

Coupled-mode equations and gap solitons in a two-dimensional nonlinear elliptic problem with a separable periodic potential

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Abstract

We address a two-dimensional nonlinear elliptic problem with a *finite*-amplitude periodic potential. For a class of *separable symmetric* potentials, we study the bifurcation of the *first band gap* in the spectrum of the linear Schrödinger operator and the relevant *coupled-mode equations* to describe this bifurcation. The coupled-mode equations are derived by the rigorous analysis based on the Fourier–Bloch decomposition and the Implicit Function Theorem in the space of bounded continuous functions vanishing at infinity. Persistence of *reversible localized* solutions, called *gap solitons*, beyond the coupled-mode equations is proved under a non-degeneracy assumption on the kernel of the linearization operator. Various branches of reversible localized solutions are classified numerically in the framework of the coupled-mode equations and convergence of the approximation error is verified. Error estimates on the time-dependent solutions of the Gross–Pitaevskii equation approximated by solutions of the coupled-mode equations are obtained for a finite-time interval.

1 Introduction

Interplay between nonlinearity and periodicity is the focus of recent studies in different branches of nonlinear physics and applied mathematics. Physical applications of nonlinear systems with periodic potentials range from nonlinear optics, in the dynamics of guided waves in inhomogeneous optical structures and photonic crystal lattices, to atomic physics, in the dynamics of Bose–Einstein condensate droplets in periodic potentials, and from condensed matter, in Josephson-junction ladders, to biophysics, in various models of the DNA double strand. The paramount significance for these models is the possibility of spatial localization, that is emergence of nonlinear localized structures residing in the spectral band gaps of the periodic potentials. To describe this phenomenon, the primary equations of physics are typically simplified to the Gross–Pitaevskii equation, which we shall study in our article in the space of two dimensions. More precisely, we consider the two-dimensional Gross–Pitaevskii equation in the form

$$iE_t = -\nabla^2 E + V(x)E + \sigma|E|^2 E, \quad (1.1)$$

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where $E(x, t) : \mathbb{R}^2 \times \mathbb{R} \mapsto \mathbb{C}$, $\nabla^2 = \partial_{x_1}^2 + \partial_{x_2}^2$, $V(x) : \mathbb{R}^2 \mapsto \mathbb{R}$, and $\sigma = \pm 1$. Time-periodic solutions of the Gross–Pitaevskii equation are found from the solutions of the nonlinear elliptic problem

$$\nabla^2 \phi(x) + \omega \phi(x) = V(x)\phi + \sigma |\phi(x)|^2 \phi(x), \quad (1.2)$$

where $\phi(x) : \mathbb{R}^2 \mapsto \mathbb{C}$ and $\omega \in \mathbb{R}$ arise in the substitution $E(x, t) = \phi(x)e^{-i\omega t}$. It is known that localized solutions of the elliptic problem (1.2) with a periodic potential $V(x)$, called *gap solitons*, exist in *every* finite gap of the spectrum of the Schrödinger operator $L = -\nabla^2 + V(x)$ and in the semi-infinite gap for $\sigma = -1$ [27, 19]. Bifurcations of localized solutions from edges of the spectral bands were studied earlier in [15, 17].

Coupled-mode equations were used by physicists for the analysis of existence, stability and dynamics of gap solitons [18, 26]. A justification of the one-dimensional coupled-mode equations in the context of the elliptic problem (1.2) with $x \in \mathbb{R}$ was carried out in [21] in the limit of *small-amplitude* periodic potentials $V(x)$. (A justification of time-dependent coupled-mode equations on finite-time intervals was done earlier in [13, 24].) In the limit of small-amplitude potentials, narrow gaps of the spectrum of the Schrödinger operator $L = -\partial_x^2 + V(x)$ bifurcate from resonant points of the spectrum of $L_0 = -\partial_x^2$, while the Bloch modes of L bifurcate from the Fourier modes of L_0 . In other words, photonic band gaps open generally for small-amplitude one-dimensional periodic potentials $V(x)$. *Small-amplitude* gap solitons of the elliptic problem (1.2) in $x \in \mathbb{R}$ reside in the narrow gaps of L for $V(x) \neq 0$ according to the approximation obtained from the coupled-mode equations [21].

We refer to the opening of a spectral gap under a small change of the potential $V(x)$ as to the bifurcation of the band gap. Bifurcations of band gaps do not occur for small-amplitude multi-dimensional periodic potentials. This is caused by an overlap of the spectral bands of $L_0 = -\nabla^2$ in the first Brillouin zone if $x \in \mathbb{R}^N$ and $N \geq 2$ [16]. As a result, photonic band gaps in multi-dimensional potentials open only at some finite amplitudes of the periodic potential $V(x)$ and the resonant eigenfunctions are given by the Bloch modes of $L = -\nabla^2 + V(x)$ rather than by the Fourier modes of L_0 . Although the coupled-mode equations were also derived for multi-dimensional problems with small periodic potentials [1, 2, 3, 4, 8] and the resonant Fourier modes were used for the approximation of the full solution, the applicability of these coupled-mode equations remains an open issue for a rigorous analysis. Bloch mode decomposition has been also used in one dimension for finite-amplitude periodic potentials to derive coupled-mode equations [9]. The corresponding unperturbed one-dimensional potential, however, has to be of a special type to admit a finite number of open gaps, such that a new gap is opened under a small perturbation.

In this paper we derive coupled-mode equations for wavepackets in narrow band gaps of a *finite-amplitude* periodic potential by using the Fourier–Bloch decomposition and the rigorous analysis based on the Implicit Function Theorem in the space of bounded continuous functions vanishing at infinity. The coupled-mode equations we derive here take the form of coupled nonlinear Schrödinger (NLS) equations. These equations differ from the first-order coupled-mode equations exploited earlier [26]. Similar coupled NLS equations have been recently derived in [25] near band edges of the well-separated spectral bands and in [6] for tunnelling problems. Unlike these works relying on numerical approximations, we justify the derivation of the coupled-mode equations and prove the persistence of localized solutions in the full nonlinear problem (1.2). Although details of our analysis are given only for the bifurcation of the first band gap in the spectrum of L , a similar analysis can be developed for bifurcations of other band gaps and for bifurcations of the localized solutions near band edges of the well-separated spectral bands.

Our derivation is developed for the class of *separable* potentials

$$V(x_1, x_2) = \eta [W(x_1) + W(x_2)], \quad \eta \in \mathbb{R}, \quad (1.3)$$

where the function $W(x)$ is assumed to be real-valued, bounded, piecewise-continuous, and 2π -periodic on $x \in \mathbb{R}$. To simplify the details of our analysis, we assume that $W(-x) = W(x)$ on $x \in \mathbb{R}$, such that the solution set of the elliptic problem (1.2) includes functions satisfying one of the following two *reversibility* constraints

$$\phi(x_1, x_2) = s_1 \bar{\phi}(-x_1, x_2) = s_2 \bar{\phi}(x_1, -x_2) \quad (1.4)$$

or

$$\phi(x_1, x_2) = s_1 \bar{\phi}(x_2, x_1) = s_2 \bar{\phi}(-x_2, -x_1), \quad (1.5)$$

where $s_1, s_2 = \pm 1$.

Our strategy is to show that there may exist a value $\eta = \eta_0$, for which the first band gap opens due to the resonance of three lowest-order Bloch modes for three spectral bands of the operator $L = -\nabla^2 + V(x)$. The new small parameter $\epsilon := \eta - \eta_0$ is then used for the bifurcation theory of Bloch modes which results in the *algebraic* coupled-mode equations for nonlinear interaction of the three resonant modes. The Fourier–Bloch decomposition is used for the approximation of localized solutions and for the derivation of the *differential* coupled-mode equations with the second-order derivative terms. The main idea behind our technique is that a differential operator after the Fourier–Bloch decomposition becomes a pseudo-differential operator whose symbol is the multiple-valued dispersion relation. Then only the relevant (three) branches of the resonant modes can be taken into account, which leads to a coupled-mode system.

If the linearization operator of the coupled NLS equations at the localized solutions is non-degenerate, the persistence of the localized symmetric solutions in the full nonlinear problem (1.2) is proved with the Implicit Function Theorem. Localized symmetric solutions of the coupled NLS equations are approximated numerically and the convergence rate for the error of approximation is studied. Finally, we study time-dependent localized solutions of the Gross–Pitaevskii equation and the coupled-mode system and control smallness of the distance between the two solutions on a finite-time interval.

The article is structured as follows. Section 2 reviews elements of the Sturm–Liouville theory for the separable potentials. Section 3 contains a derivation of the algebraic coupled-mode equations for three resonant Bloch modes. Section 4 gives details of the projection technique for the derivation of the differential coupled-mode equations for localized solutions. The persistence of localized reversible solutions under a non-degeneracy assumption on the linearization operator is proved in Section 5. Numerical approximations of the localized solutions, the associated linearization operators, and the convergence of the approximation error are obtained in Section 6. Section 7 extends the results to the time-dependent case for finite time intervals. Section 8 discusses relevant generalizations.

2 Sturm–Liouville theory for separable potentials

It is typically expected that the band gaps in the spectrum of the linear Schrödinger operator with a two-dimensional periodic potential open at the extremal values of the Bloch band surfaces [16]. For a general potential, however, the extremal values may occur anywhere within the first irreducible Brillouin zone B_0 in the quasi-momentum space (k_1, k_2) [14]. We will show here that the extremal values for a separable potential occur only at the vertex points Γ , X and M on the boundary ∂B_0 . Figure 1 shows the irreducible Brillouin zone B_0 and the vertex points for a two-dimensional separable potential $V(x)$.

Let us consider the spectral problem for the linear Schrödinger operator associated with the separable periodic potential (1.3):

$$-\nabla^2 u(x_1, x_2) + \eta [W(x_1) + W(x_2)] u(x_1, x_2) = \omega u(x_1, x_2). \quad (2.1)$$

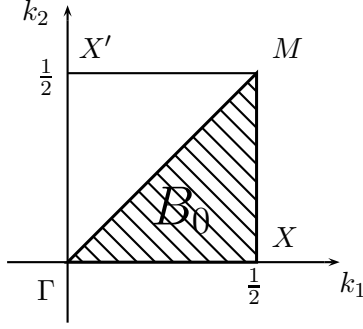


Figure 1: The first irreducible Brillouin zone B_0 for a two-dimensional separable potential.

By using the separation of variables $u(x_1, x_2) = f_1(x_1)f_2(x_2)$ and the parametrization $\omega = \xi_1 + \xi_2$, we obtain the uncoupled eigenvalue problems

$$-f_j''(x_j) + \eta W(x_j)f_j(x_j) = \xi_j f_j(x_j), \quad j = 1, 2. \quad (2.2)$$

The Bloch modes and the band surfaces for the one-dimensional problems (2.2) are introduced according to the regular Sturm–Liouville problem

$$\begin{cases} -u''(x) + \eta W(x)u(x) = \rho u(x), & 0 \leq x \leq 2\pi, \\ u(2\pi) = e^{i2\pi k}u(0), \end{cases} \quad (2.3)$$

where k is a quasi-momentum defined on the interval $\mathbb{T} = [-\frac{1}{2}, \frac{1}{2}]$. The eigenfunctions of the Sturm–Liouville problem (2.3) are periodic with respect to k with the period one. By Theorem 2.4.3 in [10], there exists a countable infinite set of eigenvalues $\{\rho_n(k)\}_{n \in \mathbb{N}}$ for each $k \in \mathbb{T}$, which can be ordered as

$$\rho_1(k) \leq \rho_2(k) \leq \rho_3(k) \leq \dots$$

By Theorem 4.2.3 in [10], if $W(x)$ is a bounded and 2π -periodic potential, eigenvalues $\{\rho_n(k)\}_{n \in \mathbb{N}}$ have a uniform asymptotic distribution on $k \in \mathbb{T}$, such that

$$C_- n^2 \leq |\rho_n(k)| \leq C_+ n^2, \quad \forall n \in \mathbb{N}, \quad \forall k \in \mathbb{T}, \quad (2.4)$$

for some constants $C_{\pm} > 0$.

Let $\{u_n(x; k)\}_{l \in \mathbb{N}}$ be the corresponding set of eigenfunctions of the Sturm–Liouville problem (2.3), such that $u_n(x + 2\pi; k) = u_n(x; k)e^{2\pi i k}$. By Theorem XIII.89 in [23], if $W(x)$ is a bounded, piecewise-continuous and 2π -periodic potential, then the eigenvalue $\rho_n(k)$ and the Bloch function $u_n(x; k)$ are analytic in $k \in \mathbb{T} \setminus \{0, \pm \frac{1}{2}\}$ and continuous at the points $k = 0$ and $k = \pm \frac{1}{2}$. By Theorem XIII.95 in [23], the eigenvalue $\rho_n(k)$ is extended on a smooth Riemann surface in the neighborhood of the points $k = 0$ and $k = \frac{1}{2}$ if the n^{th} spectral band is disjoint from the adjacent $(n \pm 1)^{\text{th}}$ spectral bands by a non-empty band gap.

By Theorem XIII.90 in [23], if $W(x)$ is a bounded, piecewise-continuous and 2π -periodic potential, then the spectrum of $L_{1D} = -\partial_x^2 + \eta W(x)$ in $L^2(\mathbb{R})$ is absolutely continuous and consists of the union of the intervals in the range of the functions $\rho_n(k)$ on $k \in \mathbb{T}$ for $n \in \mathbb{N}$, where $\rho_n(-k) = \rho_n(k)$. Moreover, the extremal values of $\rho_n(k)$ occur only at the points $k = 0$ and $k = \pm \frac{1}{2}$. These points correspond to an

alternating sequence of the maximum and minimum values of the eigenvalues $\{\rho_n(k)\}_{n \in \mathbb{N}}$ according to the following formula

$$\arg \min_{k \in \mathbb{S}} \rho_{2m-1}(k) = 0, \arg \max_{k \in \mathbb{S}} \rho_{2m-1}(k) = \pm \frac{1}{2}, \arg \min_{k \in \mathbb{S}} \rho_{2m}(k) = \pm \frac{1}{2}, \arg \max_{k \in \mathbb{S}} \rho_{2m}(k) = 0,$$

for all $m \in \mathbb{N}$. The Bloch function $u_n(x; k)$ is 2π -periodic if $k = 0$ and 2π -antiperiodic if $k = \pm \frac{1}{2}$. Let us denote the periodic and antiperiodic eigenfunctions and the corresponding eigenvalues by

$$\psi_n(x) = u_n(x; 0), \quad \lambda_n = \rho_n(0) \quad \text{and} \quad \varphi_n(x) = u_n\left(x; \pm \frac{1}{2}\right), \quad \mu_n = \rho_n\left(\pm \frac{1}{2}\right), \quad n \in \mathbb{N}. \quad (2.5)$$

By Theorems 2.3.1 and 3.1.2 in [10], these eigenvalues are ordered by $\lambda_1 < \lambda_2 \leq \lambda_3 \leq \dots$ and $\mu_1 < \mu_2 \leq \mu_3 \leq \dots$, while the corresponding eigenfunctions $\psi_n(x)$ and $\varphi_n(x)$ have precisely $n - 1$ zeros (nodes) on the interval $(-\pi, \pi)$. If $W(-x) = W(x)$, the eigenfunctions $\psi_n(x)$ and $\varphi_n(x)$ are even for odd n and odd for even n . Each set of the eigenfunctions $\{\psi_n(x)\}_{n \in \mathbb{Z}}$ and $\{\varphi_n(x)\}_{n \in \mathbb{Z}}$ is orthogonal in $L^2([-\pi, \pi])$.

Eigenvalues of the same one-dimensional operator $L_{1D} = -\partial_x^2 + \eta W(x)$ for 4π -periodic eigenfunctions consist of the union of the eigenvalues $\{\lambda_n\}_{n \in \mathbb{N}}$ and $\{\mu_n\}_{n \in \mathbb{N}}$. Since there are at most two eigenvalues of the second-order operator L_{1D} and by Theorem 2.3.1 of [10], we obtain that

$$\lambda_1 < \mu_1 < \mu_2 < \lambda_2 \leq \lambda_3 < \mu_3 \leq \mu_4 < \lambda_4 \leq \lambda_5 < \dots \quad (2.6)$$

In particular, the first band gap is always non-empty for a non-constant potential $W(x)$ (see Theorem XIII.91(a) in [23]). Due to this ordering, the lowest value of $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$ for the crossing of the Bloch band surfaces associated with the two-dimensional separable potential $V(x_1, x_2)$ occurs at $\omega = \omega_0 = \lambda_1 + \mu_2 = 2\mu_1$. Using these facts, we obtain the following results.

Lemma 1 *Extremal values of the Bloch band surfaces $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$ for $(k_1, k_2) \in B_0$ occur only at the vertex points of the boundary ∂B_0 .*

Proof. Because $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$ for a separable potential (1.3), we have $\nabla \omega = [\rho'_{n_1}(k_1), \rho'_{n_2}(k_2)]^T$, where $\rho_n(k)$ are analytic on $k \in \mathbb{T} \setminus \{0, \pm \frac{1}{2}\}$. If an extremal point occurs in the interior of the Brillouin zone B_0 , then $\nabla \omega = 0$ at $k = k_0 \in B_0$. However, $\rho'_n(k) \neq 0$ for any $0 < |k| < \frac{1}{2}$ and any $n \in \mathbb{N}$ by Theorem XIII.90 in [23]. Similarly, the extremal points cannot occur in the interior of the boundary ∂B_0 . Therefore, the extremal values of ω occur only at the vertex points Γ , X and M on ∂B_0 . $\square$

Remark 1 The derivative $\rho'_n(k)$ may be non-zero at $k = 0$ and $k = \frac{1}{2}$ if the n^{th} spectral band touches the adjacent $(n \pm 1)^{\text{th}}$ spectral bands. This happens when the corresponding eigenvalue λ_n or μ_n is double degenerate with the equality sign in the ordering (2.6). However, λ_1 , μ_1 and μ_2 are always simple and, therefore, $\nabla \omega = 0$ at least for the first three spectral bands $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$ at $\omega = \omega_0 = \lambda_1 + \mu_2 = 2\mu_1$.

Lemma 2 *Assume that the resonant condition $\lambda_1 + \mu_2 = 2\mu_1 \equiv \omega_0$ for the 2π -periodic eigenvalue λ_1 and the 2π -antiperiodic eigenvalues μ_1, μ_2 of $L_{1D} = -\partial_x^2 + \eta W(x)$ is satisfied for $\eta = \eta_0$. Then there are exactly three resonant Bloch modes at $\omega = \omega_0$ and $\eta = \eta_0$ in the spectral problem (2.1):*

$$\Phi_1 = \psi_1(x_1)\varphi_2(x_2), \quad \Phi_2 = \varphi_2(x_1)\psi_1(x_2), \quad \Phi_3 = \varphi_1(x_1)\varphi_1(x_2).$$

The three resonant modes are orthogonal to each other with respect to the 4π -periodic inner product

$$(f, g) = \int_{-2\pi}^{2\pi} \int_{-2\pi}^{2\pi} \bar{f}(x_1, x_2) g(x_1, x_2) dx_1 dx_2.$$

Proof. There are exactly three resonant modes for *any* separable potential (1.3) because λ_1 and μ_1 are the smallest non-degenerate eigenvalues of the operator L_{1D} and the double degeneracy $\lambda_1 + \mu_2 = \mu_2 + \lambda_1$ is due to the symmetry with respect to the interchange of the variables x_1 and x_2 . The eigenfunctions $\{\psi_n(x)\}_{n \in \mathbb{N}}$ and $\{\varphi_n(x)\}_{n \in \mathbb{N}}$ are all orthogonal to each other in $L^2([-2\pi, 2\pi])$, which leads to the orthogonality of the three resonant modes. $\square$

Remark 2 We note that the eigenfunctions $\psi_1(x)$ and $\varphi_1(x)$ are not orthogonal on the interval $[-\pi, \pi]$ since both of them are positive by Theorem 3.1.2 in [10]. However, a linear combination of $\psi_1(x)$ and $\varphi_1(x)$ belongs to the class of 4π -periodic functions and the two eigenfunctions are orthogonal on the double-length interval $[-2\pi, 2\pi]$.

Remark 3 By Theorem 6.10.5 in [10], there are finitely many gaps in the spectral problem (2.1) with a separable potential. (In fact, there are finitely many gaps for general smooth periodic potentials in dimension 2 or higher [20].) Lemma 2 indicates a bifurcation when one of these gaps at the lowest value of ω may open. It is observed for many examples of the separable potential (1.3) that this bifurcation leads to the *first* band gap in the spectrum of $L = -\nabla^2 + \eta[W(x_1) + W(x_2)]$ if η is increased from $\eta = 0$.

Example 1 Let $W(x) = 1 - \cos x$. Numerical approximations of the eigenvalues of the Sturm–Liouville problem (2.3) are computed with the use of the second-order central difference method. The eigenfunctions $\psi_n(x)$ and $\varphi_n(x)$ are plotted in Figure 2 for $n = 1, 2, 3$, while the dependence of the first eigenvalues λ_n and μ_n on η is plotted in Figure 3(a). Figure 3(b) shows the intersection of $2\mu_1$ and $\lambda_1 + \mu_2$ at the bifurcation value $\eta = \eta_0 \approx 0.1745$, when $\lambda_1 \approx 0.1595$, $\mu_1 \approx 0.3336$ and $\mu_2 \approx 0.5077$, such that $\omega_0 = \lambda_1 + \mu_2 = 2\mu_1 \approx 0.6672$. The perturbation behavior shown in Figure 3 was studied analytically in [5]. Figure 4 illustrates the band structure along ∂B_0 of the full spectral problem (2.1) with $\eta = 0.1745$ clearly revealing the resonance at $\omega \approx 0.6672$ and the two resonant modes at the points X and M . The third resonant mode lies at X' because the symmetry $V(x_1, x_2) = V(x_2, x_1)$ implies $\omega(k_1, k_2) = \omega(k_2, k_1)$.

In what follows, we consider the bifurcation of non-trivial solutions of the nonlinear elliptic problem (1.2) with the separable potential (1.3) in the lowest band gap described by Lemma 2. Let $\epsilon = \eta - \eta_0$, $\omega = \omega_0 + \epsilon\Omega$, $\phi(x) = \sqrt{\epsilon}\Phi(x)$ and rewrite the nonlinear elliptic problem (1.2) in the form

$$\mathcal{L}_0 \Phi(x) = \epsilon \Omega \Phi(x) - \epsilon [W(x_1) + W(x_2)] \Phi(x) - \epsilon \sigma |\Phi(x)|^2 \Phi(x), \quad (2.7)$$

where $\Phi : \mathbb{R}^2 \mapsto \mathbb{C}$ and $\mathcal{L}_0 = -\nabla^2 + \eta_0 [W(x_1) + W(x_2)] - \omega_0$. Two classes of non-trivial solutions of the bifurcation problem (2.7) are considered for small ϵ : bounded 4π -periodic solutions (Section 3) and bounded decaying solutions (Sections 4–6).

3 Algebraic coupled-mode equations

We consider here bounded periodic solutions $\Phi(x)$ of the bifurcation problem (2.7) for small ϵ . Our results depend on the period of the periodic solutions $\Phi(x)$. Since the potential $V(x)$ is separable, the

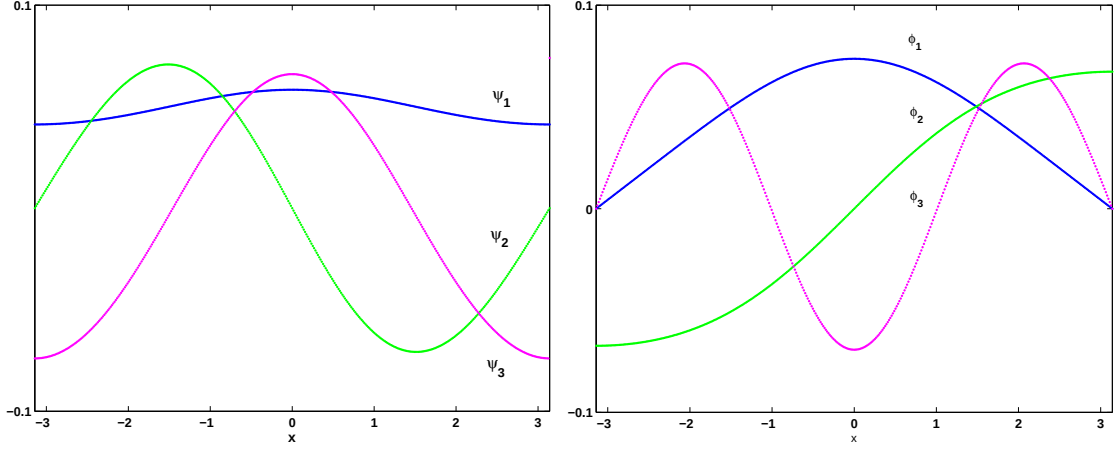


Figure 2: The 2π -periodic (left) and 2π -antiperiodic (right) eigenfunctions of $L_{1D} = -\partial_x^2 + \eta_0 W(x)$ with $W(x) = 1 - \cos x$.

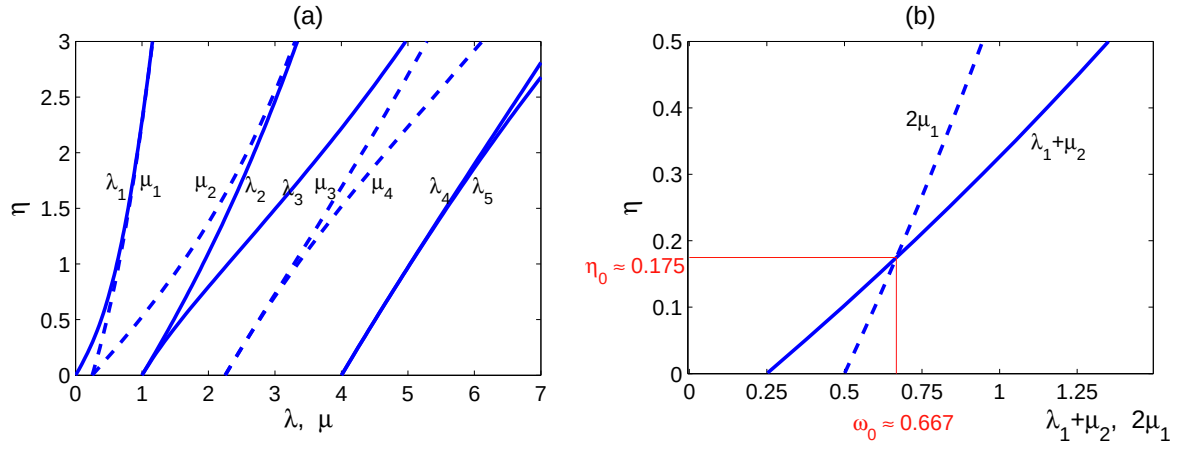


Figure 3: (a) Eigenvalues of $L_{1D} = -\partial_x^2 + \eta(1 - \cos x)$ for 2π -periodic (solid) and 2π -antiperiodic (dashed) boundary conditions. (b) The lowest resonance occurs at $\omega = \omega_0$ and $\eta = \eta_0$ when $\lambda_1 + \mu_2 = 2\mu_1$.

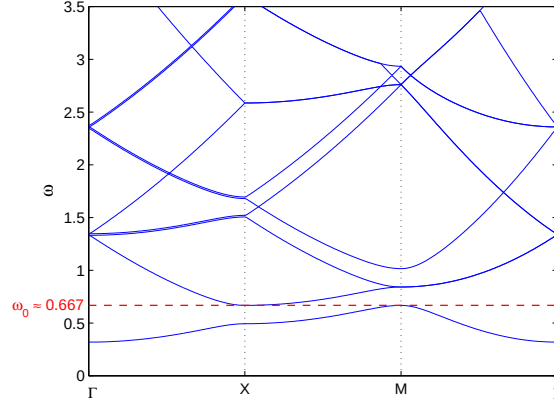


Figure 4: Band diagram along ∂B_0 for the spectral problem (2.1) with $W(x) = 1 - \cos x$ and $\eta = \eta_0$.

2π -periodic (2π -antiperiodic) function $\Phi(x)$ can be represented by the series of Bloch modes associated with the eigenvalue problem (2.3) on $x \in \mathbb{R}$ for $k = 0$ ($k = \pm \frac{1}{2}$), while the 4π -periodic functions $\Phi(x)$ can be represented by the series of both 2π -periodic and 2π -antiperiodic Bloch modes. In what follows, we shall use symbols $L^2(\mathbb{P}_k)$, $H^s(\mathbb{P}_k)$ and $C_b^0(\mathbb{P}_k)$ to denote the corresponding spaces of functions $u(x)$ on the interval $[0, 2\pi]$ satisfying the boundary conditions $u(2\pi) = e^{i2\pi k}u(0)$. We shall also use symbol $\vec{\phi}$ to denote the vector of elements of the sequence $\{\phi_n\}_{n \in \mathbb{N}}$.

Proposition 1 *Let $W(x)$ be a bounded and 2π -periodic function. Let $\{\rho_n(k)\}_{n \in \mathbb{N}}$ and $\{u_n(x; k)\}_{n \in \mathbb{N}}$ be sets of eigenvalues and eigenfunctions of the Sturm–Liouville problem (2.3) that depends on $k \in \mathbb{T}$, such that*

$$\langle u_n(\cdot; k), u_{n'}(\cdot; k) \rangle_{2\pi} = \delta_{n,n'}, \quad \forall n, n' \in \mathbb{N}, \quad \forall k \in \mathbb{T}, \quad (3.1)$$

where $\langle f, g \rangle_{2\pi} = \int_0^{2\pi} \bar{f}(x)g(x)dx$ and $\delta_{n,n'}$ is the Kronecker symbol. For any fixed $k \in \mathbb{T}$, the set of eigenfunctions is complete in $L^2(\mathbb{P}_k)$, such that there exists a unique set of coefficients $\{\phi_n\}_{n \in \mathbb{N}}$ in the decomposition

$$\forall \phi(x) \in L^2(\mathbb{P}_k) : \quad \phi(x) = \sum_{n \in \mathbb{N}} \phi_n u_n(x; k), \quad (3.2)$$

given by $\phi_n = \langle u_n(\cdot; k), \phi \rangle_{2\pi}$.

Proof. The statement of the proposition follows by Theorem XIII.88 of [23]. $\square$

Lemma 3 *Let $\phi(x)$ be defined by the decomposition (3.2), where $\vec{\phi}$ belongs to the vector space $l_s^1(\mathbb{N})$ with the norm*

$$\|\vec{\phi}\|_{l_s^1(\mathbb{N})} = \sum_{n \in \mathbb{N}} (1+n)^s |\phi_n| < \infty. \quad (3.3)$$

If $s > \frac{1}{2}$, then $\phi(x)$ is a continuous function on $x \in \mathbb{R}$ and $\phi(x) = \psi(x)e^{ikx}$ with $\psi(x+2\pi) = \psi(x)$.

Proof. By the triangle inequality, we obtain

$$\|\phi\|_{C_b^0(\mathbb{R})} \leq \sum_{n \in \mathbb{N}} |\phi_n| \|u_n(\cdot; k)\|_{C_b^0(\mathbb{P}_k)}.$$

By Sobolev's Embedding Theorem, there exists a $C > 0$ such that $\|u_n(\cdot; k)\|_{C_b^0(\mathbb{P}_k)} \leq C \|u_n(\cdot; k)\|_{H^s(\mathbb{P}_k)}$ for any $s > \frac{1}{2}$, $n \in \mathbb{N}$ and $k \in \mathbb{T}$. Since $W(x)$ is a bounded potential, the squared norm $\|u_n(\cdot; k)\|_{H^s(\mathbb{P}_k)}^2$ is equivalent to the integral

$$\int_0^{2\pi} \left| (c_\eta + L_{1D})^{s/2} u_n(x; k) \right|^2 dx = (c_\eta + \rho_n(k))^s,$$

where $c_\eta > -\eta \min_{x \in \mathbb{R}} W(x)$ and $(c_\eta + L_{1D})^{s/2}$ is defined using the spectral family associated with the Sturm-Liouville operator $L_{1D} = -\partial_x^2 + \eta W(x)$ in $L^2(\mathbb{P}_k)$. By the asymptotic distribution of eigenvalues (2.4), we obtain that

$$\|\phi\|_{C_b^0(\mathbb{P}_k)} \leq C \sum_{n \in \mathbb{N}} |\phi_n| \|u_n(\cdot; k)\|_{H^s(\mathbb{P}_k)} \leq \tilde{C} \sum_{n \in \mathbb{N}} (1+n)^s |\phi_n|$$

for some $\tilde{C} > 0$ and any $s > \frac{1}{2}$. □

If the potential $\eta W(x)$ is continued with respect to the parameter η , the perturbation theory for an eigenvalue $\rho_n(k)$ depends on whether $\rho_n(k)$ is simple or multiple. The following lemma is a trivial statement of the perturbation theory, so we omit its proof.

Lemma 4 *Let $W(x)$ be a bounded and 2π -periodic function of $x \in \mathbb{R}$. Fix $k \in \mathbb{T}$, $\eta_0 \in \mathbb{R}$, and $n \in \mathbb{N}$. If $\rho_{n-1}(k) < \rho_n(k) < \rho_{n+1}(k)$, then $\rho_n(k)$ and $u_n(x; k)$ depend analytically on η near $\eta = \eta_0$, such that*

$$\partial_\eta \rho_n(k)|_{\eta=\eta_0} = \langle u_n(\cdot; k)|_{\eta=\eta_0}, W u_n(\cdot; k)|_{\eta=\eta_0} \rangle_{2\pi} \quad (3.4)$$

and

$$|\rho_n(k) - \rho_n(k)|_{\eta=\eta_0} - \partial_\eta \rho_n(k)|_{\eta=\eta_0} (\eta - \eta_0)| \leq C(\eta - \eta_0)^2 \quad (3.5)$$

for some $C > 0$ and sufficiently small $|\eta - \eta_0|$.

Due to the construction of the spectrum of the two-dimensional spectral problem (2.1), the results of Lemma 4 settle the question of the splitting of the three resonant bands near the point $\omega = \omega_0$ described in Lemma 2. Indeed, each Bloch band surface (the graph of $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$) corresponding to the three resonant bands includes a different vertex point (X' , X , and M) at $\omega = \omega_0$ for different values of k in the set $\{(0, \frac{1}{2}); (\frac{1}{2}, 0); (\frac{1}{2}, \frac{1}{2})\}$. Each eigenvalue of the spectral problem (2.1) is simple and isolated if k is fixed, such that the continuation of each Bloch band surface in η near $\eta = \eta_0$ is determined by the expression (3.4) and the separation of variables in $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$. In other words, bifurcation of the lowest band gap that occurs at $\omega = \omega_0$ can not be studied if the function space is restricted to $L^2(\mathbb{P}_{k_1} \times \mathbb{P}_{k_2})$ for a fixed value of $(k_1, k_2) \in \mathbb{T}^2$. To detect the bifurcation, we shall work in the function space $L_{\text{per}}^2([-2\pi, 2\pi] \times [-2\pi, 2\pi])$, where all three vertex points X' , X and M correspond to the same 4π -periodic boundary conditions on the function $\Phi(x)$. According to Lemma 2, the three resonant Bloch modes are orthogonal to each other in this space.

To work with the 4π -periodic eigenfunctions, we shall introduce a number of notations. Let $\{\nu_n\}_{n \in \mathbb{N}}$ and $\{v_n(x)\}_{n \in \mathbb{N}}$ denote the sets of eigenvalues and the corresponding 4π -periodic eigenfunctions of the one-dimensional spectral problem (2.3). These sets consist of the union of eigenvalues and eigenfunctions defined by (2.5). Suppose that the eigenvalues are sorted in non-decreasing order, such that $\nu_1 = \lambda_1$, $\nu_2 = \mu_1$, $\nu_3 = \mu_2$, $\nu_4 = \lambda_2$, $\nu_5 = \lambda_3$ and so on, and that the eigenfunctions $v_1 = \psi_1, v_2 = \varphi_1, v_3 = \varphi_2, v_4 = \psi_2, v_5 = \psi_3$, etc., are normalized such that $\langle v_i, v_j \rangle_{4\pi} = \delta_{i,j}$, where $\langle f, g \rangle_{4\pi} = \int_{-2\pi}^{2\pi} \bar{f}(x)g(x)dx$.

The statements of Proposition 1 and Lemma 3 extend naturally to the new sets of eigenfunctions in space $L_{\text{per}}^2([-2\pi, 2\pi])$. To develop the nonlinear analysis of bifurcations of a non-trivial 4π -periodic solution $\Phi(x)$ on $x \in \mathbb{R}^2$, we shall study first the nonlinear vector field $|\Phi(x)|^2\Phi(x)$ acting on the decomposition $\Phi(x) = \sum_{n \in \mathbb{N}} \phi_n v_n(x)$, where $\vec{\phi}$ belongs to the vector space $l_s^1(\mathbb{N})$.

Lemma 5 *Let $W(x)$ be a bounded and 2π -periodic function. Let $\phi(x) = \sum_{n \in \mathbb{N}} \phi_n v_n(x)$ and $|\phi(x)|^2\phi(x) = \sum_{n \in \mathbb{N}} g_n v_n(x)$. If $0 < s < 1$, then there exists a $C > 0$ such that $\|\vec{g}\|_{l_s^1(\mathbb{N})} \leq C \|\vec{\phi}\|_{l_s^1(\mathbb{N})}^3$.*

Proof. We only need to prove that the space $l_s^1(\mathbb{N})$ with $0 < s < 1$ forms a Banach algebra in the sense

$$\forall \vec{\phi}, \vec{\varphi} \in l_s^1(\mathbb{N}) : \quad \|\vec{\phi} \star \vec{\varphi}\|_{l_s^1(\mathbb{N})} \leq C \|\vec{\phi}\|_{l_s^1(\mathbb{N})} \|\vec{\varphi}\|_{l_s^1(\mathbb{N})}, \quad (3.6)$$

for some $C > 0$, where

$$(\vec{\phi} \star \vec{\varphi})_n = \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} K_{n,i,j} \phi_i \varphi_j, \quad \forall n \in \mathbb{N}$$

and

$$K_{n,i,j} = \langle v_n, v_i v_j \rangle_{4\pi}, \quad \forall (n, i, j) \in \mathbb{N}^3.$$

According to Lemmas A.1 and A.2 of Appendix A of [7], if $W \in L_{\text{per}}^2([-2\pi, 2\pi])$ and $\|v_n\|_{L_{\text{per}}^2([-2\pi, 2\pi])}^2 = 1$ for any $n \in \mathbb{N}$, then there exists an n -independent constant $C > 0$, such that

$$|K_{n,i,j}| \leq \frac{C}{(1 + |n - i - j|)^p}, \quad \forall (n, i, j) \in \mathbb{N}^3, \quad (3.7)$$

for any $0 < p < 2$. By explicit computation, we obtain

$$\begin{aligned} \|\vec{\phi} \star \vec{\varphi}\|_{l_s^1(\mathbb{N})} &\leq \sum_{n \in \mathbb{N}} (1 + n)^s \sum_{i \in \mathbb{N}} \sum_{j \in \mathbb{N}} |K_{n,i,j}| |\phi_i| |\varphi_j| \\ &\leq C \sum_{i \in \mathbb{N}} (1 + i)^s |\phi_i| \sum_{j \in \mathbb{N}} (1 + j)^s |\varphi_j| \sum_{n \in \mathbb{N}} \left(\frac{1 + n}{(1 + i)(1 + j)} \right)^s \frac{1}{(1 + |n - i - j|)^p} \\ &\leq \tilde{C} \sum_{i \in \mathbb{N}} (1 + i)^s |\phi_i| \sum_{j \in \mathbb{N}} (1 + j)^s |\varphi_j| \sum_{n \in \mathbb{N}} \left(1 + \frac{n^s}{(1 + i)^s (1 + j)^s} \right) \frac{1}{(1 + n)^p} \end{aligned}$$

for some $\tilde{C} > 0$. If $p > 1$ and $p - s > 1$, the bound is completed as follows

$$\|\vec{\phi} \star \vec{\varphi}\|_{l_s^1(\mathbb{N})} \leq \tilde{C}_1 \|\vec{\phi}\|_{l_s^1(\mathbb{N})} \|\vec{\varphi}\|_{l_s^1(\mathbb{N})} + \tilde{C}_2 \|\vec{\phi}\|_{l^1(\mathbb{N})} \|\vec{\varphi}\|_{l^1(\mathbb{N})} \leq (\tilde{C}_1 + \tilde{C}_2) \|\vec{\phi}\|_{l_s^1(\mathbb{N})} \|\vec{\varphi}\|_{l_s^1(\mathbb{N})}$$

for some $\tilde{C}_1, \tilde{C}_2 > 0$. Since $1 < p < 2$, the parameter s must satisfy $0 < s < 1$. $\square$

By using this construction, we prove the first main result of our analysis.

Theorem 1 *Let $W(x)$ be a bounded, even and 2π -periodic function on $x \in \mathbb{R}$. The nonlinear elliptic problem (2.7) has a continuous and 4π -periodic solution $\Phi(x)$ for sufficiently small ϵ if there exists a solution for $(A_1, A_2, A_3) \in \mathbb{C}^3$ of the algebraic coupled-mode equations*

$$\begin{cases} (\Omega - \beta_1)A_1 &= \sigma [\gamma_1 |A_1|^2 A_1 + \gamma_2 (2|A_2|^2 A_1 + A_2^2 \bar{A}_1) + \gamma_3 (2|A_3|^2 A_1 + A_3^2 \bar{A}_1)] + \epsilon R_1(A_1, A_2, A_3), \\ (\Omega - \beta_1)A_2 &= \sigma [\gamma_1 |A_2|^2 A_2 + \gamma_2 (2|A_1|^2 A_2 + A_1^2 \bar{A}_2) + \gamma_3 (2|A_3|^2 A_2 + A_3^2 \bar{A}_2)] + \epsilon R_2(A_1, A_2, A_3), \\ (\Omega - \beta_2)A_3 &= \sigma [\gamma_4 |A_3|^2 A_3 + 2\gamma_3 (|A_1|^2 + |A_2|^2) A_3 + \gamma_3 (A_1^2 + A_2^2) \bar{A}_3] + \epsilon R_3(A_1, A_2, A_3), \end{cases} \quad (3.8)$$

where parameters are given by

$$\beta_1 = \langle \psi_1, W\psi_1 \rangle_{4\pi} + \langle \varphi_2, W\varphi_2 \rangle_{4\pi}, \quad \beta_2 = 2\langle \varphi_1, W\varphi_1 \rangle_{4\pi}$$

and

$$\gamma_1 = \langle \psi_1^2, \psi_1^2 \rangle_{4\pi} \langle \varphi_2^2, \varphi_2^2 \rangle_{4\pi}, \quad \gamma_2 = |\langle \psi_1^2, \varphi_2^2 \rangle_{4\pi}|^2, \quad \gamma_3 = \langle \psi_1^2, \varphi_1^2 \rangle_{4\pi} \langle \varphi_1^2, \varphi_2^2 \rangle_{4\pi}, \quad \gamma_4 = |\langle \varphi_1^2, \varphi_1^2 \rangle_{4\pi}|^2$$

and the residual terms $R_{1,2,3}(A_1, A_2, A_3)$ are analytic functions of ϵ near $\epsilon = 0$ satisfying the bounds

$$\forall |\epsilon| < \epsilon_0 : \quad |R_{1,2,3}(A_1, A_2, A_3)| \leq C_{1,2,3}(|A_1| + |A_2| + |A_3|),$$

for some constants $C_{1,2,3} > 0$ and sufficiently small ϵ_0 . Moreover, there exists an ϵ -independent constant $C > 0$ such that

$$\|\Phi - A_1\Phi_1 - A_2\Phi_2 - A_3\Phi_3\|_{C_b^0(\mathbb{R}^2)} \leq C\epsilon,$$

where (Φ_1, Φ_2, Φ_3) are the modes defined by Lemma 2.

Proof. 4π -periodic solutions of the nonlinear elliptic problem (2.7) are expanded in the form

$$\Phi(x) = \sum_{(n_1, n_2) \in \mathbb{N}^2} \Phi_{n_1, n_2} v_{n_1}(x_1) v_{n_2}(x_2). \quad (3.9)$$

Let the vector $\vec{\Phi}$ with the elements of the sequence $\{\Phi_{n_1, n_2}\}_{(n_1, n_2) \in \mathbb{N}^2}$ belong to the vector space $l_s^1(\mathbb{N}^2)$ equipped with the norm

$$\|\vec{\Phi}\|_{l_s^1(\mathbb{N}^2)} = \sum_{(n_1, n_2) \in \mathbb{N}^2} (1 + n_1)^s (1 + n_2)^s |\Phi_{n_1, n_2}| < \infty. \quad (3.10)$$

Similarly to Lemma 3, it follows that the function $\Phi(x)$ is continuous if $\vec{\Phi} \in l_s^1(\mathbb{N}^2)$ with $s > \frac{1}{2}$. Indeed,

$$\begin{aligned} \|\Phi\|_{C_b^0(\mathbb{R}^2)} &\leq \sum_{(n_1, n_2) \in \mathbb{N}^2} |\Phi_{n_1, n_2}| \|v_{n_1}\|_{C_b^0([-2\pi, 2\pi])} \|v_{n_2}\|_{C_b^0([-2\pi, 2\pi])} \\ &\leq C \sum_{(n_1, n_2) \in \mathbb{N}^2} |\Phi_{n_1, n_2}| \|v_{n_1}\|_{H_{\text{per}}^s([-2\pi, 2\pi])} \|v_{n_2}\|_{H_{\text{per}}^s([-2\pi, 2\pi])} \\ &\leq \tilde{C} \sum_{(n_1, n_2) \in \mathbb{N}^2} (1 + n_1)^s (1 + n_2)^s |\Phi_{n_1, n_2}| \end{aligned}$$

for some $C, \tilde{C} > 0$ and any $s > \frac{1}{2}$. By construction, the solution $\Phi(x)$ is 4π -periodic in both coordinates of $x \in \mathbb{R}^2$. The partial differential equation (2.7) is rewritten in the lattice form, which is diagonal with respect to the linear terms

$$[\nu_{n_1} + \nu_{n_2} - \omega_0 - \epsilon\Omega] \Phi_n = -\epsilon\sigma \sum_{(m, i, j) \in \mathbb{N}^6} M_{n, m, i, j} \Phi_m \bar{\Phi}_i \Phi_j, \quad \forall n = (n_1, n_2) \in \mathbb{N}^2, \quad (3.11)$$

where ν_n depend on $\eta = \eta_0 + \epsilon$ and

$$M_{n, m, i, j} = \langle v_{n_1} v_{i_1}, v_{m_1} v_{j_1} \rangle_{4\pi} \langle v_{n_2} v_{i_2}, v_{m_2} v_{j_2} \rangle_{4\pi}, \quad \forall (n_1, n_2, m_1, m_2, i_1, i_2, j_1, j_2) \in \mathbb{N}^8.$$

Since $M_{n,m,i,j}$ is a product of one-dimensional inner products and the weights in the norm in $l_s^1(\mathbb{N}^2)$ are separable, Lemma 5 applies and guarantees that the nonlinear vector field of the lattice equations (3.11) is closed in $l_s^1(\mathbb{N}^2)$ for $0 < s < 1$. Therefore, solutions of the lattice equations (3.11) can be considered in the space $l_s^1(\mathbb{N}^2)$ for any $\frac{1}{2} < s < 1$.

By Lemma 2, the three resonant modes are isolated from all other 4π -periodic modes. By Lemma 4, the eigenvalues $\nu_{n_1} + \nu_{n_2}$ are then analytic in η near $\eta = \eta_0$. The three resonant modes correspond to the values of n in the set $\{(1,3); (3,1); (2,2)\}$. Therefore, we decompose the solution $\vec{\Phi}$ of the lattice equations (3.11) into

$$\vec{\Phi} = A_1 \mathbf{e}_{1,3} + A_2 \mathbf{e}_{3,1} + A_3 \mathbf{e}_{2,2} + \vec{\Psi}, \quad (3.12)$$

where $\{\mathbf{e}_{1,3}, \mathbf{e}_{3,1}, \mathbf{e}_{2,2}\}$ are unit vectors on $\mathbb{N}^2$, $\text{Span}(\mathbf{e}_{1,3}, \mathbf{e}_{3,1}, \mathbf{e}_{2,2})$ is the kernel of the linearized system at the zero solution for $\epsilon = 0$, and $\vec{\Psi}$ lies in the orthogonal complement of the kernel such that $\Psi_{1,3} = \Psi_{3,1} = \Psi_{2,2} = 0$. The linearized operator projected onto the orthogonal complement of the kernel is continuously invertible for sufficiently small ϵ . By the Implicit Function Theorem in the space $l_s^1(\mathbb{N}^2)$ for any $\frac{1}{2} < s < 1$, there exists a unique map $\vec{\Psi}_\epsilon(A_1, A_2, A_3) : \mathbb{C}^3 \mapsto l_s^1(\mathbb{N}^2)$ for sufficiently small ϵ . Moreover, the map is locally analytic in ϵ near $\epsilon = 0$, such that $\vec{\Psi}_0(A_1, A_2, A_3) = \mathbf{0}$. In addition, $\vec{\Psi}_\epsilon(0, 0, 0) = \mathbf{0}$ for any $\epsilon \in \mathbb{R}$ and $(\partial_\epsilon \vec{\Psi}_\epsilon(A_1, A_2, A_3))|_{\epsilon=0}$ is a homogeneous cubic polynomial of (A_1, A_2, A_3) . Let $\delta \equiv |A_1| + |A_2| + |A_3| < \delta_0$ for a fixed ϵ -independent $\delta_0 > 0$. Then the map $\vec{\Psi}_\epsilon(A_1, A_2, A_3)$ satisfies the bound

$$\forall |\epsilon| < \epsilon_0 : \quad \|\vec{\Psi}_\epsilon(A_1, A_2, A_3)\|_{l_s^1(\mathbb{N}^2)} \leq \epsilon C (|A_1| + |A_2| + |A_3|), \quad (3.13)$$

where $\epsilon_0 > 0$ is sufficiently small, $\delta_0 > 0$ is finite, and the constant $C > 0$ is independent of ϵ and δ .

We can now consider the three equations of the system (3.11) for $n = \{(1,3); (3,1); (2,2)\}$. After the Taylor expansion of (3.11) in ϵ the formula (3.4) yields the coefficients β_1, β_2 since $\partial_\eta = \partial_\epsilon$. Note that the 2π -inner product in (3.4) is replaced by the 4π -inner product. Although the Bloch modes $v_n(x)$ are now normalized over the 4π -long interval, the value of (3.4) is unchanged. Using the bound (3.13) and the fact that the lattice equations are closed in $l_s^1(\mathbb{N}^2)$, we derive the algebraic coupled-mode equations in Theorem 1. The coefficients of these equations can be simplified due to the fact that $W(x)$ is even on $x \in \mathbb{R}$, such that the eigenfunctions $\psi_1(x)$ and $\varphi_1(x)$ are even while $\varphi_2(x)$ is odd on $x \in \mathbb{R}$. As a result, many coefficients of the coupled-mode system are identically zero, for instance $\langle \psi_1 \varphi_2, \varphi_1^2 \rangle_{4\pi} = 0$, $\langle \varphi_1^2, \varphi_1 \varphi_2 \rangle_{4\pi} = 0$ and so on. The residual terms $R_{1,2,3}(A_1, A_2, A_3)$ are estimated from the map $\vec{\Psi}_\epsilon(A_1, A_2, A_3)$ with the bound (3.13). The last estimate in the statement of Theorem 1 is obtained from (3.13) and Lemma 3. $\square$

We shall refer to the system (3.8) without remainder terms $\epsilon R_{1,2,3}(A_1, A_2, A_3)$ as to the truncated coupled-mode system.

Corollary 1 *There exist five invariant reductions of the truncated coupled-mode system, namely (i) $A_1 = A_2 = 0$, (ii) $A_1 = A_3 = 0$, (iii) $A_2 = A_3 = 0$, (iv) $A_1 = 0$, and (v) $A_2 = 0$, which persist in the full lattice equations (3.11).*

Proof. Any of the five invariant reductions implies symmetry constraints on the function $\Phi(x)$ at the leading order of the decomposition (3.12). For instance, if $A_1 = A_2 = 0$, then $\Phi(x)$ is 2π -antiperiodic with respect to both x_1 and x_2 ; if $A_1 = 0$, then $\Phi(x)$ is 2π -antiperiodic in x_1 and 4π -periodic in x_2 , and so on. By the completeness results of Proposition 1, all other terms of the decomposition (3.9) which violate the symmetry constraints on the solution $\Phi(x)$ can be set to be identically zero. By the Implicit Function Theorem, the zero solution is unique near $\epsilon = 0$. Therefore, the series (3.9) shrinks to fewer terms, the reduction persists for sufficiently small ϵ , and the proof of Theorem 1 applies. $\square$

Remark 4 The invariant reduction $A_3 = 0$ of the truncated coupled-mode system may not satisfy the full lattice equations (3.11) since the solution $\Phi(x)$ with $A_3 = 0$ is still a 4π -periodic function of both x_1 and x_2 and the series (3.9) can not be shrunk to fewer terms for $A_3 = 0$.

Remark 5 The Fourier–Bloch decomposition needed in Theorem 1 can be alternatively developed for $\vec{\phi}$ in the vector space $l_s^2(\mathbb{N})$ equipped with the squared norm

$$\|\vec{\phi}\|_{l_s^2(\mathbb{N})}^2 = \sum_{n \in \mathbb{N}} (1 + n^2)^s |\phi_n|^2 < \infty. \quad (3.14)$$

Indeed, the squared norm $\|\phi\|_{H^s(\mathbb{P}_k)}^2$ is equivalent to the integral

$$\begin{aligned} \int_0^{2\pi} \left| (c_\eta + L_{1D})^{s/2} \phi(x) \right|^2 dx &= \sum_{n_1 \in \mathbb{N}} \sum_{n_2 \in \mathbb{N}} \phi_{n_1} \bar{\phi}_{n_2} (c_\eta + \rho_n(k))^s \langle u_{n_1}(\cdot; k), u_{n_2}(\cdot; k) \rangle_{2\pi} \\ &= \sum_{n \in \mathbb{N}} (c_\eta + \rho_n(k))^s |\phi_n|^2, \end{aligned}$$

where we have used the orthogonality relation (3.1). By the asymptotic distribution (2.4), $\|\phi\|_{H^s(\mathbb{P}_k)}^2$ is thus equivalent to $\|\vec{\phi}\|_{l_s^2(\mathbb{N})}^2$. By Sobolev’s Embedding Theorem, $\|\phi\|_{C_b^0(\mathbb{P}_k)} \leq C \|\phi\|_{H^s(\mathbb{P}_k)}$ for some $C > 0$ and any $s > \frac{1}{2}$. Therefore, the decomposition (3.2) produces a continuous function $\phi(x)$ on $x \in \mathbb{R}$ if $\vec{\phi} \in l_s^2(\mathbb{N})$ with $s > \frac{1}{2}$. Furthermore, using Lemma 3.4 in [7], one can prove that the nonlinear term maps $l_s^2(\mathbb{N})$ to $l_s^2(\mathbb{N})$ for any $s > \frac{1}{2}$, such that the arguments of the Lyapunov–Schmidt reductions of Theorem 1 will work in the space $l_s^2(\mathbb{N})$ for any $s > \frac{1}{2}$. Note that this approach would lift the upper bound on the index s in Theorem 1, where $\frac{1}{2} < s < 1$.

Example 2 For $W(x) = 1 - \cos x$ and $\eta = \eta_0 \approx 0.1745$, the parameters of the algebraic coupled-mode equations (3.8) are approximated numerically as follows:

$$\beta_1 \approx 2.2835, \quad \beta_2 \approx 0.9183$$

and

$$\gamma_1 \approx 9.4829 \times 10^{-3}, \quad \gamma_2 \approx 4.5196 \times 10^{-3}, \quad \gamma_3 \approx 3.7942 \times 10^{-3}, \quad \gamma_4 \approx 1.5981 \times 10^{-2}.$$

The algebraic coupled-mode equations describe both linear and nonlinear corrections to the eigenvalues $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$ for fixed values of (k_1, k_2) at the vertex points X , X' and M . In particular, these corrections show how the band edges of the three resonant bands split for $\epsilon \neq 0$ and deform due to nonlinear interactions between resonant Bloch modes. We skip further analysis of the algebraic coupled-mode equations and proceed with the decaying solutions of the nonlinear elliptic problem (2.7) described by the differential coupled-mode equations.

4 Differential coupled-mode equations

We consider here bounded and decaying solutions $\Phi(x)$ of the bifurcation problem (2.7) for small ϵ . The decomposition of the decaying solution $\Phi(x)$ depends now on the completeness of the Bloch modes of the one-dimensional Sturm–Liouville problem (2.3) in $L^2(\mathbb{R})$, where all Bloch modes for all $k \in \mathbb{T}$ must be incorporated in the Fourier–Bloch decomposition.

Proposition 2 Let $W(x)$ be a bounded and 2π -periodic function. Let $\{\rho_n(k)\}_{n \in \mathbb{N}}$ and $\{u_n(x; k)\}_{n \in \mathbb{N}}$ be sets of eigenvalues and eigenfunctions of the Sturm–Liouville problem (2.3) on $k \in \mathbb{T}$, such that

$$\langle u_n(\cdot; k), u_{n'}(\cdot; k') \rangle_{\mathbb{R}} = \delta_{n, n'} \delta(k - k'), \quad \forall n, n' \in \mathbb{N}, \quad \forall k, k' \in \mathbb{T}, \quad (4.1)$$

where $\langle f, g \rangle_{\mathbb{R}} = \int_{\mathbb{R}} \bar{f}(x)g(x)dx$ and $\delta(x)$ is the Dirac's delta function in the distribution sense. Then, there exists a unitary transformation $\mathcal{T} : L^2(\mathbb{R}) \mapsto l^2(\mathbb{N}, L^2(\mathbb{T}))$ given by

$$\forall \phi \in L^2(\mathbb{R}) : \quad \hat{\phi}(k) = \mathcal{T}\phi, \quad \hat{\phi}_n(k) = \int_{\mathbb{R}} \bar{u}_n(y; k) \phi(y) dy, \quad \forall n \in \mathbb{N}, \quad \forall k \in \mathbb{T}, \quad (4.2)$$

where $l^2(\mathbb{N}, L^2(\mathbb{T}))$ is equipped with the squared norm

$$\|\hat{\phi}\|_{l^2(\mathbb{N}, L^2(\mathbb{T}))}^2 = \sum_{n \in \mathbb{N}} \int_{\mathbb{T}} |\hat{\phi}_n(k)|^2 dk.$$

The inverse transformation is given by

$$\forall \hat{\phi} \in l^2(\mathbb{N}, L^2(\mathbb{T})) : \quad \phi(x) = \mathcal{T}^{-1}\hat{\phi} = \sum_{n \in \mathbb{N}} \int_{\mathbb{T}} \hat{\phi}_n(k) u_n(x; k) dk, \quad \forall x \in \mathbb{R}. \quad (4.3)$$

Proof. The original proof of the proposition can be found in [11]. Orthogonality and completeness of the Bloch wave functions $\{u_n(x; k)\}_{n \in \mathbb{N}}$ on $k \in \mathbb{T}$ is summarized in Theorem XIII.98 on p.304 in [23]. Existence of the unitary transformation (4.2) with the inverse transformation (4.3) is summarized in Theorems XIII.97 and XIII.98 on pp. 303–304 in [23]. $\square$

Lemma 6 Let $\phi(x)$ be defined by the decomposition (4.3), where $\hat{\phi}$ belongs to the vector space $l_s^1(\mathbb{N}, L^1(\mathbb{T}))$ with the norm

$$\|\hat{\phi}\|_{l_s^1(\mathbb{N}, L^1(\mathbb{T}))} = \sum_{n \in \mathbb{N}} (1+n)^s \|\hat{\phi}_n\|_{L^1(\mathbb{T})} = \sum_{n \in \mathbb{N}} (1+n)^s \int_{\mathbb{T}} |\hat{\phi}_n(k)| dk < \infty. \quad (4.4)$$

If $s > \frac{1}{2}$, then $\phi(x)$ is a continuous function on $x \in \mathbb{R}$ such that $\phi(x) \rightarrow 0$ as $|x| \rightarrow \infty$.

Proof. The proof is similar to that of Lemma 3 since the asymptotic bound (2.4) is uniform on $k \in \mathbb{T}$. Therefore,

$$\|\phi\|_{C_b^0(\mathbb{R})} \leq \sum_{n \in \mathbb{N}} \int_{\mathbb{T}} |\hat{\phi}_n(k)| \|u_n(\cdot; k)\|_{C_b^0(\mathbb{P}_k)} dk \leq C \sum_{n \in \mathbb{N}} \int_{\mathbb{T}} |\hat{\phi}_n(k)| \|u_n(\cdot; k)\|_{H^s(\mathbb{P}_k)} dk \leq \tilde{C} \|\hat{\phi}\|_{l_s^1(\mathbb{N}, L^1(\mathbb{T}))},$$

for some $C, \tilde{C} > 0$ and any $s > \frac{1}{2}$. The decay of $\phi(x)$ as $|x| \rightarrow \infty$ follows from the Riemann–Lebesgue Lemma applied to the Fourier–Bloch transform. Indeed, the summation in $n \in \mathbb{N}$ of the integrals on $k \in \mathbb{T}$ can be written as an integral on $k \in \mathbb{R}$ in the form

$$\phi(x) = \int_{\mathbb{R}} \hat{\phi}(k) v(x; k) dk,$$

where $v(x; k)$ for $k \in \mathbb{R}$ is related to the Bloch functions $u_n(x; k)$ for $k \in \mathbb{T}$ (see [7] for details). Since $v(x; k) = e^{ikx} w(x; k)$, where $w(x; k)$ is periodic in x with period 2π and is uniformly bounded in $C_b^0(\mathbb{R})$ with respect to both x and k , the Riemann–Lebesgue Lemma applies to the Fourier–Bloch transform in the same manner as it applies to the standard Fourier transform if $\hat{\phi} \in L^1(\mathbb{R})$. $\square$

Lemma 7 Let $W(x)$ be a bounded, piecewise-continuous and 2π -periodic function. Let $\rho_n(k_0)$ be the extremal value of $\rho_n(k)$ for either $k_0 = 0$ or $k_0 = \pm\frac{1}{2}$ and assume that the adjacent bands are bounded away from the value $\rho_n(k_0)$. Then, $\rho_n(k)$ is an analytic function at the point $k = k_0$, such that

$$\rho'(k_0) = 0, \quad \rho''(k_0) \neq 0, \quad \left| \rho_n(k) - \rho_n(k_0) - \frac{1}{2}\rho''(k_0)(k - k_0)^2 \right| \leq C(k - k_0)^4 \quad (4.5)$$

for some $C > 0$ uniformly in $k \in \mathbb{T}$.

Proof. By Theorem XIII.95 in [23], the function $\rho_n(k)$ for an isolated spectral band can be extended onto a smooth Riemann surface which has no singularities other than square root branch points at $k = 0$ and $k = \pm\frac{1}{2}$. Therefore, the function $\rho_n(k)$ is expanded in even powers of $(k - k_0)$ for $k_0 = 0$ or $k_0 = \pm\frac{1}{2}$ and $\rho''(k_0) \neq 0$. $\square$

Lemma 8 Let $W(x)$ be a bounded and 2π -periodic function. Let $\hat{\phi} = \mathcal{T}\phi$ and $\hat{g} = \mathcal{T}(|\phi|^2\phi)$. If $0 < s < 1$, then there exists a $C > 0$ such that $\|\hat{g}\|_{l_s^1(\mathbb{N}, L^1(\mathbb{T}))} \leq C\|\hat{\phi}\|_{l_s^1(\mathbb{N}, L^1(\mathbb{T}))}^3$.

Proof. The proof is similar to that of Lemma 5 since the asymptotic bound (3.7) is uniform on $k \in \mathbb{T}$ [7] and the length of $\mathbb{T}$ is finite. The Banach algebra property (3.6) holds in space $l_s^1(\mathbb{N}, L^1(\mathbb{T}))$ for any $0 < s < 1$. Indeed, let

$$(\hat{\phi} \star \hat{\phi})_n(k) = \sum_{j_1 \in \mathbb{N}} \sum_{j_2 \in \mathbb{N}} \int_{\mathbb{T}} \int_{\mathbb{T}} K_{n, j_1, j_2}(k, k_1, k_2) \hat{\phi}_{j_1}(k_1) \hat{\phi}_{j_2}(k_2) dk_1 dk_2, \quad n \in \mathbb{N}, k \in \mathbb{T},$$

where $K_{n, j_1, j_2}(k, k_1, k_2) = \langle u_n(\cdot; k), u_{j_1}(\cdot; k_1) u_{j_2}(\cdot; k_2) \rangle_{\mathbb{R}^1}$ for all $(n, j_1, j_2) \in \mathbb{N}^3$ and $(k, k_1, k_2) \in \mathbb{T}^3$. By an explicit computation, we obtain

$$\begin{aligned} \|\hat{\phi} \star \hat{\phi}\|_{l_s^1(\mathbb{N}, L^1(\mathbb{T}))} &\leq \sum_{n \in \mathbb{N}} (1+n)^s \sum_{j_1 \in \mathbb{N}} \sum_{j_2 \in \mathbb{N}} \int_{\mathbb{T}} \int_{\mathbb{T}} \int_{\mathbb{T}} |K_{n, j_1, j_2}(k, k_1, k_2)| |\hat{\phi}_{j_1}(k_1)| |\hat{\phi}_{j_2}(k_2)| dk dk_1 dk_2 \\ &\leq C \sum_{j_1 \in \mathbb{N}} \sum_{j_2 \in \mathbb{N}} (1+j_1)^s (1+j_2)^s \int_{\mathbb{T}} \int_{\mathbb{T}} |\hat{\phi}_{j_1}(k_1)| |\hat{\phi}_{j_2}(k_2)| dk_1 dk_2 \\ &\quad \times \sum_{n \in \mathbb{N}} \left(\frac{1+n}{(1+j_1)(1+j_2)} \right)^s \frac{1}{(1+|n-j_1-j_2|)^p} \end{aligned}$$

for some $C > 0$ and any $0 < p < 2$. The last sum is finite if $p > 1$ and $p - s > 1$ (that is $0 < s < 1$), similarly to the proof of Lemma 5. $\square$

We shall now define the coupled-mode system, which is a central element of our paper. Let $A_{1,2,3}(y)$ be functions of $y = \sqrt{\epsilon}x$ on $x \in \mathbb{R}^2$ which satisfy the differential coupled-mode equations

$$\begin{cases} (\Omega - \beta_1)A_1 + (\alpha_1 \partial_{y_1}^2 + \alpha_2 \partial_{y_2}^2) A_1 &= \sigma [\gamma_1 |A_1|^2 A_1 + \gamma_2 (2|A_2|^2 A_1 + A_2^2 \bar{A}_1) + \gamma_3 (2|A_3|^2 A_1 + A_3^2 \bar{A}_1)] \\ (\Omega - \beta_1)A_2 + (\alpha_2 \partial_{y_1}^2 + \alpha_1 \partial_{y_2}^2) A_2 &= \sigma [\gamma_1 |A_2|^2 A_2 + \gamma_2 (2|A_1|^2 A_2 + A_1^2 \bar{A}_2) + \gamma_3 (2|A_3|^2 A_2 + A_3^2 \bar{A}_2)] \\ (\Omega - \beta_2)A_3 + \alpha_3 (\partial_{y_1}^2 + \partial_{y_2}^2) A_3 &= \sigma [\gamma_4 |A_3|^2 A_3 + 2\gamma_3 (|A_1|^2 + |A_2|^2) A_3 + \gamma_3 (A_1^2 + A_2^2) \bar{A}_3], \end{cases} \quad (4.6)$$

where parameters $\beta_{1,2}$ and $\gamma_{1,2,3,4}$ are the same as in Theorem 1, while

$$\alpha_1 = \frac{1}{2}\rho_1''(0), \quad \alpha_2 = \frac{1}{2}\rho_2''\left(\frac{1}{2}\right), \quad \alpha_3 = \frac{1}{2}\rho_1''\left(\frac{1}{2}\right).$$

Since $\lambda_1 = \rho_1(0)$, $\mu_1 = \rho_1\left(\frac{1}{2}\right)$, and $\mu_2 = \rho_2\left(\frac{1}{2}\right)$ are non-degenerate eigenvalues in the ordering (2.6), the values of $\alpha_{1,2,3}$ are non-zero according to Lemma 7.

Example 3 For $W(x) = 1 - \cos x$ and $\eta = \eta_0 = 0.1745$, the parameters of the differential coupled-mode equations are approximated numerically as follows:

$$\alpha_1 \approx 0.9422, \quad \alpha_2 \approx 6.7813, \quad \alpha_3 \approx -4.7890.$$

Let $\hat{A}_{1,2,3}(p)$ on $p \in \mathbb{R}^2$ denote the Fourier transforms of the functions $A_{1,2,3}(y)$ on $y \in \mathbb{R}^2$ such that

$$A_{1,2,3}(y) = \frac{1}{2\pi} \int_{\mathbb{R}^2} \hat{A}_{1,2,3}(p) e^{ip \cdot y} dp, \quad \hat{A}_{1,2,3}(p) = \frac{1}{2\pi} \int_{\mathbb{R}^2} A_{1,2,3}(y) e^{-ip \cdot y} dy. \quad (4.7)$$

We shall use the standard norm in $L_q^1(\mathbb{R}^2)$ for the Fourier transforms $\hat{A}_{1,2,3}(p)$ with any $q \geq 0$:

$$\|\hat{A}\|_{L_q^1(\mathbb{R}^2)} = \int_{\mathbb{R}^2} (1 + |p|^2)^{q/2} |\hat{A}(p)| dp. \quad (4.8)$$

The differential coupled-mode equations (4.6) are converted to the equivalent integral form

$$\begin{cases} (\Omega - \beta_1 - \alpha_1 p_1^2 - \alpha_2 p_2^2) \hat{A}_1(p) &= \sigma \hat{N}_1[\hat{A}_1, \hat{A}_2, \hat{A}_3](p), \\ (\Omega - \beta_1 - \alpha_2 p_1^2 - \alpha_1 p_2^2) \hat{A}_2(p) &= \sigma \hat{N}_2[\hat{A}_1, \hat{A}_2, \hat{A}_3](p), \\ (\Omega - \beta_2 - \alpha_3 p_1^2 - \alpha_3 p_2^2) \hat{A}_3(p) &= \sigma \hat{N}_3[\hat{A}_1, \hat{A}_2, \hat{A}_3](p), \end{cases} \quad (4.9)$$

where $\hat{N}_{1,2,3}[\hat{A}_1, \hat{A}_2, \hat{A}_3](p)$ denote the Fourier transform of the cubic nonlinear terms of the differential coupled-mode equations. We now prove the second main result of our analysis.

Theorem 2 *Let $W(x)$ be a bounded, piecewise-continuous, even and 2π -periodic function on $x \in \mathbb{R}$. Let $\frac{1}{4} < r < \frac{1}{2}$. The nonlinear elliptic problem (2.7) has a continuous and decaying solution $\Phi(x)$ for sufficiently small $\epsilon > 0$ if there exists a solution $(\hat{B}_1, \hat{B}_2, \hat{B}_3) \in L^1(D_\epsilon, \mathbb{C}^3)$, compactly supported on the disk $D_\epsilon = \{p \in \mathbb{R}^2 : |p| < \epsilon^{r-\frac{1}{2}}\} \subset \mathbb{R}^2$, which satisfies the extended coupled-mode equations in the integral form*

$$\begin{cases} (\Omega - \beta_1 - \alpha_1 p_1^2 - \alpha_2 p_2^2) \hat{B}_1(p) - \sigma \hat{Q}_1(p) &= \epsilon^{\tilde{r}} \hat{R}_1(p), \\ (\Omega - \beta_1 - \alpha_2 p_1^2 - \alpha_1 p_2^2) \hat{B}_2(p) - \sigma \hat{Q}_2(p) &= \epsilon^{\tilde{r}} \hat{R}_2(p), \\ (\Omega - \beta_2 - \alpha_3 p_1^2 - \alpha_3 p_2^2) \hat{B}_3(p) - \sigma \hat{Q}_3(p) &= \epsilon^{\tilde{r}} \hat{R}_3(p), \end{cases} \quad (4.10)$$

where $\tilde{r} = \min(4r - 1, 1 - 2r)$, $\hat{Q}_{1,2,3}(p)$ denote the cubic nonlinear terms $\hat{N}_{1,2,3}[\hat{B}_1, \hat{B}_2, \hat{B}_3](p)$ truncated on $p \in D_\epsilon$, and $\hat{R}_{1,2,3}(p)$ are bounded by

$$\forall 0 < \epsilon < \epsilon_0 : \quad \|\hat{R}_{1,2,3}\|_{L^1(D_\epsilon)} \leq C_{1,2,3} \left(\|\hat{B}_1\|_{L^1(D_\epsilon)} + \|\hat{B}_2\|_{L^1(D_\epsilon)} + \|\hat{B}_3\|_{L^1(D_\epsilon)} \right), \quad (4.11)$$

for some constants $C_{1,2,3} > 0$ and sufficiently small ϵ_0 . Moreover, there exists an ϵ -independent constant $C > 0$ such that

$$\|\Phi - B_1 \Phi_1 - B_2 \Phi_2 - B_3 \Phi_3\|_{C_b^0(\mathbb{R}^2)} \leq C \epsilon^{1-2r}, \quad (4.12)$$

where $\Phi_{1,2,3}(x)$ are modes defined by Lemma 2 and $B_{1,2,3}(y)$ are defined by the Fourier transform (4.7).

Proof. Solutions of the nonlinear elliptic problem (2.7) are expanded in the form

$$\Phi(x) = \sum_{(n_1, n_2) \in \mathbb{N}^2} \int_{\mathbb{T}^2} \hat{\Phi}_{n_1, n_2}(k_1, k_2) u_{n_1}(x_1; k_1) u_{n_2}(x_2; k_2) dk_1 dk_2. \quad (4.13)$$

Let $\hat{\Phi}$ denote the union of functions $\hat{\Phi}_{n_1, n_2}(k_1, k_2)$ for all $(n_1, n_2) \in \mathbb{N}^2$ and $(k_1, k_2) \in \mathbb{T}^2$ and consider the vector space $l_s^1(\mathbb{N}^2, L^1(\mathbb{T}^2))$ equipped with the norm

$$\|\hat{\Phi}\|_{l_s^1(\mathbb{N}^2, L^1(\mathbb{T}^2))} = \sum_{(n_1, n_2) \in \mathbb{N}^2} (1 + n_1)^s (1 + n_2)^s \int_{\mathbb{T}} \int_{\mathbb{T}} |\hat{\Phi}_{n_1, n_2}(k_1, k_2)| dk_1 dk_2 < \infty. \quad (4.14)$$

One can show similarly to the proof of Theorem 1 that the statements of Lemmas 6 and 8 extend in two dimensions to the vector space with the norm (4.14). Therefore, we convert the partial differential equation (2.7) to the integral form, which is diagonal with respect to the linear terms

$$\begin{aligned} & [\rho_{n_1}(k_1) + \rho_{n_2}(k_2) - \omega_0 - \epsilon\Omega] \hat{\Phi}_n(k) \\ &= -\epsilon\sigma \sum_{(m, i, j) \in \mathbb{N}^6} \int_{\mathbb{T}^6} M_{n, m, i, j}(k, l, \kappa, \lambda) \hat{\Phi}_m(l) \bar{\hat{\Phi}}_i(\kappa) \hat{\Phi}_j(\lambda) dl d\kappa d\lambda \end{aligned} \quad (4.15)$$

for all $n = (n_1, n_2) \in \mathbb{N}^2$ and $k = (k_1, k_2) \in \mathbb{T}^2$, where

$$M_{n, m, i, j}(k, l, \kappa, \lambda) = \langle u_{n_1}(\cdot; k_1) u_{i_1}(\cdot; \kappa_1), u_{m_1}(\cdot; l_1) u_{j_1}(\cdot; \lambda_1) \rangle_{\mathbb{R}} \langle u_{n_2}(\cdot; k_2) u_{i_2}(\cdot; \kappa_2), u_{m_2}(\cdot; l_2) u_{j_2}(\cdot; \lambda_2) \rangle_{\mathbb{R}},$$

for all $(n_1, n_2, m_1, m_2, i_1, i_2, j_1, j_2) \in \mathbb{N}^8$ and $(k_1, k_2, l_1, l_2, \kappa_1, \kappa_2, \lambda_1, \lambda_2) \in \mathbb{T}^8$. In view of Lemmas 6 and 8 we consider solutions of the integral equations (4.15) in the space $l_s^1(\mathbb{N}^2, L^1(\mathbb{T}^2))$ for any $\frac{1}{2} < s < 1$.

When $\eta = \eta_0$, the multiplication operator $\rho_{n_1}(k_1) + \rho_{n_2}(k_2) - \omega_0$ vanishes at the points X' , X , and M , where the values of k are given by

$$\left\{ \left(0, \frac{1}{2}\right); \left(\frac{1}{2}, 0\right); \left(\frac{1}{2}, \frac{1}{2}\right) \right\} \subset \mathbb{T}^2, \quad (4.16)$$

with $n \in \{(1, 3); (3, 1); (2, 2)\} \subset \mathbb{N}^2$ resp. Therefore, we apply the method of Lyapunov–Schmidt reductions [12] and decompose the solution $\hat{\Phi}$ of the integral equations (4.15) into

$$\hat{\Phi}(k) = \hat{U}_1(k) \chi_{D_1}(k) \mathbf{e}_{1,3} + \hat{U}_2(k) \chi_{D_2}(k) \mathbf{e}_{3,1} + \hat{U}_3(k) \chi_{D_3}(k) \mathbf{e}_{2,2} + \hat{\Psi}(k), \quad (4.17)$$

where $\{\mathbf{e}_{1,3}, \mathbf{e}_{3,1}, \mathbf{e}_{2,2}\}$ are unit vectors on $\mathbb{N}^2$, $D_{1,2,3}$ are disks of radius ϵ^r centered at the points k of the set (4.16), see Figure 5. Since $k \in \mathbb{T}^2$, where $\mathbb{T}^2$ is the first Brillouin zone, we map D on $\mathbb{T}^2$ by periodic continuation and denote the resulting object by $D \cap \mathbb{T}^2$. In the representation (4.17), $\chi_D(k)$ is the characteristic function on $k \in \mathbb{T}^2$ ($\chi_D(k) = 1$ if $k \in D \cap \mathbb{T}^2$ and $\chi_D(k) = 0$ if $k \notin D \cap \mathbb{T}^2$), and $\hat{\Psi}(k)$ is zero identically on $k \in D_{1,2,3}$ for the corresponding values of n :

$$\hat{\Psi}_{(1,3)} = 0 \text{ on } D_1, \quad \hat{\Psi}_{(3,1)} = 0 \text{ on } D_2, \quad \hat{\Psi}_{(2,2)} = 0 \text{ on } D_3.$$

For any of the three resonant points of k , it follows by Lemma 7 that $\rho'_{n_j}(k_j) = 0$ and $\rho''_{n_j}(k_j) \neq 0$ for $j = 1, 2$ with the n corresponding to the resonance point k . As a result, there exists a constant $C > 0$ such that

$$\min_{\substack{(k_1, k_2) \in \text{supp}(\hat{\Psi}) \\ (n_1, n_2) \in \mathbb{N}^2}} |\rho_{n_1}(k_1)|_{\eta=\eta_0} + \rho_{n_2}(k_2)|_{\eta=\eta_0} - \omega_0| \geq C\epsilon^{2r}. \quad (4.18)$$

Note that the minimal values of the multiplication operator occur for the three resonant bands with the indices n in the set $\{(1, 3); (3, 1); (2, 2)\}$. For all other non-resonant bands, the multiplication operator is continuously invertible uniformly in ϵ for sufficiently small ϵ . If $2r < 1$, the lower bound (4.18) is still larger than the perturbation terms of order ϵ . By the Implicit Function Theorem in the space $l_s^1(\mathbb{N}^2, L^1(\mathbb{T}^2))$ for

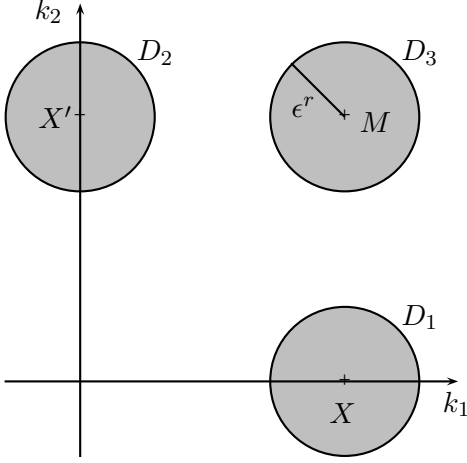


Figure 5: Decomposition of the k -space

any $\frac{1}{2} < s < 1$, there exists a unique map $\hat{\Psi}_\epsilon(\hat{U}_1, \hat{U}_2, \hat{U}_3) : L^1(D_1) \times L^1(D_2) \times L^1(D_3) \mapsto l_s^1(\mathbb{N}^2, L^1(\mathbb{T}^2))$ for sufficiently small $\epsilon > 0$. The right-hand side of the integral equation (4.15) is a homogeneous cubic polynomial of $\hat{\Psi}(k)$ and $\hat{U}_1, \hat{U}_2, \hat{U}_3$ multiplied by ϵ . Let $\delta \equiv \|\hat{U}_1\|_{L^1(D_1)} + \|\hat{U}_2\|_{L^1(D_2)} + \|\hat{U}_3\|_{L^1(D_3)} < \delta_0$ for a fixed ϵ -independent $\delta_0 > 0$. The map $\hat{\Psi}_\epsilon(\hat{U}_1, \hat{U}_2, \hat{U}_3)$ satisfies the bound

$$\|\hat{\Psi}_\epsilon(\hat{U}_1, \hat{U}_2, \hat{U}_3)\|_{l_s^1(\mathbb{N}^2, L^1(\mathbb{T}^2))} \leq \epsilon^{1-2r} C \left(\|\hat{U}_1\|_{L^1(D_1)} + \|\hat{U}_2\|_{L^1(D_2)} + \|\hat{U}_3\|_{L^1(D_3)} \right), \quad (4.19)$$

for sufficiently small $0 < \epsilon < \epsilon_0$, finite $0 < \delta < \delta_0$, and the (ϵ, δ) -independent constant $C > 0$.

We shall now map the disks $D_{1,2,3}$ to the same disk $D_\epsilon \subset \mathbb{R}^2$ in the stretched variable p centered at the origin. To do so, we apply the scaling transformation

$$\hat{B}_j(p) = \epsilon \hat{U}_j(k), \quad p = \frac{k - k_0}{\epsilon^{1/2}}, \quad \forall k \in D_j \cap \mathbb{T}^2, \quad j = 1, 2, 3, \quad (4.20)$$

where k_0 is the corresponding point of the set (4.16). The new disk D_ϵ is now $D_\epsilon = \{p \in \mathbb{R}^2 : |p| < \epsilon^{r-\frac{1}{2}}\}$ and it covers the entire plane $p \in \mathbb{R}^2$ in the limit $\epsilon \rightarrow 0$ if $2r < 1$. Note that the L^1 -norm of $\hat{U}_j(k)$ on $k \in D_j \cap \mathbb{T}^2$ is invariant with respect to the transformation (4.20) in the new variable $\hat{B}_j(p)$ on $p \in D_\epsilon \subset \mathbb{R}^2$, such that $\|\hat{U}_j\|_{L^1(D_j)} = \|\hat{B}_j\|_{L^1(D_\epsilon)}$ for any $j = 1, 2, 3$.

When the integral equations (4.15) are considered on the compact domains D_1, D_2, D_3 for the three resonant modes and the scaling transformation (4.20) is applied to map these domains into the domain D_ϵ , we obtain the extended coupled-mode system (4.10), where remainder terms occur due to three different sources. The first source comes from the component $\hat{\Psi} = \hat{\Psi}_\epsilon(\hat{U}_1, \hat{U}_2, \hat{U}_3)$ and it is estimated with the bound (4.19). The remainder terms have the order of ϵ^{1-2r} and are small if $2r < 1$. The second source comes from the expansion of $\rho_n(k)$ and $M_{n,m,i,j}(k, l, \kappa, \lambda)$ in powers of ϵ and it is estimated with Lemma 4. The remainder terms have the order of ϵ^1 . The third source comes from the expansion of $\rho_n(k)$ and $M_{n,m,i,j}(k, l, \kappa, \lambda)$ in powers of $k - k_0$ and it is estimated with Lemma 7. The remainder terms have the order of ϵ^{4r-1} because of the following estimate:

$$\epsilon \| |p|^4 \hat{B}_j \|_{L^1(D_\epsilon)} = \epsilon \int_{D_\epsilon} |p|^4 |\hat{B}_j(p)| dp \leq \epsilon^{4r-1} \|\hat{B}_j\|_{L^1(D_\epsilon)}, \quad j = 1, 2, 3.$$

The remainder terms are small if $4r > 1$. Thus, the statement is proved if $\frac{1}{4} < r < \frac{1}{2}$ and the largest remainder terms have the order $\epsilon^{\tilde{r}}$ with $\tilde{r} = \min(4r - 1, 1 - 2r)$. $\square$

Remark 6 If $r = \frac{1}{3}$, then $\tilde{r} = r = \frac{1}{3}$ and both remainder terms of the extended coupled-mode equations are of the same order in ϵ . The fastest convergence rate of the remainder terms is $\epsilon^{1/3}$ because $\max_{r \in (1/4, 1/2)}(\tilde{r}) = 1/3$.

The differential coupled-mode system on $A_{1,2,3}(y)$ has invariant reductions when one or two components of $A_{1,2,3}$ are identically zero. In particular, the reduction $A_3 = 0$ recovers coupled-mode equations near the band edge C derived in [25], while the reduction $A_1 = A_2 = 0$ recovers coupled-mode equations near the band edge B in [25]. However, these reductions do not generally persist in the extended coupled-mode equations near $\eta = \eta_0$ since the reductions do not imply any symmetry constraints on the function $\Phi(x)$.

The coupled-mode equations (4.9) linearized at the zero solution describe the expansions of the function $\omega = \rho_{n_1}(k_1) + \rho_{n_2}(k_2)$ near the vertex points X' , X , and M in terms of the perturbation parameter $\epsilon = \eta - \eta_0$ and the small deviation of $k = (k_1, k_2)$ from the value $k_0 = (k_{1,0}, k_{2,0})$ in the set (4.16)

$$\omega = \omega_0 + \epsilon \partial_\eta \omega|_{\eta=\eta_0, k=k_0} + \frac{1}{2} \rho''_{n_1}(k_{1,0})(k_1 - k_{1,0})^2 + \frac{1}{2} \rho''_{n_2}(k_{2,0})(k_2 - k_{2,0})^2 + \mathcal{O}(|k - k_0|^4). \quad (4.21)$$

We note that the values of $\partial_\eta \omega|_{\eta=\eta_0}$ are equal for the vertex points X and X' , while the values of $\rho''_{n_1}(k_{1,0})$ and $\rho''_{n_2}(k_{2,0})$ have the same sign for all points X , X' and M . Moreover, $\text{sign}(\rho''_{n_j}(X_j)) = \text{sign}(\rho''_{n_j}(X'_j))$, $j = 1, 2$. A simple analysis of (4.21) shows that the band gap between the three resonant Bloch band surfaces exists if

$$\rho''_{n_1}(k_1)|_X > 0, \quad \rho''_{n_1}(k_1)|_M < 0, \quad \text{for } \epsilon \partial_\eta \omega|_X > \epsilon \partial_\eta \omega|_M$$

or

$$\rho''_{n_1}(k_1)|_X < 0, \quad \rho''_{n_1}(k_1)|_M > 0, \quad \text{for } \epsilon \partial_\eta \omega|_X < \epsilon \partial_\eta \omega|_M.$$

Examples 2 and 3 show that the first case occurs for the particular potential $W(x) = 1 - \cos x$ if $\eta > \eta_0$, such that the band gap opens for $\epsilon > 0$ in the interval $\beta_2 < \Omega < \beta_1$, in a correspondence with a narrow band gap for $\eta > \eta_0$ in Figure 3(b).

5 Persistence of localized reversible solutions

The coupled-mode system in the integral form (4.9) is different from the extended coupled-mode system (4.10) in two aspects. First, the convolution integrals are truncated in (4.10) on the domain D_ϵ for $|p| < \epsilon^{r-\frac{1}{2}}$, where $\frac{1}{4} < r < \frac{1}{2}$. Second, the remainder terms of order $\epsilon^{\tilde{r}}$ with $\tilde{r} = \min(4r - 1, 1 - 2r)$ are present in (4.10). The first source is small if solutions of the extended coupled-mode system are considered on $p \in \mathbb{R}^2$ in the space $L^1_q(\mathbb{R}^2)$ for some $q \geq 0$. The second source is handled with the Implicit Function Theorem. We shall consider here a special class of decaying solutions of the coupled-mode system (4.9) on $p \in \mathbb{R}^2$ which lead to the corresponding solutions of the extended coupled-mode system (4.10) on $p \in D_\epsilon$.

Definition 1 A solution (A_1, A_2, A_3) of the differential coupled-mode system (4.6) on $y \in \mathbb{R}^2$ is called reversible if it satisfies one of the two constraints (1.4) and (1.5) for each function $A_1(y)$, $A_2(y)$ and $A_3(y)$.

For notational simplicity, we write the differential coupled-mode equations (4.6) in the form $\mathbf{F}(\mathbf{A}) = \mathbf{0}$, where $\mathbf{F}$ is a nonlinear operator on $(A_1, A_2, A_3) \in C^2(\mathbb{R}^2, \mathbb{C}^3)$ with the range in $C^0(\mathbb{R}^2, \mathbb{C}^3)$. The Jacobian

of the operator $\mathbf{F}(\mathbf{A})$ denoted by $D_{\mathbf{A}}\mathbf{F}(\mathbf{A})$ is a matrix differential operator, which is diagonal with respect to the unbounded differential part and full with respect to the local potential part. In many cases, the Jacobian operator $D_{\mathbf{A}}\mathbf{F}(\mathbf{A})$ can be block-diagonalized and simplified but we can work with a general operator to prove the third main result of our analysis.

Theorem 3 *Let $W(x)$ satisfy the same assumptions as in Theorem 2. Let Ω belong to the interior of the band gap of the coupled-mode system $\mathbf{F}(\mathbf{A}) = \mathbf{0}$. Let (A_1, A_2, A_3) on $y \in \mathbb{R}^2$ be a reversible solution of the differential coupled-mode system $\mathbf{F}(\mathbf{A}) = \mathbf{0}$ in the sense of Definition 1 such that their Fourier transforms satisfy $\hat{\mathbf{A}} \in L_q^1(\mathbb{R}^2, \mathbb{C}^3)$ for all $q \geq 0$. Assume that the Jacobian operator $D_{\mathbf{A}}\mathbf{F}(\mathbf{A})$ has a three-dimensional kernel with the eigenvectors $\{\partial_{y_1}\mathbf{A}, \partial_{y_2}\mathbf{A}, i\mathbf{A}\}$. Then, there exists a solution $(\hat{B}_1, \hat{B}_2, \hat{B}_3) \in L^1(D_\epsilon, \mathbb{C}^3)$ of the extended coupled-mode system (4.10) such that*

$$\forall 0 < \epsilon < \epsilon_0 : \quad \|\hat{B}_j - \hat{A}_j\|_{L^1(D_\epsilon)} \leq C_j \epsilon^{\tilde{r}}, \quad \forall j = 1, 2, 3, \quad (5.1)$$

for some ϵ -independent constant $C_j > 0$ and sufficiently small ϵ_0 .

Proof. First, we consider system (4.10) on the entire plane $p \in \mathbb{R}^2$ in the space $L_q^1(\mathbb{R}^2)$ for a fixed $q \geq 0$ by extending the right-hand-side functions $\hat{R}_{1,2,3}(p)$ on $\mathbb{R}^2$ with a compact support on D_ϵ . Thanks to the assumption on the existence of a solution $\hat{\mathbf{A}}$ of $\hat{\mathbf{F}}(\hat{\mathbf{A}}) = \mathbf{0}$ and its fast decay in $L_q^1(\mathbb{R}^2)$ for all $q \geq 0$, we decompose the solution of the extended system $\hat{\mathbf{F}}(\hat{\mathbf{B}}) = \epsilon^{\tilde{r}} \hat{\mathbf{R}}(\hat{\mathbf{B}})$ on $p \in \mathbb{R}^2$ into $\hat{\mathbf{B}} = \hat{\mathbf{A}} + \hat{\mathbf{b}}$, where $\hat{\mathbf{b}}$ solves the nonlinear problem in the form

$$\hat{J}\hat{\mathbf{b}} = \hat{\mathbf{N}}(\hat{\mathbf{b}}), \quad \hat{J} = D_{\hat{\mathbf{A}}}\hat{\mathbf{F}}(\hat{\mathbf{A}}), \quad \hat{\mathbf{N}}(\hat{\mathbf{b}}) = \epsilon^{\tilde{r}} \hat{\mathbf{R}}(\hat{\mathbf{A}} + \hat{\mathbf{b}}) - [\hat{\mathbf{F}}(\hat{\mathbf{A}} + \hat{\mathbf{b}}) - \hat{J}\hat{\mathbf{b}}], \quad (5.2)$$

where $\hat{J}$ is a linearized operator, $\hat{\mathbf{F}}(\hat{\mathbf{A}} + \hat{\mathbf{b}}) - \hat{J}\hat{\mathbf{b}}$ is quadratic in $\hat{\mathbf{b}}$, and $\hat{\mathbf{R}}(\hat{\mathbf{A}} + \hat{\mathbf{b}})$ maps an element $L_q^1(\mathbb{R}^2)$ to itself. The kernel of the Jacobian operator $J = D_{\mathbf{A}}\mathbf{F}(\mathbf{A})$ is exactly three-dimensional, by the assumption, and it is generated by the two-dimensional group of translations in $y \in \mathbb{R}^2$ and a one-dimensional gauge invariance in $\arg(\mathbf{A})$. If Ω belongs to the interior of the band gap of the coupled-mode system, the continuous spectrum of $D_{\mathbf{A}}\mathbf{F}(\mathbf{A})$ is bounded away from zero and the triple zero eigenvalue is isolated from other eigenvalues of the discrete spectrum of $D_{\mathbf{A}}\mathbf{F}(\mathbf{A})$. The nonlinear elliptic problem (1.2) with a real-valued symmetric potential $V(x)$ admits the gauge invariance $\phi(x) \rightarrow e^{i\alpha}\phi(x)$ for any $\alpha \in \mathbb{R}$ and the reversibility symmetries (1.4) and (1.5). The extended coupled-mode system (4.10) obtained from the integral system (4.15) after the Lyapunov–Schmidt decomposition (4.17) and the scaling transformation (4.20) inherits all the symmetries, such that after restriction of $\mathbf{B}$ to functions satisfying (1.4) or (1.5) and after setting uniquely the phase, e.g. by $\mathbf{B}(0) \in \mathbb{R}$, system (5.2) is formulated in the orthogonal complement of the kernel of $\hat{J}$. Therefore, the linearized operator is continuously invertible for sufficiently small $\epsilon > 0$ under this restriction. By the Implicit Function Theorem, there exists a unique reversible solution in the form $\hat{\mathbf{b}} = \hat{J}^{-1}\hat{\mathbf{N}}(\hat{\mathbf{b}})$ such that $\|\hat{\mathbf{b}}\|_{L_q^1(\mathbb{R}^2, \mathbb{C}^3)} \leq C\epsilon^{\tilde{r}}$ for some $C > 0$ and any $q \geq 0$. This result implies the desired bound (5.1) for $\hat{B}_j$ as a solution of (4.10) on $p \in \mathbb{R}^2$.

Next, we consider the error between system (4.10) on the disk $p \in D_\epsilon$ and the same system on the plane $p \in \mathbb{R}^2$. The error comes from the terms $\|\hat{\mathbf{b}}\|_{L_{q+2}^1(D_\epsilon^\perp, \mathbb{C}^3)}$ and $\|\hat{\mathbf{b}}\|_{L_q^1(D_\epsilon^\perp, \mathbb{C}^3)}$, where $D_\epsilon^\perp = \mathbb{R}^2 \setminus D_\epsilon$, since $\hat{\mathbf{A}} \in L_q^1(\mathbb{R}^2, \mathbb{C}^2)$ for all $q \geq 0$ and the cubic nonlinear terms $\hat{\mathbf{N}}_j(\hat{\mathbf{b}})$ of the coupled-mode system (4.9) map elements of $L_q^1(\mathbb{R}^2)$ to elements of $L_q^1(\mathbb{R}^2)$. Since $\hat{\mathbf{b}} = \hat{J}^{-1}\hat{\mathbf{N}}(\hat{\mathbf{b}})$ and $\hat{J}^{-1}$ is a map from $L_q^1(\mathbb{R}^2, \mathbb{C}^3)$ to $L_{q+2}^1(\mathbb{R}^2, \mathbb{C}^3)$ for any $q \geq 0$, we obtain that

$$\forall \hat{\mathbf{b}} = \hat{J}^{-1}\hat{\mathbf{N}}(\hat{\mathbf{b}}) \in L_q^1(\mathbb{R}^2, \mathbb{C}^3) : \quad \|\hat{\mathbf{b}}\|_{L_{q+2}^1(D_\epsilon^\perp, \mathbb{C}^3)} \leq \|\hat{\mathbf{b}}\|_{L_{q+2}^1(\mathbb{R}^2, \mathbb{C}^3)} \leq C\|\hat{\mathbf{N}}(\hat{\mathbf{b}})\|_{L_q^1(\mathbb{R}^2, \mathbb{C}^3)} \leq \tilde{C}\epsilon^{\tilde{r}}$$

for some $C, \tilde{C} > 0$. Since $\|\hat{\mathbf{b}}\|_{L_q^1(D_\epsilon^\perp, \mathbb{C}^3)} \leq \|\hat{\mathbf{b}}\|_{L_q^1(\mathbb{R}^2, \mathbb{C}^3)} \leq C\epsilon^{\tilde{r}}$, the error between system (4.10) on the disk $p \in D_\epsilon$ and the same system on the plane $p \in \mathbb{R}^2$ is of the same order as the right-hand-side terms of system (4.10), such that the desired bound (5.1) holds on $p \in D_\epsilon$. $\square$

Corollary 2 *The solution $\Phi(x)$ constructed in Theorems 2 and 3 is a reversible localized solution of the bifurcation problem (2.7) satisfying one of the two constraints (1.4) and (1.5) on $x \in \mathbb{R}^2$.*

Proof. Since the modes $\Phi_{1,2,3}(x)$ of Lemma 2 and the solution $B_{1,2,3}(y)$ of Theorem 3 satisfy one of the two reversibility constraints (1.4) and (1.5), the leading-order part of the representation (4.17) produces a solution $\Phi(x)$ which satisfies the same constraint. Since the symmetry is also preserved in the integral equation (4.15), the map $\hat{\Psi}_\epsilon(\hat{U}_1, \hat{U}_2, \hat{U}_3)$ constructed in Theorem 2 inherits the symmetry and produces the remainder term in the decomposition (4.17) satisfying the same reversibility constraint. $\square$

There are several classes of localized reversible solutions of the differential coupled-mode equations which satisfy the assumptions of Theorem 3. These solutions are numerically approximated in Section 6. According to Theorem 3, all these solutions persist as localized reversible solutions of the nonlinear elliptic problem (1.2).

Corollary 3 *The solution $\Phi(x)$ constructed in Theorems 2 and 3 satisfy the bound:*

$$\|\Phi - A_1\Phi_1 - A_2\Phi_2 - A_3\Phi_3\|_{C_b^0(\mathbb{R}^2)} \leq C\epsilon^{\tilde{r}}, \quad \tilde{r} = \min(4r - 1, 1 - 2r), \quad (5.3)$$

where $\frac{1}{4} < r < \frac{1}{2}$. The fastest convergence rate is $\epsilon^{1/3}$, which is obtained at $r = \frac{1}{3}$. Consequently, the solution $\phi(x) = \sqrt{\epsilon}\Phi(x)$ of the nonlinear elliptic problem (1.2) is $\mathcal{O}(\epsilon^{\tilde{r}+1/2})$ accurate to the approximation $\phi^{(1)}(x) = \sqrt{\epsilon}(A_1\Phi_1 + A_2\Phi_2 + A_3\Phi_3)$, with the fastest convergence rate being $\epsilon^{5/6}$.

Proof. Using the triangle inequality and the bound (4.12), we obtain

$$\|\Phi - A_1\Phi_1 - A_2\Phi_2 - A_3\Phi_3\|_{C_b^0(\mathbb{R}^2)} \leq C_1\epsilon^{1-2r} + C_2 \sum_{j=1}^3 \|A_j - B_j\|_{C_b^0(\mathbb{R}^2)},$$

for some $C_1, C_2 > 0$. By the Hölder inequality we have

$$\|A_j - B_j\|_{C_b^0(\mathbb{R}^2)} \leq \|\hat{A}_j - \hat{B}_j\|_{L^1(\mathbb{R}^2)} = \|\hat{A}_j - \hat{B}_j\|_{L^1(D_\epsilon)} + \|\hat{A}_j\|_{L^1(\mathbb{R}^2 \setminus D_\epsilon)},$$

with the last equality due to a compact support of $\hat{B}_{1,2,3}(p)$ on $p \in D_\epsilon$. The first term in the upper bound is $\mathcal{O}(\epsilon^{\tilde{r}})$ by the bound (5.1) and the second term is smaller than any power of ϵ if $\hat{\mathbf{A}} \in L_q^1(\mathbb{R}^2, \mathbb{C}^3)$ for all $q \geq 0$. $\square$

6 Numerical approximations of localized reversible solutions

We approximate here several classes of localized reversible solutions of the differential coupled-mode system (4.6) numerically. We use the same potential as in the Examples 1–3, i.e. $W(x) = 1 - \cos(x)$ so that the bifurcation takes place for $\eta_0 \approx 0.1745$. For selected representative cases we also verify the convergence rate of Corollary 3 and the conditions of Theorem 3 on the Jacobian operator, which guarantees persistence of these solutions in the full system (1.2). We limit our attention to the following classes of reversible solutions:

- (A) defocusing case $\sigma = 1$: $A_1 = A_2 = 0$, $A_3 = R(r)e^{im\theta}$, $r = \frac{1}{\sqrt{\alpha_3}}\sqrt{y_1^2 + y_2^2}$, $\theta = \arg(y_1 + iy_2)$
 $m = 0 \dots$ radially symmetric positive soliton
 $m = 1 \dots$ vortex of charge one
- (B) focusing case $\sigma = -1$: $A_3 = 0$
- (i) $A_2 = 0$, $A_1 = R(r)e^{im\theta}$, $r = \sqrt{\frac{y_1^2}{\alpha_1} + \frac{y_2^2}{\alpha_2}}$, $\theta = \arg(\alpha_2 y_1 + i\alpha_1 y_2)$
 $m = 0 \dots$ ellipsoidal positive soliton
 $m = 1 \dots$ ellipsoidal vortex of charge one
- (ii) $A_1(y_1, y_2) = \pm A_2(y_2, y_1) \in \mathbb{R}$, $A_1(y_1, y_2) = A_1(-y_1, y_2) = A_1(y_1, -y_2)$
 $\dots$ symmetric real coupled soliton
- (iii) $A_1(y_1, y_2) = \pm i A_2(y_2, y_1) \in i\mathbb{R}$, $A_1(y_1, y_2) = A_1(-y_1, y_2) = A_1(y_1, -y_2)$
 $\dots \pi/2$ -phase delay coupled soliton
- (iv) $A_1(y_1, y_2) = \pm i \bar{A}_2(y_2, y_1) \in \mathbb{C}$, $A_1(y_1, y_2) = -\bar{A}_1(-y_1, y_2) = \bar{A}_1(y_1, -y_2)$
 $\dots$ coupled vortex of charge one

We will see that the localized solutions with $A_3 = 0$ bifurcate at $\sigma = -1$ from the upper edge $\Omega = \beta_1$ of the band gap and the localized solutions with $A_1 = A_2 = 0$ bifurcate at $\sigma = +1$ from the lower edge $\Omega = \beta_2$ of the band gap. All solutions above satisfy the reversibility condition of Definition 1. Provided the assumptions of Theorem 3 are satisfied, Corollary 2 then guarantees that these solutions correspond to reversible solutions of the nonlinear elliptic problem (1.2). Using the symmetries of ψ_1 , φ_1 and φ_2 , we can see that the function $\phi(x)$ satisfies the following symmetry:

- (A) $\phi(x_1, x_2) = \phi(-x_1, x_2) = \phi(x_1, -x_2) \in \mathbb{R}$ ($m = 0$)
 $\phi(x_1, x_2) = -\bar{\phi}(-x_1, x_2) = \bar{\phi}(x_1, -x_2) \in \mathbb{C}$ ($m = 1$)
- (B-i) $\phi(x_1, x_2) = \phi(-x_1, x_2) = -\phi(x_1, -x_2) \in \mathbb{R}$ ($m = 0$)
 $\phi(x_1, x_2) = -\bar{\phi}(-x_1, x_2) = -\bar{\phi}(x_1, -x_2) \in \mathbb{C}$ ($m = 1$)
- (B-ii) $\phi(x_1, x_2) = \pm \phi(x_2, x_1) = \mp \phi(-x_2, -x_1) \in \mathbb{R}$
- (B-iii) $\phi(x_1, x_2) = \pm i \bar{\phi}(x_2, x_1) = \mp i \bar{\phi}(-x_2, -x_1) \in \mathbb{C}$
- (B-iv) $\phi(x_1, x_2) = \pm i \bar{\phi}(x_2, x_1) = \pm i \bar{\phi}(-x_2, -x_1) \in \mathbb{C}$

Note that (B-iii) and (B-iv) agree with the reversibility constraint (1.5) after multiplication by $e^{-i\pi/4}$.

The above solutions do not include any three-component gap solitons with all A_1 , A_2 and A_3 nonzero. Such solutions do not bifurcate from either upper or lower edge $\Omega = \beta_1$ or $\Omega = \beta_2$, respectively, and it is thus hard to capture such solutions numerically. It is, nevertheless, possible that the three-component solitons still exist in the interior of the gap $\beta_2 < \Omega < \beta_1$ but we do not attempt here to locate these special solutions.

6.1 One-component solutions

One-component solutions correspond to classes (A) and (B-i). The function $R(r)$ for class (A) satisfies the ODE

$$R'' + \frac{1}{r}R' + (\Omega - \beta_2)R - \frac{m^2}{r^2}R - \sigma\gamma_4 R^3 = 0, \quad (6.1)$$

where $R(0) > 0$, $R'(0) = 0$ for $m = 0$ and $R(0) = 0$, $R'(0) > 0$ for $m = 1$. For $m \neq 0$ the initial-value problem for the ODE (6.1) is ill-posed but can be turned into a well-posed one via the transformation $Q = r^{-m}R(r)$ leading to

$$Q'' + \frac{2m+1}{r}Q' + (\Omega - \beta_2)Q - \sigma\gamma_4 r^{2m}Q^3 = 0, \quad (6.2)$$

with $Q(0) > 0$, such that $R(r) \sim r^{|m|}$ as $r \rightarrow 0$. Similarly, the function $R(r)$ for class (B-i) satisfies the ODE

$$R'' + \frac{1}{r}R' + (\Omega - \beta_1)R - \frac{m^2}{r^2}R - \sigma\gamma_1 R^3 = 0. \quad (6.3)$$

We solve these equations numerically via a shooting method searching for $R(r)$ vanishing at infinity as $r \rightarrow \infty$.

Figure 6 shows the solution families in the frequency-amplitude space for both solutions with $m = 0$ and $m = 1$. Class (A) families bifurcate from the lower edge $\Omega = \beta_2$ and class (B-i) families from the upper edge $\Omega = \beta_1$. Examples of the gap solitons ($m = 0$) are in Figure 7 and of the vortices ($m = 1$) in Figure 8. As expected, the class (A) solutions are radially symmetric and the class (B) solutions ellipsoidal.

For the case of one-component solutions, the coupled-mode equations reduce to a scalar two-dimensional NLS equation. Conditions of Theorem 3 on the kernel of the Jacobian operator are known to be satisfied for $m = 0$ [28] and, therefore, do not need to be checked numerically.

Figure 9 presents the computed ϵ -convergence of the error term $\phi(x) - \phi^{(1)}(x)$ described by Corollary 3 for the solution classes (A) and (B-i) with $m = 0$. The convergence rate is seen around $\epsilon^{1.07}$ and $\epsilon^{1.08}$, which is higher than the fastest convergence rate $\epsilon^{5/6}$ predicted by Corollary 3. The observed rate is close to ϵ^1 , which is the rate predicted by a formal multiple scales asymptotic expansion of $\phi(x)$, for which $\phi^{(1)}(x)$ is the leading order term.

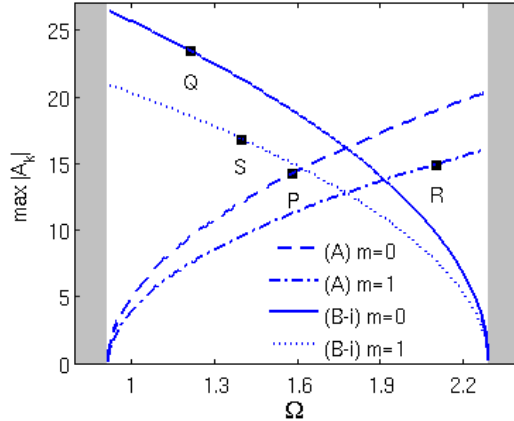


Figure 6: Continuation curves of one-component solutions (A) and (B-i). The marked points P, Q, R and S at $\Omega \approx 1.6, 1.22, 2.1$ and 1.4 correspond to the profiles in Fig. 7 and 8.

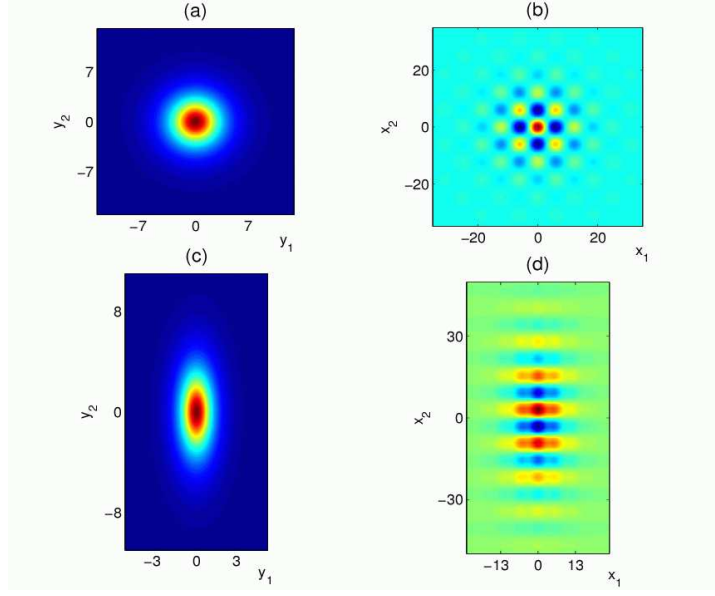


Figure 7: Profiles of the one-component real gap soliton ($m = 0$). (a) A_3 at point P in Fig. 6; (b) the corresponding leading-order term $A_3(y_1, y_2)\Phi_3(x_1, x_2)$ for $\epsilon = 0.1$; (c) A_1 at point Q in Fig. 6; (d) the corresponding leading-order term $A_1(y_1, y_2)\Phi_1(x_1, x_2)$ for $\epsilon = 0.02$.

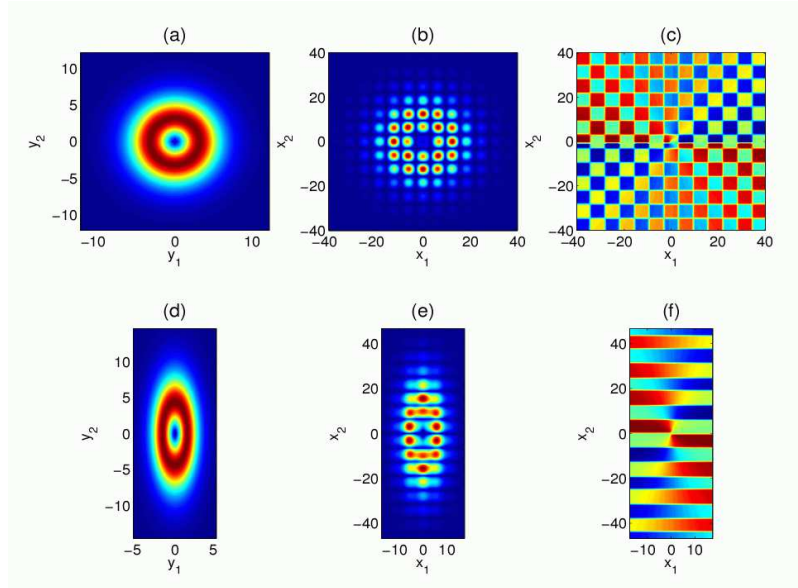


Figure 8: Profiles of the one-component vortex ($m = 1$). (a) $|A_3|$ at point R in Fig. 6; (b) and (c) the modulus and phase, respectively, of the corresponding leading-order term $A_3(y_1, y_2)\Phi_3(x_1, x_2)$ for $\epsilon = 0.1$; (d) $|A_1|$ at point S in Fig. 6; (e) and (f) the modulus and phase, respectively, of the corresponding leading-order term $A_1(y_1, y_2)\Phi_1(x_1, x_2)$ for $\epsilon = 0.1$.

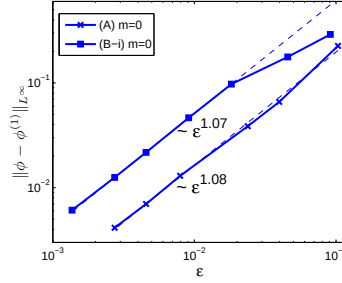


Figure 9: ϵ -convergence of the error term for the gap soliton ($m = 0$) corresponding to (A) at $\Omega \approx 1.22$ and (B-i) at $\Omega \approx 1.25$.

6.2 Two-component solutions

The following algorithm is used to compute two-component solutions of classes (B-ii), (B-iii) and (B-iv). First, α_1 and α_2 are replaced by $\bar{\alpha} = \frac{1}{2}(\alpha_1 + \alpha_2)$ so that the first two equations of the coupled-mode system (4.6) admit a reduction $A_1 = A_2$, where $A_1 = R(r)e^{im\theta}$ solves a one-component problem. The function $R(r)$ is then computed as in Section 6.1. Next, homotopy in the coefficients α_1 and α_2 is employed to gradually deform the computed solution with $\alpha_1 = \alpha_2 = \bar{\alpha}$ into the one with the original values of α_1 and α_2 . In this homotopy continuation the full coupled-mode system needs to be solved numerically and this is done via Newton's method on a central finite-difference discretization with zero Dirichlet boundary conditions.

Figure 10 shows the solution families of classes (B-ii), (B-iii) and (B-iv) as curves in the frequency-amplitude space. Profiles of examples of these solutions corresponding to the marked points in Figure 10 appear in Figures 11, 12 and 13. Note that the coupled vortex in Figure 13 has been obtained via the above described homotopy continuation from a vortex of charge one with $\alpha_1 = \alpha_2$. As the phase plots of A_1 and A_2 show, the resulting coupled vortex is also of charge one.

In order to verify the persistence conditions of Theorem 3 for the two-component solutions, the kernel of the Jacobian operator J has to be studied numerically. When rewritten in the real variables (for real and imaginary part) the first two equations of the coupled-mode system (4.6) give rise to a Jacobian operator J . For the cases (B-ii) and (B-iii), the Jacobian operator can be block-diagonalized to the form

$$\begin{pmatrix} J_+ & 0 \\ 0 & J_- \end{pmatrix}$$

such that $\dim(\text{Ker}(J)) = \dim(\text{Ker}(J_+)) + \dim(\text{Ker}(J_-))$. The elements of $\text{Ker}(J)$ can, moreover, be easily reconstructed from the elements of $\text{Ker}(J_+)$ and $\text{Ker}(J_-)$. This diagonalization reduces the expense of the eigenvalue solver.

Figure 14 shows the four smallest (in modulus) eigenvalues $\lambda_{J_1}, \dots, \lambda_{J_4}$ of the 4th order central finite-difference approximation of J for examples of solutions (B-ii) and (B-iii) as functions of D , where D is the size of the computational box $[-D, D] \times [-D, D] \subset \mathbb{R}^2$ with the step sizes $dy_1 = dy_2 \approx 0.14$ and with zero Dirichlet boundary conditions. Clearly, the three smallest eigenvalues converge to zero as D grows while the fourth eigenvalue converges to a nonzero value. Therefore, the assumptions of Theorem 3 are verified for these solutions. We have also checked that the corresponding eigenvectors of the three zero eigenvalues are approximations of $\partial_{y_1} \mathbf{A}$, $\partial_{y_2} \mathbf{A}$ and $i\mathbf{A}$.

For the case (B-iv) the Jacobian operator J has to be treated in full because it cannot be block-diagonalized for complex-valued solutions. Figure 15 shows the four smallest eigenvalues of the discretized Jacobian operator for an example of the solution (B-iv). The fourth-order central finite-difference discretization was used once again with the step sizes $dy_1 = dy_2 \approx 0.12$. The fourth eigenvalue λ_{J_4} converges approximately to 0.005 as D grows, while the second and third eigenvalues $\lambda_{J_{2,3}}$ converge to 0.0002. We have checked that the limit of $\lambda_{J_{2,3}}$ decreases as $dy_1 = dy_2$ is decreased while the limit of λ_{J_4} remains practically unchanged.

Finally, Figure 16 verifies the ϵ -convergence of the error term $\phi(x) - \phi^{(1)}(x)$ described by Corollary 3 for the gap soliton of class (B-ii) at $\Omega \approx 0.944$. The observed convergence rate is $\epsilon^{0.95}$, which is, once again, close to ϵ^1 expected from the formal asymptotic expansion. The ϵ -convergence has not been checked for any complex-valued solutions of classes (B-iii) and (B-iv) due to four times larger memory requirements compared to the real case. The memory use grows rapidly as ϵ decreases since domains of the size $(2D/\sqrt{\epsilon}) \times (2D/\sqrt{\epsilon})$ need to be discretized to compute the solution $\phi(x)$ of the elliptic problem (1.2) and each period $[0, 2\pi] \times [0, 2\pi]$ of the potential function $V(x)$ requires about 100 grid points.

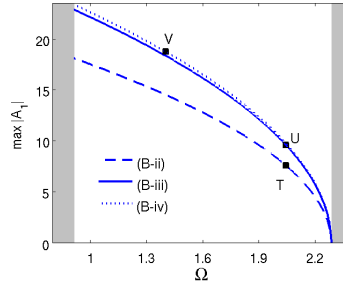


Figure 10: Continuation curves of two-component solutions (B-ii), (B-iii) and (B-iv). The marked points T and U at $\Omega \approx 2.04$ correspond to the profiles in Figs. 11 and 12, while the point V at $\Omega \approx 1.4$ corresponds to the profiles in Fig. 13.

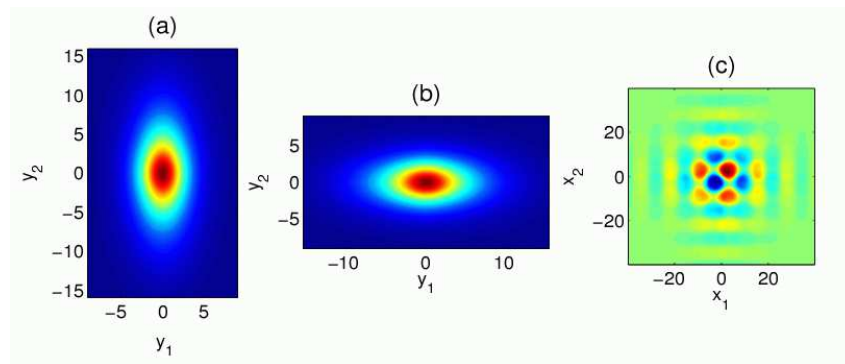


Figure 11: Two-component real gap soliton (B-ii) at point T in Fig. 10. (a) A_1 ; (b) A_2 ; (c) the leading-order term $A_1(y_1, y_2)\Phi_1(x_1, x_2) + A_2(y_1, y_2)\Phi_2(x_1, x_2)$ for $\epsilon = 0.1$.

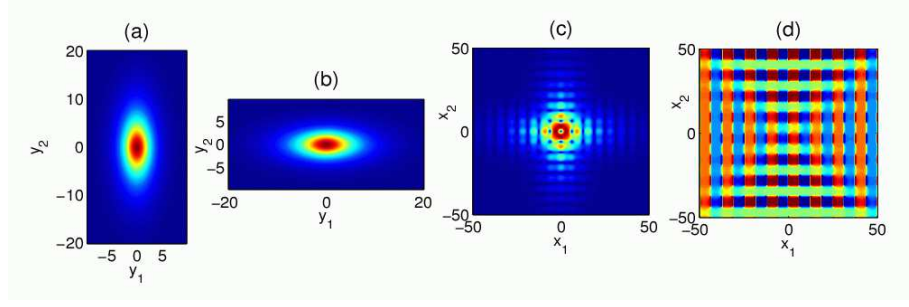


Figure 12: Two-component $\pi/2$ -phase delay gap soliton (B-iii) at point U in Fig. 10. (a) A_1 ; (b) $-iA_2$; (c) and (d) modulus and phase, respectively, of the leading-order term $A_1(y_1, y_2)\Phi_1(x_1, x_2) + A_2(y_1, y_2)\Phi_2(x_1, x_2)$ for $\epsilon = 0.1$.

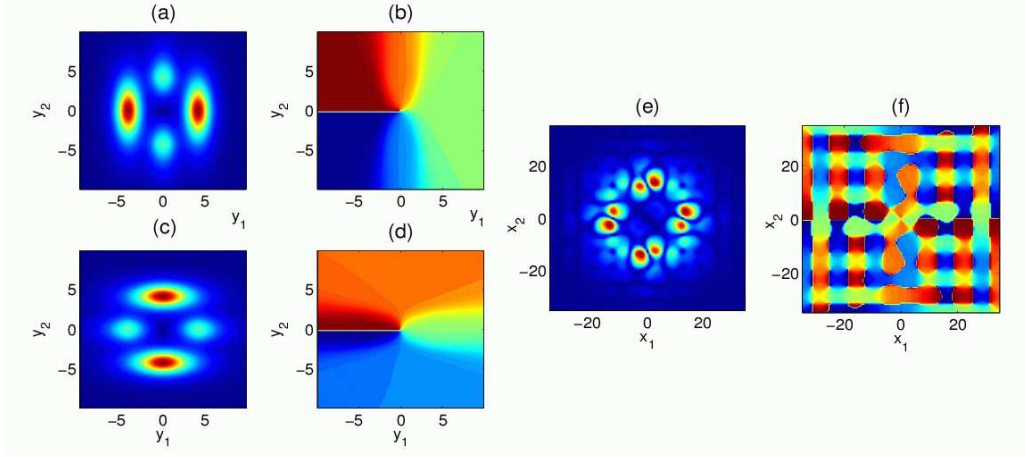


Figure 13: Two-component vortex (B-iv) at point V in Fig. 10. (a) and (b) modulus and phase of A_1 ; (c) and (d) modulus and phase of A_2 ; (e) and (f) modulus and phase of the leading-order term $A_1(y_1, y_2)\Phi_1(x_1, x_2) + A_2(y_1, y_2)\Phi_2(x_1, x_2)$ for $\epsilon = 0.1$.

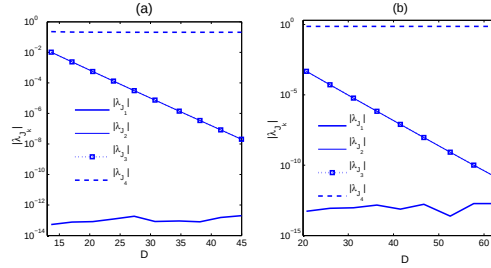


Figure 14: The four smallest eigenvalues of the Jacobian operator J for (a) the two-component real gap soliton (B-ii) and (b) the two-component $\pi/2$ -phase delay gap soliton (B-iii) for $\Omega \approx 1.19$.

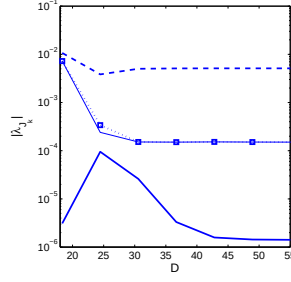


Figure 15: The four smallest eigenvalues of the Jacobian operator J for the two-component vortex (B-iv) at $\Omega \approx 1.2$.

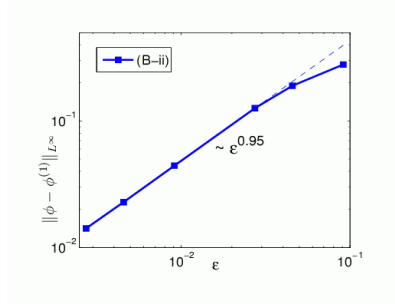


Figure 16: ϵ -convergence of the error term for the gap soliton (B-ii) with $\Omega \approx 0.94$.

7 The time-dependent case

We show here that dynamics of non-stationary localized solutions of the Gross–Pitaevskii equation (1.1) are close to the dynamics of the time-dependent coupled-mode equations for finite time intervals. These results are similar to the ones in [7, 24] and they give a rigorous basis for formal asymptotic results in [6, 25]. According to a formal asymptotic multiple scales expansion, solutions of the Gross–Pitaevskii equation (1.1) in the form

$$E_{\text{ans}}(x, t) = \sqrt{\epsilon} E_1(x, t) + \mathcal{O}(\epsilon),$$

where

$$E_1 = [A_1(\sqrt{\epsilon}x, \epsilon t)\psi_1(x_1)\varphi_2(x_2) + A_2(\sqrt{\epsilon}x, \epsilon t)\varphi_2(x_1)\psi_1(x_2) + A_3(\sqrt{\epsilon}x, \epsilon t)\varphi_1(x_1)\varphi_1(x_2)] e^{i\omega_0 t},$$

are approximated by solutions of the time-dependent coupled-mode equations

$$\begin{cases} (i\partial_T - \beta_1)A_1 + (\alpha_1\partial_{y_1}^2 + \alpha_2\partial_{y_2}^2)A_1 &= \sigma [\gamma_1|A_1|^2A_1 + \gamma_2(2|A_2|^2A_1 + A_2^2\bar{A}_1) + \gamma_3(2|A_3|^2A_1 + A_3^2\bar{A}_1)], \\ (i\partial_T - \beta_1)A_2 + (\alpha_2\partial_{y_1}^2 + \alpha_1\partial_{y_2}^2)A_2 &= \sigma [\gamma_1|A_2|^2A_2 + \gamma_2(2|A_1|^2A_2 + A_1^2\bar{A}_2) + \gamma_3(2|A_3|^2A_2 + A_3^2\bar{A}_2)], \\ (i\partial_T - \beta_2)A_3 + \alpha_3(\partial_{y_1}^2 + \partial_{y_2}^2)A_3 &= \sigma [\gamma_4|A_3|^2A_3 + 2\gamma_3(|A_1|^2 + |A_2|^2)A_3 + \gamma_3(A_1^2 + A_2^2)\bar{A}_3], \end{cases} \quad (7.1)$$

where $y = \sqrt{\epsilon}x$ and $T = \epsilon t$. Under the non-resonance condition

$$\inf_{\substack{(n_1, n_2) \in \mathbb{N}^2 \\ j_1, j_2, j_3 \in \{\pm 5, \pm 3, \pm 1\}}} \left| \rho_{n_1} \left(\frac{j_2 + j_3}{2} \right) + \rho_{n_2} \left(\frac{j_1 + j_3}{2} \right) - |j_1 + j_2 + j_3|\omega_0 \right| > 0, \quad (7.2)$$

where $|j_1 + j_2 + j_3| \leq 5$ and the infimum does not include direct resonances that give the nonlinear terms in system (7.1), the following theorem states the approximation result on the time-dependent solutions.

Theorem 4 *Let $s > 1, s_* \geq \max\{3, s\}$, and assume that the non-resonance condition (7.2) holds. Then for all C_1 and $T_0 > 0$ there exist $\epsilon_0 > 0$ and $C_2 > 0$ such that for all solutions $A_1, A_2, A_3 \in C([0, T_0], H^{s_*}(\mathbb{R}^2))$ of the time-dependent coupled-mode system with*

$$\sup_{T \in [0, T_0]} \|\mathbf{A}(\cdot, T)\|_{H^{s_*}(\mathbb{R}^2)} \leq C_1,$$

there exist solutions $E \in C([0, T_0/\epsilon], H^s(\mathbb{R}^2))$ of the Gross–Pitaevskii equation (1.1) with

$$\sup_{t \in [0, T_0/\epsilon]} \|E(\cdot, t) - E_{\text{ans}}(\cdot, t)\|_{H^s(\mathbb{R}^2)} \leq C_2 \epsilon^{3/2}.$$

for all $\epsilon \in (0, \epsilon_0)$.

Proof. The proof is very similar to the one given for a scalar nonlinear Schrödinger equation in the one-dimensional case in [7]. The non-resonance condition (7.2) differs from [7, Eq.(4)] by including the terms with $j_1, j_2, j_3 = \pm 5$. This is necessary to make the residual formally of order $\mathcal{O}(\epsilon^3)$. Due to the fact that we are working here on $x \in \mathbb{R}^2$, we lose $\epsilon^{-1/2}$ due to the scaling of the L^2 -norm in contrast to [7], where we would only lose $\epsilon^{-1/4}$ on $x \in \mathbb{R}$ with the same scaling. Assuming that the non-resonance condition (7.2) is satisfied, the $\mathcal{O}(\epsilon)$ terms in E_{ans} can be chosen in such a way that all terms up to order $\mathcal{O}(\epsilon^{5/2})$ in the residual

$$\text{Res}(E_{\text{ans}}) = -iE_t - \nabla^2 E + V(x)E + \sigma|E|^2 E$$

can be eliminated. By [7, Lemma 3.3] Bloch transform is an isomorphism between $H^s(\mathbb{R}^2)$ and $l_s^2(\mathbb{N}^2, L^2(\mathbb{T}^2))$. Hence, similarly to [7, Lemma 3.4] the nonlinearity $E \mapsto |E|^2 E$ maps $l_s^2(\mathbb{N}^2, L^2(\mathbb{T}^2))$ in Bloch space, or $H^s(\mathbb{R}^2)$ in physical space, into itself for $s > 1$ due to Sobolev’s embedding theorem in two dimensions. Moreover, $L = -\nabla^2 + V(x)$ generates a uniformly bounded semigroup in $l_s^2(\mathbb{N}^2, L^2(\mathbb{T}^2))$, or respectively in $H^s(\mathbb{R}^2)$, according to [7, page 927]. Hence, the error function $R = \epsilon^{-3/2}(E - E_{\text{ans}})$ satisfies an equation of the form

$$\partial_t R = LR + \mathcal{O}(\epsilon).$$

Using the variation of constant formula and Gronwall’s inequality gives the required $\mathcal{O}(1)$ bound for R . For more details see [7, Section 4.2]. $\square$

8 Various generalizations

We have given a detailed justification of the three coupled-mode equations which describe gap solitons bifurcating in the first band gap of a two-dimensional separable periodic potential. These equations are generic (structurally stable) for the considered bifurcation but they can be modified for other relevant bifurcation problems. We review here several examples of other bifurcations, where the justification analysis is expected to be applicable in a similar manner.

Bifurcations from band edges. If the band edge separates the existing band gap of finite length and a single or double-degenerate spectral band, the coupled-mode equations persist without any modifications. A formal derivation is given in the recent paper [25], where a scalar NLS equation is derived for a single

band and two coupled NLS equations are derived for a double band. Note that the coupled NLS equations for a double band may have terms destroying the reduction $A_1 = 0$ or $A_2 = 0$ in the truncated system of equations. This happens, for instance, at the band edge E in the second band gap of a separable symmetric potential [25]. Since the analysis of separable potentials relies on the construction of one-dimensional Bloch modes and one-dimensional spectral bands, the same analysis is valid for bifurcations from band edges in one-dimensional problems. The formal derivation of the NLS equation for a band edge of a single spectral band in the one-dimensional GP equation was reported in [22].

Bifurcations in the higher-order band gaps. With larger values of the parameter η in the separable potential (1.3), more band gaps open, although the number of band gaps is always finite for finite η , see Theorem 6.10.5 in [10]. Since the bifurcation of new band gaps occurs due to the resonance of finitely many Bloch modes in the separable potential, a system of finitely-many coupled-mode equations can be derived similarly in the higher-order band gaps. For instance, the bifurcation of the second band gap in the symmetric separable potential may occur for a resonance of either three modes when $\lambda_2 + \mu_1 = 2\mu_2 < \lambda_1 + \lambda_3$ or four modes when $\lambda_2 + \mu_1 = \lambda_1 + \lambda_3 > 2\mu_2$ or five modes when $\lambda_2 + \mu_1 = \lambda_1 + \lambda_3 = 2\mu_2$.

Bifurcations in asymmetric separable potentials. If the separable potential is asymmetric, such that

$$V(x) = \eta (W_1(x_1) + W_2(x_2)),$$

where W_1 and W_2 are two different functions on $x \in \mathbb{R}$, the degeneracy of spectral bands is broken and bifurcations of the band gaps occur with a smaller number of resonant Bloch modes. Our analysis remains valid but the spectrum of two different one-dimensional Sturm–Liouville problems must be incorporated in the Fourier–Bloch decomposition. In this case, two coupled-mode equations occur generally for the bifurcation of the first band gap in the anisotropic separable potential.

Bifurcations in finite-gap potentials. Finite-gap potentials lead to the degeneracy of eigenvalues of the one-dimensional Sturm–Liouville problem and non-zero derivatives of the functions $\rho_n(k)$ at the extremal points $k = 0$ and $k = \pm \frac{1}{2}$. Adding a generic potential breaks the symmetry of the finite-gap potential and leads to the bifurcation of narrow band gaps in the space of one dimension. The corresponding coupled-mode equations must have first-order than second-order derivative operators. A formal derivation of such coupled-mode equations from the Bloch mode decomposition was considered in [9]. Our analysis provides a rigorous justification of these coupled-mode equations.

Bifurcation in super-lattices. Let the potential $V(x)$ be represented in the form

$$V(x) = \eta_0 (W(x_1) + W(x_2)) + \epsilon (\tilde{W}(x_1) + \tilde{W}(x_2)),$$

where $W(x)$ and η_0 are the same as in the separable potential (1.3) and $\tilde{W}(x)$ is a 4π -periodic potential. The perturbation term $\tilde{W}(x)$ couples resonant Bloch modes of the potential $W(x)$ by linear terms and destroys reductions $A_1 = 0$, $A_2 = 0$ and $A_3 = 0$ in the differential coupled-mode system. The system is still formulated in the form of the coupled NLS equations with various (linear and nonlinear) coupling terms.

Bifurcations in three-dimensional periodic problems. The same analysis holds in three-dimensional separable potentials, since the spectral bands are still enumerated by a countable number of spectral bands of the one-dimensional potentials. Bifurcations of new band gaps occur again due to a resonance of finitely many Bloch modes of the one-dimensional potentials.

Bifurcations in non-separable periodic potentials. At the present time, the generalization of the analysis for non-separable periodic potentials meets a technical obstacle that the bound (3.7) obtained in [7] is needed to be extended to problems with two-dimensional periodic potentials.

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