

BIFURCATION OF NONLINEAR BOUND STATES IN THE PERIODIC GROSS-PITAEVSKII EQUATION WITH \mathcal{PT} -SYMMETRY

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ABSTRACT. The stationary Gross–Pitaevskii equation in one dimension is considered with a complex periodic potential satisfying the conditions of the \mathcal{PT} (parity-time reversal) symmetry. Under rather general assumptions on the potentials we prove bifurcations of \mathcal{PT} -symmetric nonlinear bound states from the end points of a real interval in the spectrum of the non-selfadjoint linear Schrödinger operator with a complex \mathcal{PT} -symmetric periodic potential. The nonlinear bound states are approximated by the effective amplitude equation, which bears the form of the cubic nonlinear Schrödinger equation. In addition we provide sufficient conditions for the appearance of complex spectral bands when the complex \mathcal{PT} -symmetric potential has an asymptotically small imaginary part.

1. INTRODUCTION

We consider the stationary Gross-Pitaevskii (GP) equation

$$-\frac{d^2u}{dx^2} + V(x)u + \sigma(x)|u|^2u = \omega u, \quad x \in \mathbb{R} \quad (1.1)$$

with complex 2π -periodic potentials V and σ and with a real parameter ω . The periodic potentials satisfy the conditions of the \mathcal{PT} (parity-time reversal) symmetry given by

$$V(-x) = \overline{V(x)}, \quad \sigma(-x) = \overline{\sigma(x)}, \quad \text{for all } x \in \mathbb{R}. \quad (1.2)$$

Assumption (I). Assume $V \in L^\infty_{\text{per}}(0, 2\pi)$ and $\sigma \in H^s_{\text{per}}(0, 2\pi)$ with $s > 1/2$ satisfy the \mathcal{PT} -symmetry condition (1.2).

Consider the linear Schrödinger operator

$$\mathcal{L} := -\frac{d^2}{dx^2} + V : \quad H^2(\mathbb{R}) \rightarrow L^2(\mathbb{R}), \quad (1.3)$$

which is not self-adjoint if V is complex. Nevertheless, we assume the existence of a real spectral interval in the spectrum of \mathcal{L} and prove the existence of $H^s(\mathbb{R})$ -solutions (with $s > 1/2$) to the stationary GP equation (1.1) bifurcating from an edge $\omega_* \in \mathbb{R}$ of the spectral interval. We call these solutions nonlinear bound states. They correspond to standing waves $\psi(x, t) = e^{-i\omega t}u(x)$ of the t -dependent Gross-Pitaevskii (GP) equation

$$i\partial_t\psi = -\partial_x^2\psi + V(x)\psi + \sigma(x)|\psi|^2\psi. \quad (1.4)$$

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The bifurcating solutions u are approximated via a slowly varying envelope ansatz. In a generic case (non-vanishing second derivative of the spectral function at the edge and non-vanishing coefficient in front of the cubic nonlinear term) the effective envelope equation is a nonlinear Schrödinger equation with constant coefficients.

We work in the Sobolev space $H^s(\mathbb{R})$ with $s > 1/2$ in order to enjoy the algebra property and the embedding of $H^s(\mathbb{R})$ to the space of bounded and continuous functions decaying to zero at infinity. Besides the Banach fixed point theorem the main analytical tool in the justification of the effective amplitude equation is the Bloch transformation \mathcal{B} given formally by

$$\tilde{u}(x, k) = (\mathcal{B}u)(x, k) = \sum_{n \in \mathbb{Z}} u(x + 2\pi n) e^{-ikx - 2\pi ink}. \quad (1.5)$$

The Bloch transformation was introduced by Gelfand [12] and was used in the analysis of the Schrödinger operator \mathcal{L} with a real periodic potential V [27]. With $\mathbb{B} := (-1/2, 1/2]$ being the so-called Brillouin zone, the Bloch transform

$$\mathcal{B} : H^s(\mathbb{R}) \rightarrow \mathcal{X}_s := L^2(\mathbb{B}, H^s(0, 2\pi))$$

is an isomorphism for $s \geq 0$, see [27], with the inverse given by

$$u(x) = (\mathcal{B}^{-1}\tilde{u})(x) = \int_{\mathbb{B}} e^{ikx} \tilde{u}(x, k) dk. \quad (1.6)$$

As the norm in \mathcal{X}_s we choose

$$\|\tilde{u}\|_{\mathcal{X}_s} = \left(\int_{\mathbb{B}} \|\tilde{u}(\cdot, k)\|_{H^s(0, 2\pi)}^2 dk \right)^{1/2}.$$

Under the Bloch transform the linear Schrödinger operator (1.3) is represented by the family of linear operators parameterized by $k \in \mathbb{B}$ and given by

$$L(k) := - \left(\frac{d}{dx} + ik \right)^2 + V : H^2(0, 2\pi) \rightarrow L^2(0, 2\pi). \quad (1.7)$$

Consider the family of Bloch eigenvalue problems

$$\begin{cases} L(k)p(\cdot, k) = \omega(k)p(\cdot, k), \\ p(x + 2\pi, k) = p(x, k) \end{cases} \quad \text{for all } x \in \mathbb{R}, \quad (1.8)$$

under the normalization condition $\|p(\cdot, k)\|_{L^2(0, 2\pi)} = 1$. In what follows we denote the eigenpairs of the Bloch eigenvalue problem (1.8) by $(\omega_m(k), p_m(x, k))$, $m \in \mathbb{N}$, where the ordering can be done, *e.g.*, according to the real part of the eigenvalues $\omega_m(k)$ (including their multiplicity).

We assume the existence of a real spectral interval given by an eigenvalue family $\{\omega_m(k)\}_{k \in \mathbb{B}}$ of the periodic eigenvalue problem (1.8) for some $m \in \mathbb{N}$. We also assume that this interval is disjoint from the rest of the spectrum of \mathcal{L} given by (1.3) and that the end points of the spectral interval have non-vanishing second derivative of ω_m . In summary we pose the following.

Assumption (II). For some $m \in \mathbb{N}$ the eigenvalue family ω_m is real with the spectral interval

$$\omega_m(\mathbb{B}) = [a, b] \subset \mathbb{R} \quad (1.9)$$

and with $[a, b]$ separated from the rest of the spectrum $\cup_{k \in \mathbb{B}} \sigma(L(k))$. Moreover, the eigenvalue $\omega_m(k)$ is simple for each $k \in \mathbb{B}$. For an end point $\omega_* \in \{a, b\}$ we assume that

$$\omega_m''(k_0) \neq 0, \quad (1.10)$$

where $k_0 \in \mathbb{B}$ is the preimage of ω_* under the mapping ω_m .

In Fig. 1 we plot the first (with respect to the real part) several eigenvalues of the spectral problem (1.8) with

$$V(x) = 2 \cos(x) + \cos(2x) + \gamma i \sin(2x)$$

for $\gamma = 1$ (a) and $\gamma = 3/2$ (b,c). They have been computed via a finite difference discretization. For $\gamma = 1$ all the lower spectral intervals appear real while for $\gamma = 3/2$ a symmetry breaking has occurred where the two lowest eigenvalue functions have collided and bifurcated into a complex conjugate pair. The third spectral function remains real for $\gamma = 3/2$ and its image is the marked interval $[a, b]$. At $\omega = a$ we have $k_0 = 0$ and at $\omega = b$ it is $k_0 = 1/2$. The fourth and fifth spectral functions also produce unstable eigenvalues in a small neighborhood of $k = 0$.

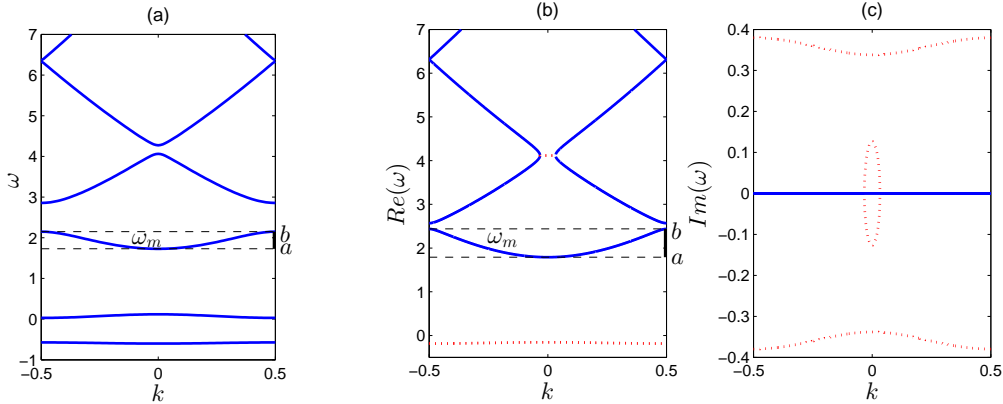


FIGURE 1. The smallest (with respect to the real part) several eigenvalues $\omega_n(k)$ of the spectral problem (1.8) with $V(x) = 2 \cos(x) + \cos(2x) + i\gamma \sin(2x)$, where $\gamma = 1$ in (a) and $\gamma = 3/2$ in (b) and (c). Purely real eigenvalues are plotted with the full blue line, complex eigenvalues are in dotted red. A real spectral interval $[a, b] = \omega_m(\mathbb{B})$ is marked in both (a) and (b).

For real potentials $V \in L_{\text{per}}^\infty((0, 2\pi), \mathbb{R})$, the eigenvalue family $\{\omega_m(k)\}_{k \in \mathbb{B}}$ cannot have an extremum for $k \notin \{0, 1/2\}$ due to the symmetry $\omega_m(-k) = \omega_m(k)$, the 1-periodicity of ω_m and the fact that the differential equation $\mathcal{L}u = \lambda u$ posed for the Schrödinger operator (1.3) on the infinite line is of the second order [27]. Because the spectral interval $[a, b]$ is isolated from the rest of the spectrum of \mathcal{L} , the eigenvalue family $\{\omega_m(k)\}_{k \in \mathbb{B}}$ then must have an extremum at either $k_0 = 0$ or $k_0 = 1/2$ and due to the smoothness of simple eigenvalues with respect to parameters one has $\omega_m'(k_0) = 0$.

The extension of these properties to general non-self-adjoint operator \mathcal{L} with complex potentials $V \in L_{\text{per}}^\infty(0, 2\pi)$ is not obvious. Nevertheless, for \mathcal{PT} -symmetric potentials we show in Section 2 that the reflection symmetry

$$\omega_m(-k) = \omega_m(k) \quad \text{for all } k \in \mathbb{B}, \quad (1.11)$$

still holds for the eigenvalue family $\{\omega_m(k)\}_{k \in \mathbb{B}}$ in Assumption (II). The 1-periodicity and smoothness of ω_m in k hold clearly as well. Finally, the possibility of an extremum of the eigenvalue family $\{\omega_m(k)\}_{k \in \mathbb{B}}$ at $k_0 \in (0, 1/2)$ is excluded by the same argument as in the case of real potentials. Indeed, if an extremum of ω_m exists at k_0 , it also occurs at $-k_0$ by symmetry (1.11). Therefore, on one side of the extremal value of ω_m , we have four bounded linearly independent solutions of the eigenvalue problem $\mathcal{L}u = \lambda u$ on the infinite line, which contradicts the fact that the eigenvalue problem is given by a second-order differential equation. Hence, if the spectral band $[a, b]$ is isolated, then the eigenvalue family $\{\omega_m(k)\}_{k \in \mathbb{B}}$ has an extremum at either $k_0 = 0$ or $k_0 = 1/2$ and

$$\omega'_m(k_0) = 0 \quad \text{for } k_0 = 0 \text{ or } k_0 = \frac{1}{2}. \quad (1.12)$$

For any eigenpair $(\omega(k), p(\cdot, k))$ of the spectral problem (1.8), the pair $(\overline{\omega(k)}, q(\cdot, k))$ with $q(x, k) := p(-x, k)$ for all $x \in \mathbb{R}$ is also an eigenpair of the same eigenvalue problem. This can be seen by complex conjugating $L(k)p(\cdot, k) = \omega(k)p(\cdot, k)$,

$$\left[- \left(\frac{d}{dx} - ik \right)^2 + V(x) \right] p(x, k) = \omega(k) p(x, k),$$

using the \mathcal{PT} -symmetry (1.2), and transforming $x \rightarrow -x$,

$$\left[- \left(\frac{d}{dx} + ik \right)^2 + V(x) \right] p(-x, k) = \overline{\omega(k)} p(-x, k),$$

hence $L(k)q(\cdot, k) = \overline{\omega(k)}q(\cdot, k)$. If $\omega(k) \in \mathbb{R}$ is simple for some $k \in \mathbb{B}$, then $p(\cdot, k)$ and $q(\cdot, k)$ are linearly dependent and, thanks to the normalization condition, the eigenfunction $p(\cdot, k)$ can be chosen to satisfy the \mathcal{PT} -symmetry condition,

$$\overline{p(-x, k)} = p(x, k), \quad \text{for all } x \in \mathbb{R}. \quad (1.13)$$

In what follows, we say that the solution u to the stationary GP equation (1.1) is \mathcal{PT} -symmetric if it satisfies the same \mathcal{PT} -symmetry condition,

$$\overline{u(-x)} = u(x), \quad \text{for all } x \in \mathbb{R}. \quad (1.14)$$

We study the bifurcation of \mathcal{PT} -symmetric solutions to the stationary GP equation (1.1) from an endpoint ω_* of the real interval $[a, b]$ into a spectral gap. Hence, we pick $\omega_* \in \{a, b\}$ as in Assumption (II) and set

$$\omega = \omega_* + \varepsilon^2 \Omega, \quad (1.15)$$

where ε is a formal small parameter and $\Omega = -1$ if $\omega_* = a$ or $\Omega = +1$ if $\omega_* = b$.

We prove in Section 3 that similarly to the case of real potentials V and σ [7, 9] (see also a review in Chapter 2 in [25]), the family of nonlinear bound states in $H^s(\mathbb{R})$ with $s > 1/2$ bifurcating from ω_* can be approximated via the slowly varying envelope ansatz

$$u(x) \sim u_{\text{form}}(x) := \varepsilon A(\varepsilon x) e^{ik_0 x} p_m(x, k_0) \quad \text{as } \varepsilon \rightarrow 0, \quad (1.16)$$

where $A \in H^{s_A}(\mathbb{R})$ with $s_A \geq 1$ satisfies the effective amplitude equation given by the stationary nonlinear Schrödinger (NLS) equation,

$$-\frac{1}{2} \omega_m''(k_0) \frac{d^2 A}{dX^2} + \Gamma |A|^2 A = \Omega A, \quad (1.17)$$

with

$$\Gamma := \int_{-\pi}^{\pi} \sigma(x) p_m(x, k_0) |p_m(x, k_0)|^2 \overline{p_m(-x, -k_0)} dx. \quad (1.18)$$

The coefficient Γ is real due to the \mathcal{PT} -symmetry of σ and $p_m(\cdot, \pm k_0)$ in (1.2) and (1.13).

If the effective equation (1.17) has a bound state, we may expect the same for the GP equation (1.1). It follows from the elementary phase-plane analysis that bound states of the stationary NLS equation (1.17) exist if and only if

$$\Gamma \neq 0 \quad \text{and} \quad \text{sign}(\Gamma) = -\text{sign}(\omega''(k_0)) = \text{sign}(\Omega). \quad (1.19)$$

Real even bound states A are unique and have an explicit sech-function form, see Lemma 6.15 in [11]. They belong to $H^{s_A}(\mathbb{R})$ for every $s_A \geq 0$. For the justification of the effective equation we need the invertibility of the linearization operator of the NLS equation at the bound state A . For this the translational and gauge invariances of the differential equation (1.17) need to be eliminated, which is achieved if A satisfies the \mathcal{PT} -symmetry condition

$$\overline{A(-x)} = A(x), \quad \text{for all } x \in \mathbb{R}. \quad (1.20)$$

The following theorem justifies the effective amplitude equation (1.17) used for the approximation (1.16) and constitutes the main result of this article.

Theorem 1. *Let $1/2 < s \leq 2$ and $0 < r < 1/2$ and assume (I) and (II). Let $A \in H^{s_A}(\mathbb{R})$ be a \mathcal{PT} -symmetric solution to the stationary NLS equation (1.17) with $s_A \geq 1$ satisfying (1.20). Then there are constants $c > 0$ and $\varepsilon_0 > 0$ such that for each $\varepsilon \in (0, \varepsilon_0)$ there exists a \mathcal{PT} -symmetric solution $u \in H^s(\mathbb{R})$ of the stationary GP equation (1.1) with $\omega = \omega_* + \varepsilon^2 \Omega$ satisfying (1.14) and*

$$\|u - u_{\text{form}}\|_{H^s(\mathbb{R})} \leq c\varepsilon^{r+1/2},$$

where u_{form} is defined in (1.16).

Remark 2. Condition (1.19) for the existence of NLS bound states implies that the bifurcation is always into a spectral gap. At the lower spectral edge $\omega_* = a$, where $\omega''(k_0) > 0$, one has $\Omega < 0$ and the bifurcation in ω is down from a ; analogously at the upper edge b , where $\omega''(k_0) < 0$, one has $\Omega > 0$ and the bifurcation in ω is up from b .

Remark 3. Theorem 1 guarantees that the error $u - u_{\text{form}}$ is indeed smaller than the approximation u_{form} itself because $\|u_{\text{form}}\|_{H^s(\mathbb{R})} \sim c\varepsilon^{1/2}$ as $\varepsilon \rightarrow 0$ for an ε -independent c .

Remark 4. The statement of Theorem 1 can be generalized in a number of ways. First, one can prove existence of smoother solutions with $s > 2$ provided that $p(\cdot, k_0)$ belongs to $H_{\text{per}}^s(0, 2\pi)$. This would require a smoother potential V than the one in (I). Second, the spectral interval $[a, b]$ does not have to be real entirely, as in (II). For the justification result, it is sufficient that a little segment of $[a, b]$ near the end point ω_* be real. Similarly, the simplicity assumption of the eigenvalue $\omega_m(k)$ has to be satisfied only near the end point that corresponds to $k = k_0$.

Remark 5. Assumption (II) is not satisfied for an arbitrary complex V . Propositions 9, 11 and 13 in Section 4 give sufficient conditions for the occurrence of complex spectral bands if $V(x) = U(x) + i\gamma W(x)$ with U even and W odd and with $\gamma > 0$ arbitrarily small. The sufficient conditions detect bifurcations of double eigenvalues at $\gamma = 0$ into complex pairs of simple eigenvalues for $\gamma > 0$.

Remark 6. Recent interest in \mathcal{PT} -symmetric periodic potentials is explained by the experimental realization of such optical lattices in physical experiments [13, 20]. Several computational works were devoted to the existence and spectral stability of standing waves in the GP equation with complex periodic potentials [14, 22, 23] (see also the review in [19]). Persistence of real spectrum in honeycomb \mathcal{PT} -symmetric potentials was studied in [5]. Small \mathcal{PT} -symmetric perturbations of honeycomb periodic potentials were considered in [6] and their effect on the nonlinear dynamics of the GP equation was studied. A heuristic asymptotic method was used in [24] to approximate the standing waves of the GP equation by sech-solitons of the stationary NLS equation. Our work is the first one, to the best of our knowledge, which gives a rigorous proof of the existence of nonlinear bound states and their approximation by an effective equation for the bifurcation from an edge of a real interval in the spectrum of a \mathcal{PT} -symmetric non-selfadjoint linear Schrödinger operator.

Remark 7. The bifurcation from simple eigenvalues is a more classical problem. The bifurcation of nonlinear bound states from possibly complex eigenvalues of non-selfadjoint Fredholm operators is covered in the pioneering works [4, 15]. The bifurcation of nonlinear bound states from simple real eigenvalues under an antilinear symmetry (which includes the \mathcal{PT} -symmetry) has been shown for a large class of nonlinear problems in [8]. Earlier, in [17] this bifurcation was proved for the special case of a discrete NLS equation on a finite lattice. The main difference between the bifurcation from a simple eigenvalue and from the edge of a spectral interval is that in the former case the existence of the bifurcation is automatic due to the separation of a simple eigenvalue from the rest of the spectrum while in the latter case the edge is connected to the spectral band. In the case of simple eigenvalues a bifurcation occurs even without symmetry assumptions and \mathcal{PT} -symmetry is used only to show that the nonlinear bound state corresponds to real eigenvalue parameter. In the case of a spectral *interval* the symmetry is crucial for proving the bifurcation itself.

The rest of the article is organized as follows. Section 2 covers the technical results associated with the adjoint eigenvalue problem and with the Bloch transform. Section 3 gives a proof of Theorem 1. Section 4 reports results based on perturbation theory which give sufficient conditions on when Assumption (II) is not satisfied.

2. THE ADJOINT EIGENVALUE PROBLEM AND THE BLOCH TRANSFORM REVISITED

Since the spectral problem (1.8) is not self-adjoint in the presence of complex periodic potentials, we also introduce the adjoint eigenvalue problem. By the Fredholm theory (see Remark 6.23 in Chapter III.6.6 [16]), eigenvalues of the adjoint operator $L^*(k)$ are related to the eigenvalues of the operator $L(k)$ by complex conjugation. The adjoint eigenvalue problem is written by

$$\begin{cases} L^*(k)p^*(\cdot, k) = \overline{\omega(k)}p^*(\cdot, k), \\ p^*(x + 2\pi, k) = p^*(x, k) \end{cases} \quad \text{for all } x \in \mathbb{R}, \quad (2.1)$$

where

$$L^*(k) := - \left(\frac{d}{dx} + ik \right)^2 + \bar{V} : \quad H^2(0, 2\pi) \rightarrow L^2(0, 2\pi) \quad (2.2)$$

is the adjoint operator and $p^*(\cdot, k)$ is the adjoint eigenfunction.

If $\omega(k)$ is a simple eigenvalue of the spectral problem (1.8), then $\overline{\omega(k)}$ is a simple eigenvalue of the adjoint spectral problem (2.1) and the adjoint eigenfunction can be uniquely normalized by $\langle p^*(\cdot, k), p(\cdot, k) \rangle = 1$. Indeed, if $\omega(k)$ is a simple eigenvalue, then $\langle p^*(\cdot, k), p(\cdot, k) \rangle = 0$ leads to a contradiction. In detail, if $\langle p^*(\cdot, k), p(\cdot, k) \rangle = 0$, then we have

$$p(\cdot, k) \in \text{Ker}(L(k) - \omega(k)) \cap \text{Ran}(L(k) - \omega(k)).$$

Therefore, there exists $\varphi \in H^2(0, 2\pi) \setminus \{0\}$ such that $(L(k) - \omega(k))\varphi = p(\cdot, k)$. At the same time, $\omega(k)$ being simple implies

$$\text{Ker}(L(k) - \omega(k))^2 = \text{Ker}(L(k) - \omega(k)),$$

so that $\varphi = c p(\cdot, k)$ with $c \in \mathbb{R}$, which contradicts equation $(L(k) - \omega(k))\varphi = p(\cdot, k)$. Thus, $\langle p^*(\cdot, k), p(\cdot, k) \rangle \neq 0$, and the normalization $\langle p^*(\cdot, k), p(\cdot, k) \rangle = 1$ can be used.

In the case of simple eigenvalues, the eigenpair $(\omega(k), p(\cdot, k))$ of the spectral problem (1.8) and the eigenpair $(\overline{\omega(k)}, p^*(\cdot, k))$ of the adjoint problem (2.1) are related via

$$\overline{\omega(k)} = \omega(-k), \quad p^*(x, k) = p(-x, -k). \quad (2.3)$$

This follows from the \mathcal{PT} -symmetry of V in (1.2) such that after the transformation $x \rightarrow -x$ and $k \rightarrow -k$, the adjoint problem $L^*(k)p^*(\cdot, k) = \overline{\omega(k)}p^*(\cdot, k)$ becomes

$$\left[-\left(\frac{d}{dx} + ik\right)^2 + V(x) \right] p^*(-x, -k) = \overline{\omega(-k)}p^*(-x, -k),$$

which coincides with the spectral problem (1.8). As a result of the symmetry reflection (2.3) we obtain

$$\omega(-k) = \omega(k) \quad \text{for all } k \in \mathbb{B}, \quad (2.4)$$

for every simple real eigenvalue family $\{\omega(k)\}_{k \in \mathbb{B}}$. In addition, the eigenvalue family can be continued as a 1-periodic function of k on \mathbb{R} . This symmetry and the k -smoothness of simple eigenvalues $\omega(k)$ justify (1.11) and (1.12) claimed in Section 1.

Before we proceed with the proof of Theorem 1, let us also elaborate properties of the Bloch transform defined by (1.5) and (1.6). Let \hat{u} be the standard Fourier transform of u given by

$$\hat{u}(\xi) = (\mathcal{F}u)(\xi) = \frac{1}{2\pi} \int_{\mathbb{R}} u(x) e^{-i\xi x} dx, \quad u(x) = (\mathcal{F}^{-1}\hat{u})(x) = \int_{\mathbb{R}} \hat{u}(\xi) e^{i\xi x} d\xi.$$

Then, the Bloch transform (1.5) can also be related to the Fourier transform as follows:

$$\tilde{u}(x, k) = \sum_{j \in \mathbb{Z}} e^{ijx} \hat{u}(k + j), \quad (2.5)$$

see [2] or Section 2.1.2 in [25].

By construction of \tilde{u} in the definition of the Bloch transform in (1.5), we have the continuation property for all $x \in \mathbb{R}$ and $k \in \mathbb{R}$:

$$\tilde{u}(x + 2\pi, k) = \tilde{u}(x, k) \quad \text{and} \quad \tilde{u}(x, k + 1) = e^{-ix} \tilde{u}(x, k). \quad (2.6)$$

For two functions $u, v \in H^s(\mathbb{R})$ with $s > 1/2$, the product uv is also in $H^s(\mathbb{R})$, thanks to the Banach algebra of $H^s(\mathbb{R})$ with respect to the pointwise multiplication [1, Thm.4.39]. In the Bloch space the multiplication operator is conjugate to the convolution operator:

$$(\mathcal{B}(uv))(x, k) = (\tilde{u} *_{\mathbb{B}} \tilde{v})(x, k) := \int_{\mathbb{B}} \tilde{u}(x, k - l) \tilde{v}(x, l) dl = \int_{\mathbb{B} + k_0} \tilde{u}(x, k - l) \tilde{v}(x, l) dl$$

for any $k_0 \in \mathbb{R}$, where the last equality holds due to the 1-quasi-periodicity of the Bloch transform in the variable k . The convolution property follows from relation (2.5). Note that due to the algebra property of $H^s(\mathbb{R})$ for $s > 1/2$ and the above identity we have also the algebra property

$$\|\tilde{u} *_\mathbb{B} \tilde{v}\|_{\mathcal{X}_s} \leq c \|\tilde{u}\|_{\mathcal{X}_s} \|\tilde{v}\|_{\mathcal{X}_s} \quad \text{for any } \tilde{u}, \tilde{v} \in \mathcal{X}_s \quad \text{if } s > 1/2, \quad (2.7)$$

where the constant $c > 0$ depends on s .

Finally, for any 2π -periodic and bounded function σ we have the property

$$(\mathcal{B}(\sigma u))(x, k) = \sigma(x)(\mathcal{B}u)(x, k) \quad \text{for all } x \in \mathbb{R} \text{ and } k \in \mathbb{R}. \quad (2.8)$$

The commutativity property follows directly from the representation (1.5).

3. NONLINEAR ESTIMATES; PROOF OF THEOREM 1

Problem (1.1) transforms via the Bloch transform \mathcal{B} to the form

$$(L(k) - \omega)\tilde{u}(x, k) + \sigma(x)(\tilde{u} *_\mathbb{B} \tilde{u} *_\mathbb{B} \tilde{\tilde{u}})(x, k) = 0, \quad (3.1)$$

where property (2.8) has been used.

We decompose \tilde{u} into the part corresponding to the spectral band ω_m and the rest. Note that we cannot use a full spectral decomposition of $\tilde{u}(\cdot, k)$ as this is not available for non-selfadjoint problems. For our decomposition we define the projections

$$P_k : H^s(0, 2\pi) \rightarrow \text{span}\{p_m(\cdot, k)\}$$

and

$$Q_k = I - P_k : H^s(0, 2\pi) \rightarrow \text{span}\{p_m(\cdot, k)\}^\perp$$

with $m \in \mathbb{N}$ fixed by assumption (II), such that $(P_k \tilde{u})(\cdot, k) := \langle \tilde{u}(\cdot, k), p_m^*(\cdot, k) \rangle p_m(\cdot, k)$, where $\langle \cdot, \cdot \rangle$ is the standard $L^2(0, 2\pi)$ -inner product. Decomposing now the solution into

$$\tilde{u}(x, k) = \tilde{u}_1(x, k) + \tilde{u}_2(x, k),$$

where

$$\begin{aligned} \tilde{u}_1(\cdot, k) &= P_k \tilde{u}(\cdot, k) = U_1(k) p_m(\cdot, k) \quad \text{with } U_1(k) \in \mathbb{C}, \\ \tilde{u}_2(\cdot, k) &= Q_k \tilde{u}(\cdot, k), \end{aligned}$$

and using $\omega = \omega_* + \varepsilon^2 \Omega$ as is given by (1.15), equation (3.1) is written as a system of two equations given by

$$(\omega_m(k) - \omega_* - \varepsilon^2 \Omega) U_1(k) + \langle F(\tilde{u})(\cdot, k), p_m^*(\cdot, k) \rangle = 0 \quad (3.2)$$

and

$$Q_k(L(k) - \omega_* - \varepsilon^2 \Omega) Q_k \tilde{u}_2(x, k) + Q_k F(\tilde{u}_1) + Q_k(F(\tilde{u}) - F(\tilde{u}_1)) = 0, \quad (3.3)$$

where $F(\tilde{v})(x, k) := \sigma(x)(\tilde{v} *_\mathbb{B} \tilde{v} *_\mathbb{B} \tilde{\tilde{v}})(x, k)$. We note that U_1 is 1-periodic because $\tilde{u}(x, \cdot)$ and $p(x, \cdot)$ are 1-quasiperiodic.

Since $Q_k F(\tilde{u}_1)$ in (3.3) produces a large output, we need to perform a near-identity transformation before we can proceed with the nonlinear estimates. See the pioneering work [18] that explains this procedure. We hence decompose \tilde{u}_2 into

$$\tilde{u}_2(x, k) = \tilde{u}_{2,1}(x, k) + \tilde{u}_R(x, k),$$

where $\tilde{u}_{2,1}$ and \tilde{u}_R solve equations

$$Q_k(L(k) - \omega_* - \varepsilon^2 \Omega) Q_k \tilde{u}_{2,1}(x, k) + Q_k F(\tilde{u}_1) = 0 \quad (3.4)$$

and

$$Q_k(L(k) - \omega_* - \varepsilon^2\Omega)Q_k\tilde{u}_R(x, k) + Q_k(F(\tilde{u}) - F(\tilde{u}_1)) = 0. \quad (3.5)$$

The resulting system of equations is given by (3.2), (3.4) and (3.5).

The component \tilde{u}_1 is supposed to approximately recover the Bloch transform of the formal ansatz (1.16). Note that because $\mathcal{F}(A(\varepsilon\cdot)e^{ik_0\cdot})(k) = \varepsilon^{-1}\hat{A}(\varepsilon^{-1}(k - k_0))$, we have

$$\mathcal{B}(u_{\text{form}})(x, k) = \sum_{j \in \mathbb{Z}} \hat{A}\left(\frac{k - k_0 + j}{\varepsilon}\right) p_m(x, k_0) e^{ijx}, \quad (3.6)$$

where we have used properties (2.5) and (2.8). Since $\hat{A}(\varepsilon^{-1}(k - k_0))$ is concentrated near $k = k_0$, we decompose U_1 on $\mathbb{B} + k_0$ into a part compactly supported near k_0 and the rest. We write

$$U_1(k) = \hat{D}\left(\frac{k - k_0}{\varepsilon}\right) := \hat{B}\left(\frac{k - k_0}{\varepsilon}\right) + \hat{C}\left(\frac{k - k_0}{\varepsilon}\right), \quad k \in \mathbb{B} + k_0, \quad (3.7)$$

and continue U_1 outside $\mathbb{B} + k_0$ periodically with period one. For all ε small enough the components \hat{B} and \hat{C} are defined by their support

$$\begin{aligned} \text{supp}\left(\hat{B}\left(\frac{\cdot - k_0}{\varepsilon}\right)\right) &\subset (k_0 - \varepsilon^r, k_0 + \varepsilon^r), \\ \text{supp}\left(\hat{C}\left(\frac{\cdot - k_0}{\varepsilon}\right)\right) &\subset (k_0 + \mathbb{B}) \setminus (k_0 - \varepsilon^r, k_0 + \varepsilon^r), \end{aligned}$$

where $r \in (0, 1)$ is a parameter to be specified to suit the nonlinear estimates. Equivalently, defining

$$I_{\varepsilon^{r-1}} := (-\varepsilon^{r-1}, \varepsilon^{r-1}),$$

we have $\text{supp}(\hat{B}) \subset I_{\varepsilon^{r-1}}$ and $\text{supp}(\hat{C}) \subset \varepsilon^{-1}\mathbb{B} \setminus I_{\varepsilon^{r-1}}$. We note that neither \hat{B} , \hat{C} , nor \hat{D} refer to the Fourier transform, since they are defined in the Bloch space. On the other hand, \hat{A} denotes the Fourier transform of the amplitude variable A that satisfies the effective amplitude equation (1.17). In the Fourier variable κ the amplitude \hat{A} satisfies the effective amplitude equation in the form

$$\left(\frac{1}{2}\omega_m''(k_0)\kappa^2 - \Omega\right) \hat{A}(\kappa) + \Gamma\left(\hat{A} * \hat{A} * \hat{A}\right)(\kappa) = 0. \quad (3.8)$$

We aim at constructing a solution \tilde{u} with \hat{B} close to \hat{A} on $I_{\varepsilon^{r-1}}$ and with the other components \hat{C} , $\tilde{u}_{2,1}$ and \tilde{u}_R being small corrections. Hence, due to (3.6) ansatz (3.7) corresponds formally to the slowly varying envelope ansatz (1.16).

Obviously, system (3.2), (3.4) and (3.5) is coupled in the components \hat{B} , \hat{C} , $\tilde{u}_{2,1}$ and \tilde{u}_R . Nevertheless, it can be approached by treating each problem independently with consistent assumptions on the form and size of the remaining components. In brief, our steps to construct such a solution $\tilde{u} \in \mathcal{X}_s$ of (3.1), i.e. of the original equation in the Bloch space, are as follows:

- (1) For any given \tilde{u}_1 small, solve (3.4) uniquely to produce a small $\tilde{u}_{2,1}$ due to the invertibility of $Q_k(L(k) - \omega_* - \varepsilon^2\Omega)Q_k$ in $Q_k\mathcal{X}_s$ for ε small enough.
- (2) For any given \tilde{u}_1 small, apply the Banach fixed point theorem to (3.5) in a neighborhood of zero to find a small solution \tilde{u}_R .
- (3) For any given \hat{B} decaying sufficiently fast, apply the Banach fixed point theorem to (3.2) on the support of \hat{C} to find a small \hat{C} .

- (4) Prove the existence of such solutions \hat{B} to equation (3.2) (with the component \hat{C} given by step 3) on the support of \hat{B} that are close to a solution \hat{A} of equation (3.8). It is in this step where a restriction to the \mathcal{PT} -symmetric solutions is necessary. It allows for the invertibility of the Jacobian operator at \hat{A} associated with equation (3.8).

The rest of this section explains the details of each step in the justification analysis. We denote a generic, positive, ε -independent constant by c . It may change from one line to another line. We also restrict our work to the space \mathcal{X}_s with $1/2 < s \leq 2$.

3.1. Preliminary estimates. We assume that for all $\varepsilon > 0$ sufficiently small

$$\|\hat{B}\|_{L^2_{s_B}(\mathbb{R})} + \|\hat{C}\|_{L^2_{s_C}(\mathbb{R})} \leq c, \quad (3.9)$$

where $s_B, s_C \geq 0$ are to be determined later and the space $L^2_s(\mathbb{R})$ for $s \geq 0$ is

$$L^2_s(\mathbb{R}) := \{f \in L^2(\mathbb{R}) : \|f\|_{L^2_s(\mathbb{R})} := \|(1 + |\cdot|)^s f\|_{L^2(\mathbb{R})} < \infty\}.$$

We estimate first $\|\tilde{u}_1\|_{\mathcal{X}_s}$. Since $p_m(\cdot, k) \in H^2(0, 2\pi)$ in the domain of $L(k)$ given by (1.7), there is a positive constant c such that for all $\varepsilon > 0$ sufficiently small and any $1/2 < s \leq 2$, we have

$$\|\tilde{u}_1\|_{\mathcal{X}_s} \leq \sup_{k \in \mathbb{B}} \|p_m(\cdot, k)\|_{H^2(0, 2\pi)} \left\| \hat{D} \left(\frac{\cdot - k_0}{\varepsilon} \right) \right\|_{L^2(\mathbb{B})} \leq c\varepsilon^{1/2} \|\hat{D}\|_{L^2(\varepsilon^{-1}\mathbb{B})}. \quad (3.10)$$

Next, let us consider the \mathcal{X}_s -norm of $F(\tilde{u}_1)$ given by

$$F(\tilde{u}_1) = \sigma(x) \int_{\mathbb{B}} \int_{\mathbb{B}} U_1(k-l) U_1(l-t) \overline{U_1(-t)} p_m(x, k-l) p_m(x, l-t) \overline{p_m(x, -t)} dt dl,$$

which appears in equations (3.4) and (3.5). By assumption (I) we get

$$\begin{aligned} \|F(\tilde{u}_1)\|_{\mathcal{X}_s} &\leq \|\sigma\|_{H^s(0, 2\pi)} \sup_{k \in \mathbb{B}} \|p_m(\cdot, k)\|_{H^2(0, 2\pi)}^3 \|U_1 *_{\mathbb{B}} U_1 *_{\mathbb{B}} \overline{U_1(-\cdot)}\|_{L^2(\mathbb{B})} \\ &\leq c \|U_1 *_{\mathbb{B}} U_1 *_{\mathbb{B}} \overline{U_1(-\cdot)}\|_{L^2(\mathbb{B})}. \end{aligned}$$

Next, we estimate

$$\|U_1 *_{\mathbb{B}} U_1 *_{\mathbb{B}} \overline{U_1(-\cdot)}\|_{L^2(\mathbb{B})} = \varepsilon^{5/2} \|\hat{B} * \hat{B} * \hat{\overline{B}}\|_{L^2(-3\varepsilon^{r-1}, 3\varepsilon^{r-1})} + \|E\|_{L^2(\mathbb{B}+k_0)},$$

where

$$\begin{aligned} E &:= 2W_1 *_{\mathbb{B}} \hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \hat{\overline{B}} \left(\frac{\cdot + k_0}{\varepsilon} \right) + \hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \overline{W_1(-\cdot)} \\ &\quad + \text{h.o.t.} \end{aligned} \quad (3.11)$$

with

$$W_1(k) = \begin{cases} \hat{C} \left(\frac{k-k_0}{\varepsilon} \right), & k - k_0 \in \mathbb{B} \\ U_1(k), & k - k_0 \in \mathbb{R} \setminus \mathbb{B} \end{cases}$$

and with ‘‘h.o.t.’’ containing the remaining convolution terms, *i.e.* those quadratic and cubic in W_1 . A direct calculation yields

$$\begin{aligned} &\left(W_1 *_{\mathbb{B}} \hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \hat{\overline{B}} \left(\frac{\cdot + k_0}{\varepsilon} \right) \right) (k) = \\ &\sum_{n \in \{-1, 0, 1\}} \int_{\substack{|l| < 2\varepsilon^r \\ |k-l-k_0-n| < 1/2}} \int_{(-k_0-\varepsilon^r, -k_0+\varepsilon^r) \cap \mathbb{B}} \hat{C} \left(\frac{k-l-k_0-n}{\varepsilon} \right) \hat{B} \left(\frac{l-t-k_0}{\varepsilon} \right) \hat{\overline{B}} \left(\frac{t+k_0}{\varepsilon} \right) dt dl, \end{aligned}$$

such that

$$\left\| W_1 *_{\mathbb{B}} \hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \hat{B} \left(\frac{\cdot + k_0}{\varepsilon} \right) \right\|_{L^2(\mathbb{B}+k_0)} \leq c\varepsilon^{5/2} \|\hat{C}\|_{L^2(\mathbb{R})} \|\hat{B}\|_{L^1(\mathbb{R})}^2,$$

where we have used Young's inequality for convolutions. Next, we use the estimate

$$\|\hat{B}\|_{L^1(\mathbb{R})} = \int_{\mathbb{R}} (1 + |\kappa|)^{-s_B} (1 + |\kappa|)^{s_B} |\hat{B}| d\kappa \leq c \|\hat{B}\|_{L^2_{s_B}(\mathbb{R})}, \quad (3.12)$$

which holds for any $s_B > 1/2$ because $\int_{\mathbb{R}} (1 + |\kappa|)^{-2s_B} d\kappa < \infty$ for $s_B > 1/2$. Besides, due to the support of \hat{C} we have

$$\|\hat{C}\|_{L^2(\mathbb{R})} \leq \sup_{|\kappa| > \varepsilon^{r-1}} (1 + |\kappa|)^{-s_C} \|\hat{C}\|_{L^2_{s_C}(\mathbb{R})} \leq c\varepsilon^{s_C(1-r)} \|\hat{C}\|_{L^2_{s_C}(\mathbb{R})} \quad (3.13)$$

for any $s_C > 0$. With (3.12) and (3.13) we obtain

$$\left\| W_1 *_{\mathbb{B}} \hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \hat{B} \left(\frac{\cdot + k_0}{\varepsilon} \right) \right\|_{L^2(\mathbb{B}+k_0)} \leq c\varepsilon^{5/2+s_C(1-r)} \|\hat{C}\|_{L^2_{s_C}(\mathbb{R})} \|\hat{B}\|_{L^2_{s_B}(\mathbb{R})}^2$$

for any $s_B > 1/2$ and $s_C > 0$. Using similar computations for the higher-order terms in (3.11) with the use of the estimate (3.12) for \hat{C} , we obtain

$$\|E\|_{L^2(\mathbb{B}+k_0)} \leq c\varepsilon^{5/2+s_C(1-r)} \|\hat{C}\|_{L^2_{s_C}(\mathbb{R})} \left(\|\hat{B}\|_{L^2_{s_B}(\mathbb{R})} + \|\hat{C}\|_{L^2_{s_C}(\mathbb{R})} \right)^2, \quad (3.14)$$

for any $s_B > 1/2$ and $s_C > 1/2$. By using the estimate

$$\|\hat{B} * \hat{B} * \hat{B}\|_{L^2(-3\varepsilon^{r-1}, 3\varepsilon^{r-1})} \leq \|\hat{B}\|_{L^2(\mathbb{R})} \|\hat{B}\|_{L^1(\mathbb{R})}^2 \leq c \|\hat{B}\|_{L^2_{s_B}(\mathbb{R})}^3,$$

which follows from Young's inequality and estimate (3.12), we arrive at

$$\|F(\tilde{u}_1)\|_{\mathcal{X}_s} \leq c\varepsilon^{5/2} \left(\|\hat{B}\|_{L^2_{s_B}(\mathbb{R})} + \|\hat{C}\|_{L^2_{s_C}(\mathbb{R})} \right)^3 \quad (3.15)$$

for any $s_B > 1/2$ and $s_C > 1/2$.

3.2. Component $\tilde{u}_{2,1}$. We solve now equation (3.4) for $\tilde{u}_{2,1}$ under assumption (3.9). Recall that the operator

$$M_k := Q_k(L(k) - \omega_* - \varepsilon^2\Omega)Q_k, \quad (3.16)$$

is invertible in $Q_k\mathcal{X}_s$ with a bounded inverse. Thanks to estimate (3.15) there exists a unique solution $\tilde{u}_{2,1}$ of (3.4) which satisfies

$$\|\tilde{u}_{2,1}\|_{\mathcal{X}_s} \leq P\varepsilon^{5/2}, \quad (3.17)$$

where P depends polynomially on $\|\hat{B}\|_{L^2_{s_B}(\mathbb{R})}$ and $\|\hat{C}\|_{L^2_{s_C}(\mathbb{R})}$.

3.3. Component \tilde{u}_R . Next, we solve equation (3.5) for \tilde{u}_R via a Banach fixed point argument with \tilde{u}_1 satisfying (3.9) and $\tilde{u}_{2,1}$ given as above. We write

$$\tilde{u}_R = M_k^{-1} Q_k (F(\tilde{u}_1) - F(\tilde{u}_1 + \tilde{u}_{2,1} + \tilde{u}_R)) =: G(\tilde{u}_R) \quad (3.18)$$

We show the contraction property of G in

$$B_{K\varepsilon^\eta}^{\mathcal{X}_s} := \{f \in \mathcal{X}_s : \|f\|_{\mathcal{X}_s} \leq K\varepsilon^\eta\}$$

for some $K > 0$ and $\eta > 0$ to be determined. First, using (2.7), we estimate

$$\begin{aligned} \|G(\tilde{u}_R)\|_{\mathcal{X}_s} &\leq c [\|\tilde{u}_1\|_{\mathcal{X}_s}^2 (\|\tilde{u}_{2,1}\|_{\mathcal{X}_s} + \|\tilde{u}_R\|_{\mathcal{X}_s}) + \|\tilde{u}_{2,1}\|_{\mathcal{X}_s}^2 (\|\tilde{u}_1\|_{\mathcal{X}_s} + \|\tilde{u}_R\|_{\mathcal{X}_s}) \\ &\quad + \|\tilde{u}_R\|_{\mathcal{X}_s}^2 (\|\tilde{u}_{2,1}\|_{\mathcal{X}_s} + \|\tilde{u}_1\|_{\mathcal{X}_s}) + \|\tilde{u}_1\|_{\mathcal{X}_s} \|\tilde{u}_{2,1}\|_{\mathcal{X}_s} \|\tilde{u}_R\|_{\mathcal{X}_s} + \|\tilde{u}_{2,1}\|_{\mathcal{X}_s}^3 + \|\tilde{u}_R\|_{\mathcal{X}_s}^3]. \end{aligned}$$

Together with (3.10) and (3.17) we obtain for $\tilde{u}_R \in B_{K\varepsilon^\eta}^{\mathcal{X}_s}$

$$\|G(\tilde{u}_R)\|_{\mathcal{X}_s} \leq P (\varepsilon^{7/2} + \varepsilon^{\eta+1} + \varepsilon^{2\eta+1/2} + \varepsilon^{3\eta}), \quad (3.19)$$

where P depends polynomially on $\|\hat{B}\|_{L_{s_B}^2(\mathbb{R})}$ and $\|\hat{C}\|_{L_{s_C}^2(\mathbb{R})}$. Clearly, if $5/2 \leq \eta \leq 7/2$, then $G : B_{K\varepsilon^\eta}^{\mathcal{X}_s} \rightarrow B_{K\varepsilon^\eta}^{\mathcal{X}_s}$ and

$$\|G(\tilde{u}_R)\|_{\mathcal{X}_s} \leq K\varepsilon^{7/2}, \quad (3.20)$$

with K dependent on $\|\hat{B}\|_{L_{s_B}^2(\mathbb{R})}$ and $\|\hat{C}\|_{L_{s_C}^2(\mathbb{R})}$. We set $\eta = 7/2$ for a balance.

For the contraction estimate, we consider $\tilde{u} := \tilde{u}_1 + \tilde{u}_{2,1} + \tilde{u}_R$ and $\tilde{v} := \tilde{u}_1 + \tilde{u}_{2,1} + \tilde{v}_R$. A straightforward calculation leads to

$$\begin{aligned} \|G(\tilde{u}_R) - G(\tilde{v}_R)\|_{\mathcal{X}_s} &\leq P (\|\tilde{u}_1\|_{\mathcal{X}_s}^2 + \|\tilde{u}_{2,1}\|_{\mathcal{X}_s}^2 + \|\tilde{u}_R\|_{\mathcal{X}_s}^2 + \|\tilde{v}_R\|_{\mathcal{X}_s}^2) \|\tilde{u}_R - \tilde{v}_R\|_{\mathcal{X}_s} \\ &\leq \varepsilon P \|\tilde{u}_R - \tilde{v}_R\|_{\mathcal{X}_s}, \end{aligned}$$

such that the contraction holds for $\varepsilon > 0$ small enough.

By the Banach fixed-point theorem, there exists a unique solution to equation (3.18) for \tilde{u}_R , which satisfies the estimate

$$\|\tilde{u}_R\|_{\mathcal{X}_s} \leq K\varepsilon^{7/2}, \quad (3.21)$$

where K depends polynomially on $\|\hat{B}\|_{L_{s_B}^2(\mathbb{R})}$ and $\|\hat{C}\|_{L_{s_C}^2(\mathbb{R})}$.

3.4. Component \hat{C} . Equation (3.2) on the compact support of \hat{C} can be rewritten as

$$\hat{C} \left(\frac{k - k_0}{\varepsilon} \right) = (\omega_* + \varepsilon^2 \Omega - \omega_m(k))^{-1} (1 - \chi_{(-\varepsilon^r, \varepsilon^r)}(k - k_0)) \langle F(\tilde{u})(\cdot, k), p_m^*(\cdot, k) \rangle \quad (3.22)$$

with $k - k_0 \in \mathbb{B} \setminus (-\varepsilon^r, \varepsilon^r)$. Recall the decomposition $\tilde{u}_1(x, k) = \tilde{u}_{1,B}(x, k) + \tilde{u}_{1,C}(x, k)$, where for $k - k_0 \in \mathbb{B}$ we have

$$\tilde{u}_{1,B}(x, k) = \hat{B} \left(\frac{k - k_0}{\varepsilon} \right) p_m(x, k), \quad \tilde{u}_{1,C}(x, k) = \hat{C} \left(\frac{k - k_0}{\varepsilon} \right) p_m(x, k).$$

Equation (3.22) can be rewritten in the form

$$\tilde{u}_{1,C}(x, k) = H(\tilde{u}_{1,C})(x, k), \quad k - k_0 \in \mathbb{B} \setminus (-\varepsilon^r, \varepsilon^r), \quad (3.23)$$

where

$$\begin{aligned} H(\tilde{u}_{1,C})(x, k) &:= \nu(k) (1 - \chi_{(-\varepsilon^r, \varepsilon^r)}(k - k_0)) [h^{-1}(k) \langle h(k) F(\tilde{u}_{1,B})(\cdot, k), p_m^*(\cdot, k) \rangle \\ &\quad + \langle (F(\tilde{u}) - F(\tilde{u}_{1,B}))(\cdot, k), p_m^*(\cdot, k) \rangle] p_m(x, k), \end{aligned}$$

with $\nu(k) := (\omega_* + \varepsilon^2 \Omega - \omega_m(k))^{-1}$ and $h(k) := (1 + \varepsilon^{-1}|k - k_0|)^{s_B}$ for some $s_B > 1/2$ to be determined. We note that

$$\sup_{k-k_0 \in \mathbb{B} \setminus (-\varepsilon^r, \varepsilon^r)} \nu(k) = c\varepsilon^{-2r} \quad \text{and} \quad \sup_{k-k_0 \in \mathbb{B} \setminus (-\varepsilon^r, \varepsilon^r)} h^{-1}(k) = c\varepsilon^{(1-r)s_B}.$$

The first term in $H(\tilde{u}_{1,C})$ denoted as T_1 is estimated as follows

$$\begin{aligned} \|T_1\|_{\mathcal{X}_s} &\leq c\varepsilon^{(1-r)s_B-2r} \|hF(\tilde{u}_{1,B})\|_{\mathcal{X}_s} \\ &\leq c\varepsilon^{(1-r)s_B-2r} \left\| h\hat{B}\left(\frac{\cdot - k_0}{\varepsilon}\right) *_{\mathbb{B}} \hat{B}\left(\frac{\cdot - k_0}{\varepsilon}\right) *_{\mathbb{B}} \hat{B}\left(\frac{\cdot + k_0}{\varepsilon}\right) \right\|_{L^2(k_0-3\varepsilon^r, k_0+3\varepsilon^r)} \\ &\leq c\varepsilon^{5/2+(1-r)s_B-2r} \left\| \hat{B} * \hat{B} * \hat{B} \right\|_{L^2_{s_B}(-3\varepsilon^{r-1}, 3\varepsilon^{r-1})} \\ &\leq c\varepsilon^{5/2+(1-r)s_B-2r} \|\hat{B}\|_{L^2_{s_B}(-3\varepsilon^{r-1}, 3\varepsilon^{r-1})}^3, \end{aligned}$$

if $s_B > 1/2$. The last inequality follows from $\hat{B} * \hat{B} * \hat{B} = \widehat{|B|^2 B}$, the fact that the Fourier transform \mathcal{F} is an isomorphism $\mathcal{F} : H^s(\mathbb{R}) \rightarrow L^2_s(\mathbb{R})$ for any $s \geq 0$ and from the algebra property of H^s for $s > 1/2$.

The second term in $H(\tilde{u}_{1,C})$, denoted as T_2 , is estimated with the help of the algebra property (2.7) of \mathcal{X}_s for $s > 1/2$,

$$\begin{aligned} \|T_2\|_{\mathcal{X}_s} &\leq c\varepsilon^{-2r} [\|\tilde{u}_{1,C}\|_{\mathcal{X}_s}^3 + \|\tilde{u}_{1,C}\|_{\mathcal{X}_s}^2 (\|\tilde{u}_{1,B}\|_{\mathcal{X}_s} + \|\tilde{u}_2\|_{\mathcal{X}_s}) \\ &\quad + \|\tilde{u}_{1,C}\|_{\mathcal{X}_s} (\|\tilde{u}_{1,B}\|_{\mathcal{X}_s}^2 + \|\tilde{u}_2\|_{\mathcal{X}_s}^2) + \|\tilde{u}_{1,B}\|_{\mathcal{X}_s}^2 \|\tilde{u}_2\|_{\mathcal{X}_s} + \|\tilde{u}_{1,B}\|_{\mathcal{X}_s} \|\tilde{u}_2\|_{\mathcal{X}_s}^2 + \|\tilde{u}_2\|_{\mathcal{X}_s}^3]. \end{aligned}$$

We have the equivalence

$$c_1 \varepsilon^{1/2} \|\hat{B}\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \|\tilde{u}_{1,B}\|_{\mathcal{X}_s} \leq c_2 \varepsilon^{1/2} \|\hat{B}\|_{L^2(\varepsilon^{-1}\mathbb{B})} \quad (3.24)$$

and

$$c_1 \varepsilon^{1/2} \|\hat{C}\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \|\tilde{u}_{1,C}\|_{\mathcal{X}_s} \leq c_2 \varepsilon^{1/2} \|\hat{C}\|_{L^2(\varepsilon^{-1}\mathbb{B})} \quad (3.25)$$

for some $c_1, c_2 > 0$. Using (3.17) and (3.21), we further have

$$\|\tilde{u}_2\|_{\mathcal{X}_s} \leq K\varepsilon^{5/2},$$

where K depends polynomially on $\|\hat{B}\|_{L^2_{s_B}}$ and $\|\hat{C}\|_{L^2_{s_C}}$. As a result, we obtain

$$\|T_2\|_{\mathcal{X}_s} \leq \rho \varepsilon^{-2r} (\|\tilde{u}_{1,C}\|_{\mathcal{X}_s}^3 + \varepsilon^{1/2} \|\tilde{u}_{1,C}\|_{\mathcal{X}_s}^2 + \varepsilon \|\tilde{u}_{1,C}\|_{\mathcal{X}_s} + \varepsilon^{7/2}) + \text{h.o.t.},$$

where ρ depends on $\|\hat{B}\|_{L^2_{s_B}}$ only, $\rho = \mathcal{O}(1)$ as $\varepsilon \rightarrow 0$, and where h.o.t. includes terms of higher order in ε or higher powers of $\|\tilde{u}_{1,C}\|_{\mathcal{X}_s}$.

Combining the estimates for T_1 and T_2 , we obtain

$$\begin{aligned} \|H(\tilde{u}_{1,C})\|_{\mathcal{X}_s} &\leq \rho (\varepsilon^{5/2+(1-r)s_B-2r} + \varepsilon^{7/2-2r} + \varepsilon^{1-2r} \|\tilde{u}_{1,C}\|_{\mathcal{X}_s} + \varepsilon^{1/2-2r} \|\tilde{u}_{1,C}\|_{\mathcal{X}_s}^2 \\ &\quad + \varepsilon^{-2r} \|\tilde{u}_{1,C}\|_{\mathcal{X}_s}^3) + \text{h.o.t.} \end{aligned}$$

Similarly one gets

$$\begin{aligned} \|H(\tilde{u}_{1,C}) - H(\tilde{v}_{1,C})\|_{\mathcal{X}_s} &\leq \rho (\varepsilon^{1-2r} + \varepsilon^{1/2-2r} (\|\tilde{u}_{1,C}\|_{\mathcal{X}_s} + \|\tilde{v}_{1,C}\|_{\mathcal{X}_s}) \\ &\quad + \varepsilon^{-2r} (\|\tilde{u}_{1,C}\|_{\mathcal{X}_s}^2 + \|\tilde{v}_{1,C}\|_{\mathcal{X}_s}^2)) \|\tilde{u}_{1,C} - \tilde{v}_{1,C}\|_{\mathcal{X}_s}. \end{aligned}$$

Thus, the contraction holds for $\tilde{u}_{1,C}$ in the ball

$$\|\tilde{u}_{1,C}\|_{\mathcal{X}_s} \leq \rho (\varepsilon^{5/2+(1-r)s_B-2r} + \varepsilon^{7/2-2r}) \quad (3.26)$$

if $r \in (0, 1/2)$ and if $\varepsilon > 0$ is small enough. By the Banach fixed-point theorem, there exists a unique \tilde{u}_{1_C} satisfying equation (3.23) and the bound (3.26).

We also get an estimate for $\|\hat{C}\|_{L^2(\varepsilon^{-1}\mathbb{B})}$ by using (3.25),

$$\|\hat{C}\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \rho \left(\varepsilon^{2+(1-r)s_B-2r} + \varepsilon^{3-2r} \right), \quad (3.27)$$

and an estimate of $\|\hat{C}\|_{L^2_{s_C}(\varepsilon^{-1}\mathbb{B})}$ by using

$$\|\hat{C}\|_{L^2_{s_C}(\varepsilon^{-1}\mathbb{B})} \leq \sup_{|\kappa| < \frac{1}{2\varepsilon}} (1 + |\kappa|)^{s_C} \|\hat{C}\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \rho \left(\varepsilon^{2+(1-r)s_B-2r-s_C} + \varepsilon^{3-2r-s_C} \right), \quad (3.28)$$

where ρ in both estimates (3.27) and (3.28) depends polynomially on $\|\hat{B}\|_{L^2_{s_B}}$.

3.5. Component \hat{B} . Finally, we turn to the leading order component $\hat{B}(\frac{k-k_0}{\varepsilon})p_m(x, k)$ of the solution $\tilde{u}(x, k)$ and prove the existence of \hat{B} close to \hat{A} , a solution of the effective amplitude equation (3.8).

Equation (3.2) on the compact support of \hat{B} can be rewritten as

$$(\omega_m(k) - \omega_* - \varepsilon^2\Omega)\hat{B}\left(\frac{k-k_0}{\varepsilon}\right) + \chi_{(-\varepsilon^r, \varepsilon^r)}(k-k_0)\langle F(\tilde{u})(\cdot, k), p_m^*(\cdot, k) \rangle = 0 \quad (3.29)$$

with $k - k_0 \in (-\varepsilon^r, \varepsilon^r)$. Once again, we use a fixed point argument to solve for \hat{B} . In order to close the procedure for constructing \tilde{u} , we need the constants in all estimates to depend only on norms of \hat{B} and not on norms of \hat{C} . As all constants are polynomials in $\|\hat{B}\|_{L^2_{s_B}}$ and $\|\hat{C}\|_{L^2_{s_C}}$, we can employ (3.28) to get rid of the dependence on $\|\hat{C}\|_{L^2_{s_C}}$. We need to ensure, however,

$$\min\{2 + (1-r)s_B - 2r - s_C, 3 - 2r - s_C\} > 0.$$

Hence, $s_C > 1/2$ is further restricted by

$$s_C < \min\{2 + (1-r)s_B - 2r, 3 - 2r\}.$$

Since $r < 1/2$ and $s_B > 1/2$, we can choose $s_C = 1 > 1/2$ to satisfy this restriction.

As we show below, the reduced bifurcation equation (3.29) is a perturbation of equation (3.8). To this end, we expand the band function satisfying assumption (II) by

$$\omega_m(k) = \omega_* + \frac{1}{2}\omega_m''(k_0)(k-k_0)^2 + \omega_r(k),$$

where the remainder term satisfies the cubic estimate

$$|\omega_r(k)| \leq c|k-k_0|^3 \text{ for all } k \in \mathbb{B} + k_0. \quad (3.30)$$

By substituting this decomposition into equation (3.29), we can rewrite the problem for \hat{B} in the form

$$\begin{aligned} & \left(\frac{1}{2}\omega_m''(k_0) \left(\frac{k-k_0}{\varepsilon}\right)^2 - \Omega \right) \hat{B}\left(\frac{k-k_0}{\varepsilon}\right) + \varepsilon^{-2}\chi_{(-\varepsilon^r, \varepsilon^r)}(k-k_0)\langle F(\tilde{u}_1)(\cdot, k), p_m^*(\cdot, k) \rangle \\ & + \varepsilon^{-2}\chi_{(-\varepsilon^r, \varepsilon^r)}(k-k_0) \left[\langle (F(\tilde{u}) - F(\tilde{u}_1))(\cdot, k), p_m^*(\cdot, k) \rangle - \omega_r(k)\hat{B}\left(\frac{k-k_0}{\varepsilon}\right) \right] = 0. \end{aligned} \quad (3.31)$$

The second term in equation (3.31) recovers the nonlinearity coefficient in equation (3.8). Indeed, when we isolate the \hat{B} -component in U_1 and approximate all Bloch waves by those

at $k = k_0$, we get

$$\begin{aligned} \langle F(\tilde{u}_1)(\cdot, k), p_m^*(\cdot, k) \rangle &= \Gamma \left(\hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \hat{B} \left(\frac{\cdot - k_0}{\varepsilon} \right) *_{\mathbb{B}} \hat{B} \left(\frac{\cdot + k_0}{\varepsilon} \right) \right) (k) \\ &\quad + \Gamma E(k) + H(k), \end{aligned}$$

where Γ is given by (1.18), $E(k)$ is given in (3.11), and

$$H(k) := \int_{\mathbb{B}} \int_{\mathbb{B}} (\beta(k, k-l, l-t, t) - \Gamma) U_1(k-l) U_1(l-t) \overline{U_1(-t)} dt dl$$

with

$$\beta(k, k-l, l-t, t) := \langle \sigma p_m(\cdot, k-l) p_m(\cdot, l-t) \overline{p_m(\cdot, -t)}, p_m^*(\cdot, k) \rangle.$$

Note that $\Gamma = \beta(k_0, k_0, k_0, -k_0)$.

Next, we show the smallness of E , H and the terms in the square brackets in (3.31). With the help of (3.30) we obtain

$$\begin{aligned} \left\| \omega_r(k_0 + \varepsilon \cdot) \hat{B} \right\|_{L^2(\varepsilon^{-1}\mathbb{B})}^2 &\leq c\varepsilon^6 \int_{-\varepsilon^{r-1}}^{\varepsilon^{r-1}} |\hat{B}(\kappa)|^2 |\kappa|^6 d\kappa \\ &\leq c\varepsilon^6 \sup_{|\kappa| < \varepsilon^{r-1}} \frac{|\kappa|^6}{(1+|\kappa|)^4} \int_{-\varepsilon^{r-1}}^{\varepsilon^{r-1}} (1+|\kappa|)^4 |\hat{B}(\kappa)|^2 d\kappa \\ &\leq c\varepsilon^{4+2r} \|\hat{B}\|_{L^2_2(\mathbb{R})}^2, \end{aligned}$$

so that

$$\left\| \omega_r(k_0 + \varepsilon \cdot) \hat{B} \right\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq c\varepsilon^{2+r} \|\hat{B}\|_{L^2_2(\mathbb{R})}. \quad (3.32)$$

Estimate (3.32) dictates the choice of s_B , namely $s_B = 2 > 1/2$. Hence, from now on we work with

$$s_B = 2 \text{ and } s_C = 1,$$

in addition to $r < 1/2$.

To estimate H , we substitute the ansatz $U_1(k) = \hat{D} \left(\frac{k-k_0}{\varepsilon} \right)$ for $k \in \mathbb{B} + k_0$ into $H(k)$ and use the transformations $t' := \varepsilon^{-1}(t+k_0-m_3)$, $l' := \varepsilon^{-1}(l+m_2-m_3)$ and $\kappa := \varepsilon^{-1}(k-k_0)$. Then we get

$$H(k_0 + \varepsilon \kappa) = \varepsilon^2 \sum_{m_{1,2,3} \in \{0,1\}} \int_{\varepsilon^{-1}(\mathbb{B}+m_2-m_3)} \int_{\varepsilon^{-1}(\mathbb{B}+k_0-m_3)} g dt' dl',$$

where

$$\begin{aligned} g &= (\beta(k_0 + \varepsilon \kappa, k_0 + \varepsilon(\kappa - l'), k_0 + \varepsilon(l' - t'), -k_0 + \varepsilon t') - \Gamma) \\ &\quad \times \chi_{\varepsilon^{-1}(\mathbb{B}-m_1-m_2+m_3)}(\kappa - l') \hat{D}(\kappa - l' + \varepsilon^{-1}(m_1 + m_2 - m_3)) \\ &\quad \times \chi_{\varepsilon^{-1}\mathbb{B}}(l' - t') \hat{D}(l' - t') \chi_{\varepsilon^{-1}\mathbb{B}}(t') \overline{\hat{D}(t')}. \end{aligned}$$

Due to the analyticity of $k \mapsto p_m(\cdot, k)$ (recall that the eigenvalue family ω_m is simple) the coefficient β is certainly Lipschitz continuous in each variable and we have

$$\begin{aligned} &|\beta(k_0 + \varepsilon \kappa, k_0 + \varepsilon(\kappa - l'), k_0 + \varepsilon(l' - t'), -k_0 + \varepsilon t') - \beta(k_0, k_0, k_0, -k_0)| \\ &\leq c\varepsilon(|\kappa| + |\kappa - l'| + |l' - t'| + |t'|) \\ &\leq 2c\varepsilon(|\kappa - l'| + |l' - t'| + |t'|). \end{aligned}$$

This leads to the estimate

$$|H(k_0 + \varepsilon\kappa)| \leq c\varepsilon^3 \left(2|h\hat{D}| * |\hat{D}| * |\hat{D}| + |\hat{D}| * |\hat{D}| * |h\hat{D}| \right) (\kappa) \text{ with } h(\kappa) := \kappa,$$

where $*$ is the convolution over the whole real line. Applying Young's inequality for convolutions, we have

$$\|H(k_0 + \varepsilon\cdot)\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq c\varepsilon^3 \|\hat{D}\|_{L^2_1(\mathbb{R})} \|\hat{D}\|_{L^1(\mathbb{R})}^2 \leq c\varepsilon^3 \left(\|\hat{B}\|_{L^2_1(\mathbb{R})} + \|\hat{C}\|_{L^2_1(\mathbb{R})} \right)^3,$$

where we have used estimate (3.12) and the triangle inequality. Employing now estimate (3.28) with $r < 1/2$, $s_B = 2$, and $s_C = 1$, we finally obtain

$$\|H(k_0 + \varepsilon\cdot)\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \rho\varepsilon^3, \quad (3.33)$$

where ρ depends on $\|\hat{B}\|_{L^2_{s_B}(\mathbb{R})}$ only.

To estimate E , we use (3.14) and (3.28) again and obtain for $r < 1/2$, $s_B = 2$, and $s_C = 1$

$$\|E(k_0 + \varepsilon\cdot)\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \rho\varepsilon^4,$$

where ρ depends on $\|\hat{B}\|_{L^2_{s_B}(\mathbb{R})}$ only.

By using (3.20) and (3.28) again, we obtain for $\delta F(k) := \langle (F(\tilde{u}) - F(\tilde{u}_1))(\cdot, k), p_m^*(\cdot, k) \rangle$,

$$\|\delta F(k_0 + \varepsilon\cdot)\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \rho\varepsilon^3$$

where ρ depends on $\|\hat{B}\|_{L^2_{s_B}(\mathbb{R})}$ only.

Comparing estimates for E , H and the terms in the square bracket in (3.31), we conclude that the estimate (3.32) yields the leading order term. In summary, equation (3.31) reads

$$\left(\frac{1}{2}\omega_m''(k_0)\kappa^2 - \Omega \right) \hat{B}(\kappa) + \Gamma(\hat{B} * \hat{B} * \hat{B})(\kappa) = \hat{R}(\hat{B})(\kappa), \quad (3.34)$$

where $\kappa \in I_{\varepsilon^{r-1}} := (-\varepsilon^{r-1}, \varepsilon^{r-1})$ and the remainder term satisfies

$$\|\hat{R}(\hat{B})\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq \rho\varepsilon^r, \quad (3.35)$$

with ρ depending on $\|\hat{B}\|_{L^2_2(\mathbb{R})}$ only.

Equation (3.34) is a perturbed stationary NLS equation written in the Bloch form on the compact support. In the following, we prove the existence of solutions \hat{B} to equation (3.34) close to $\chi_{I_{\varepsilon^{r-1}}}\hat{A}$, where \hat{A} satisfies (3.8).

We define

$$F_{\text{NLS}}(\hat{B}) := \left(\frac{1}{2}\omega_m''(k_0)\kappa^2 - \Omega \right) \hat{B} + \Gamma(\hat{B} * \hat{B} * \hat{B})$$

and write (3.34) as

$$F_{\text{NLS}}(\hat{B})(\kappa) = \hat{R}(\hat{B})(\kappa), \quad \kappa \in I_{\varepsilon^{r-1}},$$

where $\text{supp}(\hat{B}) \subset I_{\varepsilon^{r-1}}$. Letting

$$\hat{B} = \hat{A}_\varepsilon + \hat{b}, \text{ where } \hat{A}_\varepsilon := \chi_{I_{\varepsilon^{r-1}}}\hat{A} \text{ and } \text{supp}(\hat{b}) \subset I_{\varepsilon^{r-1}},$$

we finally reformulate (3.34) as

$$\hat{J}_\varepsilon \hat{b} = W(\hat{b}), \quad (3.36)$$

where

$$\begin{aligned}\hat{J}_\varepsilon(\kappa) &:= \chi_{I_{\varepsilon^{r-1}}}(\kappa) D_{\hat{A}} F_{\text{NLS}}(\hat{A}_\varepsilon)(\kappa) \chi_{I_{\varepsilon^{r-1}}}(\kappa), \\ W(\hat{b})(\kappa) &:= \chi_{I_{\varepsilon^{r-1}}}(\kappa) \hat{R}(\hat{A}_\varepsilon + \hat{b})(\kappa) - \chi_{I_{\varepsilon^{r-1}}}(\kappa) \left(F_{\text{NLS}}(\hat{A}_\varepsilon + \hat{b}) - \hat{J}_\varepsilon \hat{b} \right)(\kappa).\end{aligned}$$

Here $D_{\hat{A}} F_{\text{NLS}}(\hat{A})$ is a symbolic notation for the Jacobian of F_{NLS} . Note that F_{NLS} is not complex differentiable but it is differentiable in real variables (after isolating the real and imaginary parts).

The Taylor expansion yields

$$F_{\text{NLS}}(\hat{A}_\varepsilon + \hat{b}) - \hat{J}_\varepsilon \hat{b} = F_{\text{NLS}}(\hat{A}_\varepsilon) + (D_{\hat{A}} F_{\text{NLS}}(\hat{A}_\varepsilon) - \hat{J}_\varepsilon) \hat{b} + Q(\hat{b}),$$

where Q is quadratic in \hat{b} . The term $F_{\text{NLS}}(\hat{A}_\varepsilon)$ does not vanish exactly due to the convolution structure of the nonlinearity but we have

$$F_{\text{NLS}}(\hat{A}_\varepsilon) = \Gamma \left(\hat{A}_\varepsilon * \hat{A}_\varepsilon * \hat{\bar{A}}_\varepsilon - \hat{A} * \hat{A} * \hat{\bar{A}} \right),$$

where the right-hand-side includes terms of the form

$$\hat{a}_\varepsilon * \hat{A}_\varepsilon * \hat{\bar{A}}_\varepsilon, \text{ where } \hat{a}_\varepsilon := \hat{A} - \hat{A}_\varepsilon = (1 - \chi_{I_{\varepsilon^{r-1}}}) \hat{A}$$

and terms quadratic and cubic in \hat{a}_ε . Similarly to estimates of \hat{C} , we have

$$\begin{aligned}|\hat{a}_\varepsilon(\kappa)| &\leq (1 + |\kappa|)^{s_A} |\hat{a}_\varepsilon(\kappa)| \sup_{|\kappa| > \varepsilon^{r-1}} (1 + |\kappa|)^{-s_A} \\ &\leq c \varepsilon^{s_A(1-r)} (1 + |\kappa|)^{s_A} |\hat{a}_\varepsilon(\kappa)|,\end{aligned}$$

where $s_A > 0$ is to be specified. By using Young's inequality, we obtain

$$\begin{aligned}\|\hat{a}_\varepsilon * \hat{A}_\varepsilon * \hat{\bar{A}}_\varepsilon\|_{L^2(\mathbb{R})} &\leq c \varepsilon^{s_A(1-r)} \|(1 + |\cdot|)^{s_A} \hat{A}\|_{L^2(\mathbb{R})} \|\hat{A}_\varepsilon\|_{L^1(\mathbb{R})}^2 \\ &\leq c \varepsilon^{s_A(1-r)} \|\hat{A}\|_{L_{s_A}^2(\mathbb{R})}^3,\end{aligned}$$

where the last estimate holds if $s_A > 1/2$, see (3.12). Thus, we have

$$\|F_{\text{NLS}}(\hat{A}_\varepsilon)\|_{L^2(\mathbb{R})} \leq c \varepsilon^{s_A(1-r)} \|\hat{A}\|_{L_{s_A}^2(\mathbb{R})}^3. \quad (3.37)$$

Similarly, we obtain

$$\|(\chi_{I_{\varepsilon^{r-1}}} D_{\hat{A}} F_{\text{NLS}}(\hat{A}_\varepsilon) - \hat{J}_\varepsilon) \hat{b}\|_{L^2(\mathbb{R})} \leq c \varepsilon^{s_A(1-r)} \|\hat{A}\|_{L_{s_A}^2(\mathbb{R})}^2 \|\hat{b}\|_{L_{s_B}^2(\mathbb{R})} \quad (3.38)$$

for any $s_A > 1/2$.

Combining (3.35), (3.37), and (3.38), we have

$$\|W(\hat{b})\|_{L^2(\mathbb{R})} \leq c_A \left(\varepsilon^r + \varepsilon^{s_A(1-r)} + (\varepsilon^r + \varepsilon^{s_A(1-r)}) \|\hat{b}\|_{L_{s_B}^2(\mathbb{R})} + \|\hat{b}\|_{L_{s_B}^2(\mathbb{R})}^2 + \|\hat{b}\|_{L_{s_B}^2(\mathbb{R})}^3 \right),$$

where c_A depends on $\|\hat{A}\|_{L_{s_A}^2}$ only. Clearly, if $s_A \geq r/(1-r) \geq 1$ (so that $s_A \geq 1$ is used from now on), then there exist positive constants c_1 and c_2 that only depend on $\|\hat{A}\|_{L_{s_A}^2}$ such that for all $\varepsilon > 0$ small enough

$$W : B_{c_1 \varepsilon^r}^{2,2} \rightarrow B_{c_1 \varepsilon^r}^{2,2}, \quad (3.39)$$

and

$$\|W(\hat{b}_1) - W(\hat{b}_2)\|_{L^2(\mathbb{R})} \leq c_2 \varepsilon^r \|\hat{b}_1 - \hat{b}_2\|_{L_{s_B}^2(\varepsilon^{-1}\mathbb{B})} \text{ for all } \hat{b}_1, \hat{b}_2 \in B_{c_1 \varepsilon^r}^{2,2}, \quad (3.40)$$

where

$$B_{c_1 \varepsilon^r}^{2,2} := \{\hat{b} \in L_2^2(\varepsilon^{-1}\mathbb{B}) : \|\hat{b}\|_{L_2^2(\varepsilon^{-1}\mathbb{B})} \leq c_1 \varepsilon^r\}. \quad (3.41)$$

We wish to solve (3.36) in $B_{c_1 \varepsilon^r}^{2,2}$ via the Banach fixed point iteration by writing $\hat{b} = \hat{J}_\varepsilon^{-1}W(\hat{b})$, where

$$\hat{J}_\varepsilon^{-1} : L^2(\varepsilon^{-1}\mathbb{B}) \rightarrow L_2^2(\varepsilon^{-1}\mathbb{B}).$$

The operator \hat{J}_ε^{-1} is, however, not bounded uniformly in ε (in a neighborhood of $\varepsilon = 0$) because the Jacobian $\hat{J}_0 := D_{\hat{A}}F_{\text{NLS}}(\hat{A})$ has a nontrivial kernel due to the shift and phase invariances of the stationary NLS equation (1.17).

Indeed, as is well known (see Chapter 4 in [25]), the Jacobian J_0 at a bound state A of the stationary NLS equation (1.17) is a diagonal operator of two Schrödinger operators

$$L_+ := -\frac{1}{2}\omega_m''(k_0)\frac{d^2}{dX^2} - \Omega + 3\Gamma|A(X)|^2 : H^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$$

and

$$L_- := -\frac{1}{2}\omega_m''(k_0)\frac{d^2}{dX^2} - \Omega + \Gamma|A(X)|^2 : H^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$$

which act on the real and imaginary parts of the perturbation to A . By the shift and phase invariances, both operators have kernels, namely

$$\text{Ker}(L_+) = \text{span}\left(\frac{dA}{dX}\right) \quad \text{and} \quad \text{Ker}(L_-) = \text{span}(A),$$

and the simple zero eigenvalue of L_+ and L_- is isolated from the rest of their spectra. By using the Fourier transform and the dualism between $H^2(\mathbb{R})$ and $L_2^2(\mathbb{R})$ spaces, these facts imply that if $A \neq 0$ is a bound state to equation (1.17) in $H^{s_A}(\mathbb{R})$ with $s_A \geq 1$, then the kernel of $\hat{J}_0 : L_2^2(\mathbb{R}) \rightarrow L^2(\mathbb{R})$ is two-dimensional and the double zero eigenvalue is bounded away from the rest of the spectrum of \hat{J}_0 . In a suitably selected subspace defined by a symmetry of the stationary NLS equation (1.17), such that the invariances do not hold within this subspace, the Jacobian \hat{J}_0 is invertible. The two invariances are avoided if we restrict to \mathcal{PT} -symmetric A and b , *i.e.*

$$A(-x) = \overline{A(x)}, \quad b(-x) = \overline{b(x)},$$

or equivalently

$$\hat{A}(\kappa), \hat{b}(\kappa) \in \mathbb{R} \text{ for all } \kappa \in \mathbb{R}.$$

Hence, for any given \mathcal{PT} -symmetric solution A to equation (1.17), we consider a solution to the fixed-point equation (3.36) in $B_{c_1 \varepsilon^r}^{2,2}$ for real \hat{b} . By the \mathcal{PT} -symmetry of the original problem (1.1), all components of the decomposition of u inherit the \mathcal{PT} -symmetry if \hat{b} is real, so that if \hat{b} is real, then $\hat{J}_\varepsilon^{-1}W(\hat{b})$ is real, and the fixed-point equation (3.36) is closed in the space of \mathcal{PT} -symmetric solutions. Then, thanks to (3.39), (3.40), and (3.41), there exists a unique real solution $\hat{b} \in B_{c_1 \varepsilon^r}^{2,2}$ of the fixed-point equation (3.36).

In order to understand the above inheritance property in more detail, note that u is \mathcal{PT} -symmetric if and only if $\tilde{u}(\cdot, k)$ is \mathcal{PT} -symmetric for all $k \in \mathbb{B}$. Hence, we can check the inheritance in the Bloch variable \tilde{u} . Clearly, we need to only check that M_k and F commute with the \mathcal{PT} -symmetry, where M_k is given by (3.16). We write

$$\mathcal{PT}(\tilde{u})(x, k) := \overline{\tilde{u}(-x, k)}.$$

For M_k first note that $Q_k \mathcal{PT} = \mathcal{PT} Q_k$ because the eigenfunctions $p_m(\cdot, k)$ and $p_m^*(\cdot, k)$ are \mathcal{PT} -symmetric, such that

$$\begin{aligned} Q_k \mathcal{PT}(\tilde{u})(x, k) &= \mathcal{PT}(\tilde{u})(x, k) - \langle \mathcal{PT}(\tilde{u})(\cdot, k), p_m^*(\cdot, k) \rangle p_m(x, k) \\ &= \mathcal{PT}(\tilde{u})(x, k) - \langle \mathcal{PT}(\tilde{u})(\cdot, k), \mathcal{PT}(p_m^*(\cdot, k)) \rangle \mathcal{PT}(p_m)(x, k) \\ &= \mathcal{PT}(\tilde{u})(x, k) - \overline{\langle \tilde{u}(\cdot, k), p_m^*(\cdot, k) \rangle} \mathcal{PT}(p_m)(x, k) \\ &= \mathcal{PT}(Q_k \tilde{u})(x, k). \end{aligned}$$

Due to the \mathcal{PT} -symmetry of V we get also $L(k) \mathcal{PT}(\tilde{u}) = \mathcal{PT}(L(k) \tilde{u})$. As a result $M_k \mathcal{PT} = \mathcal{PT} M_k$. Similarly, due to the \mathcal{PT} -symmetry of σ we get $F(\mathcal{PT}(\tilde{u})) = \mathcal{PT}(F(\tilde{u}))$.

Therefore, for each component of \tilde{u} the Banach fixed point argument can be carried out in the \mathcal{PT} -symmetric subspace. All the resulting components of the decomposition are \mathcal{PT} -symmetric and hence the full solution u is \mathcal{PT} -symmetric.

3.6. Difference between the formal ansatz and $\tilde{u}_{1,B}$. To prove the inequality in Theorem 1, it remains to estimate the difference $u_{\text{form}} - \tilde{u}_{1,B}$. The formal ansatz u_{form} in (1.16) translates in Bloch variables to the decomposition (3.6). We seek now an estimate of $\|\tilde{u}_{\text{form}} - \tilde{u}_{1,B}\|_{\mathcal{X}_s}$, where for all $k - k_0 \in \mathbb{B}$ we have

$$\tilde{u}_{1,B}(x, k) = \hat{B}\left(\frac{k-k_0}{\varepsilon}\right) p_m(x, k) = \left(\chi_{(-\varepsilon^r, \varepsilon^r)}(k - k_0) \hat{A}\left(\frac{k-k_0}{\varepsilon}\right) + \hat{b}\left(\frac{k-k_0}{\varepsilon}\right)\right) p_m(x, k).$$

The estimate is carried out as follows:

$$\begin{aligned} \|\tilde{u}_{\text{form}} - \tilde{u}_{1,B}\|_{\mathcal{X}_s}^2 &\leq c\varepsilon \|\hat{b}\|_{L^2(\varepsilon^{-1}\mathbb{B})}^2 + \int_{k_0 - \varepsilon^r}^{k_0 + \varepsilon^r} \left| \hat{A}\left(\frac{k-k_0}{\varepsilon}\right) \right|^2 \|p_m(\cdot, k) - p_m(\cdot, k_0)\|_{H^s(0, 2\pi)}^2 dk \\ &\quad + \int_{\mathbb{B} + k_0} (1 - \chi_{k_0 - \varepsilon^r, k_0 + \varepsilon^r}(k)) \left| \hat{A}\left(\frac{k-k_0}{\varepsilon}\right) \right|^2 dk \|p_m(\cdot, k_0)\|_{H^s(0, 2\pi)}^2 \\ &\quad + \sum_{j \in \mathbb{Z} \setminus \{0\}} \int_{\mathbb{B} + k_0} \left| \hat{A}\left(\frac{k-k_0+j}{\varepsilon}\right) \right|^2 dk \|p_m(\cdot, k_0) e^{ij\cdot}\|_{H^s(0, 2\pi)}^2, \end{aligned}$$

from which we obtain

$$\begin{aligned} \|\tilde{u}_{\text{form}} - \tilde{u}_{1,B}\|_{\mathcal{X}_s}^2 &\leq c\varepsilon \left(\|\hat{b}\|_{L^2(\varepsilon^{-1}\mathbb{B})}^2 + \varepsilon^2 \int_{|\kappa| < \varepsilon^{r-1}} |\kappa|^2 |\hat{A}(\kappa)|^2 d\kappa \right. \\ &\quad + \sup_{|\kappa| > \varepsilon^{r-1}} (1 + |\kappa|)^{-2s_A} \int_{|\kappa| > \varepsilon^{r-1}} (1 + |\kappa|)^{2s_A} |\hat{A}(\kappa)|^2 d\kappa \\ &\quad \left. + \sum_{j \in \mathbb{Z} \setminus \{0\}} \sup_{\kappa \in \varepsilon^{-1}(\mathbb{B}+j)} (1 + |\kappa|)^{-2s_A} \int_{\kappa \in \varepsilon^{-1}(\mathbb{B}+j)} (1 + |\kappa|)^{2s_A} |\hat{A}(\kappa)|^2 d\kappa \right) \end{aligned}$$

and hence

$$\|\tilde{u}_{\text{form}} - \tilde{u}_{1,B}\|_{\mathcal{X}_s}^2 \leq c\varepsilon \left(\|\hat{b}\|_{L^2(\varepsilon^{-1}\mathbb{B})}^2 + \varepsilon^2 \|\hat{A}\|_{L^2(\mathbb{R})}^2 + \varepsilon^{2s_A(1-r)} \|\hat{A}\|_{L^2_{s_A}(\mathbb{R})}^2 \right).$$

Together with $\|\hat{b}\|_{L^2(\varepsilon^{-1}\mathbb{B})} \leq c_1 \varepsilon^r$ (recall that $\hat{b} \in \mathbb{B}_{c_1 \varepsilon^r}^{2,2}$), this estimate yields

$$\|\tilde{u}_{\text{form}} - \tilde{u}_{1,B}\|_{\mathcal{X}_s} \leq c_A \varepsilon^{r+1/2}, \quad (3.42)$$

where the constant c_A depends polynomially on $\|\hat{A}\|_{L^2_{s_A}(\mathbb{R})}$ with $s_A \geq 1$.

Estimate (3.42) together with (3.17), (3.21) and (3.26) and the triangle inequality complete the proof of Theorem 1.

4. THE SPECTRAL ASSUMPTION REVISITED

The proof of Theorem 1 relies critically on Assumption (II) that the spectral band $[a, b]$ is real and isolated from the rest of the spectrum of the Schrödinger operator \mathcal{L} in (1.3) (although this can be generalized as explained in Remark 4 in Section 1). In real periodic potentials, every spectral band is real but the two bands may touch at a point with no spectral gap.

For our purposes we say that the point $(k_0, \mu) \in \mathbb{B} \times \mathbb{R}$ is a *Dirac point* in the one-dimensional case if two eigenvalue families $k \mapsto \omega_m(k)$ and $k \mapsto \omega_{m+1}(k)$ of the spectral problem (1.8) are real on some neighborhood around $k = k_0$, if $\omega_m(k_0) = \omega_{m+1}(k_0) = \mu$ and if ω_m and ω_{m+1} are not differentiable at k_0 .

Due to the Lipschitz continuity of all ω_m (as follows, e.g., by a direct modification of the proof for the Helmholtz equation in [3]), a Dirac point is where ω_m and ω_{m+1} are conical in shape. Moreover, at a Dirac point (k_0, μ) two linearly independent eigenvectors of the spectral problem (1.8) exist and a system of two stationary nonlinear Dirac-type equations can be derived and justified with an analogous analysis as in the case of the stationary NLS equations [26] (see also Chapter 2 in [25]).

In \mathcal{PT} -symmetric periodic potentials with the honeycomb symmetry in two spatial dimensions, a necessary and sufficient condition was derived in [5] at the Dirac point by the perturbation theory that shows when the spectral bands remain real under a complex-valued perturbation.

Here we iterate the same question for the \mathcal{PT} -symmetric potential V in Assumption (I). We derive perturbative results related to splitting of Dirac points, when the real periodic potential is perturbed by a purely imaginary perturbation potential. Therefore, we represent

$$V(x) = U(x) + i\gamma W(x), \quad (4.1)$$

where $\gamma \in \mathbb{R}$ is the perturbation parameter and the real potentials $U, W \in L^\infty_{\text{per}}(0, 2\pi)$ satisfy the symmetry conditions

$$U(-x) = U(x), \quad W(-x) = -W(x), \quad \text{for all } x \in \mathbb{R}. \quad (4.2)$$

In what follows, we derive sufficient conditions for when the two real spectral bands overlapping at a Dirac point (k_0, μ) become complex under a small perturbation. This leads to instability of the zero solution in the time-dependent NLS equation (1.4). At the same time Assumption (II) is no longer true and the formal approximation of bound states via the stationary NLS equation (1.17) cannot be justified.

Let us first note an elementary result.

Lemma 8. *Fix $\gamma = 0$ and let $\mu = \omega(k_0)$ be a Dirac point of $L(k_0)$ for either $k_0 = 0$ or $k_0 = 1/2$. The two linearly independent eigenfunctions φ_\pm of $L(k_0)$ can be chosen such that $\varphi_+(x)e^{ik_0x}$ is real and even and $\varphi_-(x)e^{ik_0x}$ is real and odd.*

Proof. At either $k_0 = 0$ or $k_0 = 1/2$ the functions $\varphi_+(x)e^{ik_0x}$ and $\varphi_-(x)e^{ik_0x}$ are two linearly independent solutions of the Hill's equation

$$\begin{cases} -u''(x) + U(x)u(x) = \mu u(x), \\ u(x + 2\pi) = \pm u(x) \quad \text{for all } x \in \mathbb{R}, \end{cases} \quad (4.3)$$

where the plus sign is chosen for $k_0 = 0$ and the minus sign is chosen for $k_0 = 1/2$. Since U is even due to (4.2), there exists one even and one odd real-valued solution of the boundary-value problem (4.3), see Theorems 1.1 and 1.2 in [21]. \square

The following proposition presents the first perturbation result on the unstable splitting of Dirac points under a \mathcal{PT} -symmetric perturbation of a real even potential.

Proposition 9. *Let the periodic potential V in Assumption (I) be given by (4.1) and (4.2). Assume that $\mu = \omega(k_0)$ is a Dirac point of $L(k_0)$ at $\gamma = 0$ for either $k_0 = 0$ or $k_0 = 1/2$ and choose the corresponding linearly independent eigenfunctions φ_{\pm} such that $\varphi_+(x)e^{ik_0x}$ is real and even and $\varphi_-(x)e^{ik_0x}$ is real and odd. If*

$$\langle W\varphi_+, \varphi_- \rangle \neq 0,$$

then, for every $\gamma \neq 0$ sufficiently small, there exist two eigenvalues $\omega_{\pm}(k_0)$ of the spectral problem (1.8) with $\text{Im}(\omega_{\pm}(k_0)) \neq 0$ and $\omega_{\pm}(k_0) \rightarrow \mu$ as $\gamma \rightarrow 0$.

Proof. The assertion follows from the perturbation theory for the Bloch eigenvalue problem

$$\begin{cases} [L_U(k_0) + i\gamma W]p(\cdot, k_0) = \omega(k_0)p(\cdot, k_0), \\ p(x + 2\pi, k_0) = p(x, k_0) \quad \text{for all } x \in \mathbb{R}, \end{cases} \quad (4.4)$$

where $L_U(k_0) := -(\frac{d}{dx} + ik_0)^2 + U$ and $\mu = \omega(k_0)$ is double at $\gamma = 0$, with two linearly independent eigenfunctions φ_{\pm} . We normalize φ_{\pm} such that $\|\varphi_{\pm}\|_{L^2(0, 2\pi)} = 1$. The eigenfunctions are orthogonal $\langle \varphi_+, \varphi_- \rangle = \langle \varphi_+ e^{ik_0 \cdot}, \varphi_- e^{ik_0 \cdot} \rangle = 0$ because $\varphi_+ e^{ik_0 \cdot}$ and $\varphi_- e^{ik_0 \cdot}$ have opposite (even and odd) symmetries.

Let us use the orthogonal projection operators P_0 and $Q_0 = I - P_0$, such that for every $f \in L^2(0, 2\pi)$ we define

$$P_0 f = \langle \varphi_+, f \rangle \varphi_+ + \langle \varphi_-, f \rangle \varphi_-.$$

Then, clearly, $\langle \varphi_+, Q_0 f \rangle = \langle \varphi_-, Q_0 f \rangle = 0$. Therefore, we write

$$\begin{cases} p(\cdot, k_0) = c_+ \varphi_+ + c_- \varphi_- + \gamma \varphi, & \langle \varphi_+, \varphi \rangle = \langle \varphi_-, \varphi \rangle = 0, \\ \omega(k_0) = \mu + \gamma \Omega, \end{cases} \quad (4.5)$$

where $c_+, c_- \in \mathbb{C}$ are coordinates of the decomposition over the eigenfunctions φ_+ , φ_- and φ , Ω are the remainder terms (which depend on γ). By using projection operators P_0 and Q_0 , we project the eigenvalue problem (4.4) into the two blocks

$$iM_W \mathbf{c} + i\gamma \begin{bmatrix} \langle \varphi_+, W\varphi \rangle \\ \langle \varphi_-, W\varphi \rangle \end{bmatrix} = \Omega \mathbf{c} \quad (4.6)$$

and

$$[L_U(k_0) - \mu] \varphi = H_W := Q_0(\Omega - iW) [c_+ \varphi_+ + c_- \varphi_- + \gamma \varphi], \quad (4.7)$$

where $\mathbf{c} := (c_+, c_-)^T$ and

$$M_W := \begin{bmatrix} \langle W\varphi_+, \varphi_+ \rangle & \langle W\varphi_-, \varphi_+ \rangle \\ \langle W\varphi_+, \varphi_- \rangle & \langle W\varphi_-, \varphi_- \rangle \end{bmatrix}. \quad (4.8)$$

Because W is odd and $|\varphi_{\pm}(x)|^2 = \varphi_{\pm}(x)e^{ik_0x}\overline{\varphi_{\pm}(x)e^{ik_0x}}$ are even, we get $\langle W\varphi_{\pm}, \varphi_{\pm} \rangle = 0$. Hence,

$$M_W = \begin{bmatrix} 0 & \langle W\varphi_-, \varphi_+ \rangle \\ \langle W\varphi_+, \varphi_- \rangle & 0 \end{bmatrix}.$$

Since M_W is hermitian, the two eigenvalues Ω of the truncated eigenvalue problem

$$iM_W\mathbf{c} = \Omega\mathbf{c} \tag{4.9}$$

are purely imaginary, $\Omega_{1,2} = i\lambda_{1,2} := \pm i|\langle W\varphi_+, \varphi_- \rangle|$. They are nonzero and distinct if $\langle W\varphi_+, \varphi_- \rangle \neq 0$. The eigenvectors \mathbf{c} for the two distinct eigenvalues are linearly independent.

Since the double eigenvalue μ is isolated from the rest of the spectrum of $L_U(k_0)$ in $L^2(0, 2\pi)$, a positive constant C_0 exists such that

$$\|Q_0(L_U(k_0) - \mu)^{-1}Q_0\|_{L^2(0,2\pi) \rightarrow L^2(0,2\pi)} \leq C_0.$$

Let us assume that \mathbf{c} and Ω are bounded by a γ -independent positive constant in the limit $\gamma \rightarrow 0$. Since $H_W \in \text{Ran}(L_U(k_0) - \mu)$, fixed-point iterations can be applied to system (4.7) for any finite \mathbf{c} , finite Ω , and sufficiently small $\gamma > 0$. There exists a unique solution $\varphi = \varphi(\gamma, \Omega, \mathbf{c}) \in L^2(0, 2\pi)$ to system (4.7) satisfying the bound

$$\|\varphi\|_{L^2(0,2\pi)} \leq C(\|\mathbf{c}\| + |\Omega|),$$

for $\gamma > 0$ sufficiently small and a γ -independent constant $C > 0$.

We substitute now $\varphi = \varphi(\gamma, \Omega, \mathbf{c})$ into (4.6) and close the construction via an implicit function argument. Let us define

$$G(\gamma, \Omega, \mathbf{c}) := iM_W\mathbf{c} + i\gamma \begin{bmatrix} \langle \varphi_+, W\varphi \rangle \\ \langle \varphi_-, W\varphi \rangle \end{bmatrix} - \Omega\mathbf{c}.$$

We have $G(0, \Omega_1, \mathbf{c}_1) = G(0, \Omega_2, \mathbf{c}_2) = 0$, where $\Omega_{1,2} = i\lambda_{1,2}$ are the two eigenvalues of the truncated eigenvalue problem (4.9) with the eigenvectors $\mathbf{c}_{1,2} \in \mathbb{C}^2$. The Jacobian with respect to Ω and \mathbf{c} is given by

$$J_j(\tilde{\Omega}, \tilde{\mathbf{c}}) := (D_{(\Omega, \mathbf{c})}G)|_{(0, i\lambda_j, \mathbf{c}_j)}(\tilde{\Omega}, \tilde{\mathbf{c}}) = i(M_W - \lambda_j)\tilde{\mathbf{c}} - \tilde{\Omega}\mathbf{c}_j, \quad j = 1, 2.$$

For every $\mathbf{b} \in \mathbb{C}^2$, there is a unique $\tilde{\Omega} \in \mathbb{C}$ and $\tilde{\mathbf{c}} \in C_j^{\perp} := \{\mathbf{c} \in \mathbb{C}^2 : \mathbf{c} \perp \mathbf{c}_j\}$ such that $J_j(\tilde{\Omega}, \tilde{\mathbf{c}}) = \mathbf{b}$. Indeed, each $\mathbf{b} \in \mathbb{C}^2$ can be uniquely decomposed into C_j and C_j^{\perp} via $\mathbf{b} = b_j\mathbf{c}_j + \mathbf{b}_j^{\perp}$ for some b_j and $\mathbf{b}_j^{\perp} \perp \mathbf{c}_j$. Then, $\tilde{\Omega}_j = -b_j$ and $\tilde{\mathbf{c}} \in C_j^{\perp}$ is the unique solution of the linear inhomogeneous equation $i(M_W - \lambda_j)\tilde{\mathbf{c}} = \mathbf{b}_j^{\perp}$.

Hence, the implicit function theorem produces two unique roots for $\mathbf{c} \neq \mathbf{0}$ and Ω in system (4.6) which converge as $\gamma \rightarrow 0$ respectively to the eigenpairs $(i\lambda_1, \mathbf{c}_1)$ and $(i\lambda_2, \mathbf{c}_2)$ of the truncated problem (4.9). \square

Remark 10. For a general choice of the orthogonal and normalized eigenfunctions φ_+ and φ_- , the matrix M_W in (4.8) is no longer anti-diagonal. However, eigenvalues of M_W are invariant with respect to rotation of the basis in \mathbb{C}^2 and therefore the two eigenvalues are still distinct. The proof of Proposition 9 can be applied for a general choice of eigenfunctions φ_+ and φ_- and the sufficient condition for splitting of the Dirac points is given by invertibility of the matrix M_W .

If $U = 0$, there are infinitely many Dirac points in the Bloch eigenvalue problem (4.4) for $\gamma = 0$. The following proposition gives a sufficient condition that one of these Dirac points splits and gives rise to instability under the \mathcal{PT} -symmetric potential W .

Proposition 11. *Let $U = 0$. At $\gamma = 0$ Dirac points exist at each $\mu_n = \frac{1}{4}n^2, n \in \mathbb{N}$. The k -coordinate of the Dirac point at μ_n is $k_0 = 0$ for n even and $k_0 = \frac{1}{2}$ for n odd. Let $W \in L_{\text{per}}^\infty(0, 2\pi)$ be defined by the Fourier sine series*

$$W(x) = \sum_{j \in \mathbb{N}} b_j \sin(jx) \quad (4.10)$$

with $b_j \in \mathbb{R}$ for every $j \in \mathbb{N}$. If $b_n \neq 0$ for some $n \in \mathbb{N}$, then for every $\gamma \neq 0$ sufficiently small the Dirac point at $\mu_n = \frac{1}{4}n^2$ breaks into two complex eigenvalues $\omega_\pm(k_0)$ of the spectral problem (1.8) with $\text{Im}(\omega_\pm(k_0)) \neq 0$ and $\omega_\pm(k_0) \rightarrow \mu_n$ as $\gamma \rightarrow 0$.

Proof. For $U = 0$ and $\gamma = 0$, the eigenvalues of the Bloch eigenvalue problem (1.8) are

$$\tilde{\omega}_{2m-1}(k) = (k - m)^2, \quad \tilde{\omega}_{2m}(k) = (k + m)^2, \quad m \in \mathbb{N}, \quad k \in \mathbb{B},$$

which give the location of the Dirac points at $(k_0, \mu) = (0, m^2)$, i.e. the crossing point of $\tilde{\omega}_{2m-1}(k)$ and $\tilde{\omega}_{2m}(k)$, and at $(k_0, \mu) = (\frac{1}{2}, \frac{(2m-1)^2}{4})$, i.e. the crossing point of $\tilde{\omega}_{2m-2}(k)$ and $\tilde{\omega}_{2m-1}(k)$. Note that in contrast to ω_n the eigenvalues $\tilde{\omega}_n$ are not ordered according to the magnitude (of the real part) but rather according to the Fourier series index. We enumerate the Dirac points by $\mu_n := \frac{1}{4}n^2$ for $n \in \mathbb{N}$.

If $n = 2m - 1$ with $m \in \mathbb{N}$, the two linearly independent normalized eigenfunctions of the Bloch eigenvalue problem (1.8) with the symmetry properties as in Lemma 8 are given by

$$\varphi_+(x) = \frac{1}{2\sqrt{\pi}} (e^{i(m-1)x} + e^{-imx}), \quad \varphi_-(x) = \frac{1}{2i\sqrt{\pi}} (e^{i(m-1)x} - e^{-imx}). \quad (4.11)$$

If $n = 2m$ with $m \in \mathbb{N}$, the two eigenfunctions are

$$\varphi_+(x) = \frac{1}{\sqrt{\pi}} \cos(mx), \quad \varphi_-(x) = \frac{1}{\sqrt{\pi}} \sin(mx). \quad (4.12)$$

In both (4.11) and (4.12) we have

$$\langle W\varphi_+, \varphi_- \rangle = \frac{1}{2}b_n,$$

where b_n is the Fourier coefficient in (4.10) for either $n = 2m - 1$ or $n = 2m$. If $b_n \neq 0$ for some $n \in \mathbb{N}$, the two eigenvalues $\omega_\pm(k_0)$ are complex by Proposition 9. \square

Figure 2 illustrates Proposition 11 with the example $W(x) = \sin(2x)$ for $\gamma = 0$ (a) and $\gamma = 0.2$ (b,c). The eigenvalue families in (b,c) were computed numerically using a finite difference discretization.

Remark 12. If $b_j \neq 0$ for all $j \in \mathbb{N}$ in the Fourier series (4.10), then all Dirac points split into two complex eigenvalues and none of the spectral bands is completely real for γ small.

The final result shows that if U is smoother than W and W is not too smooth, then the high-energy bands split generally and become unstable for every nonzero γ . This means that the \mathcal{PT} -symmetry breaking threshold discussed in many publications (see, e.g., the review in [19]) is identically zero even if the real potential U is generic and has no Dirac

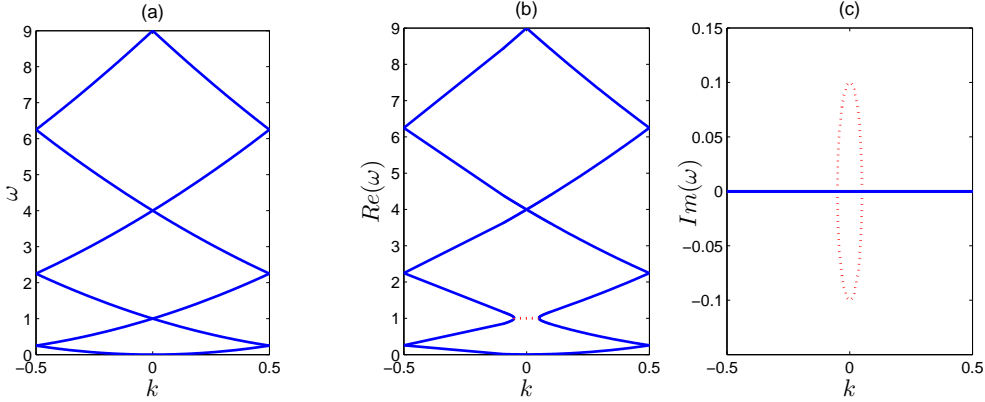


FIGURE 2. Eigenvalues $\omega_n(k)$, $n = 1, \dots, 6$ of the Bloch eigenvalue problem (1.8) with $V \equiv 0$ in (a) and $V(x) = 0.2i \sin(2x)$ in (b) and (c) computed numerically. The Dirac point at the intersection of $\tilde{\omega}_2$ and $\tilde{\omega}_3$ with $V \equiv 0$ splits into a complex conjugate pair when $V(x) = 0.2i \sin(2x)$. Purely real eigenvalues are plotted with the full blue line, complex eigenvalues are in dotted red.

points. To simplify the proof of the following proposition, we assume that U has zero mean.

Proposition 13. *Let U and W be defined by the Fourier series*

$$U(x) = 2 \sum_{j \in \mathbb{N}} a_j \cos(jx), \quad W(x) = 2 \sum_{j \in \mathbb{N}} b_j \sin(jx), \quad (4.13)$$

where $\{a_j\}_{j \in \mathbb{N}}, \{b_j\}_{j \in \mathbb{N}} \in \ell^1(\mathbb{N}, \mathbb{R})$ satisfy

$$\lim_{j \rightarrow \infty} \frac{|a_j|}{|b_j|} = 0, \quad \lim_{j \rightarrow \infty} \frac{1}{j^2 |b_j|} = 0, \quad \lim_{j \rightarrow \infty} \frac{\sum_{k=j+1}^{\infty} |b_k|^2}{j^2 |b_j|^2} = 0. \quad (4.14)$$

Then for every $\gamma \neq 0$ there is a sufficiently large $N \in \mathbb{N}$ such that for every $n \geq N$ two complex eigenvalues $\omega_{\pm(n)}(k_0)$ of the spectral problem (1.8) with $k_0 \in \{0, 1/2\}$ exist, which satisfy

- (i) $\text{Im}(\omega_{\pm(n)}(k_0)) \neq 0$,
- (ii) $|\omega_{\pm(n)}(k_0) - n^2/4| \rightarrow 0$ as $n \rightarrow \infty$.

Proof. By the asymptotic theory in [10, Chapter 4] for $\gamma = 0$, the band edge points converge at infinity to the Dirac points of the homogenous problem (1.8) with $V = 0$. Therefore, in order to prove the assertion, we will treat U and W as perturbation terms in the Bloch eigenvalue problem

$$\begin{cases} [L_0(k_0) + U + i\gamma W] p(\cdot, k_0) = \omega(k_0) p(\cdot, k_0), \\ p(x + 2\pi, k_0) = p(x, k_0) \quad \text{for all } x \in \mathbb{R}, \end{cases} \quad (4.15)$$

where $L_0(k_0) := -(\frac{d}{dx} + ik_0)^2$. The two eigenfunctions of $L_0(k_0)$ are given by either (4.11) or (4.12) for the double eigenvalue $\omega(k_0) = \frac{1}{4}n^2$ with either $n = 2m - 1$ and $k_0 = 1/2$ or $n = 2m$ and $k_0 = 0$.

We present here the even case $n = 2m$, $m \in \mathbb{N}$. The odd case is analogous. We represent

$$\omega(k_0) = m^2 + \Omega,$$

where Ω is shown to be small as $m \rightarrow \infty$. Let us write $p(\cdot, k_0)$ in the Fourier series form

$$p(x, k_0) = \sum_{j \in \mathbb{Z}} c_j e^{ijx}.$$

Substituting these representations in the Bloch eigenvalue problem (4.15), we obtain the discrete eigenvalue problem

$$(j^2 - m^2 - \Omega)c_j + \sum_{k \in \mathbb{Z}} (a_k + \gamma b_k)c_{j-k} = 0, \quad (4.16)$$

where $a_{-k} = a_k$ and $b_{-k} = -b_k$ for $k \in \mathbb{N}$ and $a_0 = b_0 = 0$. Singling out the resonant terms at $j = \pm m$, we project the eigenvalue problem (4.16) into two blocks

$$\begin{bmatrix} 0 & a_m + \gamma b_m \\ a_m - \gamma b_m & 0 \end{bmatrix} \mathbf{C}_m + \begin{bmatrix} \sum_{j \in \mathbb{Z} \setminus \{0, 2m\}} (a_j + \gamma b_j)c_{m-j} \\ \sum_{j \in \mathbb{Z} \setminus \{0, -2m\}} (a_j + \gamma b_j)c_{-m-j} \end{bmatrix} = \Omega \mathbf{C}_m \quad (4.17)$$

and

$$c_j = \frac{1}{m^2 + \Omega - j^2} \sum_{k \in \mathbb{Z}} (a_k + \gamma b_k)c_{j-k}, \quad j \in \mathbb{Z} \setminus \{m, -m\}, \quad (4.18)$$

where $\mathbf{C}_m := (c_m, c_{-m})^T$. The two eigenvalues of the matrix in the first term of the left-hand side of (4.17) are given by

$$\Omega_{\pm}^{(0)} := \pm \sqrt{a_m^2 - \gamma^2 b_m^2}. \quad (4.19)$$

Since $\lim_{m \rightarrow \infty} |a_m|/|b_m| = 0$ by the first assumption in (4.14), for any $\gamma \neq 0$ there exists a sufficiently large N such that $a_m^2 - \gamma^2 b_m^2 < 0$ for any $m \geq N$. The corresponding eigenvalues $\Omega_{\pm}^{(0)}$ are distinct and complex. In what follows, we prove persistence of this complex splitting of the double zero eigenvalue Ω in the block (4.17).

We assume that \mathbf{C}_m and Ω are bounded by an m -independent positive constant in the limit $m \rightarrow \infty$. We denote $\mathbf{c}_m := \{c_j\}_{j \in \mathbb{Z}_m}$ with $\mathbb{Z}_m := \mathbb{Z} \setminus \{m, -m\}$ and work in the sequence space $\ell^2(\mathbb{Z}_m)$, which represents the space $L^2(0, 2\pi)$ for the original problem (4.15).

Since the spacing between m^2 and $(m \pm 1)^2$ grows like m as $m \rightarrow \infty$, we set

$$K_j := \frac{1}{m^2 + \Omega - j^2} \sum_{k \in \mathbb{Z} \setminus \{j-m, j+m\}} (a_k + \gamma b_k)c_{j-k}, \quad j \in \mathbb{Z}_m$$

and obtain

$$\|K\|_{\ell^2(\mathbb{Z}_m)} \leq C m^{-1} (\|a\|_{\ell^1} + |\gamma| \|b\|_{\ell^1}) \|\mathbf{c}_m\|_{\ell^2(\mathbb{Z}_m)}, \quad (4.20)$$

by using Young's inequality for convolutions

$$\|x * y\|_{\ell^r} \leq \|x\|_{\ell^p} \|y\|_{\ell^q}, \quad r, p, q \geq 1, \quad 1 + \frac{1}{r} = \frac{1}{p} + \frac{1}{q}, \quad (4.21)$$

with $r = 2$, $p = 1$, and $q = 2$. The positive constant C is m -independent but may depend on Ω and γ . In what follows, we use the same notation for the generic constant C that may change from one line to another line.

Thanks to the bound (4.20), the inverse operator can be constructed for system (4.18) in $\ell^2(\mathbb{Z}_m)$ for any finite \mathbf{C}_m and Ω if m is sufficiently large. By the inverse function theorem, there exists a unique solution $\mathbf{c}_m \in \ell^2(\mathbb{Z}_m)$ to system (4.18), which can be represented in the form

$$\mathbf{c}_m = c_m \mathbf{P}_m(\Omega, \gamma) + c_{-m} \mathbf{Q}_m(\Omega, \gamma), \quad (4.22)$$

where the unique vectors $\mathbf{P}_m, \mathbf{Q}_m \in \ell^2(\mathbb{Z}_m)$ depend on m, Ω , and γ and satisfy the bounds

$$\|\mathbf{P}_m(\Omega, \gamma)\|_{\ell^2(\mathbb{Z}_m)} + \|\mathbf{Q}_m(\Omega, \gamma)\|_{\ell^2(\mathbb{Z}_m)} \leq Cm^{-1} \quad (4.23)$$

for an m -independent positive constant C .

By the symmetry of system (4.18), we note that

$$[\mathbf{Q}_m(\Omega, \gamma)]_{-j} = [\mathbf{P}_m(\Omega, -\gamma)]_j, \quad j \in \mathbb{Z}_m. \quad (4.24)$$

Moreover, solving system (4.18) by iterations, we can write

$$[\mathbf{P}_m(\Omega, \gamma)]_j = \frac{a_{j-m} + \gamma b_{j-m}}{m^2 + \Omega - j^2} + [\tilde{\mathbf{P}}_m(\Omega, \gamma)]_j, \quad j \in \mathbb{Z}_m. \quad (4.25)$$

where $\tilde{\mathbf{P}}_m$ satisfies the system

$$\left[\tilde{\mathbf{P}}_m(\Omega, \gamma) \right]_j = (m^2 + \Omega - j^2)^{-1} \sum_{k \in \mathbb{Z}_m \setminus \{j-m, j+m\}} (a_k + \gamma b_k) [\mathbf{P}_m(\Omega, \gamma)]_{j-k}, \quad j \in \mathbb{Z}_m.$$

Thanks to Young's inequality (4.21), the higher order terms satisfy the bound

$$\|\tilde{\mathbf{P}}\|_{\ell^2(\mathbb{Z}_m)} \leq Cm^{-1} \|\mathbf{P}_m\|_{\ell^2(\mathbb{Z}_m)} \leq Cm^{-2}, \quad (4.26)$$

for another m -independent positive constant C .

Substituting (4.22) to (4.17), we obtain the matrix nonlinear eigenvalue problem in the form

$$\begin{bmatrix} E_m(\Omega, \gamma) & a_m + \gamma b_m + F_m(\Omega, \gamma) \\ a_m - \gamma b_m + G_m(\Omega, \gamma) & H_m(\Omega, \gamma) \end{bmatrix} \mathbf{C}_m = \Omega \mathbf{C}_m, \quad (4.27)$$

where

$$\begin{aligned} E_m(\Omega, \gamma) &:= \sum_{j \in \mathbb{Z} \setminus \{0, 2m\}} (a_j + \gamma b_j) [\mathbf{P}_m(\Omega, \gamma)]_{m-j}, \\ F_m(\Omega, \gamma) &:= \sum_{j \in \mathbb{Z} \setminus \{0, 2m\}} (a_j + \gamma b_j) [\mathbf{Q}_m(\Omega, \gamma)]_{m-j}, \\ G_m(\Omega, \gamma) &:= \sum_{j \in \mathbb{Z} \setminus \{0, -2m\}} (a_j + \gamma b_j) [\mathbf{P}_m(\Omega, \gamma)]_{-m-j}, \\ H_m(\Omega, \gamma) &:= \sum_{j \in \mathbb{Z} \setminus \{0, -2m\}} (a_j + \gamma b_j) [\mathbf{Q}_m(\Omega, \gamma)]_{-m-j}. \end{aligned}$$

By the symmetry in (4.24), we obtain

$$E_m(\Omega, \gamma) = H_m(\Omega, -\gamma), \quad F_m(\Omega, \gamma) = G_m(\Omega, -\gamma).$$

Eigenvalues Ω are found as roots of the characteristic equation for (4.27), namely

$$[\Omega - E_m^+(\Omega, \gamma)]^2 = [a_m + F_m^+(\Omega, \gamma)]^2 - [\gamma b_m + F_m^-(\Omega, \gamma)]^2 + [E_m^-(\Omega, \gamma)]^2 \quad (4.28)$$

where E_m^\pm and F_m^\pm define the symmetric and anti-symmetric combinations of E_m and F_m respectively, e.g.

$$E_m^\pm(\Omega, \gamma) := \frac{E_m(\Omega, \gamma) \pm E_m(\Omega, -\gamma)}{2}.$$

Substituting the leading order (4.25), we find

$$\begin{aligned} E_m(\Omega, \gamma) &= \sum_{j \in \mathbb{Z} \setminus \{0, 2m\}} \frac{a_j^2 - \gamma^2 b_j^2}{m^2 + \Omega - (m-j)^2} + \text{h.o.t.}, \\ F_m(\Omega, \gamma) &= \sum_{j \in \mathbb{Z} \setminus \{0, 2m\}} \frac{(a_j + \gamma b_j)(a_{j-2m} - \gamma b_{j-2m})}{m^2 + \Omega - (m-j)^2} + \text{h.o.t.}, \end{aligned}$$

where the higher-order terms are convolutions of $\mathbf{a} + \gamma \mathbf{b}$ and $\tilde{\mathbf{P}}$ estimated in (4.26). Hence, by Young's inequality, h.o.t. is bounded in the ℓ^∞ norm by C/m^2 .

Since the leading order of $E_m(\Omega, \gamma)$ is even in γ , we obtain the estimates:

$$\begin{aligned} |E_m^+(\Omega, \gamma)| &\leq C_1 m^{-1}, \\ |E_m^-(\Omega, \gamma)| &\leq C_2 |\gamma| m^{-2}, \end{aligned}$$

for m -independent constants C_1, C_2 , where the factor of γ is included for convenience. On the other hand, the leading order of $F_m(\Omega, \gamma)$ can be estimated as follows:

$$\begin{aligned} \left| \sum_{j \in \mathbb{Z} \setminus \{0, 2m\}} \frac{a_j a_{j-2m}}{m^2 + \Omega - (m-j)^2} \right| &= \left| \frac{a_m^2}{m^2 + \Omega} + 2 \sum_{j \geq m+1, j \neq 2m} \frac{a_j a_{j-2m}}{m^2 + \Omega - (m-j)^2} \right| \\ &\leq C \left(\frac{a_m^2}{m^2} + \frac{(\sum_{j \in \mathbb{N}} |a_j|^2)^{1/2} (\sum_{j \geq m+1} |a_j|^2)^{1/2}}{m} \right), \end{aligned}$$

with similar estimates for the other parts of the leading order of $F_m(\Omega, \gamma)$. Combining with the higher-order terms and recalling the first assumption in (4.14), we obtain the estimates

$$\begin{aligned} |F_m^+(\Omega, \gamma)| &\leq C_3 m^{-1} \left(\sum_{j \geq m+1} |b_j|^2 \right)^{1/2} + C_4 m^{-2}, \\ |F_m^-(\Omega, \gamma)| &\leq C_5 |\gamma| m^{-1} \left(\sum_{j \geq m+1} |b_j|^2 \right)^{1/2} + C_6 |\gamma| m^{-2}, \end{aligned}$$

for m -independent constants C_3, C_4, C_5, C_6 .

The right-hand side of the nonlinear characteristic equation (4.28) is

$$R_m := b_m^2 \left(-\gamma^2 + \frac{a_m^2}{b_m^2} + 2 \frac{a_m F_m^+}{b_m^2} + \frac{(F_m^+)^2}{b_m^2} - 2 \frac{\gamma F_m^-}{b_m} - \frac{(F_m^-)^2}{b_m^2} + \frac{(E_m^-)^2}{b_m^2} \right).$$

Using the three assumptions in (4.14), we conclude that $R_m = b_m^2(-\gamma^2 + \delta_m)$, where $|\delta_m| \rightarrow 0$ as $m \rightarrow \infty$. Therefore, $R_m < 0$ if m is sufficiently large.

We note next that the roots Ω of the characteristic equation (4.28) are bounded in m as they are fixed points of

$$\Omega = E_m^+(\Omega, \gamma) \pm \sqrt{R_m(\Omega, \gamma)},$$

where $|E_m^+(\Omega, \gamma)|$ is estimated above and $|\sqrt{R_m(\Omega, \gamma)}| \leq C|b_m|(|\gamma| + \sqrt{|\delta_m|})$. Hence

$$|\Omega| \leq C_7 m^{-1}$$

for some $C_7 > 0$ independent of m . This leads to an estimate on the imaginary part of E_m^+ . Namely, since

$$\operatorname{Im}(E_m^+) = -\operatorname{Im}(\Omega) \left(\sum_{j \in \mathbb{Z} \setminus \{0, 2m\}} \frac{a_j^2 - \gamma^2 b_j^2}{(m^2 + \operatorname{Re}(\Omega) - (m-j)^2)^2 + \operatorname{Im}(\Omega)^2} + \text{h.o.t.} \right),$$

we have

$$|\operatorname{Im}(E_m^+)| \leq C/m^3.$$

Finally, thanks to the second assumption in (4.14), the imaginary part of the two roots of Ω is nonzero if m is so large that $|\delta_m|/\gamma^2 < 1$ because then the following asymptotics hold

$$\operatorname{Im}(\Omega) \sim \pm |\gamma b_m| \sqrt{1 - \delta_m/\gamma^2} \quad (m \rightarrow \infty).$$

The assertion of the proposition is thus proved. Note that $\Omega_{\pm}^{(0)}$ given by (4.19) may be smaller than the leading order term for Ω given by $E_m^+ = \mathcal{O}(m^{-1})$. \square

As an example for the assumptions in Proposition 13, we consider the periodic potentials U and W such that

$$\begin{aligned} |a_m| &= \mathcal{O}(m^{-5/2}) \quad \text{for } m \rightarrow \infty, \\ C_- m^{-3/2} \leq |b_m| \leq C_+ m^{-3/2} \quad &\text{for all } m \text{ sufficiently large} \end{aligned}$$

with some $0 < C_- \leq C_+ < \infty$. Since $\sum_{j \geq m+1} |b_j|^2 = \mathcal{O}(m^{-2})$, the assumptions in (4.14) are satisfied and by Proposition 13, for every $\gamma > 0$, there exists N such that eigenvalues (4.19) are complex for every $m \geq N$. Moreover, there is a positive constant C such that $N \geq C\gamma^{-2}$. The latter estimate follows from $|\delta_m| \leq c(m^{-1} + \gamma^2 m^{-1/2})$ obtained from the previous estimates on E_m^{\pm} and F_m^{\pm} as well as the definition of δ_m . If C is sufficiently large in $N \geq C\gamma^{-2}$, then $|\delta_m|/\gamma^2$ is small for every $m \geq N$.

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