, \tag{7.22}$$

which corresponds to (7.8). Then we have that

$$\widetilde{\operatorname{Res}}(\varepsilon\widetilde{\Psi}) = -\partial_t^2\widetilde{U}(t,\ell,\xi) - \widetilde{L}(\ell)\widetilde{U}(t,\ell,\xi) - \left(\widetilde{U}\star\widetilde{U}\star\widetilde{U}\right)(t,\ell,\xi)$$

is of order $\mathcal{O}(\varepsilon^4)$ in $\mathcal{H}^2$ in physical space:

**Lemma 7.5.** *Let $A \in C([0,T_0],H^4)$ be a solution of the effective equation (7.4) for some $T_0 > 0$. Then there exists a $C_{\text{Res}} > 0$ that only depends on the norm of the solution $A$ such that*

$$\sup_{t\in[0,T_0/\varepsilon^2]}\left\|\widetilde{\operatorname{Res}}(\varepsilon\widetilde{\Psi})\right\|_{\widetilde{\mathcal{H}}^2} \leq C_{\text{Res}}\varepsilon^4, \tag{7.23}$$

*or equivalently,*

$$\sup_{t\in[0,T_0/\varepsilon^2]}\|\operatorname{Res}(\varepsilon\Psi)\|_{\mathcal{H}^2} \leq C_{\text{Res}}\varepsilon^4. \tag{7.24}$$

*Proof.* The proof is straightforward and follows [20, Section 5.3] almost line for line. □

*Remark* 7.6. Compared to Remark 7.3 on the formal order in physical $(\mathcal{O}(\varepsilon^5))$ and Bloch space $(\mathcal{O}(\varepsilon^3))$, we note that bounds (7.23) and (7.24) are identical in physical and Bloch space. This is because we gain $\varepsilon$ in the $\widetilde{\mathcal{H}}^2$-norm due to the concentration, and lose $\varepsilon^{-1}$ in the $\mathcal{H}^2$-norm due to the long wave scaling.

## 7.4 | Estimates for the error

The remainder of the proof of Theorem 7.1 is based on energy estimates and an application of Gronwall's inequality. To do so we introduce another space. By construction, the leading-order approximation $\widetilde{V}_{\text{app}} f^{(m_0)}$ is of the order $\mathcal{O}(1)$ in $\widetilde{\mathcal{H}}^2$ due to the scaling properties of the $L^2$-norm, and thus we lose $\varepsilon^{-1}$ in naive convolution estimates in $\widetilde{\mathcal{H}}^2$. In order to avoid this, we introduce as in [20] an $L^1$-based space, namely

$$\widetilde{\mathcal{C}}^2 = \left\{\widetilde{U} \in L^1(\mathbb{T}_1^2, L^2_\Gamma) \,:\, \widetilde{u}^\zeta_{m,n} \in L^1(\mathbb{T}_1^2, H^2(\Gamma^\zeta_{m,n})), (\zeta, m, n) \in I_b, \text{(3.7)–(3.10) are satisfied}\right\},$$

equipped with the norm

$$\left\|\widetilde{U}\right\|_{\widetilde{\mathcal{C}}^2} = \sum_{(\zeta,m,n)\in I_b} \int_{-1/2}^{1/2}\int_{-1/2}^{1/2} \left\|\widetilde{u}^\zeta_{m,n}(k,l,\cdot,\cdot)\right\|_{H^2(\Gamma^\zeta_{m,n})} dk\, dl.$$

By Young's inequality we have $\|\widetilde{V}\star\widetilde{W}\|_{\widetilde{\mathcal{H}}^2} \le \|\widetilde{V}\|_{\widetilde{\mathcal{C}}^2}\|\widetilde{W}\|_{\widetilde{\mathcal{H}}^2}$, and, similar to [20, Lemma 5.7]:

**Lemma 7.7.** *Let $A \in C([0, T_0], H^4)$ be a solution of the NLS equation (7.4) for some $T_0 > 0$. Then there exist $C, C_\Psi > 0$ that only depend on the norm of the solution $A$ such that*

$$\sup_{t\in[0,T_0/\varepsilon^2]} \left\|\varepsilon\widetilde{\Psi}\right\|_{\widetilde{\mathcal{C}}^2} \le C_\Psi \varepsilon \tag{7.25}$$

*and*

$$\sup_{t\in[0,T_0/\varepsilon^2]} \|\varepsilon\Psi - \varepsilon\Psi_{\text{nls}}\|_{L^\infty} \le C\varepsilon^{3/2}. \tag{7.26}$$

In order to establish the error estimates we write the solution $U$ of (2.6) as a sum of the approximation $\varepsilon\Psi$ and an error $\varepsilon^\vartheta R$, i.e.,

$$U = \varepsilon\Psi + \varepsilon^\vartheta R, \tag{7.27}$$

and obtain

$$\partial_t^2 R = -LR + G(\Psi, R), \tag{7.28}$$

with the linear operator $L = -\Delta + 1$ and the remainder

$$G(\Psi, R) = \varepsilon^{-\vartheta}\text{Res}(\varepsilon\Psi) + 3\varepsilon^2\Psi^2 R + 3\varepsilon^{1+\vartheta}\Psi R^2 + \varepsilon^{2\vartheta}R^3.$$

The product terms in the definition of $G(\Psi, R)$ have to be understood componentwise with $R = (r^x, r^y)$ and $\Psi = (\psi^x, \psi^y)$. Using

$$\|\Psi R\|_{\mathcal{H}^2} \le C\left\|\widetilde{\Psi} * \widetilde{R}\right\|_{\widetilde{\mathcal{H}}^2} \le C\left\|\widetilde{\Psi}\right\|_{\widetilde{\mathcal{C}}^2}\left\|\widetilde{R}\right\|_{\widetilde{\mathcal{H}}^2} \le CC_\Psi\left\|\widetilde{R}\right\|_{\widetilde{\mathcal{H}}^2} \le C^2C_\Psi\|R\|_{\mathcal{H}^2},$$

we estimate the terms of $G$ as

$$\left\|\varepsilon^{-\vartheta}\text{Res}(\varepsilon\Psi)\right\|_{\mathcal{H}^2} \le C_{\text{Res}}\varepsilon^2, \quad \|3\varepsilon^2\Psi^2 R\|_{\mathcal{H}^2} \le 3C_3\varepsilon^2\|R\|_{\mathcal{H}^2},$$

$$\left\|3\varepsilon^{1+\vartheta}\Psi R^2\right\|_{\mathcal{H}^2} \leq 3C_3\varepsilon^{1+\vartheta}\|R\|^2_{\mathcal{H}^2}, \quad \left\|\varepsilon^{2\vartheta}R^3\right\|_{\mathcal{H}^2} \leq C_3\varepsilon^{2\vartheta}\|R\|^3_{\mathcal{H}^2},$$

where $C_3$ is a constant independent of $\|R\|_{\mathcal{H}^2}$ and the small parameter $\varepsilon > 0$. Therefore,

$$\|G(\Psi, R)\|_{\mathcal{H}^2} \leq C_{\mathrm{Res}}\varepsilon^2 + 3C_3\varepsilon^2\|R\|_{\mathcal{H}^2} + 3C_3\varepsilon^{1+\vartheta}\|R\|^2_{\mathcal{H}^2} + C_3\varepsilon^{2\vartheta}\|R\|^3_{\mathcal{H}^2}. \tag{7.29}$$

The local existence and uniqueness of solutions $R$ of (7.28) works exactly as for the original cKG equation in §5, cf. Remark 5.4. Our goal is to use energy estimates to show that $R$ stays $\mathcal{O}(1)$ bounded on the long time interval $0 \leq t \leq t_0 = T_0/\varepsilon^2$. Let $E_R = \langle LR, LR\rangle_{\mathcal{L}^2} + \|\partial_t\Omega R\|^2_{\mathcal{L}^2}$ be the energy, which is equivalent to the $\mathcal{H}^2 \times \mathcal{H}^1$ norm, i.e., there exists $C_{E,1}$ and $C_{E,2}$ such that

$$C_{E,1}\left(\|\partial_t R\|^2_{H^1(\Gamma^\xi_{m,n})} + \|R\|^2_{H^2(\Gamma^\xi_{m,n})}\right) \leq E_R \leq C_{E,2}\left(\|\partial_t R\|^2_{H^1(\Gamma^\xi_{m,n})} + \|R\|^2_{H^2(\Gamma^\xi_{m,n})}\right). \tag{7.30}$$

We take the $\mathcal{L}^2$ scalar product of (7.28) with $\partial_t LR$ and obtain

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

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

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

we obtain

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}E_R &\leq 2E_R^{1/2}\left(C_{\mathrm{Res}}\varepsilon^2 + 3C_3\varepsilon^2E_R^{1/2} + 3C_3\varepsilon^{1+\vartheta}E_R + C_3\varepsilon^{2\vartheta}E_R^{3/2}\right)\\ &\leq 2C_{\mathrm{Res}}\varepsilon^2 + 2\left(3C_3 + C_{\mathrm{Res}}\right)\varepsilon^2E_R + 6C_3\varepsilon^{1+\vartheta}E_R^{3/2} + 2C_3\varepsilon^{2\vartheta}E_R^2.\end{aligned}$$

From (7.9) and (7.30) we obtain $E_R(0) \leq C_{E,2}C_1$, and as long as

$$6C_3\varepsilon^{\vartheta-1}E_R^{1/2} + 2C_3\varepsilon^{2\vartheta-2}E_R \leq 1 \tag{7.31}$$

we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}E_R \leq 2C_{\mathrm{Res}}\varepsilon^2 + \beta\varepsilon^2E_R \tag{7.32}$$

with $\beta = \left(6C_3 + C_{\mathrm{Res}} + 1\right)$. Gronwall's inequality, see, e.g., [36, Lemma 2.2.8] yields, for $0 \leq t \leq t_0 = T_0/\varepsilon^2$,

$$E_R(t) \leq E_R(0)\mathrm{e}^{\beta\varepsilon^2t} + \frac{2C_{\mathrm{Res}}}{\beta}\left(\mathrm{e}^{\beta\varepsilon^2t} - 1\right) \leq \left(E_R(0) + \frac{2C_{\mathrm{Res}}}{\beta}\right)\mathrm{e}^{\beta T_0} =: M. \tag{7.33}$$

Now choosing $\varepsilon_0 > 0$ so small that $6C_3\varepsilon^{\vartheta-1}M^{1/2} + 2C_3\varepsilon^{2\vartheta-2}M \leq 1$ yields (7.33) for all $0 < \varepsilon \leq \varepsilon_0$. Sobolev's embedding theorem, bound (7.26), and the decomposition (7.27) complete the proof of Theorem 7.1. □

## 8 | EFFECTIVE EQUATIONS AT THE DIRAC POINTS

The Dirac points are of high relevance from a physical point of view and attracted recently a lot of interest, cf. [16, 28]. In [20], effective equations describing the dynamics of solutions which are concentrated in Bloch space near the Dirac points have been derived via multiple scaling analysis in the 1D case. The validity question of this so called Dirac approximation for 2D quantum graphs is more involved and has not been discussed before.

Similar results in the above sense also exist for linear and nonlinear Schrödinger equations over $\mathbb{R}^2$ with honeycomb symmetric potentials. For the linear case it has been shown in [19] that a linear Dirac equation makes correct predictions about the dynamics over a long time scale. For the nonlinear case, a nonlinear Dirac system has been derived in [18], and an approach to prove its validity has been discussed. A rigorous approximation result with the NLS equation as original

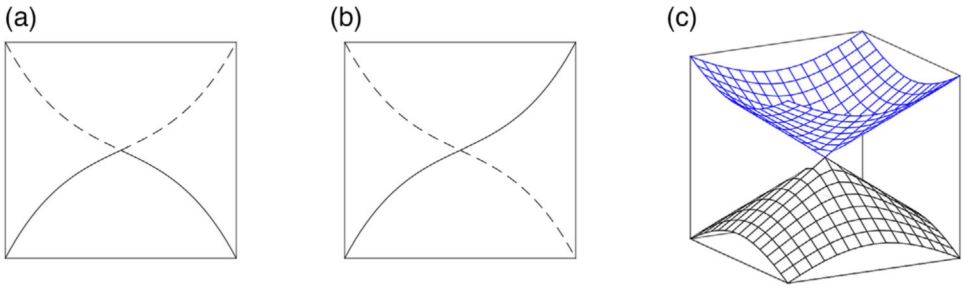


**FIGURE 5** At the Dirac points the non smooth curves in (a) obtained for the 1D dispersion relation can be made smooth by relabeling the curves leading to (b). This is not possible in the 2D case (c). Only directional smoothness can be obtained.

system has been established in [3], and similar to that result, we derive effective equations for the dynamics near the Dirac points and prove their validity for the cKG equation on 2D quantum graphs.

Suppose now that $\ell_D = (k_D, l_D)$ is a Dirac point, cf. Figure 2 and Figure 5. For a Dirac approximation we assume that the Bloch transform of the solution is concentrated in an $\mathcal{O}(\varepsilon^2)$-neighborhood of $\ell_D = (k_D, l_D)$. In this point the two surfaces of eigenvalues $\lambda_{m_D}$ and $\lambda_{m_D+1}$ of $\widetilde{L}(\ell)$ meet and form approximately a cone. In contrast to the NLS equation as original system where due to the $-U|U|^2$ nonlinearity no other modes are amplified by nonlinear coupling, for the cKG equation, with its real-valued solutions and its $U^3$ nonlinearity, other modes, in particular the second Dirac point at $\ell_{\overline{D}} = -\ell_D$, cf. Figure 2, have to be taken into account when deriving the Dirac approximation.

In contrast to all other points $\ell = (k, l)$, in a Dirac point no smooth expansion of the surfaces of eigenvalues is possible. This is fundamentally different from the 1D case where by relabeling the curves of eigenvalues the non-smooth curves of eigenvalues and the non-smooth kernels in the nonlinear convolution integrals, can be made smooth at the Dirac points, cf. Figure 5 and Remark 8.6. Hence, we have to proceed differently than in the derivation of the Dirac system in the 1D case or than in the derivation of the NLS equations above.

The starting point for the derivation of the approximation equations is again system (6.6) in Bloch space, namely

$$\partial_t^2 \widetilde{U}(t,\ell) = -\widetilde{L}(\ell)\widetilde{U}(t,\ell) - \big(\widetilde{U} \star \widetilde{U} \star \widetilde{U}\big)(t,\ell). \tag{8.1}$$

In this representation we obviously have smoothness of all linear and nonlinear operators w.r.t. the Bloch wave numbers. We recall that resolvents and spectral projections on isolated subsets of the spectrum are smooth w.r.t. $\ell$, cf. [22].

For extracting the Dirac modes at the cone around $\ell_D$ we define an $\widetilde{L}(\ell)$-invariant projection $\widetilde{P}_D(\ell)$ on the two-dimensional subspace associated to the two eigenvalues $\lambda_{m_D}(\ell)$ and $\lambda_{m_D+1}(\ell)$ which are separated from the rest of the spectrum of $\widetilde{L}(\ell)$ for $|\ell - \ell_D|$ sufficiently small. For fixed $\ell$ in a neighborhood of $\ell_D$ we set

$$\widetilde{P}_D(\ell) = \frac{1}{2\pi} \int_\Gamma \big(\lambda - \widetilde{L}(\ell)\big)^{-1} d\lambda,$$

where for this fixed $\ell$ the smooth curve $\Gamma$ surrounds the two eigenvalues $\lambda_{m_D}(\ell)$ and $\lambda_{m_D+1}(\ell)$. By Neumann's series we have a smooth expansion of $\widetilde{P}_D(\ell)$ near $\ell_D$, i.e.,

$$\widetilde{P}_D(\ell) = \widetilde{P}_D(\ell_D) + \mathcal{O}(|\ell - \ell_D|),$$

cf. [22]. Similarly, we define projections $\widetilde{P}_{\overline{D}}$ in a neighborhood of $\ell_{\overline{D}}$. We extend these projections by zero outside their domain of definitions in the set of wave vectors. We use these projections to split (8.1) into three parts. We set $\widetilde{U} = \widetilde{U}_D + \widetilde{U}_{\overline{D}} + \widetilde{U}_\perp$, where $\widetilde{U}_D = \widetilde{P}_D\widetilde{U}$, $\widetilde{U}_{\overline{D}} = \widetilde{P}_{\overline{D}}\widetilde{U}$, and $\widetilde{U}_\perp = \widetilde{P}_\perp\widetilde{U} = (1 - \widetilde{P}_D - \widetilde{P}_{\overline{D}})\widetilde{U}$, and obtain

$$\partial_t^2 \widetilde{U}_D(t,\ell) = -\widetilde{L}(\ell)\widetilde{U}_D(t,\ell) - \widetilde{P}_D(\ell)\big(\widetilde{U}_D + \widetilde{U}_{\overline{D}} + \widetilde{U}_\perp\big)^{\star 3}(t,\ell), \tag{8.2}$$

$$\partial_t^2 \widetilde{U}_{\overline{D}}(t,\ell) = -\widetilde{L}(\ell)\widetilde{U}_{\overline{D}}(t,\ell) - \widetilde{P}_{\overline{D}}(\ell)\big(\widetilde{U}_D + \widetilde{U}_{\overline{D}} + \widetilde{U}_\perp\big)^{\star 3}(t,\ell), \tag{8.3}$$

$$\partial_t^2 \widetilde{U}_\perp(t,\ell) = -\widetilde{L}(\ell)\widetilde{U}_\perp(t,\ell) - \widetilde{P}_\perp(\ell)\big(\widetilde{U}_D + \widetilde{U}_{\overline{D}} + \widetilde{U}_\perp\big)^{\star 3}(t,\ell). \tag{8.4}$$

Since $\widetilde{U}_D$ and $\widetilde{U}_{\overline{D}}$ will be of order $\mathcal{O}(\varepsilon)$, and $\widetilde{U}_\perp$ of order $\mathcal{O}(\varepsilon^3)$, for the derivation of the effective equations we set $\widetilde{U}_\perp = 0$ and make the ansatz

$$\widetilde{U}_D(t,\ell) = \varepsilon^{-4}\varepsilon\widetilde{V}_D^+(t,\ell)\big(\varepsilon^2 t, \varepsilon^{-2}(\ell-\ell_D)\big)e^{i\omega_{m_D}(\ell_D)t} + \varepsilon^{-4}\varepsilon\widetilde{V}_D^-(t,\ell)\big(\varepsilon^2 t, \varepsilon^{-2}(\ell-\ell_D)\big)e^{-i\omega_{m_D}(\ell_D)t}, \tag{8.5}$$

$$\widetilde{U}_{\overline{D}}(t,\ell) = \varepsilon^{-4}\varepsilon\widetilde{V}_{\overline{D}}^+(t,\ell)\big(\varepsilon^2 t, \varepsilon^{-2}(\ell+\ell_D)\big)e^{i\omega_{m_D}(\ell_D)t} + \varepsilon^{-4}\varepsilon\widetilde{V}_{\overline{D}}^-(t,\ell)\big(\varepsilon^2 t, \varepsilon^{-2}(\ell+\ell_D)\big)e^{-i\omega_{m_D}(\ell_D)t}, \tag{8.6}$$

where $\omega_m = \sqrt{-\lambda_m}$ as above and with $\widetilde{V}_D^\pm = \widetilde{P}_D\widetilde{V}_D^\pm$ and $\widetilde{V}_{\overline{D}}^\pm = \widetilde{P}_{\overline{D}}\widetilde{V}_{\overline{D}}^\pm$. The pre-factor $\varepsilon^{-4}$ comes from the Bloch transform, cf. Remark 7.3. We find with $T = \varepsilon^2 t$, $\underline{k} = \varepsilon^{-2}(k-k_D)$, $\underline{l} = \varepsilon^{-2}(l-l_D)$, and $\underline{\ell} = (\underline{k},\underline{l})$ the effective equations

$$\begin{aligned}2i\omega_{m_D}(\ell_D)\partial_T\widetilde{V}_D^+(T,\underline{\ell}) &= \big(i\underline{k}\widetilde{P}_D(\ell_D)\partial_k\widetilde{L}(\ell_D) + i\underline{l}\widetilde{P}_D(\ell_D)\partial_l\widetilde{L}(\ell_D)\big)\widetilde{V}_D^+(T,\underline{\ell})\\ &\quad + \widetilde{P}_D(\ell_D)\big(3\widetilde{V}_D^+ * \widetilde{V}_D^+ * \widetilde{V}_{\overline{D}}^- + 6\widetilde{V}_D^+ * \widetilde{V}_D^- * \widetilde{V}_{\overline{D}}^+\big)(T,\underline{\ell}),\end{aligned} \tag{8.7}$$

$$\begin{aligned}-2i\omega_\pm(\ell_D)\partial_T\widetilde{V}_D^-(T,\underline{\ell}) &= \big(i\underline{k}\widetilde{P}_D(\ell_D)\partial_k\widetilde{L}(\ell_D) + i\underline{l}\widetilde{P}_D(\ell_D)\partial_l\widetilde{L}(\ell_D)\big)\widetilde{V}_D^-(T,\underline{\ell})\\ &\quad + \widetilde{P}_D^-(\ell_D)\big(3\widetilde{V}_D^- * \widetilde{V}_D^- * \widetilde{V}_{\overline{D}}^+ + 6\widetilde{V}_D^- * \widetilde{V}_+^+ * \widetilde{V}_{\overline{D}}^-\big)(T,\underline{\ell}),\end{aligned} \tag{8.8}$$

and complex conjugate equations for $\widetilde{V}_{\overline{D}}^+$ and $\widetilde{V}_{\overline{D}}^-$. Like for the NLS approximation the limit equations no longer live in Bloch space, but in Fourier space.

Our approximation theorem is as follows.

**Theorem 8.1.** *For every $C_0 > 0$ and $T_0 > 0$, there exist $\varepsilon_0 > 0$ and $C > 0$ such that for all solutions $(\widetilde{V}_D^+, \widetilde{V}_D^-) \in C\big([0,T_0], H^2(\mathbb{R})^2\big)$ of the effective equations (8.7)–(8.8) with*

$$\sup_{T\in[0,T_0]} \left\|\widetilde{V}_D^\pm(T,\cdot)\right\|_{H^2} \le C_0$$

*the following holds. For all $\varepsilon \in (0,\varepsilon_0)$ there are solutions $U \in C\big([0,T_0/\varepsilon^2], L^\infty(\mathbb{R})\big)$ of the original system (8.1) satisfying the bound*

$$\sup_{t\in[0,T_0/\varepsilon^2]}\ \sup_{(x,y)\in\Gamma} |U(t,x,y) - \varepsilon\Psi_{\mathrm{dirac}}(t,x,y)| \le C\varepsilon^{5/2}$$

*where $\varepsilon\Psi_{\mathrm{dirac}}$ is defined through (8.5)–(8.6).*

*Proof.* Since the original system contains no quadratic terms the proof is straightforward and goes along the lines of Theorem 7.1 given in Section 7.3 and in Section 7.4. Since we expand $\widetilde{L}(\ell)$ only up to linear order, we only need $H^2$ in the Dirac case instead of $H^3$ in the NLS case. Moreover, due do the different scaling, every power of $|\ell - \ell_D|$ gains $\varepsilon^2$ instead of only $\varepsilon$. The computation of the higher order approximation as in Section 7.3 is possible due to the validity of the non-resonance conditions

$$\omega^{(m)}(\ell_D) \neq \omega^{(m_D)}(\ell_D) \quad \text{for all } |m| \notin \{m_D, m_D+1\} \tag{8.9}$$

and

$$\omega^{(m)}(3\ell_D) \neq 3\omega^{(m_D)}(\ell_D) \quad \text{for all } m. \tag{8.10}$$

The equations for the error have exactly the same form as (7.28) in Section 7.4. □

*Remark* 8.2. For fixed $\underline{\ell}$ the function $\widetilde{V}_D^+(\underline{\ell},\cdot)$ is two-dimensional. Hence, up to an error of order $\mathcal{O}(|\ell-\ell_D|)$ it can be represented as a linear combination of two eigenvectors which span the two-dimensional subspace at the apex of the cone. We choose two such eigenfunctions which are called $\Phi_1$ and $\Phi_2$ in the following, i.e., $\widetilde{L}(\ell_D)\Phi_j = -\omega_{m_D}^2(\ell_D)\Phi_j$. Then we set

$$\widetilde{V}_D^+(T,\underline{\ell}) = \widetilde{A}_1(T,\underline{\ell})\Phi_1 + \widetilde{A}_2(T,\underline{\ell})\Phi_2,$$

$$\widetilde{V}_D^-(T,\underline{\ell}) = \widetilde{B}_1(T,\underline{\ell})\Phi_1 + \widetilde{B}_2(T,\underline{\ell})\Phi_2,$$

with $\widetilde{A}_1(T,\underline{\ell}),\dots,\widetilde{B}_2(T,\underline{\ell}) \in \mathbb{C}$. For such $\Phi_1$ and $\Phi_2$ we have

$$\widetilde{P}_D(\ell_D)u = \frac{1}{\det}\big(\langle\Phi_2,\Phi_2\rangle\langle\Phi_1,u\rangle - \langle\Phi_1,\Phi_2\rangle\langle\Phi_2,u\rangle\big),$$

where $\det = \langle\Phi_1,\Phi_1\rangle\langle\Phi_2,\Phi_2\rangle - \langle\Phi_1,\Phi_2\rangle\langle\Phi_2,\Phi_1\rangle$. In these coordinates the effective equation (8.7) is given by

$$\begin{aligned}2i\omega_{m_D}(\ell_D)\partial_T\widetilde{A}_1(T,\underline{\ell}) = {} & (i\underline{k}\alpha_{11} + i\underline{l}\alpha_{21})\widetilde{A}_1(T,\underline{\ell}) + (i\underline{k}\alpha_{12} + i\underline{l}\alpha_{22})\widetilde{A}_2(T,\underline{\ell})\\ & + \Big(3\beta_{111}\widetilde{A}_1 * \widetilde{A}_1 * \widetilde{\overline{A_1}} + 3\beta_{112}\widetilde{A}_1 * \widetilde{A}_1 * \overline{A_2} + 3\beta_{121}\widetilde{A}_1 * \widetilde{A}_2 * \widetilde{\overline{A_1}}\\ & + 3\beta_{122}\widetilde{A}_1 * \widetilde{A}_2 * \widetilde{\overline{A_2}} + 3\beta_{221}\widetilde{A}_2 * \widetilde{A}_2 * \widetilde{\overline{A_1}} + 3\beta_{222}\widetilde{A}_2 * \widetilde{A}_2 * \widetilde{\overline{A_2}}\\ & + 6\gamma_{111}\widetilde{A}_1 * \widetilde{B}_1 * \widetilde{\overline{B_1}} + 6\gamma_{112}\widetilde{A}_1 * \widetilde{B}_1 * \widetilde{\overline{B_2}} + 6\gamma_{121}\widetilde{A}_1 * \widetilde{B}_2 * \widetilde{\overline{B_1}}\\ & + 6\gamma_{122}\widetilde{A}_1 * \widetilde{B}_2 * \widetilde{\overline{B_2}} + 6\gamma_{221}\widetilde{A}_2 * \widetilde{B}_2 * \widetilde{\overline{B_1}} + 6\gamma_{222}\widetilde{A}_2 * \widetilde{B}_2 * \widetilde{\overline{B_2}}\Big)(T,\underline{\ell}),\end{aligned}$$

where

$$\begin{aligned}\alpha_{1j} &= \frac{1}{\det}\big(\langle\Phi_2,\Phi_2\rangle\big\langle\Phi_1,\partial_k\widetilde{L}(\ell_D)\Phi_j\big\rangle - \langle\Phi_1,\Phi_2\rangle\big\langle\Phi_2,\partial_k\widetilde{L}(\ell_D)\Phi_j\big\rangle\big),\\ \alpha_{2j} &= \frac{1}{\det}\big(\langle\Phi_2,\Phi_2\rangle\big\langle\Phi_1,\partial_l\widetilde{L}(\ell_D)\Phi_j\big\rangle - \langle\Phi_1,\Phi_2\rangle\big\langle\Phi_2,\partial_l\widetilde{L}(\ell_D)\Phi_j\big\rangle\big),\\ \beta_{j_1j_2j_3} &= \frac{1}{\det}\Big(\langle\Phi_2,\Phi_2\rangle\big\langle\Phi_1,\Phi_{j_1}\Phi_{j_2}\overline{\Phi_{j_3}}\big\rangle - \langle\Phi_1,\Phi_2\rangle\big\langle\Phi_2,\Phi_{j_1}\Phi_{j_2}\overline{\Phi_{j_3}}\big\rangle\Big),\\ \gamma_{j_1j_2j_3} &= \frac{1}{\det}\Big(\langle\Phi_2,\Phi_2\rangle\big\langle\Phi_1,\Phi_{j_1}\Phi_{j_2}\overline{\Phi_{j_3}}\big\rangle - \langle\Phi_1,\Phi_2\rangle\big\langle\Phi_2,\Phi_{j_1}\Phi_{j_2}\overline{\Phi_{j_3}}\big\rangle\Big).\end{aligned}$$

A similar equation is obtained for (8.8). In physical space these equations are given by

$$\begin{aligned}2i\omega_{m_D}(\ell_D)\partial_T A_1 = {} & (\alpha_{11}\partial_X + \alpha_{21}\partial_Y)A_1 + (\alpha_{12}\partial_X + \alpha_{22}\partial_Y)A_2\\ & + \Big(3\beta_{111}A_1A_1\overline{A_1} + 3\beta_{112}A_1A_1\overline{A_2} + 3\beta_{121}A_1A_2\overline{A_1} + 3\beta_{122}A_1A_2\overline{A_2} + 3\beta_{221}A_2A_2\overline{A_1} + 3\beta_{222}A_2A_2\overline{A_2}\\ & + 6\gamma_{111}A_1B_1\overline{B}_1 + 6\gamma_{112}A_1B_1\overline{B}_2 + 6\gamma_{121}A_1B_2\overline{B}_1 + 6\gamma_{122}A_1B_2\overline{B}_2 + 6\gamma_{221}A_2B_2\overline{B}_1 + 6\gamma_{222}A_2B_2\overline{B}_2\Big).\end{aligned}$$

For suitable chosen $\Phi_1$ and $\Phi_2$ the representation [3, eq. (1.6)] of (8.7) in [3] is simpler. There, various coefficients $\alpha_.$, $\beta_.$, and $\gamma_.$ can be shown to vanish by using the hexagonal symmetry of the NLS equation on $\mathbb{R}^2$ with the honeycomb symmetric potential. Since we have chosen our coordinate system for (2.1) parallel to the $x$- and $y$-axis the existence of eigenfunctions $\Phi_1$ and $\Phi_2$ with similar properties as used in [3] is not obvious. Even for a hexagonal coordinate system this is not obvious, since the results from [16, 28] have to be transferred to quantum graphs, first.

*Remark* 8.3. By making the ansatz

$$\begin{aligned}\widetilde{U}_D(t,\ell) = {} & \varepsilon^{-4}\varepsilon^{\alpha}\widetilde{V}_D^+(t,\ell)(\varepsilon^2 t,\varepsilon^{-2}(\ell-\ell_D))e^{i\omega_{m_D}(\ell_D)t}\\ & + \varepsilon^{-4}\varepsilon^{\alpha}\widetilde{V}_D^-(t,\ell)(\varepsilon^2 t,\varepsilon^{-2}(\ell-\ell_D))e^{-i\omega_{m_D}(\ell_D)t},\end{aligned} \tag{8.11}$$

and similar for $\widetilde{U}_{\overline{D}}$, with $\alpha > 1$, the nonlinear terms are of higher order. We then obtain the linear effective equations

$$\begin{aligned}2i\omega_\pm(\ell_D)\partial_T\widetilde{A}_1(T,\underline{\ell}) &= (i\underline{k}\alpha_{11} + i\underline{l}\alpha_{21})\widetilde{A}_1(T,\underline{\ell}) + (i\underline{k}\alpha_{12} + i\underline{l}\alpha_{22})\widetilde{A}_2(T,\underline{\ell}),\\ 2i\omega_\pm(\ell_D)\partial_T\widetilde{A}_2(T,\underline{\ell}) &= (i\underline{k}\alpha_{11}^* + i\underline{l}\alpha_{21}^*)\widetilde{A}_1(T,\underline{\ell}) + (i\underline{k}\alpha_{12}^* + i\underline{l}\alpha_{22}^*)\widetilde{A}_2(T,\underline{\ell}),\end{aligned}$$

with

$$\alpha_{1j}^* = \frac{1}{\det}\left(\langle\Phi_2,\Phi_2\rangle\left\langle\Phi_1,\widetilde{P}_D(\ell_D)\partial_k\widetilde{L}(\ell_D)\Phi_j\right\rangle - \langle\Phi_1,\Phi_2\rangle\left\langle\Phi_2,\widetilde{P}_D(\ell_D)\partial_k\widetilde{L}(\ell_D)\Phi_j\right\rangle\right),$$

$$\alpha_{2j}^* = \frac{1}{\det}\left(\langle\Phi_2,\Phi_1\rangle\left\langle\Phi_1,\widetilde{P}_D(\ell_D)\partial_l\widetilde{L}(\ell_D)\Phi_j\right\rangle + \langle\Phi_1,\Phi_1\rangle\left\langle\Phi_2,\widetilde{P}_D(\ell_D)\partial_l\widetilde{L}(\ell_D)\Phi_j\right\rangle\right).$$

The system can be diagonalized into

$$\begin{aligned} i\partial_T\widetilde{A}_+(T,\underline{\ell}) + \Omega_+(\underline{\ell})\widetilde{A}_+(T,\underline{\ell}) &= 0,\\ i\partial_T\widetilde{A}_-(T,\underline{\ell}) + \Omega_-(\underline{\ell})\widetilde{A}_-(T,\underline{\ell}) &= 0, \end{aligned} \tag{8.12}$$

where the $\Omega_\pm$ are the roots of a quadratic equation in $\Omega_\pm$, $\underline{k}$, and $\underline{l}$. Since in the apex of the cone the directional derivatives exist, we have $\Omega_-(\underline{\ell}) = -\Omega_+(-\underline{\ell})$.

We have the following approximation result which is formulated in physical space.

**Theorem 8.4.** *For every $\alpha > 1$, $C_0 > 0$ and $T_0 > 0$, there exist $\varepsilon_0 > 0$ and $C > 0$ such that for all solutions $\widetilde{A}_\pm \in C(\mathbb{R}, H^2(\mathbb{R}))$ of (8.12) with*

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

*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 (8.1) satisfying the bound*

$$\sup_{t\in[0,T_0/\varepsilon^2]}\ \sup_{(x,y)\in\Gamma} |U(t,x,y) - \varepsilon^\alpha\Psi_{\mathrm{dirac}}(t,x,y)| \le C\varepsilon^{\min(\alpha+3/2,3\alpha-2))},$$

*where $\varepsilon^\alpha\Psi_{\mathrm{dirac}}$ is defined through (8.11).*

The proof works like for the NLS approximation except for the fact that the surfaces $\omega_{m_D}$ and $\omega_{m_D+1}$ are not smooth in the center. However, we have the estimate

$$\left|\omega_{m_D}(\ell) - \omega_{m_D}(\ell_D) - \Omega_+(\ell-\ell_D)\right| \le C|\ell-\ell_D|^2$$

which is sufficient for the residual estimates.

*Remark* 8.5. The linear equations (8.12) can be transferred into the massless Dirac equations. By construction, the functions $\Omega_\pm$ in (8.12) are of the form

$$\Omega_\pm(\underline{k},\underline{l}) = s_\pm\left(\frac{\underline{k}}{\sqrt{\underline{k}^2+\underline{l}^2}}, \frac{\underline{l}}{\sqrt{\underline{k}^2+\underline{l}^2}}\right)\sqrt{\underline{k}^2+\underline{l}^2},$$

with $s_\pm : S^1 \to \mathbb{R}^+$. We introduce new coordinates

$$\widetilde{\underline{k}}_\pm = \underline{k}s_\pm\left(\frac{\underline{k}}{\sqrt{\underline{k}^2+\underline{l}^2}}, \frac{\underline{l}}{\sqrt{\underline{k}^2+\underline{l}^2}}\right), \qquad \widetilde{\underline{l}}_\pm = \underline{l}s_\pm\left(\frac{\underline{k}}{\sqrt{\underline{k}^2+\underline{l}^2}}, \frac{\underline{l}}{\sqrt{\underline{k}^2+\underline{l}^2}}\right)$$

and set

$$\widetilde{\Omega}_\pm(\widetilde{\underline{k}}_\pm,\widetilde{\underline{l}}_\pm) = \Omega_\pm(\underline{k},\underline{l}) = s_\pm\left(\frac{\underline{k}}{\sqrt{\underline{k}^2+\underline{l}^2}}, \frac{\underline{l}}{\sqrt{\underline{k}^2+\underline{l}^2}}\right)\sqrt{\left(\frac{\widetilde{\underline{k}}_\pm}{s_\pm}\right)^2 + \left(\frac{\widetilde{\underline{l}}_\pm}{s_\pm}\right)^2} = \sqrt{\widetilde{\underline{k}}_\pm^2 + \widetilde{\underline{l}}_\pm^2}.$$

Since the two equations for $\widehat{A}_+$ and $\widehat{A}_-$ decouple w.r.t. these coordinates we can write

$$i\partial_T \widehat{A}_+(T,\underset{\sim}{k},\underset{\sim}{l}) + \sqrt{\underset{\sim}{k}^2 + \underset{\sim}{l}^2}\,\widehat{A}_+(T,\underset{\sim}{k},\underset{\sim}{l}) = 0, \tag{8.13}$$

$$i\partial_T \widehat{A}_-(T,\underset{\sim}{k},\underset{\sim}{l}) - \sqrt{\underset{\sim}{k}^2 + \underset{\sim}{l}^2}\,\widehat{A}_-(T,\underset{\sim}{k},\underset{\sim}{l}) = 0. \tag{8.14}$$

The new system (8.13)–(8.14) can be replaced by equations which are local in physical space, having the same spectral surfaces, such as $\partial_T^2\phi = \Delta\phi$ or the massless Dirac equation

$$\partial_T\psi = -(\sigma_x\partial_X\psi + \sigma_y\partial_Y\psi),$$

with $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and $\sigma_y = \begin{pmatrix} 0 & \mathrm{i} \\ -\mathrm{i} & 0 \end{pmatrix}$.

*Remark* 8.6. The motivation for the approach chosen in this section was that in a Dirac point no smooth expansion of the surfaces of eigenvalues is possible. We finally remark that the situation for the nonlinear kernels

$$\beta^j_{j_1,j_2,j_3}(\ell,\ell-\ell_1,\ell_1-\ell_2,\ell_2) = \left\langle f^j(\ell,\cdot), f^{j_1}(\ell-\ell_1,\cdot)f^{j_2}(\ell_1-\ell_2,\cdot)f^{j_3}(\ell_2,\cdot)\right\rangle_{L^2_\Gamma},$$

with $j, j_1, j_2, j_3 \in \{m_D, m_D+1\}$ at the apex of the cone is even worse. They even do not have a limit at the Dirac points; instead a continuum of accumulation points occurs.

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