

# Edge States in Honeycomb Structures

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**Abstract** An edge state is a time-harmonic solution of a conservative wave system, e.g. Schrödinger, Maxwell, which is propagating (plane-wave-like) parallel to, and localized transverse to, a line-defect or “edge”. Topologically protected edge states are edge states which are stable against spatially localized (even strong) deformations of the edge. First studied in the context of the quantum Hall effect, protected edge states have attracted huge interest due to their role in the field of topological insulators. Theoretical understanding of topological protection has mainly come from discrete (tight-binding) models and direct numerical simulation. In this paper we consider a rich family of continuum PDE models for which we rigorously study regimes where topologically protected edge states exist. Our model is a class of Schrödinger operators on  $\mathbb{R}^2$  with a background two-dimensional honeycomb potential perturbed by an “edge-potential”. The edge potential is a domain-wall interpolation, transverse to a prescribed “rational” edge, between two distinct periodic structures. General conditions are given for the bifurcation of a branch of topologically protected edge states from *Dirac points* of the background honeycomb structure. The bifurcation is seeded

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by the zero mode of a one-dimensional effective Dirac operator. A key condition is a spectral no-fold condition for the prescribed edge. We then use this result to prove the existence of topologically protected edge states along zigzag edges of certain honeycomb structures. Our results are consistent with the physics literature and appear to be the first rigorous results on the existence of topologically protected edge states for continuum 2D PDE systems describing waves in a non-trivial periodic medium. We also show that the family of Hamiltonians we study contains cases where zigzag edge states exist, but which are not topologically protected.

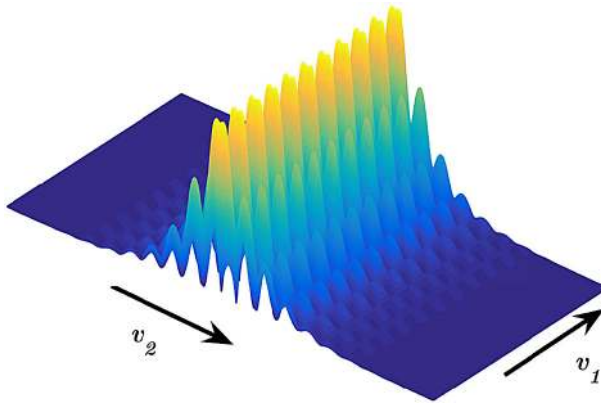
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**Mathematics Subject Classification** Primary 35J10 · 35B32; Secondary 35P · 35Q41 · 37G40

## 1 Introduction and Outline

This paper is motivated by a remarkable physical observation. When two distinct 2-dimensional materials with favorable crystalline structures are joined along an edge, there exist propagating modes, *e.g.* electronic or photonic, whose energy remains localized in a neighborhood of the edge without spreading into the “bulk”. Furthermore, these modes and their properties persist in the presence of arbitrary local, even large, perturbations of the edge. An understanding of such “protected edge states” in periodic structures has so far mainly been obtained by analyzing discrete “tight-binding” models and from numerical simulations. In this paper we prove that edge states arise from the Schrödinger equation for a class of potentials that have many features (not all) in common with the relevant experiments. A central role is played by a spectral “no-fold” condition. In the case of small amplitude (low-contrast) honeycomb potentials, this reduces to a sign condition of a particular Fourier coefficient of the potential. A combination of numerical simulation and heuristic argument suggests that if the “no-fold” condition fails, then edge states need not be topologically protected. Let us explain these ideas in more detail.

Wave transport in periodic structures with honeycomb symmetry has been an area of intense activity catalyzed by the study of graphene, a single atomic layer two-dimensional honeycomb structure of carbon atoms. The remarkable electronic properties exhibited by graphene [14, 21, 30, 44] have inspired the study of waves in general honeycomb structures or “artificial graphene” in electronic [35] and photonic [1, 17, 26, 29, 32] contexts. One such property, observed in electronic and photonic systems with honeycomb symmetry is the existence of topologically protected *edge states*. Edge states are modes which are (i) pseudo-periodic (plane-wave-like or propagating) parallel to a line-defect, and (ii) localized transverse to the line-defect; see Figure 1. *Topological protection* refers to the persistence of these modes and their properties, even when the line-defect is subjected to strong local or random perturbations. In applications, edge states are of great interest due to their potential as robust vehicles for channeling energy.



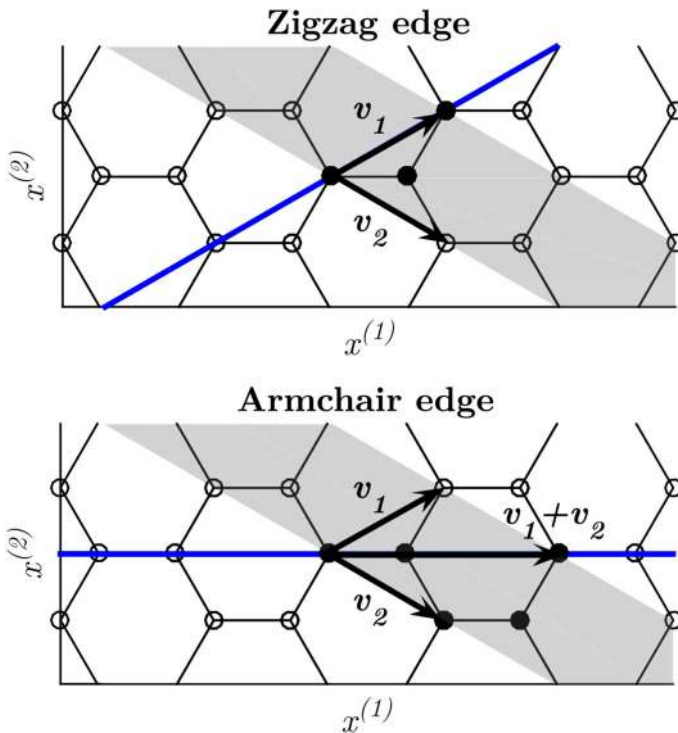
**Fig. 1** Edge state – propagating (plane-wave like) parallel to a zigzag edge ( $\mathbb{R}\mathbf{v}_1$ ) and localized transverse to the edge

The extensive physics literature on topologically robust edge states goes back to investigations of the quantum Hall effect; see, for example, [18, 19, 39, 42] and the rigorous mathematical articles [5, 6, 28, 38]. In [17, 32] a proposal for realizing *photonic edge states* in periodic electromagnetic structures which exhibit the magneto-optic effect was made. In this case, the edge is realized via a domain wall across which the Faraday axis is reversed. Since the magneto-optic effect breaks time-reversal symmetry, as does the magnetic field in the Hall effect, the resulting edge states are unidirectional.

Other realizations of edges in photonic and electromagnetic systems, *e.g.* between periodic dielectric and conducting structures, between periodic structures and free-space, have been explored through experiment and numerical simulation; see, for example [22, 27, 33, 41, 43]. In the context of tight-binding models, the existence and robustness of edge states has been related to topological invariants (Chern index or Berry/Zak phase) associated with the “bulk” (infinite periodic honeycomb) band-structure.

We are interested in exploring these phenomena in general energy-conserving wave equations in continuous media. We consider the case of the Schrödinger equation on  $\mathbb{R}^2$ ,  $i\partial_t\psi = H\psi$ , and study the existence and robustness of edge states of time-harmonic form:  $\psi = e^{-iEt}\Psi$ . Our model consists of a honeycomb background potential, the “bulk” structure, and a perturbing “edge-potential”. The edge-potential interpolates between two distinct asymptotic periodic structures, via a *domain wall* which varies transverse to a specified line-defect (“edge”) in the direction of some element of the period lattice,  $\Lambda_h$ . In the context of honeycomb structures, the most frequently studied edges are the “zigzag” and “armchair” edges; see Figure 2.

Our model of an edge is motivated by the domain-wall construction of [17, 32]. A difference is that we break spatial-inversion symmetry, while preserving time-reversal symmetry. Hence, the edge states – though topologically robust – may travel in either direction along the edge. In [7, 10] we proved that a one-dimensional variant of such edge-potentials gives rise to topologically protected edge states in periodic structures



**Fig. 2** Bulk honeycomb structure,  $\mathbf{H} = (\mathbf{A} + \Lambda_h) \cup (\mathbf{B} + \Lambda_h)$ . **Top panel:** Zigzag edge (blue line),  $\mathbb{R}v_1 = \{\mathbf{x} : \mathbf{k}_2 \cdot \mathbf{x} = 0\}$ . Shaded region is the fundamental domain of the cylinder,  $\Sigma_{ZZ}$ , corresponding to the zigzag edge. **Bottom panel:** Armchair edge (blue line),  $\mathbb{R}(v_1 + v_2) = \{\mathbf{x} : (\mathbf{k}_1 - \mathbf{k}_2) \cdot \mathbf{x} = 0\}$ . Fundamental domain of the cylinder,  $\Sigma_{AC}$ , corresponding to the armchair edge, also indicated. (Darkened vertices are sites at which zero-boundary conditions are imposed in tight-binding models of “hard” edges.)

with symmetry-induced linear band crossings, the analogue in one space dimension of Dirac points (see below). We explore a photonic realization of such states in coupled waveguide arrays in [25].

Our goal is to clarify the underlying mechanisms for the existence of topologically protected edge states. In Theorem 7.3 we give general conditions for a topologically protected bifurcation of edge states from *Dirac points* of the background (bulk) honeycomb structure. The bifurcation is seeded by the robust zero mode of a one-dimensional effective Dirac equation. A key hypothesis is a *spectral no-fold condition* for the prescribed edge, assumed to be a *rational edge*. In one-dimensional continuum models [10], this condition is a consequence of monotonicity properties of dispersion curves. For continuous  $d$ -dimensional structures, with  $d \geq 2$ , the spectral no-fold condition may or may not hold; see Section 8. Moreover, by varying a parameter, such as the lattice scale of a periodic structure, one can continuously tune between cases where the condition holds or does not hold; see Appendix A. In Theorem 8.2 and Theorem 8.5 we verify the spectral no-fold condition for the zigzag edge, for a family of Hamiltonians with weak (low-contrast) potentials, and obtain the existence of *zigzag edge states* in this setting.

In a forthcoming article [9], we study the strong binding regime (deep potentials) for a large class of honeycomb Schrödinger operators. We prove that the two lowest energy dispersion surfaces, after a rescaling by the potential well's depth, converge uniformly to those of the celebrated Wallace (1947) [40] tight-binding model of graphite. A corollary of this result is that the spectral no-fold condition, as stated in the present article, is satisfied for sufficiently deep potentials (high contrast) for a very large classes of edge directions in  $\Lambda_h$  (including the zigzag edge). In fact, we believe that the analysis of the present article can be extended and together with [9] will yield the existence of edge states which are localized, transverse to *arbitrary* edge directions  $\mathbf{v}_1 \in \Lambda_h$ . This is work in progress. For a detailed discussion of examples and motivating numerical simulations, see [8].

The types of edge states which exist for edges generated by domain walls stand in contrast to those which exist in the case of “hard edges”, *i.e.* edges defined by the tight-binding bulk Hamiltonian on one side of an edge with Dirichlet (zero) boundary condition imposed on the edge; see parenthetical remark in Figure 2. In this case, it is well-known that zigzag (hard) edges support edge states, while armchair (hard) edges do not support edge states; see, for example, [15].

Finally, we believe that failure of the spectral no-fold condition implies that there are no topologically protected edge states, although there is evidence that there are meta-stable edge states, which are localized near the edge for a long time; see Section 1.4.

## 1.1 Detailed Discussion of Main Results

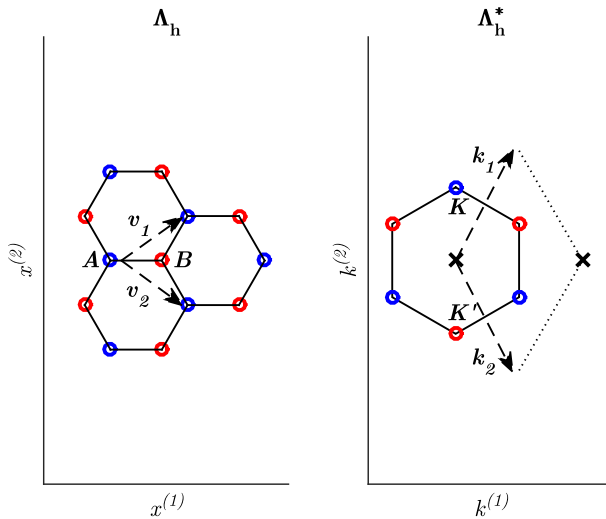
Let  $\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$  denote the regular (equilateral) triangular lattice and  $\Lambda_h^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2$  denote the associated dual lattice, with relations  $\mathbf{k}_l \cdot \mathbf{v}_m = 2\pi\delta_{lm}$ ,  $l, m = 1, 2$ . The expressions for  $\mathbf{k}_l$  and  $\mathbf{v}_m$  are displayed in Section 2.3. The honeycomb structure,  $\mathbf{H}$ , is the union of two interpenetrating triangular lattices:  $\mathbf{A} + \Lambda_h$  and  $\mathbf{B} + \Lambda_h$ ; see Figures 2 and 3.

A *honeycomb lattice potential*,  $V(\mathbf{x})$ , is a real-valued, smooth function, which is  $\Lambda_h$ -periodic and, relative to some origin of coordinates, inversion symmetric (even) and invariant under a  $2\pi/3$  rotation; see Definition 2.4. A choice of period cell is  $\Omega_h$ , the parallelogram in  $\mathbb{R}^2$  spanned by  $\{\mathbf{v}_1, \mathbf{v}_2\}$ .

We begin with the Hamiltonian for the unperturbed honeycomb structure:

$$H^{(0)} = -\Delta + V(\mathbf{x}).$$

The *band structure* of the  $\Lambda_h$ -periodic Schrödinger operator,  $H^{(0)}$ , is obtained by considering the family of eigenvalue problems, parametrized by  $\mathbf{k} \in \mathcal{B}_h$ , the Brillouin zone:  $(H^{(0)} - E)\Psi = 0$ ,  $\Psi(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{k}\cdot\mathbf{v}}\Psi(\mathbf{x})$ ,  $\mathbf{x} \in \mathbb{R}^2$ ,  $\mathbf{v} \in \Lambda_h$ . Equivalently,  $\psi(\mathbf{x}) = e^{-i\mathbf{k}\cdot\mathbf{x}}\Psi(\mathbf{x})$ , satisfies the periodic eigenvalue problem:  $(H^{(0)}(\mathbf{k}) - E(\mathbf{k}))\psi = 0$  and  $\psi(\mathbf{x} + \mathbf{v}) = \psi(\mathbf{x})$  for all  $\mathbf{x} \in \mathbb{R}^2$  and  $\mathbf{v} \in \Lambda_h$ , where  $H^{(0)}(\mathbf{k}) = -(\nabla + i\mathbf{k})^2 + V(\mathbf{x})$ . For each  $\mathbf{k} \in \mathcal{B}_h$ , the spectrum is real and consists of discrete eigenvalues  $E_b(\mathbf{k})$ ,  $b \geq 1$ , where  $E_j(\mathbf{k}) \leq E_{j+1}(\mathbf{k})$ . The maps  $\mathbf{k} \mapsto E_b(\mathbf{k}) \in \mathbb{R}$  are called the dispersion surfaces of  $H^{(0)}$ . The collection of these sur-



**Fig. 3** **Left panel:**  $\mathbf{A} = (0, 0)$ ,  $\mathbf{B} = (\frac{1}{\sqrt{3}}, 0)$ . The honeycomb structure,  $\mathbf{H}$  is the union of two interpenetrating sublattices:  $\Lambda_{\mathbf{A}} = \mathbf{A} + \Lambda_h$  (blue) and  $\Lambda_{\mathbf{B}} = \mathbf{B} + \Lambda_h$  (red). The lattice vectors  $\{\mathbf{v}_1, \mathbf{v}_2\}$  generate  $\Lambda_h$ . Colors designate sublattices; in graphene the atoms occupying  $\Lambda_{\mathbf{A}}$ - and  $\Lambda_{\mathbf{B}}$ - sites are identical. **Right panel:** Brillouin zone,  $\mathcal{B}_h$ , and dual basis  $\{\mathbf{k}_1, \mathbf{k}_2\}$ .  $\mathbf{K}$  and  $\mathbf{K}'$  are labeled. Other vertices of  $\mathcal{B}_h$  obtained via application of  $R$ , a rotation by  $2\pi/3$ .

faces constitutes the *band structure* of  $H^{(0)}$ . As  $\mathbf{k}$  varies over  $\mathcal{B}_h$ , each map  $\mathbf{k} \rightarrow E_b(\mathbf{k})$  is Lipschitz continuous and sweeps out a closed interval in  $\mathbb{R}$ . The union of these intervals is the  $L^2(\mathbb{R}^2)$ - spectrum of  $H^{(0)}$ . A more detailed discussion is presented in Section 2.

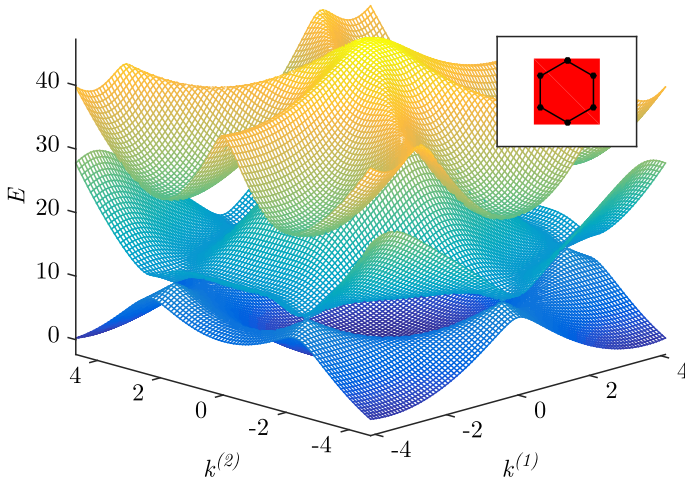
A central role is played by the *Dirac points* of  $H^{(0)}$ . These are quasi-momentum / energy pairs,  $(\mathbf{K}_\star, E_\star)$ , in the band structure of  $H^{(0)}$  at which neighboring dispersion surfaces touch conically at a point [11, 21, 30]. The existence of Dirac points, located at the six vertices of the Brillouin zone,  $\mathcal{B}_h$  (regular hexagonal dual period cell) for generic honeycomb structures was proved in [10, 11]; see also [2, 16]. The quasi-momenta of Dirac points partition into two equivalence classes; the  $\mathbf{K}$ - points consisting of  $\mathbf{K}$ ,  $R\mathbf{K}$  and  $R^2\mathbf{K}$ , where  $R$  is a rotation by  $2\pi/3$  and  $\mathbf{K}'$ - points consisting of  $\mathbf{K}' = -\mathbf{K}$ ,  $R\mathbf{K}'$  and  $R^2\mathbf{K}'$ . The time evolution of a wavepacket, with data spectrally localized near a Dirac point, is governed by a massless two-dimensional Dirac system [12].

Figure 4 displays the first three dispersion surfaces of  $H^{(0)}$  for a honeycomb potential. The lowest two of these surfaces touch conically at the six vertices of  $\mathcal{B}_h$  (inset). Associated with the Dirac point  $(\mathbf{K}_\star, E_\star)$  is a two-dimensional eigenspace of  $\mathbf{K}_\star$ -pseudo-periodic states,  $\text{span}\{\Phi_1, \Phi_2\}$ :

$$H^{(0)}\Phi_j(\mathbf{x}) = E_\star\Phi_j(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^2, \quad j = 1, 2,$$

$$\text{where } \Phi_j(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{K}_\star \cdot \mathbf{v}}\Phi_j(\mathbf{x}), \quad \mathbf{v} \in \Lambda_h;$$

see Definition 3.1. It is also shown in [11] that a  $\Lambda_h$ - periodic perturbation of  $V(\mathbf{x})$ , which breaks inversion or time-reversal symmetry lifts the eigenvalue degeneracy; a



**Fig. 4** Lowest three dispersion surfaces  $\mathbf{k} \equiv (k^{(1)}, k^{(2)}) \in \mathcal{B}_h \mapsto E(\mathbf{k})$  of the band structure of  $H^{(0)} \equiv -\Delta + V(\mathbf{x})$ , where  $V$  is the honeycomb potential:  $V(\mathbf{x}) = 10(\cos(\mathbf{k}_1 \cdot \mathbf{x}) + \cos(\mathbf{k}_2 \cdot \mathbf{x}) + \cos((\mathbf{k}_1 + \mathbf{k}_2) \cdot \mathbf{x}))$ . Dirac points occur at the intersection of the lower two dispersion surfaces, at the six vertices of the Brillouin zone,  $\mathcal{B}_h$ .

(local) gap is opened about the Dirac points and the perturbed dispersion surfaces are locally smooth. The perturbation of  $H^{(0)}$  by an edge potential (see (1.1)) takes advantage of this instability of Dirac points with symmetry breaking perturbations.

To construct our Hamiltonian, perturbed by an edge-potential, we first choose a vector  $\mathbf{v}_1 \in \Lambda_h$ , the period lattice, and consider the line  $\mathbb{R}\mathbf{v}_1$ , the “edge”. Choose  $\mathbf{v}_2$  such that  $\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$ . Also introduce dual basis vectors,  $\mathfrak{R}_1$  and  $\mathfrak{R}_2$ , satisfying  $\mathfrak{R}_l \cdot \mathbf{v}_m = 2\pi\delta_{lm}$ ,  $l, m = 1, 2$ ; see Section 4 for a detailed discussion. The choice  $\mathbf{v}_1 = \mathbf{v}_1$  (or equivalently  $\mathbf{v}_2$ ) is a zigzag edge and the choice  $\mathbf{v}_1 = \mathbf{v}_1 + \mathbf{v}_2$  is an armchair edge; see Figure 2.

Introduce the perturbed Hamiltonian:

$$H^{(\delta)} \equiv -\Delta + V(\mathbf{x}) + \delta\kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x})W(\mathbf{x}) = H^{(0)} + \delta\kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x})W(\mathbf{x}). \quad (1.1)$$

Here,  $\delta$  is real and will be taken to be sufficiently small, and  $W(\mathbf{x})$  is  $\Lambda_h$ -periodic and odd. The function  $\kappa$ , defines a domain wall. We choose  $\kappa$  to be sufficiently smooth and to satisfy  $\kappa(0) = 0$  and  $\kappa(\zeta) \rightarrow \pm\kappa_\infty \neq 0$  as  $\zeta \rightarrow \pm\infty$ . Without loss of generality, we assume  $\kappa_\infty > 0$ , e.g.  $\kappa(\zeta) = \tanh(\zeta)$ . We refer to the line  $\mathbb{R}\mathbf{v}_1$  as a  $\mathbf{v}_1$ -edge.

Note that  $H^{(\delta)}$  is invariant under translations parallel to the  $\mathbf{v}_1$ -edge,  $\mathbf{x} \mapsto \mathbf{x} + \mathbf{v}_1$ , and hence there is a well-defined parallel quasi-momentum, denoted  $k_\parallel$ . Furthermore,  $H^{(\delta)}$  transitions adiabatically between the asymptotic Hamiltonian  $H_-^{(\delta)} = H^{(0)} - \delta\kappa_\infty W(\mathbf{x})$  as  $\mathfrak{R}_2 \cdot \mathbf{x} \rightarrow -\infty$  to the asymptotic Hamiltonian  $H_+^{(\delta)} = H^{(0)} + \delta\kappa_\infty W(\mathbf{x})$  as  $\mathfrak{R}_2 \cdot \mathbf{x} \rightarrow \infty$ . In the case where  $\kappa$  changes sign once across  $\zeta = 0$ , the domain wall modulation of  $W(\mathbf{x})$  realizes a phase-defect across the edge (line-defect)  $\mathbb{R}\mathbf{v}_1$ . A

variant of this construction was used in [10] to insert a phase defect between asymptotic dimer periodic potentials.

Suppose  $H^{(0)}$  has a Dirac point at  $(\mathbf{K}_\star, E_\star)$ . It is important to note that while  $H^{(0)}$  is inversion symmetric,  $H_\pm^{(\delta)}$  is not. For  $\delta \neq 0$ ,  $H_\pm^{(\delta)}$  does not have Dirac points; its dispersion surfaces are locally smooth and for quasi-momenta  $\mathbf{k}$  such that  $|\mathbf{k} - \mathbf{K}_\star|$  is sufficiently small, there is an open neighborhood of  $E_\star$  not contained in the  $L^2(\mathbb{R}^2/\Lambda_h)$ -spectrum of  $H_\pm^{(\delta)}(\mathbf{k})$ . This ‘‘spectral gap’’ about  $E = E_\star$  may however only be local about  $\mathbf{K}_\star$  [11]. If there is a real open neighborhood of  $E_\star$ , not contained in the spectrum of  $H_\pm^{(\delta)}(\mathbf{k}) = -(\nabla + i\mathbf{k})^2 + V \pm \delta\kappa_\infty W$  for all  $\mathbf{k} \in \mathcal{B}_h$ , then  $H_\pm^{(\delta)}$  is said to have a (global) omni-directional spectral gap about  $E = E_\star$ . We’ll see, in our discussion of the *spectral no-fold condition*, that it is a ‘‘directional spectral gap’’ that plays a key role in the existence of edge states; see Section 1.3 and Definition 7.1.

Under suitable hypotheses, we shall construct  $\mathbf{v}_1$ -edge states of  $H^{(\delta)}$ , which are spectrally localized near the Dirac point,  $(\mathbf{K}_\star, E_\star)$ . These are non-trivial solutions  $\Psi$ , with energies  $E \approx E_\star$ , of the  $k_\parallel$ -eigenvalue problem:

$$H^{(\delta)}\Psi = E\Psi, \tag{1.2}$$

$$\Psi(\mathbf{x} + \mathbf{v}_1) = e^{ik_\parallel}\Psi(\mathbf{x}) \text{ (propagation parallel to } \mathbb{R}\mathbf{v}_1\text{)}, \tag{1.3}$$

$$|\Psi(\mathbf{x})| \rightarrow 0, \text{ as } |\mathfrak{R}_2 \cdot \mathbf{x}| \rightarrow \infty \text{ (localization transverse to } \mathbb{R}\mathbf{v}_1\text{)}, \tag{1.4}$$

for  $k_\parallel \approx \mathbf{K}_\star \cdot \mathbf{v}_1$ . To formulate the eigenvalue problem in an appropriate Hilbert space, we introduce the cylinder  $\Sigma \equiv \mathbb{R}^2/\mathbb{Z}\mathbf{v}_1$ . If  $f(\mathbf{x})$  satisfies the pseudo-periodic boundary condition (1.3), then  $f(\mathbf{x})e^{-i\frac{k_\parallel}{2\pi}\mathfrak{R}_1 \cdot \mathbf{x}}$  is well-defined on the cylinder  $\Sigma$ . Denote by  $H^s(\Sigma)$ ,  $s \geq 0$ , the Sobolev spaces of functions defined on  $\Sigma$ . The pseudo-periodicity and decay conditions (1.3)–(1.4) are encoded by requiring  $\Psi \in H_{k_\parallel}^s(\Sigma)$ , for some  $s \geq 0$ , where

$$H_{k_\parallel}^s = H_{k_\parallel}^s(\Sigma) \equiv \left\{ f : f(\mathbf{x})e^{-i\frac{k_\parallel}{2\pi}\mathfrak{R}_1 \cdot \mathbf{x}} \in H^s(\Sigma) \right\}.$$

Thus we formulate the EVP (1.2)–(1.4) as:

$$H^{(\delta)}\Psi = E\Psi, \quad \Psi \in H_{k_\parallel}^2(\Sigma). \tag{1.5}$$

*Remark 1.1* (Symmetry relation among  $\mathbf{K}$ - and  $\mathbf{K}'$ - points). Note that if  $\Psi(\mathbf{x}) = e^{i\mathbf{k} \cdot \mathbf{x}}Z(\mathbf{x})$  is a solution of the eigenvalue problem (1.5), then  $\psi_{\mathbf{K}} = e^{-i(Et - \mathbf{K} \cdot \mathbf{x})}Z(\mathbf{x})$ , where  $Z(\mathbf{x} + \mathbf{v}_1) = Z(\mathbf{x})$  and  $Z(\mathbf{x}) \rightarrow 0$  as  $|\mathfrak{R}_2 \cdot \mathbf{x}| \rightarrow \infty$ , is a propagating edge state of the time-dependent Schrödinger equation:  $i\partial_t\psi(\mathbf{x}, t) = H^{(\delta)}\psi(\mathbf{x}, t)$  with parallel quasi-momentum  $k_\parallel = \mathbf{K} \cdot \mathbf{v}_1$ . Since the time-dependent Schrödinger equation has the invariance  $\psi(\mathbf{x}, t) \mapsto \overline{\psi(\mathbf{x}, -t)}$ , it follows that

$$\overline{\psi_{\mathbf{K}}(\mathbf{x}, -t)} = e^{-i(Et + \mathbf{K} \cdot \mathbf{x})}\overline{Z(\mathbf{x})} = e^{-i(Et - \mathbf{K}' \cdot \mathbf{x})}\overline{Z(\mathbf{x})} = \psi_{\mathbf{K}'}(\mathbf{x}, t).$$



Thus  $\psi_{\mathbf{K}'}(\mathbf{x}, t)$  is a counterpropagating edge state with parallel quasi-momentum,  $k_{\parallel} = \mathbf{K}' \cdot \mathbf{v}_1 = -\mathbf{K} \cdot \mathbf{v}_1$ . Due to these symmetry considerations and the equivalence of  $\mathbf{K}-$  points:  $\{\mathbf{K}, R\mathbf{K}, R^2\mathbf{K}\}$ , without loss of generality, we henceforth restrict our attention to the Dirac point  $(\mathbf{K}, E_*)$ .

## 1.2 Summary of Main Results

### 1.2.1 General Conditions for the Existence of Topologically Protected Edge States; Theorem 7.3 and Corollary 7.4

In **Theorem 7.3** we formulate hypotheses on the honeycomb potential,  $V$ , domain wall function,  $\kappa(\zeta)$ , and asymptotic periodic structure,  $W(\mathbf{x})$ , which imply the existence of topologically protected  $\mathbf{v}_1-$  edge states, constructed as non-trivial eigenpairs  $\delta \mapsto (\Psi^\delta, E^\delta)$  of (1.5) with  $k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1$ , defined for all  $|\delta|$  sufficiently small. This branch of non-trivial states bifurcates from the trivial solution branch  $E \mapsto (\Psi \equiv 0, E)$  at  $E = E_*$ , the energy of the Dirac point. Key among the hypotheses is the spectral no-fold condition, discussed below in Section 1.3. At leading order in  $\delta$ , the edge state,  $\Psi^\delta(\mathbf{x})$ , is a slow modulation of the degenerate nullspace of  $H^{(0)} - E_*$ :

$$\Psi^\delta(\mathbf{x}) \approx \alpha_{\star,+}(\delta\mathfrak{R}_2 \cdot \mathbf{x})\Phi_+(\mathbf{x}) + \alpha_{\star,-}(\delta\mathfrak{R}_2 \cdot \mathbf{x})\Phi_-(\mathbf{x}) \text{ in } H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma), \tag{1.6}$$

$$E^\delta = E_* + \mathcal{O}(\delta^2), \quad 0 < |\delta| \ll 1, \tag{1.7}$$

where  $\Phi_+$  and  $\Phi_-$  are the appropriate linear combinations of  $\Phi_1$  and  $\Phi_2$ , defined in (4.14). The envelope amplitude-vector,  $\alpha_\star(\zeta) = (\alpha_{\star,+}(\zeta), \alpha_{\star,-}(\zeta))^T$ , is a zero-energy eigenstate,  $\mathcal{D}\alpha_\star = 0$ , of the one-dimensional Dirac operator (see also (6.22)):

$$\mathcal{D} \equiv -i|\lambda_{\sharp}| |\mathfrak{R}_2| \sigma_3 \partial_\zeta + \vartheta_{\sharp} \kappa(\zeta) \sigma_1,$$

where the Pauli matrices  $\sigma_j$  are displayed in (1.13). Here  $\lambda_{\sharp} \in \mathbb{C}$  (see (3.9)) depends on the unperturbed honeycomb potential,  $V$ , and is non-zero for generic  $V$ . The constant  $\vartheta_{\sharp} \equiv \langle \Phi_1, W\Phi_1 \rangle_{L^2(\Omega_h)}$  is real and is also generically nonzero.  $\mathcal{D}$  has a spatially localized zero-energy eigenstate for any  $\kappa(\zeta)$  having asymptotic limits of opposite sign at  $\pm\infty$ . Therefore, the zero-energy eigenstate, which seeds the bifurcation, persists for *localized* perturbations of  $\kappa(\zeta)$ . In this sense, the bifurcating branch of edge states is topologically protected against a class of local perturbations of the edge.

Section 6 gives an account of a formal multiple scale expansion, to any order in the small parameter,  $\delta$ , of a solution to the eigenvalue problem (1.5). The expression in (1.6) is the leading order term in this expansion. Our methods can be used to prove the validity of the multiple scale expansion, at any finite order.

**Corollary 7.4** ensures, under the conditions of Theorem 7.3, the existence of edge states,  $\Psi(\mathbf{x}; k_{\parallel}) \in H^2_{k_{\parallel}}(\Sigma)$  for all  $k_{\parallel}$  in a neighborhood of  $k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1$ , and by symmetry (see Remark 1.4) for all  $k_{\parallel}$  in a neighborhood of  $k_{\parallel} = -\mathbf{K} \cdot \mathbf{v}_1 = \mathbf{K}' \cdot \mathbf{v}_1$ . Thus, by taking a continuous superposition of states given by Corollary 7.4, one obtains states that remain localized about (and dispersing along) the zigzag edge for all time.

*Remark 1.2* A key hypothesis in Theorem 7.3 is a *spectral no-fold* condition at  $(\mathbf{K}, E_\star)$  for the  $\mathbf{v}_1$ –edge of the band-structure of  $-\Delta + V$ . This (essentially) ensures the existence of a  $L^2_{k_\parallel=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$ –spectral gap containing  $E_\star$  for the perturbed Hamiltonian,  $H^{(\delta)}$ ; see Definition 7.1 and the discussion in Section 1.3.

1.2.2 Theorem 8.5; Existence of Topologically Protected Zigzag Edge States

We consider the case of zigzag edges corresponding to the choice  $\mathbf{v}_1 = \mathbf{v}_1, \mathbf{v}_2 = \mathbf{v}_2$ , and  $\mathfrak{R}_1 = \mathbf{k}_1, \mathfrak{R}_2 = \mathbf{k}_2$ . Recall that  $\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$ . The choice  $\mathbf{v}_1 = \mathbf{v}_2$  would lead to equivalent results.

We consider the zigzag edge state eigenvalue problem

$$H^{(\varepsilon,\delta)}\Psi = E\Psi, \quad \Psi \in H^2_{k_\parallel}(\Sigma) \quad (\text{see also (1.5)}), \tag{1.8}$$

with Hamiltonian

$$H^{(\varepsilon,\delta)} \equiv -\Delta + \varepsilon V(\mathbf{x}) + \delta\kappa(\delta\mathbf{k}_2 \cdot \mathbf{x})W(\mathbf{x}) = H^{(\varepsilon)} + \delta\kappa(\delta\mathbf{k}_2 \cdot \mathbf{x})W(\mathbf{x}). \tag{1.9}$$

Here,  $\varepsilon$  and  $\delta$  are chosen to satisfy

$$0 < |\delta| \lesssim \varepsilon^2 \ll 1. \tag{1.10}$$

There are two cases, which are delineated by the sign of the distinguished Fourier coefficient,  $\varepsilon V_{1,1}$ , of the unperturbed (bulk) honeycomb potential,  $\varepsilon V(\mathbf{x})$ . Here,

$$V_{1,1} \equiv \frac{1}{|\Omega_h|} \int_{\Omega_h} e^{-i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{y}} V(\mathbf{y}) \, d\mathbf{y},$$

is assumed to be non-zero. We designate these cases:

$$\text{Case (1)} \quad \varepsilon V_{1,1} > 0 \quad \text{and} \quad \text{Case (2)} \quad \varepsilon V_{1,1} < 0.$$

In Appendix A we give two explicit families of potentials, a superposition of “bump-functions” concentrated, respectively, on a triangular lattice,  $\Lambda_h^{(a)}$ , and a honeycomb structure,  $\mathbf{H}$ , that can be tuned between these two cases by variation of a lattice scale parameter.

Under the condition  $\varepsilon V_{1,1} > 0$  (Case (1)) and (1.10), we verify the spectral no-fold condition for the zigzag edge in Theorem 8.2. The existence of zigzag edge states (Theorem 8.5) then follows from Theorem 7.3 and Corollary 7.4. In particular, for all  $\varepsilon$  and  $\delta$  satisfying (1.10) and for each  $k_\parallel$  near  $\mathbf{K} \cdot \mathbf{v}_1 = 2\pi/3$ , the zigzag edge state eigenvalue problem (1.5) has topologically protected edge states with energies sweeping out a neighborhood of  $E_\star^\varepsilon$ , where  $(\mathbf{K}, E_\star^\varepsilon)$  is a Dirac point.

*Remark 1.3* (Directional versus omnidirectional spectral gaps). While the regime of weak potentials, implied by (1.10), would at first seem to be a simplifying assumption, we wish to remark on a subtlety for  $H_\pm^{(\varepsilon,\delta)} = -\Delta + \varepsilon V \pm \delta\kappa_\infty W$  ( $\varepsilon, \delta$  small), which

arises precisely in this regime. It is well-known that for sufficiently weak periodic potentials on  $\mathbb{R}^d$ ,  $d \geq 2$ , that there are no spectral gaps; this is related to the ‘‘Bethe-Sommerfeld conjecture’’ [3,36,37]. Nevertheless, if  $\varepsilon V_{1,1} > 0$ , and  $\varepsilon$  and  $\delta$  are related as in (1.10), then a *directional* spectral gap, i.e. an  $L^2_{k_{\parallel}}(\Sigma)$ - spectral gap exists; see Theorem 8.3 and Section 1.3.

Figure 5 and Figure 6 are illustrative of Cases (1) and (2). The simulations were done for the Hamiltonian  $H^{(\varepsilon,\delta)}$  with  $\varepsilon = \pm 10$  and  $0 \leq \delta \leq 10$ :

$$\begin{aligned}
 H^{(\varepsilon,\delta)} &= -\Delta + \varepsilon V(\mathbf{x}) + \delta \kappa(\delta \mathbf{k}_2 \cdot \mathbf{x}) W(\mathbf{x}), \quad \kappa(\zeta) = \tanh(\zeta), \\
 V(\mathbf{x}) &= \sum_{j=0}^2 \cos(R^j \mathbf{k}_1 \cdot \mathbf{x}), \quad W(\mathbf{x}) = \sum_{j=0}^2 (-1)^{\delta j^2} \sin(R^j \mathbf{k}_1 \cdot \mathbf{x}). \quad (1.11)
 \end{aligned}$$

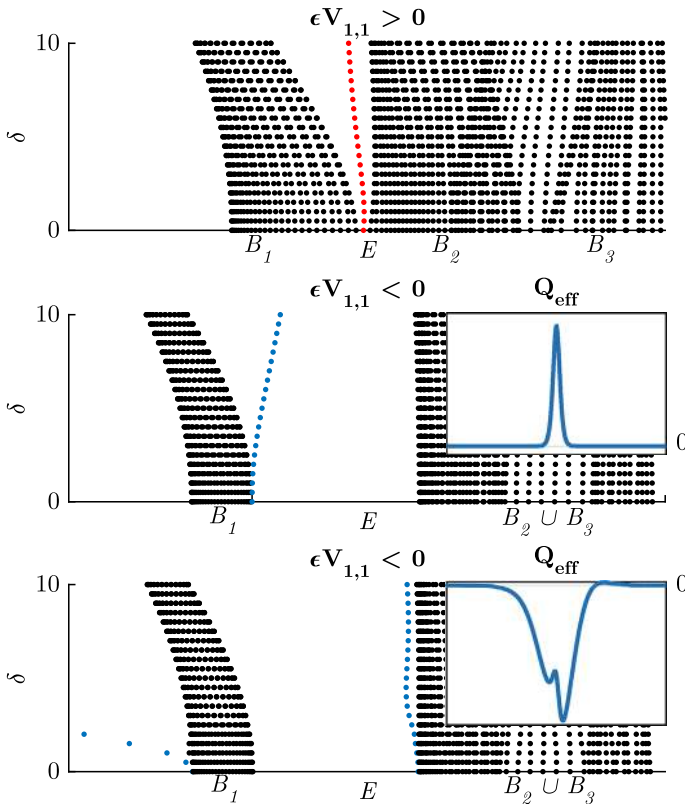
Here,  $R$  is the  $2\pi/3$ - rotation matrix displayed in (2.6). Figure 5 displays, for fixed  $\varepsilon$ , the  $L^2_{k_{\parallel}=2\pi/3}(\Sigma)$ - spectra (plotted horizontally) of  $H^{(\varepsilon,\delta)}$  corresponding to a range of  $\delta$  values (strength / scale of domain wall -perturbation) for Cases (1)  $\varepsilon V_{1,1} > 0$  (top panel) and (2)  $\varepsilon V_{1,1} < 0$  (middle and bottom panels). Figure 6 displays, for these cases, the  $L^2_{k_{\parallel}}(\Sigma)$ - spectra (plotted vertically) for a range of parallel-quasi-momentum,  $k_{\parallel}$ .

*Remark 1.4* (Symmetries of  $k_{\parallel} \mapsto E(k_{\parallel})$ ). Figure 6 exhibits some elementary symmetries. Since the boundary condition for the EVP (1.8),  $\Psi(\mathbf{x} + \mathbf{v}_1) = e^{ik_{\parallel}} \Psi(\mathbf{x})$  is  $2\pi$ - periodicity in  $k_{\parallel}$ , the mapping  $k_{\parallel} \mapsto E(k_{\parallel})$  is  $2\pi$ - periodic. Furthermore, invariance under complex conjugation, implies symmetry of  $k_{\parallel} \mapsto E(k_{\parallel})$  about  $k_{\parallel} = 0$  and  $k_{\parallel} = \pi$ .

### 1.2.3 Non-Topologically Protected Bifurcations of Edge States

In Case (2), where  $\varepsilon V_{1,1} < 0$ , **Theorem 8.4** implies that the spectral no-fold condition fails and we do not obtain a bifurcation from the Dirac point. However, through a combination of formal asymptotic analysis and numerical computations, we do find bifurcating branches of edge states. These branches do not emanate from Dirac points (the no-fold condition fails), but rather from a spectral band edge. Moreover, as we discuss below, these states are not topologically protected; they may be destroyed by an appropriate localized perturbation of the edge. Case (2) ( $\varepsilon V_{1,1} < 0$ ) is illustrated by Figures 5 (middle and bottom panels) and Figure 6 (bottom panel).

In particular, Dirac points occur at the intersection of the second and third spectral bands of  $H^{(\varepsilon,0)} = -\Delta + \varepsilon V(\mathbf{x})$  (see Theorem 3.5), and the failure of the spectral no-fold condition implies that an  $L^2_{k_{\parallel}}$ - spectral gap does not open about  $E = E^{\varepsilon}_{\star}$  for  $\delta \neq 0$  and small. However, for  $\varepsilon V_{1,1} < 0$  there is a spectral gap between the first and second spectral bands of  $H^{(\varepsilon,0)}$ . For the choice of edge-potential displayed in (1.11) with  $\varepsilon = -10$ , a family of nontrivial edge states bifurcates, for  $0 < |\delta|$  sufficiently small, from the upper edge of the first (lowest)  $L^2_{k_{\parallel}=2\pi/3}$ - spectral band into the spectral gap (dotted blue curve); see middle panel of Figure 5. A bifurcation of a similar nature is discussed in [31].

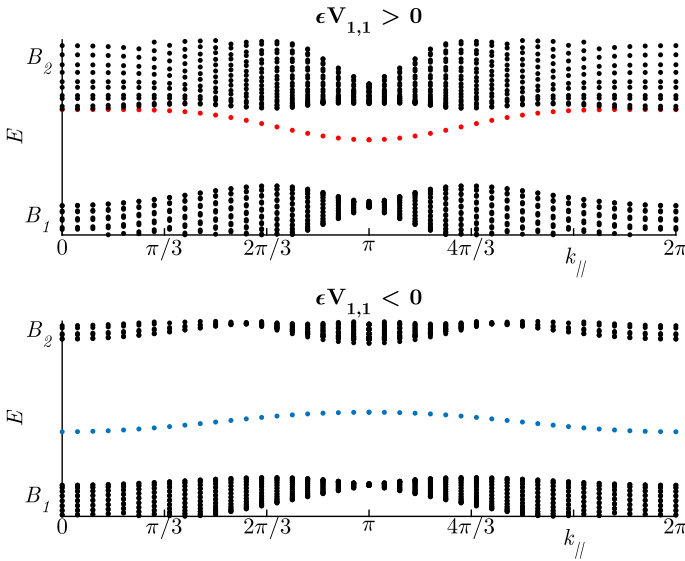


**Fig. 5**  $L^2_{k_{||}=K \cdot v_1}(\Sigma)$ — spectra, where  $K \cdot v_1 = \frac{2}{3}\pi$ , of the Hamiltonian  $H^{(\epsilon, \delta)}$  ((1.11)) for the zigzag edge ( $\mathbb{R}v_1$ ). **Top panel:** Case (1)  $\epsilon V_{1,1} > 0$ . Topologically protected bifurcation of edge states, described by Theorem 8.2 (dotted red curve), is seeded by zero-energy mode of a Dirac operator (6.22). The branch of edge states emanates from intersection of first and second bands ( $B_1$  and  $B_2$ ) at  $E = E^*$  for  $\delta = 0$ ; see discussion in Section 1.2.2. **Middle panel:** Case (2)  $\epsilon V_{1,1} < 0$  with domain wall function  $\kappa$ . Spectral no-fold condition does not hold. Bifurcation of zigzag edge states from upper endpoint,  $E = \tilde{E}^\epsilon$ , of the first spectral band. This bifurcation is seeded by a bound state of a Schrödinger operator (1.12) with effective mass  $m_{\text{eff}} < 0$  and effective potential  $Q_{\text{eff}}(\zeta)$  (displayed in the inset) and is *not* topologically protected; see discussion in Section 1.2.3. **Bottom panel:** Case (2)  $\epsilon V_{1,1} < 0$  with domain wall function  $\kappa_{\mp}$ . Bifurcation from upper endpoint of  $B_1$  is destroyed. Bound states bifurcate from the lower edges of the first two spectral bands.

A formal multiple scale analysis clarifies this latter bifurcation. For  $\mathbf{k} \in \mathcal{B}_h$ , let  $(\tilde{E}^\epsilon(\mathbf{k}), \tilde{\Phi}^\epsilon(\mathbf{x}; \mathbf{k}))$  denote the eigenpair associated with a lowest spectral band. In [8], we calculate that the edge state bifurcation is seeded by a discrete eigenvalue effective Schrödinger operator:

$$H_{\text{eff}}^\epsilon = -\frac{1}{2m_{\text{eff}}^\epsilon} \frac{\partial^2}{\partial \zeta^2} + Q_{\text{eff}}^\epsilon(\zeta; \kappa), \quad \text{where} \quad \frac{1}{m_{\text{eff}}^\epsilon} = \sum_{i,j=1,2} [D^2 \tilde{E}^\epsilon(\mathbf{K})]_{ij} \mathfrak{R}_2^i \mathfrak{R}_2^j, \tag{1.12}$$

and  $Q_{\text{eff}}^\epsilon(\zeta; \kappa, \tilde{\Phi}^\epsilon) = a \kappa'(\zeta) + b (\kappa_\infty^2 - \kappa^2(\zeta))$  is a spatially localized effective potential, depending on  $\kappa(\zeta)$ , and constants  $a$  and  $b$ , with  $b > 0$ , which depend on



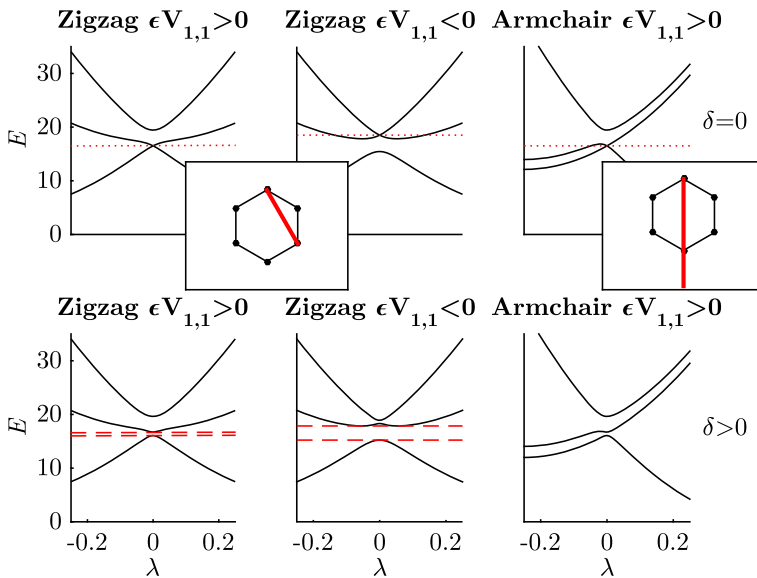
**Fig. 6** **Top panel:**  $L^2_{k_{||}}(\Sigma)$ – spectrum of protected states of  $H^{(\varepsilon,\delta)}$ , for the case  $\varepsilon V_{1,1} > 0$ . **Bottom panel:**  $L^2_{k_{||}}(\Sigma)$ – spectrum of non-protected states of  $H^{(\varepsilon,\delta)}$  for the case  $\varepsilon V_{1,1} < 0$ .  $V, W$  and  $\kappa$  are chosen as in (1.11). For each fixed  $k_{||}$ , edge states shown in the top panel ( $\varepsilon V_{1,1} > 0$ ) arise due to a protected bifurcation from a Dirac point displayed in the top panel of Figure 5. Those edge states indicated in the bottom panel ( $\varepsilon V_{1,1} < 0$ ) arise via an edge bifurcation of the type shown in the middle and bottom panels of Figure 5. The band edge energies from which this latter bifurcation takes place is well-separated from the energy of the Dirac point which, when  $\varepsilon V_{1,1} < 0$ , lies within the overlap of the second and third spectral bands.

$V, W$  and  $\tilde{\Phi}^\varepsilon$ . For the above choice of the zigzag edge-potential (middle panel of Figure 5), we have  $m_{\text{eff}}^\varepsilon < 0$  and the effective potential  $Q_{\text{eff}}^\varepsilon$ , displayed in the figure inset, induces a bifurcation into the gap above the first band.

Now, we can construct domain wall functions,  $\kappa_\pm(\zeta)$ , for which the corresponding  $H_{\text{eff}}^\varepsilon$  has no point eigenvalues in a neighborhood of the right (upper) edge of the first spectral band; see bottom panel of Figure 5. If  $\kappa(\zeta)$  is chosen as above, then  $Q_{\text{eff}}^\varepsilon(\zeta; (1 - \theta)\kappa + \theta\kappa_\pm), 0 \leq \theta \leq 1$ , provides a smooth homotopy from a Schrödinger Hamiltonian for which there is a bifurcation of edge states ( $H^{(\varepsilon,\delta)}$  with domain wall  $\kappa$ ) to one for which the branch of edge states does not exist ( $H^{(\varepsilon,\delta)}$  with domain wall  $\kappa_\pm$ ). Therefore, this type of bifurcation is not topologically protected; see [8] for a more detailed discussion. This contrast between topologically protected states and non-protected states is explained and explored numerically, in a one-dimensional setting in [25].

### 1.3 Remarks on the Spectral No-Fold Condition

The spectral no-fold hypothesis of Theorem 7.3 requires that the dispersion curves obtained by slicing the band structure (situated in  $\mathbb{R}^2_{\mathbf{k}} \times \mathbb{R}_E$ ) with a plane through the Dirac point  $(\mathbf{K}, E_*)$  containing the direction  $\mathfrak{R}_2$  (dual direction to the  $\mathbf{v}_1$ – edge)



**Fig. 7** Zigzag and armchair slices at the Dirac point  $(\mathbf{K}, E_\star^\varepsilon)$  of the band structure of  $-\Delta + \varepsilon V + \delta \kappa_\infty W$  for  $\delta = 0$  (**first row**) and  $\delta > 0$  (**second row**). Insets indicate zigzag and armchair quasi-momentum segments (one-dimensional Brillouin zones) parametrized by  $\lambda$ , for  $0 \leq \lambda \leq 1$ . See discussion of Section 1.4 and Theorem 4.2.

do not fold-over and fill out energies arbitrarily near  $E_\star$ . This essentially implies that via a small perturbation which breaks inversion symmetry (as we do with  $H^{(\delta)} = -\Delta + V(\mathbf{x}) + \delta \kappa(\delta \mathfrak{R}_2 \cdot \mathbf{x})W(\mathbf{x})$  for  $\delta \neq 0$ ) we open a  $L^2_{k_\parallel}(\Sigma)$ - spectral gap about  $E_\star$ . Figure 7 is illustrative.

In the first row of plots in Figure 7, we consider whether the spectral no-fold condition holds at the Dirac point  $(\mathbf{K}, E_\star^\varepsilon)$  for the zigzag edge, in the two cases: (1)  $\varepsilon V_{1,1} > 0$  and (2)  $\varepsilon V_{1,1} < 0$ , as well as for the armchair edge. The energy level  $E = E_\star^\varepsilon$  is indicated with the dotted line. In the left panel we see that for the zigzag edge, the spectral no-fold condition holds if  $\varepsilon V_{1,1} > 0$ . In this case, there is a topologically protected branch of edge states. In the center panel we see that the spectral no-fold condition fails if  $\varepsilon V_{1,1} < 0$ . Finally, in the right panel we see that it also fails for the armchair slice.

The second row of plots in Figure 7, illustrates that the spectral no-fold condition controls whether a full  $L^2_{k_\parallel}$ - spectral gap opens when breaking inversion symmetry. In particular, for  $\delta > 0$ ,  $H^{(\varepsilon, \delta)}$  is no longer inversion symmetric. For  $\varepsilon V_{1,1} > 0$ , a spectral gap opens about the Dirac point, between the first and second spectral bands (see Theorem 3.5). For the zigzag edge with  $\varepsilon V_{1,1} < 0$  there is no spectral gap about the Dirac point. (Note, however, that there is a spectral gap between the first and second spectral bands; see the discussion above in Section 1.2.3.) Similarly, for the armchair edge (right panel) there is no spectral gap for  $\delta > 0$ .

### 1.4 Are there Meta-stable Edge States?

Consider the Hamiltonian  $H^{(\delta)} = -\Delta_{\mathbf{x}} + V(\mathbf{x}) + \delta\kappa (\delta\mathfrak{R}_2 \cdot \mathbf{x}) W(\mathbf{x})$  (as in (1.1)), corresponding to an *arbitrary* rational edge,  $\mathbb{R}\mathbf{v}_1$ , i.e.  $\mathbf{v}_1 = a_1\mathbf{v}_1 + b_1\mathbf{v}_2$ ,  $a_1$  and  $b_1$  coprime integers, as introduced in the discussion leading up to (1.1); see also Section 4. Irrespective of whether the spectral no-fold condition holds for the  $\mathbf{v}_1$ -edge (see Section 1.3 and Definition 7.1), the multiple scale expansion of Section 6 produces a formal edge state to *any finite order* in the small parameter  $\delta$ .

*But is this formal expansion the expansion of a true edge state?* We believe the answer is no, if the spectral no-fold condition fails.

Indeed, from Theorem 4.2, we have that any  $\mathbf{v}_1$ -edge state,  $\Psi \in L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}$ , is a superposition of Floquet-Bloch modes of  $H^{(0)} = -\Delta + V$  along the quasimomentum segment:  $\mathbf{K} + \lambda\mathfrak{R}_2$ ,  $|\lambda| \leq 1/2$ . The formal expansion of Section 6 however is spectrally concentrated on Floquet-Bloch components along this segment, which are near the Dirac point, corresponding to  $|\lambda| \ll 1$ . If the spectral no-fold condition fails, the expansion does not capture the effect of resonant coupling to quasi-momenta along this segment “far from  $\mathbf{K}$ ” (corresponding to  $\lambda$  bounded away from  $\lambda = 0$  in Figure 7).

**Conjecture** *Suppose the spectral no-fold condition fails for the  $\mathbf{v}_1$ -edge  $\mathbb{R}\mathbf{v}_1$ . Then,  $H^{(\delta)}$  has topologically protected long-lived (meta-stable) edge quasi-modes,  $\Psi \in H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1, \text{loc}}(\Sigma)$ , but generically has no topologically protected edge states.*

### 1.5 Outline

In **Section 2** we review spectral theory for two-dimensional periodic Schrödinger operators, introduce the triangular lattice, the honeycomb structure and honeycomb lattice potentials.

In **Section 3** we define Dirac points and review the results on the existence of Dirac points for generic honeycomb potentials from [11, 12].

In **Section 4** we introduce the notion of an edge or line defect in a bulk (unperturbed) honeycomb structure. Honeycomb structures with edges parallel to a period lattice direction, have a translation invariance. Thus, an important tool is the Fourier decomposition of states which are  $L^2$  (localized) in the unbounded direction, transverse to the edge, and propagating (plane-wave like) parallel to the edge.

In **Section 5** we introduce our class of Hamiltonians, consisting of a bulk honeycomb potential, perturbed by a general line-defect/ $\mathbf{v}_1$ -edge potential.

In **Section 6** we give a formal multiple scale construction of edge states to any finite order in the small parameter  $\delta$ .

In **Section 7** we formulate general hypotheses which imply the existence of a branch of topologically protected  $\mathbf{v}_1$ -edge states, bifurcating from the Dirac point. The proof uses a Lyapunov-Schmidt reduction strategy, applied to a system for the Floquet-Bloch amplitudes which is equivalent to the eigenvalue problem. Such a strategy was implemented in a 1D setting in [10]. First, the edge-state eigenvalue problem is formulated in (quasi-) momentum space as an infinite system for the Floquet-Bloch mode amplitudes. We view this system as consisting of two coupled subsystems; one

is for the quasi-momentum / energy components “near” the Dirac point,  $(\mathbf{K}, E_*)$ , and the second governs the components which are “far” from the Dirac point. We next solve for the far-energy components as a functional of the near-energy components and thereby obtain a reduction to a closed system for the near-energy components. The construction of this map requires that the spectral no-fold condition holds.

In **Section 8** we consider the Hamiltonian, introduced in **Section 7**, in the weak-potential (low-contrast) regime and prove the existence of topologically protected zigzag edge states, under the condition  $\varepsilon V_{1,1} > 0$ .

In **Appendix A** we give two families of honeycomb potentials, depending on the lattice scale parameter,  $a$ , where we can tune between Case (1)  $\varepsilon V_{1,1} > 0$  and Case (2)  $\varepsilon V_{1,1} < 0$  by continuously varying the lattice scale parameter.

In a number of places, the proofs of certain assertions are very similar to those of corresponding assertions in [10]. In such cases, we do not repeat a variation on the proof in [10], but rather refer to the specific proposition or lemma in [10].

### 1.6 Notation

- (1)  $\mathbf{v}_j, j = 1, 2$  are basis vectors of the triangular lattice in  $\mathbb{R}^2, \Lambda_h. \mathbf{k}_\ell, \ell = 1, 2$  are dual basis vectors of  $\Lambda_h^*$ , which satisfy  $\mathbf{k}_\ell \cdot \mathbf{v}_j = 2\pi \delta_{\ell j}$ .
- (2) For  $\mathbf{m} = (m_1, m_2) \in \mathbb{Z}^2, \mathbf{m}\mathbf{k} = m_1\mathbf{k}_1 + m_2\mathbf{k}_2$ .
- (3)  $\mathbf{v}_1 = a_1\mathbf{v}_1 + a_2\mathbf{v}_2 \in \Lambda_h, a_1, a_2$  co-prime integers. The  $\mathbf{v}_1$ -edge is  $\mathbb{R}\mathbf{v}_1. \mathbf{v}_j, j = 1, 2$ , is an alternate basis for  $\Lambda_h$  with corresponding dual basis,  $\mathfrak{K}_\ell, \ell = 1, 2$ , satisfying  $\mathfrak{K}_\ell \cdot \mathbf{v}_j = 2\pi \delta_{\ell j}$ .
- (4)  $\mathfrak{K} = (\mathfrak{K}^{(1)}, \mathfrak{K}^{(2)}), \mathfrak{z} \equiv \mathfrak{K}^{(1)} + i\mathfrak{K}^{(2)}, |\mathfrak{z}| = |\mathfrak{K}|$ .
- (5)  $\mathcal{B}$  denotes the Brillouin Zone, associated with  $\Lambda_h$ , shown in the right panel of **Figure 3**.
- (6)  $\langle f, g \rangle = \int \bar{f}g$ .
- (7)  $x \lesssim y$  if and only if there exists  $C > 0$  such that  $x \leq Cy. x \approx y$  if and only if  $x \lesssim y$  and  $y \lesssim x$ .
- (8)  $L^{p,s}(\mathbb{R})$  is the space of functions  $F : \mathbb{R} \rightarrow \mathbb{R}$  such that  $(1 + |\cdot|^2)^{s/2}F \in L^p(\mathbb{R})$ , endowed with the norm

$$\|F\|_{L^{p,s}(\mathbb{R})} \equiv \left\| (1 + |\cdot|^2)^{s/2}F \right\|_{L^p(\mathbb{R})} \approx \sum_{j=0}^s \left\| |\cdot|^j F \right\|_{L^p(\mathbb{R})} < \infty, \quad 1 \leq p \leq \infty.$$

- (9) For  $f, g \in L^2(\mathbb{R}^d)$ , the Fourier transform and its inverse are given by

$$\mathcal{F}\{f\}(\xi) \equiv \widehat{f}(\xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} e^{-iX \cdot \xi} f(X) dX,$$

$$\mathcal{F}^{-1}\{g\}(X) \equiv \check{g}(X) = \int_{\mathbb{R}^d} e^{iX \cdot \xi} g(\xi) d\xi.$$

The Plancherel relation states:  $\int_{\mathbb{R}^d} f(x)\overline{g(x)}dx = (2\pi)^d \int_{\mathbb{R}^d} \widehat{f}(\xi)\overline{\widehat{g}(\xi)}d\xi$ .



(10)  $\sigma_j$ ,  $j = 1, 2, 3$ , denote the Pauli matrices, where

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.13)$$

## 2 Floquet-Bloch Theory and Honeycomb Lattice Potentials

We begin with a review of Floquet-Bloch theory; see, for example, [4, 23, 24, 34].

### 2.1 Fourier Analysis on $L^2(\mathbb{R}/\Lambda)$ and $L^2(\Sigma)$

Let  $\{\mathbf{v}_1, \mathbf{v}_2\}$  be a linearly independent set in  $\mathbb{R}^2$  and introduce the

$$\begin{aligned} \text{Lattice: } \Lambda &= \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2 = \{m_1\mathbf{v}_1 + m_2\mathbf{v}_2 : m_1, m_2 \in \mathbb{Z}\}; \\ \text{Fundamental period cell: } \Omega &= \{\theta_1\mathbf{v}_1 + \theta_2\mathbf{v}_2 : 0 \leq \theta_j \leq 1, j = 1, 2\}; \\ \text{Dual lattice: } \Lambda^* &= \mathbb{Z}\mathfrak{K}_1 \oplus \mathbb{Z}\mathfrak{K}_2 = \{\mathbf{m}\mathfrak{K} = m_1\mathfrak{K}_1 + m_2\mathfrak{K}_2 : m_1, m_2 \in \mathbb{Z}\}, \\ &\quad \mathfrak{K}_i \cdot \mathbf{v}_j = 2\pi\delta_{ij}, \quad 1 \leq i, j \leq 2; \end{aligned} \quad (2.1)$$

**Brillouin zone:**  $\mathcal{B}$ , a choice of fundamental dual cell;

**Cylinder:**  $\Sigma \equiv \mathbb{R}^2/\mathbb{Z}\mathbf{v}_1$ ;

**Fundamental domain for  $\Sigma$ :**  $\Omega_\Sigma \equiv \{\tau_1\mathbf{v}_1 + \tau_2\mathbf{v}_2 : 0 \leq \tau_1 \leq 1, \tau_2 \in \mathbb{R}\}$ . (2.2)

We denote by  $L^2(\Omega)$  and  $L^2(\Omega_\Sigma)$  the standard  $L^2$  spaces on the domains  $\Omega$  and  $\Omega_\Sigma$ , respectively.

**Definition 2.1** [The spaces  $L^2(\mathbb{R}^2/\Lambda)$  and  $L^2_{\mathbf{k}}$ ].

- $L^2(\mathbb{R}^2/\Lambda)$  denotes the space of  $L^2_{loc}$  functions which are  $\Lambda$ -periodic:  $f \in L^2(\mathbb{R}^2/\Lambda)$  if and only if  $f(\mathbf{x} + \mathbf{v}) = f(\mathbf{x})$  for all  $\mathbf{x} \in \mathbb{R}^2$ ,  $\mathbf{v} \in \Lambda$  and  $f \in L^2(\Omega)$ .
- $L^2_{\mathbf{k}}$  denotes the space of  $L^2_{loc}$  functions which satisfy a pseudo-periodic boundary condition:  $f(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{k} \cdot \mathbf{v}} f(\mathbf{x})$  for all  $\mathbf{x} \in \mathbb{R}^2$ ,  $\mathbf{v} \in \Lambda$  and  $e^{-i\mathbf{k} \cdot \mathbf{x}} f(\mathbf{x}) \in L^2(\mathbb{R}^2/\Lambda)$ . For  $f$  and  $g$  in  $L^2_{\mathbf{k}}$ ,  $\overline{f}g$  is in  $L^1(\mathbb{R}^2/\Lambda)$  and we define their inner product by

$$\langle f, g \rangle_{L^2_{\mathbf{k}}} = \int_{\Omega} \overline{f(\mathbf{x})} g(\mathbf{x}) d\mathbf{x}.$$

**Definition 2.2** [The spaces  $L^2(\Sigma)$  and  $L^2_{k_{\parallel}}$ ].

- $L^2(\Sigma) = L^2(\mathbb{R}^2/\mathbb{Z}\mathbf{v}_1)$  denotes the space of  $L^2_{loc}$  functions, which are periodic in the direction of  $\mathbf{v}_1$ :  $f(\mathbf{x} + \mathbf{v}_1) = f(\mathbf{x})$ , for all  $\mathbf{x} \in \mathbb{R}^2$  and such that  $f \in L^2(\Omega_\Sigma)$ , where  $\Omega_\Sigma$  is the fundamental domain for  $\Sigma$ ; see (2.2).
- $L^2_{k_{\parallel}}(\Sigma) = L^2_{k_{\parallel}}$  denotes the space of  $L^2_{loc}$  functions:

(1) which are  $k_{\parallel}$ -pseudo-periodic in the direction  $\mathbf{v}_1$ :

$$f(\mathbf{x} + \mathbf{v}_1) = e^{ik_{\parallel}} f(\mathbf{x}), \text{ for } \mathbf{x} \in \mathbb{R}^2, \text{ and}$$

(2) such that  $e^{-i(1/2\pi)k_{\parallel}\mathfrak{R}_1 \cdot \mathbf{x}} f(\mathbf{x})$ , which is defined on  $\Sigma$ , is in  $L^2(\Omega_{\Sigma})$ .

For  $f$  and  $g$  in  $L^2_{k_{\parallel}}(\Sigma)$ ,  $\overline{f}g$  is in  $L^2(\Sigma)$  and we define their inner product by

$$\langle f, g \rangle_{L^2_{k_{\parallel}}} = \int_{\Omega_{\Sigma}} \overline{f(\mathbf{x})} g(\mathbf{x}) d\mathbf{x}.$$

The respective Sobolev spaces  $H^s(\mathbb{R}^2/\Lambda)$ ,  $H^s_{\mathbf{k}}$ ,  $H^s(\Sigma)$  and  $H^s_{k_{\parallel}}(\Sigma) = H^s_{k_{\parallel}}$  are defined in a natural way.

**Simplified notational convention:** We shall do many calculations requiring us to explicitly write out inner products like  $\langle f, g \rangle_{L^2(\Sigma)}$  and  $\langle f, g \rangle_{L^2_{k_{\parallel}}(\Sigma)}$ . We shall write these as  $\int_{\Sigma} \overline{f(\mathbf{x})} g(\mathbf{x}) d\mathbf{x}$  rather than as  $\int_{\Omega_{\Sigma}} \overline{f(\mathbf{x})} g(\mathbf{x}) d\mathbf{x}$ .

If  $f \in L^2(\mathbb{R}^2/\Lambda)$ , then it can be expanded in a Fourier series:

$$f(\mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{Z}^2} f_{\mathbf{m}} e^{i\mathbf{m}\mathfrak{R} \cdot \mathbf{x}}, \quad f_{\mathbf{m}} = \frac{1}{|\Omega|} \int_{\Omega} e^{-i\mathbf{m}\mathfrak{R} \cdot \mathbf{y}} f(\mathbf{y}) d\mathbf{y}, \quad \mathbf{m}\mathfrak{R} = m_1\mathfrak{R}_1 + m_2\mathfrak{R}_2, \tag{2.3}$$

where  $|\Omega|$  denotes the area of the fundamental cell,  $\Omega$ . In Section 4.1, we show that, if  $g \in L^2(\Sigma)$ , then it can be expanded in a Fourier series in  $\mathbf{v}_1 \cdot \mathbf{x}$  and Fourier transform in  $\mathbf{v}_2 \cdot \mathbf{x}$ :

$$g(\mathbf{x}) = 2\pi \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}} \widehat{g}_n(2\pi\xi) e^{i\xi\mathfrak{R}_2 \cdot \mathbf{x}} d\xi e^{in\mathfrak{R}_1 \cdot \mathbf{x}},$$

$$2\pi \widehat{g}_n(2\pi\xi) = \frac{1}{|\mathbf{v}_1 \wedge \mathbf{v}_2|} \int_{\Sigma} e^{-i\xi\mathfrak{R}_2 \cdot \mathbf{y}} e^{-in\mathfrak{R}_1 \cdot \mathbf{y}} g(\mathbf{y}) d\mathbf{y}.$$

### 2.2 Floquet-Bloch Theory

Let  $Q(\mathbf{x})$  denote a real-valued potential which is periodic with respect to  $\Lambda$ . We shall assume throughout this paper that  $Q \in C^\infty(\mathbb{R}^2/\Lambda)$ , although we expect that this condition can be relaxed without much extra work. Introduce the Schrödinger Hamiltonian  $H \equiv -\Delta + Q(\mathbf{x})$ . For each  $\mathbf{k} \in \mathbb{R}^2$ , we study the *Floquet-Bloch eigenvalue problem* on  $L^2_{\mathbf{k}}$ :

$$H\Phi(\mathbf{x}; \mathbf{k}) = E(\mathbf{k})\Phi(\mathbf{x}; \mathbf{k}), \quad \mathbf{x} \in \mathbb{R}^2,$$

$$\Phi(\mathbf{x} + \mathbf{v}) = e^{i\mathbf{k} \cdot \mathbf{v}} \Phi(\mathbf{x}; \mathbf{k}), \quad \forall \mathbf{v} \in \Lambda. \tag{2.4}$$

An  $L^2_{\mathbf{k}}$  solution of (2.4) is called a *Floquet-Bloch state*.

Since the  $\mathbf{k}$ -pseudo-periodic boundary condition in (2.4) is invariant under translations in the dual period lattice,  $\Lambda^*$ , it suffices to restrict our attention to  $\mathbf{k} \in \mathcal{B}$ , where  $\mathcal{B}$ , the Brillouin Zone, is a fundamental cell in  $\mathbf{k}$ -space.

An equivalent formulation to (2.4) is obtained by setting  $\Phi(\mathbf{x}; \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} p(\mathbf{x}; \mathbf{k})$ . Then,

$$H(\mathbf{k})p(\mathbf{x}; \mathbf{k}) = E(\mathbf{k})p(\mathbf{x}; \mathbf{k}), \quad \mathbf{x} \in \mathbb{R}^2, \quad p(\mathbf{x} + \mathbf{v}) = p(\mathbf{x}; \mathbf{k}), \quad \mathbf{v} \in \Lambda, \quad (2.5)$$

where  $H(\mathbf{k}) \equiv -(\nabla + i\mathbf{k})^2 + Q(\mathbf{x})$  is a self-adjoint operator on  $L^2(\mathbb{R}^2/\Lambda)$ . The eigenvalue problem (2.5), has a discrete set of eigenvalues  $E_1(\mathbf{k}) \leq E_2(\mathbf{k}) \leq \dots \leq E_b(\mathbf{k}) \leq \dots$ , with  $L^2(\mathbb{R}^2/\Lambda)$ -eigenfunctions  $p_b(\mathbf{x}; \mathbf{k})$ ,  $b = 1, 2, 3, \dots$ . The maps  $\mathbf{k} \in \mathcal{B} \mapsto E_j(\mathbf{k})$  are, in general, Lipschitz continuous functions; see, for example, Appendix A of [12]. For each  $\mathbf{k} \in \mathcal{B}$ , the set  $\{p_j(\mathbf{x}; \mathbf{k})\}_{j \geq 1}$  can be taken to be a complete orthonormal basis for  $L^2(\mathbb{R}^2/\Lambda)$ .

As  $\mathbf{k}$  varies over  $\mathcal{B}$ ,  $E_b(\mathbf{k})$  sweeps out a closed real interval. The union over  $b \geq 1$  of these closed intervals is exactly the  $L^2(\mathbb{R}^2)$ -spectrum of  $-\Delta + V(\mathbf{x})$ :  $\text{spec}(H) = \bigcup_{\mathbf{k} \in \mathcal{B}} \text{spec}(H(\mathbf{k}))$ . Furthermore, the set  $\{\Phi_b(\mathbf{x}; \mathbf{k})\}_{b \geq 1, \mathbf{k} \in \mathcal{B}}$  is complete in  $L^2(\mathbb{R}^2)$ :

$$f(\mathbf{x}) = \sum_{b \geq 1} \int_{\mathcal{B}} \langle \Phi_b(\cdot; \mathbf{k}), f(\cdot) \rangle_{L^2(\mathbb{R}^2)} \Phi_b(\mathbf{x}; \mathbf{k}) d\mathbf{k} \equiv \sum_{b \geq 1} \int_{\mathcal{B}} \tilde{f}_b(\mathbf{k}) \Phi_b(\mathbf{x}; \mathbf{k}) d\mathbf{k},$$

where the sum converges in the  $L^2$  norm.

### 2.3 The Honeycomb Period Lattice, $\Lambda_h$ , and its Dual, $\Lambda_h^*$

Consider  $\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$ , the equilateral triangular lattice generated by the basis vectors:  $\mathbf{v}_1 = (\frac{\sqrt{3}}{2}, \frac{1}{2})^T$ ,  $\mathbf{v}_2 = (\frac{\sqrt{3}}{2}, -\frac{1}{2})^T$ ; see Figure 3, left panel. The dual lattice  $\Lambda_h^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2$  is spanned by the dual basis vectors:  $\mathbf{k}_1 = q(\frac{1}{2}, \frac{\sqrt{3}}{2})^T$ ,  $\mathbf{k}_2 = q(\frac{1}{2}, -\frac{\sqrt{3}}{2})^T$ , where  $q \equiv \frac{4\pi}{\sqrt{3}}$ , with the biorthonormality relations  $\mathbf{k}_i \cdot \mathbf{v}_j = 2\pi\delta_{ij}$ . Other useful relations are:  $|\mathbf{v}_1| = |\mathbf{v}_2| = 1$ ,  $\mathbf{v}_1 \cdot \mathbf{v}_2 = \frac{1}{2}$ ,  $|\mathbf{k}_1| = |\mathbf{k}_2| = q$  and  $\mathbf{k}_1 \cdot \mathbf{k}_2 = -\frac{1}{2}q^2$ . The Brillouin zone,  $\mathcal{B}_h$ , is a regular hexagon in  $\mathbb{R}^2$ . Denote by  $\mathbf{K}$  and  $\mathbf{K}'$  its top and bottom vertices (see right panel of Figure 3) given by:  $\mathbf{K} \equiv \frac{1}{3}(\mathbf{k}_1 - \mathbf{k}_2)$ ,  $\mathbf{K}' \equiv -\mathbf{K} = \frac{1}{3}(\mathbf{k}_2 - \mathbf{k}_1)$ . All six vertices of  $\mathcal{B}_h$  can be generated by application of the matrix  $R$ , which rotates a vector in  $\mathbb{R}^2$  clockwise by  $2\pi/3$ :

$$R = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}. \quad (2.6)$$

The vertices of  $\mathcal{B}_h$  fall into two groups, generated by the action of  $R$  on  $\mathbf{K}$  and  $\mathbf{K}'$ :  $\mathbf{K}$ -type-points:  $\mathbf{K}$ ,  $R\mathbf{K} = \mathbf{K} + \mathbf{k}_2$ ,  $R^2\mathbf{K} = \mathbf{K} - \mathbf{k}_1$ , and  $\mathbf{K}'$ -type-points:  $\mathbf{K}'$ ,  $R\mathbf{K}' = \mathbf{K}' - \mathbf{k}_2$ ,  $R^2\mathbf{K}' = \mathbf{K}' + \mathbf{k}_1$ .

Functions which are periodic on  $\mathbb{R}^2$  with respect to the lattice  $\Lambda_h$  may be viewed as functions on the torus,  $\mathbb{R}^2/\Lambda_h$ . As a fundamental period cell, we choose the parallelogram spanned by  $\mathbf{v}_1$  and  $\mathbf{v}_2$ , denoted  $\Omega_h$ .

*Remark 2.3* (Symmetry Reduction). Let  $(\Phi(\mathbf{x}; \mathbf{k}), E(\mathbf{k}))$  denote a Floquet-Bloch eigenpair for the eigenvalue problem (2.4) with quasi-momentum  $\mathbf{k}$ . Since  $V$  is real,  $(\overline{\Phi(\mathbf{x}; \mathbf{k})} \equiv \Phi(\mathbf{x}; -\mathbf{k}), E(\mathbf{k}))$  is a Floquet-Bloch eigenpair for the eigenvalue problem with quasi-momentum  $-\mathbf{k}$ . The above relations among the vertices of  $\mathcal{B}_h$  and the  $\Lambda_h^*$ -periodicity of:  $\mathbf{k} \mapsto E(\mathbf{k})$  and  $\mathbf{k} \mapsto \Phi(\mathbf{x}; \mathbf{k})$  imply that the local character of the dispersion surfaces in a neighborhood of any vertex of  $\mathcal{B}_h$  is determined by its character about any other vertex of  $\mathcal{B}_h$ .

### 2.4 Honeycomb Potentials

**Definition 2.4** [Honeycomb potentials] Let  $V$  be real-valued and  $V \in C^\infty(\mathbb{R}^2)$ .  $V$  is a honeycomb potential if there exists  $\mathbf{x}_0 \in \mathbb{R}^2$  such that  $\tilde{V}(\mathbf{x}) = V(\mathbf{x} - \mathbf{x}_0)$  has the following properties:

- (V1)  $\tilde{V}$  is  $\Lambda_h$ -periodic, i.e.  $\tilde{V}(\mathbf{x} + \mathbf{v}) = \tilde{V}(\mathbf{x})$  for all  $\mathbf{x} \in \mathbb{R}^2$  and  $\mathbf{v} \in \Lambda_h$ .
- (V2)  $\tilde{V}$  is even or inversion-symmetric, i.e.  $\tilde{V}(-\mathbf{x}) = \tilde{V}(\mathbf{x})$ .
- (V3)  $\tilde{V}$  is  $\mathcal{R}$ -invariant, i.e.  $\mathcal{R}[\tilde{V}](\mathbf{x}) \equiv \tilde{V}(R^*\mathbf{x}) = \tilde{V}(\mathbf{x})$ , where,  $R^*$  is the counter-clockwise rotation matrix by  $2\pi/3$ , i.e.  $R^* = R^{-1}$ , where  $R$  is given by (2.6).

N.B. Throughout this paper, we shall omit the tildes on  $V$  and choose coordinates with  $\mathbf{x}_0 = 0$ .

Introduce the mapping  $\tilde{R} : \mathbb{Z}^2 \rightarrow \mathbb{Z}^2$  which acts on the indices of the Fourier coefficients of  $V$ :  $\tilde{R}(m_1, m_2) = (-m_2, m_1 - m_2)$  and therefore  $\tilde{R}^2(m_1, m_2) = (m_2 - m_1, -m_1)$ , and  $\tilde{R}^3(m_1, m_2) = (m_1, m_2)$ . Any  $\mathbf{m} \neq 0$  lies on an  $\tilde{R}$ -orbit of length exactly three [11]. We say that  $\mathbf{m}$  and  $\mathbf{n}$  are in the same equivalence class if  $\mathbf{m}$  and  $\mathbf{n}$  lie on the same 3-cycle. Let  $\tilde{S}$  denote a set consisting of exactly one representative from each equivalence class. Honeycomb lattice potentials have the following Fourier series characterization [11]:

**Proposition 2.5** Let  $V(\mathbf{x})$  denote a honeycomb lattice potential. Then,

$$V(\mathbf{x}) = v_0 + \sum_{\mathbf{m} \in \tilde{S}} v_{\mathbf{m}} \left[ \cos(\mathbf{m}\mathbf{k} \cdot \mathbf{x}) + \cos((\tilde{R}\mathbf{m})\mathbf{k} \cdot \mathbf{x}) + \cos((\tilde{R}^2\mathbf{m})\mathbf{k} \cdot \mathbf{x}) \right],$$

where  $\mathbf{m}\mathbf{k} = m_1\mathbf{k}_1 + m_2\mathbf{k}_2$  and the  $v_{\mathbf{m}}$  are real.

### 3 Dirac Points

In this section we summarize results of [11] on *Dirac points*. These are conical singularities in the dispersion surfaces of  $H_V = -\Delta + V(\mathbf{x})$ , where  $V$  is a honeycomb lattice potential.

Let  $\mathbf{K}_\star$  denote any vertex of  $\mathcal{B}_h$ , and recall that  $L^2_{\mathbf{K}_\star}$  is the space of  $\mathbf{K}_\star$ -pseudo-periodic functions. A key property of honeycomb lattice potentials,  $V$ , is that  $H_V$  and  $\mathcal{R}$ , defined in (V3) of Definition 2.4, leave a dense subspace of  $L^2_{\mathbf{K}_\star}$  invariant. Furthermore, restricted to this dense subspace of  $L^2_{\mathbf{K}_\star}$ ,  $H_V$  commutes with  $\mathcal{R}$ :  $[\mathcal{R}, H_V] = 0$ . Since  $\mathcal{R}$  has eigenvalues 1,  $\tau$  and  $\bar{\tau}$ , it is natural to split  $L^2_{\mathbf{K}_\star}$  into the direct sum:

$$L^2_{\mathbf{K}_\star} = L^2_{\mathbf{K}_\star,1} \oplus L^2_{\mathbf{K}_\star,\tau} \oplus L^2_{\mathbf{K}_\star,\bar{\tau}}.$$

Here,  $L^2_{\mathbf{K}_\star,\sigma}$ , where  $\sigma = 1, \tau, \bar{\tau}$  and  $\tau = \exp(2\pi i/3)$ , denote the invariant eigenspaces of  $\mathcal{R}$ :

$$L^2_{\mathbf{K}_\star,\sigma} = \left\{ g \in L^2_{\mathbf{K}_\star} : \mathcal{R}g = \sigma g \right\}.$$

We next give a precise definition of a Dirac point.

**Definition 3.1** Let  $V(\mathbf{x})$  be a smooth, real-valued, even (inversion symmetric) and periodic potential on  $\mathbb{R}^2$ . Denote by  $\mathcal{B}_h$ , the Brillouin zone. Let  $\mathbf{K} \in \mathcal{B}_h$ . The energy / quasi-momentum pair  $(\mathbf{K}, E_\star) \in \mathcal{B}_h \times \mathbb{R}$  is called a *Dirac point* if there exists  $b_\star \geq 1$  such that:

- (1)  $E_\star$  is a  $L^2_{\mathbf{K}}$ -eigenvalue of  $H_V$  of multiplicity two.
- (2)  $\text{Nullspace}(H_V - E_\star I) = \text{span}\left\{ \Phi_1(\mathbf{x}), \Phi_2(\mathbf{x}) \right\}$ , where  $\Phi_1 \in L^2_{\mathbf{K},\tau}$  ( $\mathcal{R}\Phi_1 = \tau\Phi_1$ ) and  $\Phi_2(\mathbf{x}) = (\mathcal{C} \circ \mathcal{I})[\Phi_1](\mathbf{x}) = \overline{\Phi_1(-\mathbf{x})} \in L^2_{\mathbf{K},\bar{\tau}}$  ( $\mathcal{R}\Phi_2 = \bar{\tau}\Phi_2$ ), and  $\langle \Phi_a, \Phi_b \rangle_{L^2_{\mathbf{K}}(\Omega)} = \delta_{ab}$ ,  $a, b = 1, 2$ .
- (3) There exist  $\lambda_\sharp \neq 0$ ,  $\zeta_0 > 0$ , and Floquet-Bloch eigenpairs

$$\mathbf{k} \mapsto (\Phi_{b_\star+1}(\mathbf{x}; \mathbf{k}), E_{b_\star+1}(\mathbf{k})) \text{ and } \mathbf{k} \mapsto (\Phi_{b_\star}(\mathbf{x}; \mathbf{k}), E_{b_\star}(\mathbf{k})),$$

and Lipschitz functions  $e_j(\mathbf{k})$ ,  $j = b_\star, b_\star + 1$ , where  $e_j(\mathbf{K}) = 0$ , defined for  $|\mathbf{k} - \mathbf{K}| < \zeta_0$  such that

$$\begin{aligned} E_{b_\star+1}(\mathbf{k}) - E_\star &= +|\lambda_\sharp| |\mathbf{k} - \mathbf{K}| (1 + e_{b_\star+1}(\mathbf{k})), \\ E_{b_\star}(\mathbf{k}) - E_\star &= -|\lambda_\sharp| |\mathbf{k} - \mathbf{K}| (1 + e_{b_\star}(\mathbf{k})), \end{aligned} \tag{3.1}$$

where  $|e_j(\mathbf{k})| \leq C|\mathbf{k} - \mathbf{K}|$ ,  $j = b_\star, b_\star + 1$ , for some  $C > 0$ .

In [11], the authors prove the following

**Proposition 3.2** Suppose conditions 1 and 2 of Definition 3.1 hold and let  $\{c(\mathbf{m})\}_{\mathbf{m} \in \mathcal{S}}$  denote the sequence of  $L^2_{\mathbf{K},\tau}$ -Fourier-coefficients of  $\Phi_1(\mathbf{x})$  normalized as in [11]. Define the sum

$$\lambda_\sharp \equiv \sum_{\mathbf{m} \in \mathcal{S}} c(\mathbf{m})^2 \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot (\mathbf{K} + \mathbf{m}\mathbf{k}). \tag{3.2}$$

Here,  $\mathcal{S} \subset \mathbb{Z}^2$  is defined in [11]. If  $\lambda_\sharp \neq 0$ , then condition 3 of Definition 3.1 holds (see (3.1)).

Therefore Dirac points are found by verifying conditions 1 and 2 of Definition 3.1 and the additional (non-degeneracy) condition:  $\lambda_{\sharp} \neq 0$ .

Furthermore, Theorem 4.1 of [11] and Theorem 3.2 of [12] imply the following local behavior of Floquet-Bloch modes near the Dirac point:<sup>1</sup>

**Corollary 3.3**

$$\Phi_{b_{\star+1}}(\mathbf{x}; \mathbf{k}) = \frac{1}{\sqrt{2}} \left[ \frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|} \frac{(\mathbf{k} - \mathbf{K})^{(1)} + i(\mathbf{k} - \mathbf{K})^{(2)}}{|\mathbf{k} - \mathbf{K}|} \Phi_1(\mathbf{x}) + \Phi_2(\mathbf{x}) \right] + \Phi_{b_{\star+1}}^{(1)}(\mathbf{x}; \mathbf{k}), \tag{3.3}$$

$$\Phi_{b_{\star}}(\mathbf{x}; \mathbf{k}) = \frac{1}{\sqrt{2}} \left[ \frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|} \frac{(\mathbf{k} - \mathbf{K})^{(1)} + i(\mathbf{k} - \mathbf{K})^{(2)}}{|\mathbf{k} - \mathbf{K}|} \Phi_1(\mathbf{x}) - \Phi_2(\mathbf{x}) \right] + \Phi_{b_{\star}}^{(1)}(\mathbf{x}; \mathbf{k}), \tag{3.4}$$

where  $\Phi_j^{(1)}(\cdot; \mathbf{k}) = \mathcal{O}(|\mathbf{k} - \mathbf{K}|)$  in  $H^2(\Omega_h)$  as  $|\mathbf{k} - \mathbf{K}| \rightarrow 0$ .

In the next section we discuss the result of [11], that  $-\Delta + \varepsilon V$  has Dirac points for generic  $\varepsilon$ .

**3.1 Dirac Points of  $-\Delta + \varepsilon V(\mathbf{x})$ ,  $\varepsilon$  Generic**

The strategy used in [11] to produce Dirac points is based on a bifurcation theory for the operator  $-\Delta + \varepsilon V(\mathbf{x})$  acting in  $L^2_{\mathbf{K}}$ , from the  $\varepsilon = 0$  limit. We describe the setup here, since we shall make detailed use of it.

Consider  $-\Delta$  acting on  $L^2_{\mathbf{K}}$ . We note that  $E_{\star}^0 \equiv |\mathbf{K}|^2$  is an eigenvalue with multiplicity three, since the three vertices of the regular hexagon,  $\mathcal{B}_h$ :  $\mathbf{K}$ ,  $R\mathbf{K}$  and  $R^2\mathbf{K}$  are equidistant from the origin. The corresponding three-dimensional eigenspace has an orthonormal basis consisting of the functions:  $\Phi_{\sigma}(\mathbf{x}) = e^{i\mathbf{K}\cdot\mathbf{x}} p_{\sigma}(\mathbf{x}) \in L^2_{\mathbf{K},\sigma}$ ,  $\sigma = 1, \tau, \bar{\tau}$ , defined by

$$\begin{aligned} \Phi_{\sigma}(\mathbf{x}) &= e^{i\mathbf{K}\cdot\mathbf{x}} p_{\sigma}(\mathbf{x}), \quad (\sigma = 1, \tau, \bar{\tau}) \\ &= \frac{1}{\sqrt{3|\Omega|}} \left[ e^{i\mathbf{K}\cdot\mathbf{x}} + \bar{\sigma} e^{iR\mathbf{K}\cdot\mathbf{x}} + \sigma e^{iR^2\mathbf{K}\cdot\mathbf{x}} \right] \\ &= \frac{1}{\sqrt{3|\Omega|}} e^{i\mathbf{K}\cdot\mathbf{x}} \left[ 1 + \bar{\sigma} e^{i\mathbf{k}_2\cdot\mathbf{x}} + \sigma e^{-i\mathbf{k}_1\cdot\mathbf{x}} \right]. \end{aligned} \tag{3.5}$$

We note that

$$\langle \Phi_{\sigma}, \Phi_{\bar{\sigma}} \rangle_{L^2_{\mathbf{K}}} = \langle p_{\sigma}, p_{\bar{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)} = \delta_{\sigma, \bar{\sigma}}. \tag{3.6}$$

---

<sup>1</sup> The factor  $\frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|}$  in (3.3)–(3.4) corrects a typographical error in equation (3.13) of [12].

In Theorem 5.1 of [11], the authors proved that for real, small and non-zero  $\varepsilon$  and under the assumption that  $V$  satisfies the non-degeneracy condition:

$$V_{1,1} \equiv \frac{1}{|\Omega_h|} \int_{\Omega_h} e^{-i(\mathbf{k}_1+\mathbf{k}_2)\cdot\mathbf{y}} V(\mathbf{y}) d\mathbf{y} \neq 0, \tag{3.7}$$

that the multiplicity three eigenvalue,  $E_\star^0 = |\mathbf{K}|^2$ , splits into

(A) a multiplicity two eigenvalue,  $E_\star^\varepsilon$ , with two-dimensional  $L^2_{\mathbf{K},\tau} \oplus L^2_{\mathbf{K},\bar{\tau}}$ -eigenspace structure, and

(B) a simple eigenvalue,  $\tilde{E}^\varepsilon$ , with one-dimensional eigenspace, a subspace of  $L^2_{\mathbf{K},1}$ .

For all  $\varepsilon$  sufficiently small, the quasi-momentum pairs  $(\mathbf{K}, E_\star^\varepsilon)$  are Dirac points in the sense of Definition 3.1. Furthermore, a continuation argument is then used to extend this result from the regime of sufficiently small  $\varepsilon$  to the regime of arbitrary  $\varepsilon$  outside of a possible discrete set; see [11] and the refinement concerning the possible exceptional set of  $\varepsilon$  values in Appendix D of [10]. We first state the result for arbitrarily large and generic  $\varepsilon$ , and then the more refined picture for  $|\varepsilon| > 0$  and sufficiently small.

**Theorem 3.4** [Generic  $\varepsilon$ ] *Let  $V(\mathbf{x})$  be a honeycomb lattice potential and consider the parameter family of Schrödinger operators:*

$$H^{(\varepsilon)} \equiv -\Delta + \varepsilon V(\mathbf{x}),$$

where  $V$  satisfies the non-degeneracy condition (3.7). Then, there exists  $\varepsilon_0 > 0$ , such that for all real and nonzero  $\varepsilon$ , outside of a possible discrete subset of  $\mathbb{R} \setminus (-\varepsilon_0, \varepsilon_0)$ ,  $H^{(\varepsilon)}$  has Dirac points  $(\mathbf{K}, E_\star^\varepsilon)$  in the sense of Definition 3.1. Specifically, for all such  $\varepsilon$ , there exists  $b_\star \geq 1$  such that  $E_\star \equiv E_{b_\star}^\varepsilon(\mathbf{K}) = E_{b_\star+1}^\varepsilon(\mathbf{K})$  is a  $\mathbf{K}$ -pseudo-periodic eigenvalue of multiplicity two where

- (1) (a)  $E_\star^\varepsilon$  is an  $L^2_{\mathbf{K},\tau}$ -eigenvalue of  $H^{(\varepsilon)}$  of multiplicity one, with corresponding eigenfunction,  $\Phi_1^\varepsilon(\mathbf{x})$ .
- (b)  $E_\star^\varepsilon$  is an  $L^2_{\mathbf{K},\bar{\tau}}$ -eigenvalue of  $H^{(\varepsilon)}$  of multiplicity one, with corresponding eigenfunction,  $\Phi_2^\varepsilon(\mathbf{x}) = \overline{\Phi_1^\varepsilon(-\mathbf{x})}$ .
- (c)  $E_\star^\varepsilon$  is not an  $L^2_{\mathbf{K},1}$ -eigenvalue of  $H^{(\varepsilon)}$ .
- (2) There exist  $\delta_\varepsilon > 0$ ,  $C_\varepsilon > 0$  and Floquet-Bloch eigenpairs:  $(\Phi_j^\varepsilon(\mathbf{x}; \mathbf{k}), E_j^\varepsilon(\mathbf{k}))$  and Lipschitz continuous functions,  $e_j(\mathbf{k})$ ,  $j = b_\star, b_\star+1$ , defined for  $|\mathbf{k}-\mathbf{K}| < \delta_\varepsilon$ , such that

$$\begin{aligned} E_{b_\star+1}^\varepsilon(\mathbf{k}) - E^\varepsilon(\mathbf{K}) &= +|\lambda_\mp^\varepsilon| |\mathbf{k} - \mathbf{K}| (1 + e_{b_\star+1}^\varepsilon(\mathbf{k})) \quad \text{and} \\ E_{b_\star}^\varepsilon(\mathbf{k}) - E^\varepsilon(\mathbf{K}) &= -|\lambda_\mp^\varepsilon| |\mathbf{k} - \mathbf{K}| (1 + e_{b_\star}^\varepsilon(\mathbf{k})), \end{aligned} \tag{3.8}$$

and where

$$\lambda_\mp^\varepsilon \equiv \sum_{\mathbf{m} \in \mathcal{S}} c(\mathbf{m}, E_\star^\varepsilon, \varepsilon)^2 \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot (\mathbf{K} + \mathbf{m}\mathbf{k}) \neq 0 \tag{3.9}$$

is given in terms of  $\{c(\mathbf{m}, E_\star^\varepsilon, \varepsilon)\}_{\mathbf{m} \in \mathcal{S}}$ , the  $L^2_{\mathbf{K}, \tau}$ -Fourier coefficients of  $\Phi_1^\varepsilon(\mathbf{x}; \mathbf{K})$ . Furthermore,  $|e_j^\varepsilon(\mathbf{k})| \leq C_\varepsilon |\mathbf{k} - \mathbf{K}|$ ,  $j = b_\star, b_\star + 1$ . Thus, in a neighborhood of the point  $(\mathbf{k}, E) = (\mathbf{K}, E_\star^\varepsilon) \in \mathbb{R}^3$ , the dispersion surface is closely approximated by a circular cone.

### 3.2 Dirac Points of $-\Delta + \varepsilon V(\mathbf{x})$ , $\varepsilon$ Small

In this section we collect explicit information on Dirac points for the weak potential regime.

**Theorem 3.5** [Small  $\varepsilon$ ] *There exists  $\varepsilon_0 > 0$ , such that for all  $\varepsilon \in I_{\varepsilon_0} \equiv (-\varepsilon_0, \varepsilon_0) \setminus \{0\}$  the following holds:*

- (1) For  $\varepsilon \in I_{\varepsilon_0}$ ,  $-\Delta + \varepsilon V(\mathbf{x})$  has
  - (a) a multiplicity two  $L^2_{\mathbf{K}}$ -eigenvalue  $E_\star^\varepsilon$ , where  $\ker(-\Delta + \varepsilon V) \subset L^2_{\mathbf{K}, \tau} \oplus L^2_{\mathbf{K}, \bar{\tau}}$ , and
  - (b) a multiplicity one  $L^2_{\mathbf{K}}$ -eigenvalue  $\tilde{E}_\star^\varepsilon$ , where  $\ker(-\Delta + \varepsilon V) \subset L^2_{\mathbf{K}, 1}$ .
- (2) The maps  $\varepsilon \mapsto E_\star^\varepsilon$  and  $\varepsilon \mapsto \tilde{E}_\star^\varepsilon$  are well defined for all  $\varepsilon$  in the deleted neighborhood of zero,  $I_{\varepsilon_0}$ . They are constructed via perturbation theory of a simple eigenvalue in  $L^2_{\mathbf{K}, \tau}$  and in  $L^2_{\mathbf{K}, 1}$ , respectively. Therefore,  $E_\star^\varepsilon$  and  $\tilde{E}_\star^\varepsilon$  are real-analytic functions of  $\varepsilon \in I_{\varepsilon_0}$ . Moreover, they have the expansions:

$$E_\star^\varepsilon = |\mathbf{K}|^2 + \varepsilon(V_{0,0} - V_{1,1}) + \mathcal{O}(\varepsilon^2), \tag{3.10}$$

$$\tilde{E}_\star^\varepsilon = |\mathbf{K}|^2 + \varepsilon(V_{0,0} + 2V_{1,1}) + \mathcal{O}(\varepsilon^2). \tag{3.11}$$

- (3) If  $\varepsilon V_{1,1} > 0$ , then conical intersections occur between the 1<sup>st</sup> and 2<sup>nd</sup> dispersion surfaces at the vertices of  $\mathcal{B}_h$ . Specifically, (3.8) holds with  $b_\star = 1$ .
- (4) If  $\varepsilon V_{1,1} < 0$ , then conical intersections occur between the 2<sup>nd</sup> and 3<sup>rd</sup> dispersion surfaces at the vertices of  $\mathcal{B}_h$ . Specifically, (3.8) holds with  $b_\star = 2$ .  
For  $\varepsilon \in I_{\varepsilon_0}$ ,

$$|\lambda_{\sharp}^\varepsilon| = 4\pi |\Omega_h| + \mathcal{O}(\varepsilon) = 4\pi |\mathbf{v}_1 \wedge \mathbf{v}_2| + \mathcal{O}(\varepsilon). \tag{3.12}$$

The expansions (3.10), (3.11) and (3.12) are displayed in equations (6.22), (6.25) and (6.30) of [11].

The intersections of the first two dispersion surfaces for  $\varepsilon V_{1,1} > 0$ , and of the second and third dispersion surfaces for  $\varepsilon V_{1,1} < 0$ , are illustrated in the first two panels of Figure 7 along a dispersion slice corresponding to the zigzag edge.

## 4 Edges and Dual Slices

Edge states are solutions of an eigenvalue equation on  $\mathbb{R}^2$ , which are spatially localized transverse to a line-defect or “edge” and propagating (plane-wave like or pseudo-periodic) parallel to the edge. Recall that  $\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$  and  $\Lambda_h^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2$ . We



consider edges which are lines of the form  $\mathbb{R}(a_1\mathbf{v}_1 + a_2\mathbf{v}_2)$ , where  $(a_1, b_1) = 1$ , i.e.  $a_1$  and  $b_1$  are relatively prime.

We fix an edge by choosing  $\mathbf{v}_1 = a_1\mathbf{v}_1 + b_1\mathbf{v}_2$ , where  $(a_1, b_1) = 1$ . Since  $a_1, b_1$  are relatively prime, there exists a relatively prime pair of integers:  $a_2, b_2$  such that  $a_1b_2 - a_2b_1 = 1$ . Set  $\mathbf{v}_2 = a_2\mathbf{v}_1 + b_2\mathbf{v}_2$ . It follows that  $\mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2 = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2 = \Lambda_h$ . Since  $a_1b_2 - a_2b_1 = 1$ , we have dual lattice vectors  $\mathfrak{K}_1, \mathfrak{K}_2 \in \Lambda_h^*$ , given by

$$\mathfrak{K}_1 = b_2\mathbf{k}_1 - a_2\mathbf{k}_2, \quad \mathfrak{K}_2 = -b_1\mathbf{k}_1 + a_1\mathbf{k}_2,$$

which satisfy

$$\mathfrak{K}_\ell \cdot \mathbf{v}_{\ell'} = 2\pi\delta_{\ell,\ell'}, \quad 1 \leq \ell, \ell' \leq 2.$$

Note that  $\mathbb{Z}\mathfrak{K}_1 \oplus \mathbb{Z}\mathfrak{K}_2 = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2 = \Lambda_h^*$ .

Fix an edge,  $\mathbb{R}\mathbf{v}_1$ . In our construction of edge states, an important role is played by the “quasi-momentum slice” of the band structure through the Dirac point and “dual” to the given edge.

**Definition 4.1** For the edge  $\mathbb{R}\mathbf{v}_1$ , the band structure slice at quasi-momentum  $\mathbf{K}$ , dual to the edge  $\mathbb{R}\mathbf{v}_1$ , is defined to be the locus given by the union of curves:

$$\lambda \mapsto E_b(\mathbf{K} + \lambda\mathfrak{K}_2), \quad |\lambda| \leq 1/2, \quad b \geq 1.$$

We give two examples:

- (1) Zigzag:  $\mathbf{v}_1 = \mathbf{v}_1, \mathbf{v}_2 = \mathbf{v}_2$  and  $\mathfrak{K}_1 = \mathbf{k}_1$  and  $\mathfrak{K}_2 = \mathbf{k}_2$ .  
In this case, we shall refer to the *zigzag slice*.
- (2) Armchair:  $\mathbf{v}_1 = \mathbf{v}_1 + \mathbf{v}_2, \mathbf{v}_2 = \mathbf{v}_2$  and  $\mathfrak{K}_1 = \mathbf{k}_1$  and  $\mathfrak{K}_2 = \mathbf{k}_2 - \mathbf{k}_1$ .  
In this case, we shall refer to the *armchair slice*.

Figure 7 (top row) displays three cases, for  $-\Delta + \varepsilon V$ , where  $V$  is a honeycomb lattice potential. Shown are the curves  $\lambda \mapsto E_b(\mathbf{K} + \lambda\mathfrak{K}_2), b = 1, 2, 3$  for (i)  $\varepsilon V_{1,1} > 0$  and the zigzag slice (left panel), (ii)  $\varepsilon V_{1,1} < 0$  and the zigzag slice (middle panel), and (iii) the armchair slice (right panel). As discussed in the introduction, of these three examples, case (i) is the one for which the spectral no-fold condition of Definition 7.1 holds.

### 4.1 Completeness of Floquet-Bloch Modes on $L^2(\Sigma)$

For  $\mathbf{v}_1 \in \Lambda_h$ , introduce the cylinder  $\Sigma = \mathbb{R}^2/\mathbb{Z}\mathbf{v}_1$ . Consider the family of states  $\Phi_b(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{K}_2)$ ,  $b \geq 1$  for  $\lambda \in [0, 1]$  (or equivalently  $|\lambda| \leq 1/2$ ) corresponding to quasi-momenta along a line segment within  $\mathcal{B}_h$  connecting  $\mathbf{K}$  to  $\mathbf{K} + \mathfrak{K}_2$ . Since  $\mathfrak{K}_2 \cdot \mathbf{v}_1 = 0$ , all along this segment we have  $\mathbf{K} \cdot \mathbf{v}_1$  - pseudo-periodicity:

$$\Phi_b(\mathbf{x} + \mathbf{v}_1; \mathbf{K} + \lambda\mathfrak{K}_2) = e^{i(\mathbf{K} + \lambda\mathfrak{K}_2) \cdot \mathbf{v}_1} \Phi_b(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{K}_2) = e^{i\mathbf{K} \cdot \mathbf{v}_1} \Phi_b(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{K}_2).$$

The main result of this subsection is that any  $f \in L^2_{k_{\parallel}=\mathbf{K} \cdot \mathbf{v}_1}(\Sigma)$  is a superposition of these modes.

**Theorem 4.2** Let  $f \in L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma) = L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\mathbb{R}^2/\mathbb{Z}\mathbf{v}_1)$ . Then,

(1)  $f$  can be represented as a superposition of Floquet-Bloch modes of  $-\Delta + V$  with quasimomenta in  $\mathcal{B}$  located on the segment  $\left\{ \mathbf{k} = \mathbf{K} + \lambda\mathbf{K}_2 : |\lambda| \leq \frac{1}{2} \right\}$ :

$$\begin{aligned} f(\mathbf{x}) &= \sum_{b \geq 1} \int_{-\frac{1}{2}}^{\frac{1}{2}} \tilde{f}_b(\lambda) \Phi_b(\mathbf{x}; \mathbf{K} + \lambda\mathbf{K}_2) d\lambda \\ &= e^{i\mathbf{K}\cdot\mathbf{x}} \sum_{b \geq 1} \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{i\lambda\mathbf{K}_2\cdot\mathbf{x}} \tilde{f}_b(\lambda) p_b(\mathbf{x}; \mathbf{K} + \lambda\mathbf{K}_2) d\lambda, \quad \text{where} \\ \tilde{f}_b(\lambda) &= \langle \Phi_b(\cdot, \mathbf{K} + \lambda\mathbf{K}_2), f(\cdot) \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)}. \end{aligned} \tag{4.1}$$

Here, the sum representing  $e^{-i\mathbf{K}\cdot\mathbf{x}} f(\mathbf{x})$ , in (4.1) converges in the  $L^2(\Sigma)$  norm.  
 (2) In the special case where  $V \equiv 0$ :

$$f(\mathbf{x}) = \sum_{\mathbf{m} \in \mathbb{Z}^2} e^{i(\mathbf{K}+\mathbf{m}\mathbf{K})\cdot\mathbf{x}} \int_{-\frac{1}{2}}^{\frac{1}{2}} \widehat{f}_{\mathbf{m}}(\lambda) e^{i\lambda\mathbf{K}_2\cdot\mathbf{x}} d\lambda.$$

*Proof of Theorem 4.2* We introduce the parameterizations of the fundamental period cell  $\Omega$  of  $V(\mathbf{x})$ :

$$\begin{aligned} \mathbf{x} \in \Omega : \mathbf{x} &= \tau_1\mathbf{v}_1 + \tau_2\mathbf{v}_2, \quad 0 \leq \tau_1, \tau_2 \leq 1, \quad \mathbf{k}_i \cdot \mathbf{x} = 2\pi\tau_i, \\ dx_1 dx_2 &= |\mathbf{v}_1 \wedge \mathbf{v}_2| d\tau_1 d\tau_2 = |\Omega| d\tau_1 d\tau_2; \end{aligned} \tag{4.2}$$

and of the cylinder  $\Sigma = \mathbb{R}^2/\mathbb{Z}\mathbf{v}_1$ :

$$\begin{aligned} \mathbf{x} \in \Sigma : \mathbf{x} &= \tau_1\mathbf{v}_1 + \tau_2\mathbf{v}_2, \quad 0 \leq \tau_1 \leq 1, \tau_2 \in \mathbb{R}, \quad \mathbf{K}_1 \cdot \mathbf{x} = 2\pi\tau_1, \quad \mathbf{K}_2 \cdot \mathbf{x} = 2\pi\tau_2, \\ dx_1 dx_2 &= |\mathbf{v}_1 \wedge \mathbf{v}_2| d\tau_1 d\tau_2 = |\Omega| d\tau_1 d\tau_2. \end{aligned} \tag{4.3}$$

Let  $f \in L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$  be such that  $g(\mathbf{x}) = e^{-i\mathbf{K}\cdot\mathbf{x}} f(\mathbf{x})$  is defined and smooth on  $\Sigma$ , and rapidly decreasing. It suffices to prove the result for such  $f$ , and then pass to all  $L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$  by standard arguments. The function  $g(\mathbf{x})$  has the Fourier representation

$$\begin{aligned} g(\mathbf{x}) &= 2\pi \sum_{n \in \mathbb{Z}} \int_{\mathbb{R}} \widehat{g}_n(2\pi\xi) e^{i\xi\mathbf{K}_2\cdot\mathbf{x}} d\xi e^{in\mathbf{K}_1\cdot\mathbf{x}}, \\ 2\pi \widehat{g}_n(2\pi\xi) &= \frac{1}{|\mathbf{v}_1 \wedge \mathbf{v}_2|} \int_{\Sigma} e^{-i\xi\mathbf{K}_2\cdot\mathbf{y}} e^{-in\mathbf{K}_1\cdot\mathbf{y}} g(\mathbf{y}) d\mathbf{y}. \end{aligned} \tag{4.4}$$

The relation (4.4) is obtained by noting that  $G(\tau_1, \tau_2) = g(\tau_1\mathbf{v}_1 + \tau_2\mathbf{v}_2)$  is 1-periodic in  $\tau_1$  and in  $L^2(\mathbb{R}; d\tau_2)$ , and applying the standard Fourier representations.

Introduce the Gelfand-Bloch transform

$$\tilde{g}(\mathbf{x}; \lambda) = 2\pi \sum_{(m_1, m_2) \in \mathbb{Z}^2} \widehat{g}_{m_1}(2\pi(m_2 + \lambda)) e^{i(m_1 \mathfrak{R}_1 + m_2 \mathfrak{R}_2) \cdot \mathbf{x}}, \quad |\lambda| \leq 1/2. \tag{4.5}$$

Note that  $\mathbf{x} \mapsto \tilde{g}(\mathbf{x}; \lambda)$  is  $\Lambda_h$ -periodic and  $\lambda \mapsto \tilde{g}(\mathbf{x}; \lambda)$  is 1-periodic. Using (4.5) and (4.4), it is straightforward to check that

$$g(\mathbf{x}) = \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{i\lambda \mathfrak{R}_2 \cdot \mathbf{x}} \tilde{g}(\mathbf{x}; \lambda) d\lambda. \tag{4.6}$$

*Remark 4.3* For any fixed  $|\lambda| \leq 1/2$ , the mapping  $\mathbf{x} \mapsto \tilde{g}(\mathbf{x}; \lambda)$  is  $\Lambda_h$ -periodic. We wish to expand  $\mathbf{x} \mapsto \tilde{g}(\mathbf{x}; \lambda)$  in terms of a basis for  $L^2(\Omega)$ , where  $\Omega$  denotes our choice of period cell (parallelogram) for  $\mathbb{R}^2/\Lambda$  with  $\Lambda = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$ ; see (2.1). Now the eigenvalue problem  $H(\mathbf{k})p^\Omega = E^\Omega p^\Omega$  on  $\Omega$  with periodic boundary conditions has a discrete sequence of eigenvalues,  $E_j^\Omega(\mathbf{k})$ ,  $j \geq 1$  with corresponding eigenfunctions  $p_j^\Omega(\mathbf{x}; \mathbf{k})$ ,  $j \geq 1$ , which can be taken to be a complete orthonormal sequence. Recall  $p_b^{\Omega_h}(\mathbf{x}; \mathbf{k})$ ,  $b \geq 1$ , with corresponding eigenvalues,  $E_b(\mathbf{k})$ , the complete set of eigenfunctions of  $H(\mathbf{k})$  with periodic boundary conditions on  $\Omega_h$ , the elementary period parallelogram spanned by  $\{\mathbf{v}_1, \mathbf{v}_2\}$ ; see Section 2.2. By periodicity,  $p_b^{\Omega_h}(\mathbf{x}; \mathbf{k})$ ,  $b \geq 1$ , (initially defined on  $\Omega_h$ ) and  $p_j^\Omega(\mathbf{x}; \mathbf{k})$ ,  $j \geq 1$ , (initially defined on  $\Omega$ ) can be extended to all  $\mathbb{R}^2$  as periodic functions. We continue to denote these extensions by:  $p_j^\Omega(\mathbf{x}; \mathbf{k})$  and  $p_b^{\Omega_h}(\mathbf{x}; \mathbf{k})$ , respectively. Since  $\Lambda = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2 = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2 = \Lambda_h$ , both sequences of eigenfunctions are  $\Lambda_h$ -periodic. Thus, in a natural way, we can take  $p_b^\Omega(\mathbf{x}; \mathbf{k}) = A_b p_b^{\Omega_h}(\mathbf{x}; \mathbf{k})$ ,  $b \geq 1$ , where  $A_b$  is a normalization constant. Abusing notation, we henceforth drop the explicit dependence on  $\Omega$ , and simply write  $p_b(\mathbf{x}; \mathbf{k})$  for  $p_b^\Omega(\mathbf{x}; \mathbf{k})$ .

In view of Remark 4.3 we expand  $\tilde{g}(\mathbf{x}; \lambda)$  in terms of the states  $\{p_b(\cdot; \mathbf{K} + \lambda \mathfrak{R}_2)\}$ ,  $b \geq 1$ :

$$\tilde{g}(\mathbf{x}; \lambda) = \sum_{b \geq 1} \langle p_b(\cdot; \mathbf{K} + \lambda \mathfrak{R}_2), \tilde{g}(\cdot, \lambda) \rangle_{L^2(\Omega)} p_b(\mathbf{x}; \mathbf{K} + \lambda \mathfrak{R}_2). \tag{4.7}$$

Recall that  $f(\mathbf{x}) = e^{i\mathbf{K} \cdot \mathbf{x}} g(\mathbf{x})$ . We claim (and prove below) that

$$\langle p_b(\cdot; \mathbf{K} + \lambda \mathfrak{R}_2), \tilde{g}(\cdot, \lambda) \rangle_{L^2(\Omega)} = \langle \Phi_b(\cdot; \mathbf{K} + \lambda \mathfrak{R}_2), f(\cdot) \rangle_{L^2_{k_{\parallel}=\mathbf{K} \cdot \mathbf{v}_1}(\Sigma)}. \tag{4.8}$$

The assertions of Theorem 4.2 then follow from (4.6), (4.7) and the claim (4.8):

$$f(\mathbf{x}) = e^{i\mathbf{K} \cdot \mathbf{x}} g(\mathbf{x}) = e^{i\mathbf{K} \cdot \mathbf{x}} \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{i\lambda \mathfrak{R}_2 \cdot \mathbf{x}} \tilde{g}(\mathbf{x}; \lambda) d\lambda$$

$$\begin{aligned}
 &= e^{i\mathbf{K}\cdot\mathbf{x}} \sum_{b \geq 1} \int_{-\frac{1}{2}}^{\frac{1}{2}} e^{i\lambda\mathfrak{K}_2\cdot\mathbf{x}} \langle p_b(\cdot; \mathbf{K} + \lambda\mathfrak{K}_2), \tilde{g}(\cdot, \lambda) \rangle_{L^2(\Omega)} p_b(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{K}_2) d\lambda \\
 &= \sum_{b \geq 1} \int_{-\frac{1}{2}}^{\frac{1}{2}} \langle \Phi_b(\cdot; \mathbf{K} + \lambda\mathfrak{K}_2), f(\cdot) \rangle_{L^2_{\mathbf{k}_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)} \Phi_b(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{K}_2) d\lambda,
 \end{aligned}$$

where, in the final line we have used that  $\Phi_b(\mathbf{y}; \lambda) = p_b(\mathbf{y}; \lambda)e^{i(\mathbf{K}+\lambda\mathfrak{K}_2)\cdot\mathbf{x}}$ . Therefore, it remains to prove claim (4.8). We shall employ the one-dimensional Poisson summation formula:

$$2\pi \sum_{n \in \mathbb{Z}} \widehat{f}(2\pi(n + \lambda)) e^{2\pi i n y} = \sum_{n \in \mathbb{Z}} f(y + n) e^{-2\pi i \lambda(y+n)}. \tag{4.9}$$

In the following calculation we use the abbreviated notation:

$$p_b(\mathbf{y}; \lambda) \equiv p_b(\mathbf{y}; \mathbf{K} + \lambda\mathfrak{K}_2) \quad \text{and} \quad \Phi_b(\mathbf{y}; \lambda) \equiv \Phi_b(\mathbf{y}; \mathbf{K} + \lambda\mathfrak{K}_2).$$

Substituting (4.4)–(4.5) into the left hand side of (4.8) and applying (4.9) gives

$$\begin{aligned}
 &\langle p_b(\cdot; \lambda), \tilde{g}(\cdot, \lambda) \rangle_{L^2(\Omega)} \\
 &= \int_{\Omega} \overline{p_b(\mathbf{y}; \lambda)} \tilde{g}(\mathbf{y}, \lambda) d\mathbf{y} \\
 &= |\Omega| \int_0^1 \int_0^1 \frac{1}{p_b(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2; \lambda)} 2\pi \sum_{\mathbf{m} \in \mathbb{Z}^2} \widehat{g}_{m_1}(2\pi(m_2 + \lambda)) e^{2\pi i(m_1 \tau_1 + m_2 \tau_2)} d\tau_1 d\tau_2 \tag{(4.2)} \\
 &= |\Omega| \int_0^1 \int_0^1 \frac{1}{p_b(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2; \lambda)} \sum_{m_1 \in \mathbb{Z}} \left[ 2\pi \sum_{m_2 \in \mathbb{Z}} \widehat{g}_{m_1}(2\pi(m_2 + \lambda)) e^{2\pi i m_2 \tau_2} \right] e^{2\pi i m_1 \tau_1} d\tau_1 d\tau_2 \\
 &= |\Omega| \int_0^1 \int_0^1 \frac{1}{p_b(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2; \lambda)} \sum_{m_1 \in \mathbb{Z}} \left[ \sum_{m_2 \in \mathbb{Z}} g_{m_1}(\tau_2 + m_2) e^{-2\pi i \lambda(\tau_2 + m_2)} \right] e^{2\pi i m_1 \tau_1} d\tau_1 d\tau_2 \tag{(4.9)} \\
 &= |\Omega| \int_0^1 \int_{\mathbb{R}} \frac{1}{p_b(\tau_1 \mathbf{v}_1 + s \mathbf{v}_2; \lambda)} e^{-2\pi i \lambda s} \sum_{m_1 \in \mathbb{Z}} g_{m_1}(s) e^{2\pi i m_1 \tau_1} d\tau_1 ds \quad (\tau_2 + m_2 = s) \\
 &= |\Omega| \int_0^1 \int_{\mathbb{R}} \frac{1}{p_b(\tau_1 \mathbf{v}_1 + s \mathbf{v}_2; \lambda)} e^{-2\pi i \lambda s} G(\tau_1, s) d\tau_1 ds \\
 &\quad (G(\tau_1, \tau_2) = g(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2) \text{ and (4.4)}) \\
 &= \int_{\Sigma} \overline{p_b(\mathbf{y}; \lambda)} e^{-i\lambda\mathfrak{K}_2\cdot\mathbf{x}} g(\mathbf{y}) d\mathbf{y} \quad (\text{by (4.3)}).
 \end{aligned}$$

Finally, recalling that  $g = e^{-i\mathbf{K}\cdot\mathbf{x}} f$  and  $\overline{p_b(\mathbf{y}; \lambda)} e^{-i(\mathbf{K}+\lambda\mathfrak{K}_2)\cdot\mathbf{x}} = \overline{\Phi_b(\mathbf{y}; \lambda)}$ , we obtain that

$$\begin{aligned}
 \langle p_b(\cdot; \lambda), \tilde{g}(\cdot, \lambda) \rangle_{L^2(\Omega)} &= \int_{\Sigma} \overline{p_b(\mathbf{y}; \lambda)} e^{-i\lambda\mathfrak{K}_2\cdot\mathbf{x}} e^{-i\mathbf{K}\cdot\mathbf{x}} f(\mathbf{y}) d\mathbf{y} \\
 &= \int_{\Sigma} \overline{\Phi_b(\mathbf{y}; \lambda)} f(\mathbf{y}) d\mathbf{y} \\
 &= \langle \Phi_b(\cdot; \lambda), f(\cdot) \rangle_{L^2_{\mathbf{k}_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)}.
 \end{aligned}$$

This completes the proof of claim (4.8) and part 1 for the case where  $f$  is smooth and rapidly decreasing. Passing to arbitrary  $f \in L^2_{k_{\parallel}}$  is standard. In the case where  $V \equiv 0$ , the Schrödinger operator reduces to the Laplacian  $-\Delta$ . In this case the Floquet-Bloch coefficients of  $f \in L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}$  are simply its Fourier coefficients:  $\tilde{f}(\lambda) = \widehat{f}(\lambda)$ . Part 2 therefore follows from part 1, completing the proof of Theorem 4.2.  $\square$

Sobolev regularity can be measured in terms of the Floquet-Bloch coefficients. Indeed, as in Lemma 2.1 in [10], by the  $2D$ -Weyl law  $E_b(\mathbf{K} + \lambda\mathfrak{R}_2) \approx b$  for all  $\lambda \in [-1/2, 1/2]$ ,  $b \gg 1$ , we have

**Corollary 4.4**  $L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$  and  $H^s_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$ ,  $s \in \mathbb{N}$ , norms can be expressed in terms of the Floquet-Bloch coefficients  $\tilde{f}_b(\lambda)$ ,  $b \geq 1$ . For  $f \in L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma) = L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\mathbb{R}^2/\mathbb{Z}\mathbf{v}_1)$ :

$$\begin{aligned} \|f\|^2_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)} &\sim \sum_{b \geq 1} \int_{-\frac{1}{2}}^{\frac{1}{2}} |\tilde{f}_b(\lambda)|^2 d\lambda, \\ \|f\|^2_{H^s_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)} &\sim \sum_{b \geq 1} (1+b)^s \int_{-\frac{1}{2}}^{\frac{1}{2}} |\tilde{f}_b(\lambda)|^2 d\lambda. \end{aligned}$$

### 4.2 Expansion of $\mathbf{k} \mapsto E_b(\mathbf{k})$ Along a Quasi-Momentum Slice

Let  $(\mathbf{K}, E_*)$  denote a Dirac point as in Definition 3.1. In a neighborhood of the Dirac point, the eigenvalues  $E_{b_*}(\mathbf{k})$  and  $E_{b_*+1}(\mathbf{k})$  are Lipschitz continuous functions and the corresponding normalized eigenmodes,  $\Phi_{b_*}(\mathbf{x}; \mathbf{k})$  and  $\Phi_{b_*+1}(\mathbf{x}; \mathbf{k})$  are discontinuous functions of  $\mathbf{k}$ ; see [12]. Note however that what is relevant to our construction of  $\mathbf{v}_1$ -edge states are Floquet-Bloch modes along the quasi-momentum line  $\mathbf{K} + \lambda\mathfrak{R}_2$ ,  $|\lambda| \leq 1/2$ . The following proposition gives a smooth parametrization of these modes along this quasi-momentum line.

**Proposition 4.5** Let  $(\mathbf{K}, E_*)$  denote a Dirac point in the sense of Definition 3.1. Let  $\{\Phi_1(\mathbf{x}), \Phi_2(\mathbf{x})\}$  denote the basis of the  $L^2_{\mathbf{K}} = L^2_{\mathbf{K},\tau} \oplus L^2_{\mathbf{K},\bar{\tau}}$ -nullspace of  $H_V - E_*I$  in Definition 3.1. Introduce the  $\Lambda_h$ -periodic functions

$$P_1(\mathbf{x}) = e^{-i\mathbf{K}\cdot\mathbf{x}}\Phi_1(\mathbf{x}), \quad P_2(\mathbf{x}) = e^{-i\mathbf{K}\cdot\mathbf{x}}\Phi_2(\mathbf{x}). \tag{4.10}$$

For each  $|\lambda| \leq 1/2$ , there exist  $L^2_{\mathbf{K}+\lambda\mathfrak{R}_2}$ -eigenpairs  $(\Phi_{\pm}(\mathbf{x}; \lambda), E_{\pm}(\lambda))$ , real analytic in  $\lambda$ , such that  $\langle \Phi_a(\cdot; \lambda), \Phi_b(\cdot; \lambda) \rangle = \delta_{ab}$  and

$$\text{span} \{ \Phi_{-}(\mathbf{x}; \lambda), \Phi_{+}(\mathbf{x}; \lambda) \} = \text{span} \{ \Phi_{b_*}(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{R}_2), \Phi_{b_*+1}(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{R}_2) \}.$$

Introduce  $\Lambda_h$ -periodic functions  $p_{\pm}(\mathbf{x}; \lambda)$  by

$$\Phi_{\pm}(\mathbf{x}; \lambda) = e^{i(\mathbf{K}+\lambda\mathfrak{R}_2)\cdot\mathbf{x}} p_{\pm}(\mathbf{x}; \lambda), \quad \langle p_a(\cdot; \lambda), p_b(\cdot; \lambda) \rangle = \delta_{ab}, \quad a, b \in \{+, -\}. \tag{4.11}$$

There is a constant  $\zeta_0 > 0$  such that for  $|\lambda| < \zeta_0$  the following holds:

(1) The mapping  $\lambda \mapsto E_{\pm}(\lambda)$  is real analytic in  $\lambda$  with expansion

$$E_{\pm}(\lambda) = E_{\star} \pm |\lambda_{\sharp}| |\mathfrak{K}_2| \lambda + E_{2,\pm}(\lambda)\lambda^2, \tag{4.12}$$

where  $\lambda_{\sharp} \in \mathbb{C}$  is given by (3.2),  $|E_{2,\pm}(\lambda)| \leq C$  with  $C$  a positive constant independent of  $\lambda$ .

(2) Let  $\mathfrak{z}_2 = \mathfrak{K}_2^{(1)} + i\mathfrak{K}_2^{(2)}$ ,  $|\mathfrak{z}_2| = |\mathfrak{K}_2|$ . The  $\Lambda_h$ -periodic functions,  $p_{\pm}(\mathbf{x}; \lambda)$ , can be chosen to depend real analytically on  $\lambda$  and so that<sup>2</sup>

$$p_{\pm}(\mathbf{x}; \lambda) = P_{\pm}(\mathbf{x}) + \varphi_{\pm}(\mathbf{x}, \lambda) \in L^2_{\mathbf{K}}(\mathbb{R}^2/\Lambda_h), \tag{4.13}$$

where  $p_{\pm}(\mathbf{x}; 0) = P_{\pm}(\mathbf{x})$  is given by

$$P_{\pm}(\mathbf{x}) \equiv \frac{1}{\sqrt{2}} \left[ \frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|} \frac{\mathfrak{z}_2}{|\mathfrak{z}_2|} P_1(\mathbf{x}) \pm P_2(\mathbf{x}) \right],$$

and  $\Phi_{\pm}(\mathbf{x}; 0) = \Phi_{\pm}(\mathbf{x})$  is given by

$$\Phi_{\pm}(\mathbf{x}) \equiv \frac{1}{\sqrt{2}} \left[ \frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|} \frac{\mathfrak{z}_2}{|\mathfrak{z}_2|} \Phi_1(\mathbf{x}) \pm \Phi_2(\mathbf{x}) \right]. \tag{4.14}$$

Finally,  $\lambda \mapsto \varphi_{\pm}(\mathbf{x}; \lambda)$  are real analytic satisfying the bound  $|\partial_{\mathbf{x}}^{\mathfrak{N}} \varphi_{\pm}(\mathbf{x}; \lambda)| \leq C'\lambda$  for all  $\mathbf{x} \in \Lambda_h$ , where  $\mathfrak{N} = (\mathfrak{N}_1, \mathfrak{N}_2)$ ,  $|\mathfrak{N}| \leq 2$ .

N.B. We wish to point out that the subscripts  $\pm$  have a different meaning here than in [11, 12]. In [11, 12],  $E_{\pm}(\mathbf{k})$  denote ordered eigenvalues,  $E_{-}(\mathbf{k}) \leq E_{+}(\mathbf{k})$  (Lipschitz continuous) with corresponding eigenstates  $\Phi_{\pm}(\mathbf{x}; \mathbf{k})$  (discontinuous at  $\mathbf{k} = \mathbf{K}$ ); see Definition 3.1 and Corollary 3.3. In Proposition 4.5 and throughout this paper  $E_{\pm}(\lambda)$  and  $\Phi_{\pm}(\mathbf{x}; \lambda)$  refer to smooth parametrizations in  $\lambda$  of Floquet-Bloch eigenvalues and eigenfunctions of the spectral bands, which intersect at energy  $E_{\star}$ .

*Proof of Proposition 4.5* We present a proof along the lines of Theorem 3.2 in [12]; see also [13, 20]. The  $\mathbf{k}$ -pseudo-periodic Floquet-Bloch modes can be expressed in the form  $\Phi(\mathbf{x}; \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} p(\mathbf{x}; \mathbf{k})$ , where  $p(\mathbf{x}; \mathbf{k})$  is  $\Lambda_h$ -periodic. For  $\mathbf{k} = \mathbf{K} + \lambda\mathfrak{K}_2$ , consider the family of eigenvalue problems, parametrized by  $|\lambda| \leq 1/2$ :

$$H_V(\mathbf{K} + \lambda\mathfrak{K}_2) p(\mathbf{x}; \lambda) = E(\lambda) p(\mathbf{x}; \lambda), \tag{4.15}$$

$$p(\mathbf{x} + \mathbf{v}; \lambda) = p(\mathbf{x}; \lambda), \text{ for all } \mathbf{v} \in \Lambda_h, \tag{4.16}$$

where  $H_V(\mathbf{k}) \equiv -(\nabla_{\mathbf{x}} + i\mathbf{k})^2 + V(\mathbf{x})$ . Degenerate perturbation theory of the double eigenvalue  $E_{\star}$  of  $H_V(\mathbf{K})$ , yields eigenvalues:  $E_{\pm}(\lambda) = E_{\star} + E_{\pm}^{(1)}(\lambda)$ , where

$$E_{\pm}^{(1)}(\lambda) \equiv \pm |\lambda_{\sharp}| |\mathfrak{K}_2| \lambda + \mathcal{O}(\lambda^2); \text{ see [11].} \tag{4.17}$$

<sup>2</sup> The factor of  $\frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|}$  in (4.13) corrects a typographical error in equation (3.13) of [12].

Denote by  $Q_{\perp}$  the projection onto the orthogonal complement of  $\text{span}\{P_1, P_2\}$ . Then,

$$R_{\mathbf{K}}(E_{\star}) \equiv (H_V(\mathbf{K}) - E_{\star} I)^{-1} : Q_{\perp} L^2(\mathbb{R}^2/\Lambda_h) \rightarrow Q_{\perp} L^2(\mathbb{R}^2/\Lambda_h)$$

is bounded. Furthermore, via Lyapunov-Schmidt reduction analysis of the periodic eigenvalue problem (4.15)–(4.16) we obtain, corresponding to the eigenvalues (4.17), the  $\Lambda_h$ - periodic eigenstates:

$$p_{\pm}(\mathbf{x}; \lambda) = (I + R_{\mathbf{K}}(E_{\star})Q_{\perp}(2i\lambda \mathfrak{K}_2 \cdot (\nabla + i\mathbf{K}))) \times (\alpha(\lambda) P_1(\mathbf{x}) + \beta(\lambda) P_2(\mathbf{x})) + \mathcal{O}_{H^2(\mathbb{R}^2/\Lambda_h)}\left(\lambda(|\alpha|^2 + |\beta|^2)^{\frac{1}{2}}\right).$$

Here, the pair  $\alpha(\lambda), \beta(\lambda)$  satisfies the homogeneous system:

$$\mathcal{M}(E^{(1)}, \lambda) \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = 0, \quad \text{where} \\ \mathcal{M}(E^{(1)}, \lambda) \equiv \begin{pmatrix} E^{(1)} + \mathcal{O}(\lambda^2) & -\bar{\lambda}_{\pm} \lambda \mathfrak{z}_2 + \mathcal{O}(\lambda^2) \\ -\lambda_{\pm} \lambda \bar{\mathfrak{z}}_2 + \mathcal{O}(\lambda^2) & E^{(1)} + \mathcal{O}(\lambda^2) \end{pmatrix};$$

see [11]. For  $E^{(1)} = E_j^{(1)}(\lambda)$ ,  $j = \pm$ , normalized solutions,  $p_j(\mathbf{k}; \lambda)$ ,  $j = \pm$ , are obtained by choosing:

$$\begin{pmatrix} \alpha_{+}(\lambda) \\ \beta_{+}(\lambda) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \frac{\bar{\lambda}_{\pm}}{|\bar{\lambda}_{\pm}|} \frac{\mathfrak{z}_2}{|\mathfrak{z}_2|} + \mathcal{O}(\lambda) \\ +\frac{1}{\sqrt{2}} + \mathcal{O}(\lambda) \end{pmatrix}, \quad \begin{pmatrix} \alpha_{-}(\lambda) \\ \beta_{-}(\lambda) \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \frac{\bar{\lambda}_{\pm}}{|\bar{\lambda}_{\pm}|} \frac{\mathfrak{z}_2}{|\mathfrak{z}_2|} + \mathcal{O}(\lambda) \\ -\frac{1}{\sqrt{2}} + \mathcal{O}(\lambda) \end{pmatrix}.$$

Finally, we note that  $\mathcal{M}(E^{(1)}, \lambda)$  is analytic in the parameter  $\lambda$ . Therefore the eigenvalues  $E_{\pm}^{(1)}(\lambda)$  and eigenvectors  $(\alpha_{\pm}(\lambda), \beta_{\pm}(\lambda))^T$  are analytic functions of  $\lambda$ ; see, for example, [13,20]. It follows that  $E_{\pm}(\lambda)$  and  $p_{\pm}(\mathbf{x}; \lambda)$  are bounded, real analytic functions of  $\lambda \in \mathbb{R}$ . This completes the proof of Proposition 4.5.  $\square$

### 5 Model of a Honeycomb Structure with an Edge

Let  $V(\mathbf{x})$  denote a honeycomb potential in the sense of Definition 2.4. In this section we introduce a model of an edge in a honeycomb structure. A one-dimensional variant of this model was introduced and studied in [7,10,25].

Let  $W \in C^{\infty}(\mathbb{R}^2)$  be real-valued and satisfy the following properties:

- (W1)  $W$  is  $\Lambda_h$ - periodic, i.e.  $W(\mathbf{x} + \mathbf{v}) = W(\mathbf{x})$  for all  $\mathbf{x} \in \mathbb{R}^2$  and  $\mathbf{v} \in \Lambda_h$ .
- (W2)  $W$  is odd, i.e.  $W(-\mathbf{x}) = -W(\mathbf{x})$ .
- (W3)  $\vartheta_{\pm} \equiv \langle \Phi_1, W\Phi_1 \rangle_{L^2(\Omega_h)} \neq 0$ , with  $\Phi_1$  as in Definition 3.1.

The non-degeneracy condition (W3) arises in the multiple scale perturbation theory of Section 6.

Our model of a honeycomb structure with an edge is a smooth and slow interpolation between the Schrödinger Hamiltonians  $H_{-\infty}^{(\delta)} = -\Delta_{\mathbf{x}} + V(\mathbf{x}) - \delta\kappa_{\infty} W(\mathbf{x})$  and  $H_{+\infty}^{(\delta)} =$

$-\Delta_{\mathbf{x}} + V(\mathbf{x}) + \delta\kappa_{\infty}W(\mathbf{x})$ , which is transverse to a lattice direction, say  $\mathbf{v}_1$ . Here,  $\kappa_{\infty}$  is a positive constant. This interpolation is effected by a *domain wall function*.

**Definition 5.1** We call  $\kappa(\zeta) \in C^{\infty}(\mathbb{R})$  a domain wall function if  $\kappa(\zeta)$  tends to  $\pm\kappa_{\infty}$  as  $\zeta \rightarrow \pm\infty$ , and  $\Upsilon_1(\zeta) = \kappa^2(\zeta) - \kappa_{\infty}^2$  and  $\Upsilon_2(\zeta) = \kappa'(\zeta)$  satisfy:

$$\int_{\mathbb{R}} (1 + |\zeta|)^a |\Upsilon_{\ell}(\zeta)| d\zeta < \infty \text{ for some } a > 5/2 \text{ and} \\ \int_{\mathbb{R}} |\partial_{\zeta} \Upsilon_{\ell}(\zeta)| d\zeta < \infty, \quad \ell = 1, 2. \tag{5.1}$$

Without loss of generality, we assume  $\kappa_{\infty} > 0$ .

*Remark 5.2* The technical hypotheses in (5.1) are required for the boundedness of *wave operators* used in the proof of Proposition 7.15. See also Section 6.6 of [10] and, in particular, the application of Theorem 6.15.

Our model of a honeycomb structure with an edge is the domain-wall modulated Hamiltonian:

$$H^{(\delta)} = -\Delta_{\mathbf{x}} + V(\mathbf{x}) + \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x})W(\mathbf{x}),$$

where  $\kappa(\zeta)$  is a domain wall function. Suppose  $\kappa(\zeta)$  has a single zero at  $\zeta = 0$ . The “edge” is then given by  $\mathbb{R}\mathbf{v}_1 = \{\mathbf{x} : \mathfrak{K}_2 \cdot \mathbf{x} = 0\}$ .

We shall seek solutions of the eigenvalue problem

$$H^{(\delta)}\Psi = E\Psi, \tag{5.2}$$

$$\Psi(\mathbf{x} + \mathbf{v}_1) = e^{i\mathbf{K} \cdot \mathbf{v}_1} \Psi(\mathbf{x}) \quad (\text{propagation parallel to the edge, } \mathbb{R}\mathbf{v}_1), \tag{5.3}$$

$$\Psi(\mathbf{x}) \rightarrow 0 \text{ as } |\mathbf{x} \cdot \mathfrak{K}_2| \rightarrow \infty \quad (\text{localization transverse to the edge, } \mathbb{R}\mathbf{v}_1). \tag{5.4}$$

In the next section we present a formal asymptotic expansion of  $\mathbf{v}_1$ – edge states and in Section 7 we formulate a rigorous theory.

### 6 Multiple Scales and Effective Dirac Equations

We re-express the eigenvalue problem (5.2)–(5.4) in terms of an unknown function  $\Psi = \Psi(\mathbf{x}, \zeta)$ , depending on fast ( $\mathbf{x}$ ) and slow ( $\zeta = \delta\mathfrak{K}_2 \cdot \mathbf{x}$ ) spatial scales:

$$\left[ -(\nabla_{\mathbf{x}} + \delta\mathfrak{K}_2\partial_{\zeta})^2 + V(\mathbf{x}) \right] \Psi + \delta\kappa(\zeta)W(\mathbf{x})\Psi = E\Psi, \tag{6.1}$$

$$\Psi(\mathbf{x} + \mathbf{v}_1, \zeta) = e^{i\mathbf{K} \cdot \mathbf{v}_1} \Psi(\mathbf{x}, \zeta), \text{ and } \Psi(\mathbf{x}, \zeta) \rightarrow 0 \text{ as } \zeta \rightarrow \pm\infty. \tag{6.2}$$

We seek a solution to (6.1)–(6.2) in the form:

$$E^{\delta} = E^{(0)} + \delta E^{(1)} + \delta^2 E^{(2)} + \dots, \tag{6.3}$$



$$\Psi^\delta = \psi^{(0)}(\mathbf{x}, \zeta) + \delta\psi^{(1)}(\mathbf{x}, \zeta) + \delta^2\psi^{(2)}(\mathbf{x}, \zeta) + \dots \tag{6.4}$$

The conditions (5.3), (5.4) are encoded by requiring, for  $i \geq 0$ , that

$$\begin{aligned} \psi^{(i)}(\mathbf{x} + \mathbf{v}, \cdot) &= e^{i\mathbf{K}\cdot\mathbf{v}}\psi^{(i)}(\mathbf{x}, \cdot) \quad \forall \mathbf{v} \in \Lambda_h, \\ \zeta &\rightarrow \psi^{(i)}(\mathbf{x}, \zeta) \in L^2(\mathbb{R}_\zeta). \end{aligned}$$

Substituting the expansions (6.3)–(6.4) in (6.1) yields

$$\begin{aligned} &\left[ -\left( \Delta_{\mathbf{x}} + 2\delta \mathfrak{K}_2 \cdot \nabla_{\mathbf{x}} \partial_\zeta + \delta^2 |\mathfrak{K}_2|^2 \partial_\zeta^2 + \dots \right) + (V(\mathbf{x}) + \delta\kappa(\zeta)W(\mathbf{x})) \right. \\ &\quad \left. - \left( E^{(0)} + \delta E^{(1)} + \delta^2 E^{(2)} + \dots \right) \right] \left( \psi^{(0)} + \delta\psi^{(1)} + \delta^2\psi^{(2)} + \dots \right) = 0. \end{aligned}$$

Equating terms of equal order in  $\delta^j$ ,  $j \geq 0$ , yields a hierarchy of equations governing  $\psi^{(j)}(\mathbf{x}, \zeta)$ .

At order  $\delta^0$  we have that  $(E^{(0)}, \psi^{(0)})$  satisfy

$$\begin{aligned} &(-\Delta_{\mathbf{x}} + V(\mathbf{x}) - E^{(0)})\psi^{(0)} = 0, \\ \psi^{(0)}(\mathbf{x} + \mathbf{v}, \cdot) &= e^{i\mathbf{K}\cdot\mathbf{v}}\psi^{(0)}(\mathbf{x}, \cdot) \quad \forall \mathbf{v} \in \Lambda_h. \end{aligned} \tag{6.5}$$

Equation (6.5) may be solved in terms of the orthonormal basis of the  $L^2_{\mathbf{K}}(\Omega)$ –nullspace of  $H_V - E_\star$  in Definition 3.1, namely  $\{\Phi_+, \Phi_-\}$ . Expansion (4.13) in Proposition 4.5 suggests that a particularly natural orthonormal basis of the  $L^2_{\mathbf{K}}(\Omega)$ – nullspace of  $H_V - E_\star$  is given by  $\{\Phi_+, \Phi_-\}$ , where

$$\Phi_\pm(\mathbf{x}) \equiv \frac{1}{\sqrt{2}} \left[ \frac{\overline{\lambda_\sharp}}{|\lambda_\sharp|} \frac{\mathfrak{z}_2}{|\mathfrak{z}_2|} \Phi_1(\mathbf{x}) \pm \Phi_2(\mathbf{x}) \right]. \tag{6.6}$$

Here  $\lambda_\sharp$  is given in (3.2),  $\mathfrak{z}_2 = \mathfrak{K}_2^{(1)} + i\mathfrak{K}_2^{(2)}$  and  $|\mathfrak{z}_2| = |\mathfrak{K}_2|$ . We therefore solve (6.5) with

$$E^{(0)} = E_\star, \quad \psi^{(0)}(\mathbf{x}, \zeta) = \alpha_+(\zeta)\Phi_+(\mathbf{x}) + \alpha_-(\zeta)\Phi_-(\mathbf{x}). \tag{6.7}$$

Proceeding to order  $\delta^1$  we find that  $(E^{(1)}, \psi^{(1)})$  satisfies

$$\begin{aligned} &(-\Delta_{\mathbf{x}} + V(\mathbf{x}) - E_\star)\psi^{(1)}(\mathbf{x}, \zeta) = G^{(1)}(\mathbf{x}, \zeta; \psi^{(0)}) + E^{(1)}\psi^{(0)}, \\ \psi^{(1)}(\mathbf{x} + \mathbf{v}, \cdot) &= e^{i\mathbf{K}\cdot\mathbf{v}}\psi^{(1)}(\mathbf{x}, \cdot) \quad \forall \mathbf{v} \in \Lambda_h, \end{aligned} \tag{6.8}$$

where

$$\begin{aligned} &G^{(1)}(\mathbf{x}, \zeta; \psi^{(0)}) \\ &= G^{(1)}(\mathbf{x}, \zeta; \alpha_+, \alpha_-) \\ &\equiv 2\partial_\zeta\alpha_+ \mathfrak{K}_2 \cdot \nabla_{\mathbf{x}}\Phi_+ + 2\partial_\zeta\alpha_- \mathfrak{K}_2 \cdot \nabla_{\mathbf{x}}\Phi_- - \kappa(\zeta)W(\mathbf{x})(\alpha_+\Phi_+ + \alpha_-\Phi_-). \end{aligned}$$

Viewed as an equation in  $\mathbf{x}$ , (6.8) is solvable if and only if its right hand side is  $L^2_{\mathbf{K}}(\Omega; d\mathbf{x})$ - orthogonal to the nullspace of  $H_V - E_*$ . This is expressible in terms of the two orthogonality conditions:

$$-E^{(1)}\alpha_j = 2\langle \Phi_j, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_+ \rangle \partial_{\zeta}\alpha_+ + 2\langle \Phi_j, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_- \rangle \partial_{\zeta}\alpha_- - \kappa(\zeta) [\langle \Phi_j, W\Phi_+ \rangle \alpha_+ + \langle \Phi_j, W\Phi_- \rangle \alpha_-], \quad j = \pm. \tag{6.9}$$

We evaluate the inner products in (6.9) using the following two propositions.

**Proposition 6.1**

$$\langle \Phi_+, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_- \rangle_{L^2_{\mathbf{K}}(\Omega)} = 0, \tag{6.10}$$

$$\langle \Phi_-, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_+ \rangle_{L^2_{\mathbf{K}}(\Omega)} = 0, \tag{6.11}$$

$$2\langle \Phi_+, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_+ \rangle_{L^2_{\mathbf{K}}(\Omega)} = +i|\lambda_{\sharp}| |\mathfrak{R}_2|, \tag{6.12}$$

$$2\langle \Phi_-, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_- \rangle_{L^2_{\mathbf{K}}(\Omega)} = -i|\lambda_{\sharp}| |\mathfrak{R}_2|, \tag{6.13}$$

The constant,  $\lambda_{\sharp} \in \mathbb{C}$ , is generically non-zero; see Theorem 3.4.

*Proof* Let  $\mathfrak{z}_2 = \mathfrak{R}_2^{(1)} + i\mathfrak{R}_2^{(2)}$ . By (7.28)–(7.29) of [12] (see also [11]) we have:

$$\langle \Phi_1, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_2 \rangle_{L^2_{\mathbf{K}}(\Omega)} = \frac{i}{2} \bar{\lambda}_{\sharp} \mathfrak{z}_2, \tag{6.14}$$

$$\langle \Phi_2, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_1 \rangle_{L^2_{\mathbf{K}}(\Omega)} = \frac{i}{2} \lambda_{\sharp} \bar{\mathfrak{z}}_2, \tag{6.15}$$

$$\langle \Phi_b, \mathfrak{R}_2 \cdot \nabla_{\mathbf{x}}\Phi_b \rangle_{L^2_{\mathbf{K}}(\Omega)} = 0, \quad b = 1, 2. \tag{6.16}$$

Relations (6.10)–(6.13) follow from the expressions for  $\Phi_{\pm}$  in (6.6) and relations (6.14)–(6.16). □

**Proposition 6.2** Assume that  $W(\mathbf{x})$  is real-valued, odd and  $\Lambda_h$ - periodic. Let  $\vartheta_{\sharp} \equiv \langle \Phi_1, W\Phi_1 \rangle_{L^2_{\mathbf{K}}(\Omega)}$ . Then,  $\vartheta_{\sharp} \in \mathbb{R}$  and

$$\vartheta_{\sharp} = \langle \Phi_+, W\Phi_- \rangle_{L^2_{\mathbf{K}}(\Omega)} = \langle \Phi_-, W\Phi_+ \rangle_{L^2_{\mathbf{K}}(\Omega)}, \tag{6.17}$$

$$\langle \Phi_+, W\Phi_+ \rangle_{L^2_{\mathbf{K}}(\Omega)} = \langle \Phi_-, W\Phi_- \rangle_{L^2_{\mathbf{K}}(\Omega)} = 0. \tag{6.18}$$

Note that since  $\Phi_+(\mathbf{x}) = e^{i\mathbf{K}\cdot\mathbf{x}}P_+(\mathbf{x})$  and  $\Phi_-(\mathbf{x}) = e^{i\mathbf{K}\cdot\mathbf{x}}P_-(\mathbf{x})$ , relations (6.17) and (6.18) hold with  $\Phi_+$  and  $\Phi_-$  replaced, respectively, by  $P_+(\mathbf{x})$  and  $P_-(\mathbf{x})$ .

*Proof* Equations (6.17)–(6.18) follow from the relations

$$\vartheta_{\sharp} \equiv \langle \Phi_1, W\Phi_1 \rangle_{L^2_{\mathbf{K}}(\Omega)} = -\langle \Phi_2, W\Phi_2 \rangle_{L^2_{\mathbf{K}}(\Omega)}, \tag{6.19}$$

$$\langle \Phi_1, W\Phi_2 \rangle_{L^2_{\mathbf{K}}(\Omega)} = \langle \Phi_2, W\Phi_1 \rangle_{L^2_{\mathbf{K}}(\Omega)} = 0. \tag{6.20}$$

To prove (6.19) and (6.20), we begin by recalling that  $\Phi_2(\mathbf{x}) = \overline{\Phi_1(-\mathbf{x})}$ ,  $W$  is real-valued and  $W(-\mathbf{x}) = -W(\mathbf{x})$ . Since  $W$  is real-valued, it is clear that  $\vartheta_{\sharp} \in \mathbb{R}$ . Furthermore,

$$\begin{aligned} \langle \Phi_2, W\Phi_2 \rangle_{L^2_{\mathbf{K}}(\Omega)} &= \int_{\Omega} \overline{\Phi_2(\mathbf{x})} W(\mathbf{x}) \Phi_2(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \Phi_1(-\mathbf{x}) W(\mathbf{x}) \overline{\Phi_1(-\mathbf{x})} d\mathbf{x} \\ &= \int_{\Omega} \Phi_1(\mathbf{x}) W(-\mathbf{x}) \overline{\Phi_1(\mathbf{x})} d\mathbf{x} = -\vartheta_{\sharp}. \end{aligned}$$

This proves (6.17). To prove (6.18), observe that

$$\begin{aligned} \langle \Phi_2, W\Phi_1 \rangle_{L^2_{\mathbf{K}}(\Omega)} &= \int_{\Omega} \overline{\Phi_2(\mathbf{x})} W(\mathbf{x}) \Phi_1(\mathbf{x}) d\mathbf{x} = \int_{\Omega} \Phi_1(-\mathbf{x}) W(\mathbf{x}) \Phi_1(\mathbf{x}) d\mathbf{x} \\ &= \int_{\Omega} \Phi_1(\mathbf{x}) W(-\mathbf{x}) \Phi_1(-\mathbf{x}) d\mathbf{x} = - \int_{\Omega} \Phi_1(\mathbf{x}) W(\mathbf{x}) \Phi_1(-\mathbf{x}) d\mathbf{x} \\ &= -\overline{\langle \Phi_1, W\Phi_2 \rangle_{L^2_{\mathbf{K}}(\Omega)}} = -\langle \Phi_2, W\Phi_1 \rangle_{L^2_{\mathbf{K}}(\Omega)}. \end{aligned}$$

This completes the proof of Proposition 6.2. □

Propositions 6.1 and 6.2 imply that the orthogonality conditions (6.9) reduce to the following eigenvalue problem for  $\alpha(\zeta) = (\alpha_+(\zeta), \alpha_-(\zeta))^T$ :

$$(\mathcal{D} - E^{(1)})\alpha = 0, \quad \alpha \in L^2(\mathbb{R}). \tag{6.21}$$

Here,  $\mathcal{D}$  denotes the 1D Dirac operator:

$$\mathcal{D} = -i|\lambda_{\sharp}||\mathfrak{K}_2|\sigma_3\partial_{\zeta} + \vartheta_{\sharp}\kappa(\zeta)\sigma_1, \quad \text{and } \lambda_{\sharp} \times \vartheta_{\sharp} \neq 0. \tag{6.22}$$

In Section 6.1 we prove that the eigenvalue problem (6.21) has an exponentially localized eigenfunction  $\alpha_{\star}(\zeta)$  with corresponding (mid-gap) zero-energy eigenvalue  $E^{(1)} = 0$ . Moreover, this eigenvalue has multiplicity one. We impose the normalization:  $\|\alpha_{\star}\|_{L^2(\mathbb{R})} = 1$ .

Fix  $(E^{(1)}, \alpha) = (0, \alpha_{\star})$ . Then  $\alpha_{\star} \in L^2(\mathbb{R})$ ,  $\psi^{(0)}(\mathbf{x}, \zeta)$  is completely determined (up to normalization) and the solvability conditions (6.9) are satisfied. Therefore, the right hand side of (6.8) lies in the range of  $H_V - E_{\star} : H^2_{\mathbf{K}} \rightarrow L^2_{\mathbf{K}}$ , and we may invert  $(H_V - E_{\star})$  obtaining

$$\psi^{(1)}(\mathbf{x}, \zeta) = \left( R(E_{\star})G^{(1)} \right) (\mathbf{x}, \zeta) + \psi_h^{(1)}(\mathbf{x}, \zeta) \equiv \psi_p^{(1)}(\mathbf{x}, \zeta) + \psi_h^{(1)}(\mathbf{x}, \zeta), \tag{6.23}$$

where

$$R(E_{\star}) = (H_V - E_{\star})^{-1} : P_{\perp}L^2_{\mathbf{K}} \rightarrow P_{\perp}H^2_{\mathbf{K}}$$

and  $P_{\perp}$  is the  $L^2_{\mathbf{K}}(\Omega)$ - projection on to the orthogonal complement of the kernel of  $H_V - E_{\star}$ , equal to  $\text{span}\{\Phi_+, \Phi_-\}$ . Here,  $\psi_p^{(1)}$  denotes a particular solution, and

$$\psi_h^{(1)}(\mathbf{x}, \zeta) = \alpha_+^{(1)}(\zeta)\Phi_+(\mathbf{x}) + \alpha_-^{(1)}(\zeta)\Phi_-(\mathbf{x})$$

is a homogeneous solution.

Note that by exploiting the degrees of freedom coming from the  $L^2_{\mathbf{K}}$ - kernel of  $H_V - E_{\star}$ , we can continue the formal expansion to any order in  $\delta$ . Indeed, at  $\mathcal{O}(\delta^\ell)$  for  $\ell \geq 2$ , we have

$$\begin{aligned} &(-\Delta_{\mathbf{x}} + V(\mathbf{x}) - E_{\star}) \psi^{(\ell)}(\mathbf{x}, \zeta) \\ &= (2(\mathfrak{K}_2 \cdot \nabla_{\mathbf{x}}) \partial_{\zeta} - \kappa(\zeta)W(\mathbf{x})) \psi_h^{(\ell-1)}(\mathbf{x}, \zeta) + E^{(\ell)} \psi^{(0)}(\mathbf{x}, \zeta) \\ &\quad + G^{(\ell)}(\mathbf{x}, \zeta; \psi^{(0)}, \dots, \psi^{(\ell-2)}, \psi_p^{(\ell-1)}, E^{(1)}, \dots, E^{(\ell-1)}), \\ \psi^{(\ell)}(\mathbf{x} + \mathbf{v}, \cdot) &= e^{i\mathbf{K} \cdot \mathbf{v}} \psi^{(\ell)}(\mathbf{x}, \cdot) \quad \forall \mathbf{v} \in \Lambda_h, \end{aligned} \tag{6.24}$$

where, for the case  $\ell = 2$ ,

$$\begin{aligned} G^{(2)}(\mathbf{x}, \zeta; \psi^{(0)}, \psi_p^{(1)}) &= (2(\mathfrak{K}_2 \cdot \nabla_{\mathbf{x}}) \partial_{\zeta} - \kappa(\zeta)W(\mathbf{x})) \psi_p^{(1)}(\mathbf{x}, \zeta) \\ &\quad + |\mathfrak{K}_2|^2 \partial_{\zeta}^2 \psi^{(0)}(\mathbf{x}, \zeta). \end{aligned} \tag{6.25}$$

As before, (6.24) has a solution if and only if the right hand side is  $L^2_{\mathbf{K}}(\Omega; d\mathbf{x})$ -orthogonal to the functions  $\Phi_j(\mathbf{x})$ ,  $j = \pm$ . This solvability condition reduces to the inhomogeneous system:

$$\mathcal{D}\alpha^{(\ell-1)}(\zeta) = \mathcal{G}^{(\ell)}(\zeta) + E^{(\ell)}\alpha_{\star}(\zeta), \quad \alpha^{(\ell-1)} \in L^2(\mathbb{R}), \quad \text{where} \tag{6.26}$$

$$\mathcal{G}^{(\ell)}(\zeta) = \left( \begin{aligned} &\left\langle \Phi_+(\cdot), G^{(\ell)}(\cdot, \zeta; \psi^{(0)}, \dots, \psi^{(\ell-2)}, \psi_p^{(\ell-1)}, E^{(1)}, \dots, E^{(\ell-1)}) \right\rangle_{L^2_{\mathbf{K}}(\Omega)} \\ &\left\langle \Phi_-(\cdot), G^{(\ell)}(\cdot, \zeta; \psi^{(0)}, \dots, \psi^{(\ell-2)}, \psi_p^{(\ell-1)}, E^{(1)}, \dots, E^{(\ell-1)}) \right\rangle_{L^2_{\mathbf{K}}(\Omega)} \end{aligned} \right). \tag{6.27}$$

Solvability of the non-homogeneous Dirac system (6.26) in  $L^2(\mathbb{R})$ , is ensured by imposing  $L^2(\mathbb{R})$ - orthogonality of the right hand side of (6.26) to  $\alpha_{\star}(\zeta)$ . This yields:

$$E^{(\ell)} = - \left\langle \alpha_{\star}, \mathcal{G}^{(\ell)} \right\rangle_{L^2(\mathbb{R})}. \tag{6.28}$$

Thus we obtain, at  $\mathcal{O}(\delta^\ell)$ , that  $\psi^{(\ell)} = \psi_p^{(\ell)} + \psi_h^{(\ell)}$ , where  $\psi_p^{(\ell)}$  is a particular solution of (6.24) and  $\psi_h^{(\ell)}(\mathbf{x}, \zeta) = \alpha_+^{(\ell)}(\zeta)\Phi_+(\mathbf{x}) + \alpha_-^{(\ell)}(\zeta)\Phi_-(\mathbf{x})$  is a homogeneous solution.

**Summary:** Given a zero-energy  $L^2(\mathbb{R})$ - eigenstate of the Dirac operator,  $\mathcal{D}$  (see Section 6.1), we can, to any polynomial order in  $\delta$ , construct a formal solution of the eigenvalue problem  $H^{(\delta)}\psi = E\psi$ ,  $\psi \in L^2_{k_{\parallel}=\mathbf{K} \cdot \mathbf{v}_1}$ .

### 6.1 Zero-Energy Eigenstate of the Dirac Operator, $\mathcal{D}$

**Proposition 6.3** *Let  $\kappa(\zeta)$  be a domain wall function (Definition 5.1) and assume, without loss of generality, that  $\vartheta_{\sharp} > 0$ . Then,*

- (1) *The Dirac operator,  $\mathcal{D}$ , has a zero-energy eigenvalue,  $E^{(1)} = 0$ , with exponentially localized solution given by:*

$$\alpha_{\star}(\zeta) = \begin{pmatrix} \alpha_{\star,+}(\zeta) \\ \alpha_{\star,-}(\zeta) \end{pmatrix} = \gamma \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-\frac{\vartheta_{\sharp}}{|\lambda_{\sharp}||\mathfrak{z}_2|} \int_0^{\zeta} \kappa(s) ds}. \tag{6.29}$$

Here,  $\gamma \in \mathbb{C}$  is any constant for which  $\|\alpha_{\star}\|_{L^2} = 1$ .

- (2) *The solution (6.29),  $\alpha_{\star}$ , generates a leading order approximate (two-scale) edge state:*

$$\begin{aligned} \Psi^{(0)}(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) &= \alpha_{\star,+}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_+(\mathbf{x}) + \alpha_{\star,-}(\delta\mathfrak{K}_2 \cdot \mathbf{x})\Phi_-(\mathbf{x}) \end{aligned} \tag{6.30}$$

$$= e^{i\mathbf{K}\cdot\mathbf{x}} \gamma (-1 - i) \begin{bmatrix} i \frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|} \frac{\mathfrak{z}_2}{|\mathfrak{z}_2|} P_1(\mathbf{x}) - P_2(\mathbf{x}) \end{bmatrix} e^{-\frac{\vartheta_{\sharp}}{|\lambda_{\sharp}||\mathfrak{z}_2|} \int_0^{\delta\mathfrak{K}_2 \cdot \mathbf{x}} \kappa(s) ds}. \tag{6.31}$$

$\Psi^{(0)}(\mathbf{x}, \delta\mathbf{x})$  is propagating in the  $\mathbf{v}_1$  direction with parallel quasimomentum  $k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1$ , and is exponentially decaying,  $\mathfrak{K}_2 \cdot \mathbf{x} \rightarrow \pm\infty$ , in the transverse direction.

*Proof of Proposition 6.3* The system (6.21) with energy  $E^{(1)} = 0$  may be written as:

$$\partial_{\zeta} \alpha = \frac{-i\vartheta_{\sharp}}{|\lambda_{\sharp}||\mathfrak{z}_2|} \kappa(\zeta) \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \alpha, \quad \alpha = \begin{pmatrix} \alpha_+ \\ \alpha_- \end{pmatrix},$$

and has solutions:

$$\beta_1(\zeta) = \begin{pmatrix} 1 \\ i \end{pmatrix} e^{\frac{\vartheta_{\sharp}}{|\lambda_{\sharp}||\mathfrak{z}_2|} \int_0^{\zeta} \kappa(s) ds}, \quad \text{and} \quad \beta_2(\zeta) = \begin{pmatrix} 1 \\ -i \end{pmatrix} e^{-\frac{\vartheta_{\sharp}}{|\lambda_{\sharp}||\mathfrak{z}_2|} \int_0^{\zeta} \kappa(s) ds}.$$

Since  $\vartheta_{\sharp} > 0$  and  $\kappa(\zeta) \rightarrow \pm\kappa_{\infty}$  as  $\zeta \rightarrow \pm\infty$ , with  $\kappa_{\infty} > 0$ , the solution  $\beta_2(\zeta)$  decays as  $\zeta \rightarrow \pm\infty$ . Thus we set  $\alpha_{\star}(\zeta) = \gamma\beta_2(\zeta)$ , with constant  $\gamma \in \mathbb{C}$  chosen so that  $\|\alpha_{\star}\|_{L^2(\mathbb{R})} = 1$ . This yields the expression for  $\Psi^{(0)}(\mathbf{x}, \delta\mathbf{x})$  in (6.30)–(6.31), and completes the proof of Proposition 6.3.  $\square$

*Remark 6.4 (Topological Stability).* The zero-energy eigenpair, (6.29), is “topologically stable” or “topologically protected” in the sense that it (and hence the bifurcation of edge states, which it seeds) persists for any localized perturbation of  $\kappa(\zeta)$ . Such perturbations may be large but do not change the asymptotic behavior of  $\kappa(\zeta)$  as  $\zeta \rightarrow \pm\infty$ .

### 7 Existence of Edge States Localized Along an Edge

In this section we prove the existence of edge states for the eigenvalue problem:

$$\begin{aligned}
 H^{(\delta)}\Psi &= E\Psi, \quad \Psi \in H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma), \quad \text{where} \\
 H^{(\delta)} &\equiv -\Delta + V(\mathbf{x}) + \delta\kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x})W(\mathbf{x}).
 \end{aligned}
 \tag{7.1}$$

We make the following assumptions:

- (A1)  $V$  is a honeycomb potential in the sense of Definition 2.4 and  $-\Delta + V$  has a Dirac point at  $(\mathbf{K}, E_*)$ ; see Definition 3.1 and the conclusions of Theorem 3.4. In particular, the degenerate subspace of  $H^{(0)} - E_*$  has orthonormal basis of Floquet-Bloch modes  $\{\Phi_1(\mathbf{x}), \Phi_2(\mathbf{x})\}$  and

$$\lambda_{\sharp} \equiv \sum_{\mathbf{m} \in \mathcal{S}} c(\mathbf{m})^2 \begin{pmatrix} 1 \\ i \end{pmatrix} \cdot (\mathbf{K} + \mathbf{m}\mathbf{k}) \neq 0; \text{ see (3.9).}$$

- (A2)  $W$  is real-valued and  $\Lambda_h$ -periodic, odd and non-degenerate; i.e. (W1), (W2) and (W3) of Section 5 hold. In particular,

$$\vartheta_{\sharp} \equiv \langle \Phi_1, W\Phi_1 \rangle_{L^2_{\mathbf{K}}} = \langle \Phi_+, W\Phi_- \rangle_{L^2_{\mathbf{K}}} \neq 0.$$

- (A3)  $\kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x})$  is a domain wall function in the sense of Definition 5.1.

The following *spectral no-fold condition* plays a central role.

**Definition 7.1** [Spectral no-fold condition]. Let  $H_V = -\Delta + V(\mathbf{x})$ , where  $V$  is a honeycomb potential in the sense of Definition 2.4. Further, let  $(\mathbf{K}, E_*)$  be a Dirac point for  $H_V$  in the sense of Definition 3.1, in which we use the convention of labeling the dispersion maps by:  $\mathbf{k} \mapsto E_b(\mathbf{k})$ , where  $b \in \{b_*, b_* + 1\} \cup \{b \geq 1 : b \neq b_*, b_* + 1\} \equiv \{-, +\} \cup \{b \geq 1 : b \neq -, +\}$ .

To the  $\mathbf{v}_1$ -edge,  $\mathbb{R}\mathbf{v}_1$ , we associate the “ $\mathfrak{R}_2$ -slice at quasi-momentum  $\mathbf{K}$ ”, given by the union over all  $b \in \{-, +\} \cup \{b \geq 1 : b \neq -, +\}$  of the curves  $\{(\mathbf{K} + \lambda\mathfrak{R}_2, E_b(\mathbf{K} + \lambda\mathfrak{R}_2)) : |\lambda| \leq \frac{1}{2}\}$ .

We say the band structure of  $H_V$  satisfies the spectral no-fold condition for the  $\mathbf{v}_1$ -edge or, equivalently at the Dirac point and along the  $\mathfrak{R}_2$ -slice, with constants  $c_1, c_2, \mathfrak{a}_0$ , and  $\nu \in (0, 1)$  if the following holds:

There is a “modulus”,  $\omega(\mathfrak{a})$ , which is continuous, non-negative and increasing on  $0 \leq \mathfrak{a} < \mathfrak{a}_0$ , satisfying  $\omega(0) = 0$  and

$$\omega(\mathfrak{a}^\nu)/\mathfrak{a} \rightarrow \infty \text{ as } \mathfrak{a} \rightarrow 0,$$

such that for all  $0 \leq \mathfrak{a} < \mathfrak{a}_0$ :

$$\mathfrak{a}^\nu \leq |\lambda| \leq \frac{1}{2} \implies \left| E_{\pm}(\mathbf{K} + \lambda\mathfrak{R}_2) - E_* \right| \geq c_1 \omega(\mathfrak{a}^\nu), \tag{7.2}$$

$$b \neq \pm, |\lambda| \leq 1/2 \implies \left| E_b(\mathbf{K} + \lambda\mathfrak{R}_2) - E_* \right| \geq c_2 (1 + |b|). \tag{7.3}$$

Our final assumption is

- (A4)  $-\Delta + V$  satisfies the spectral no-fold condition at quasimomentum  $\mathbf{K}$  along the  $\mathfrak{K}_2$ - slice; see Definition 7.1.

*Remark 7.2* (1) Conditions (7.2)–(7.3) ensure that, restricted to the quasi-momentum slice  $\lambda \mapsto \mathbf{K} + \lambda\mathfrak{K}_2 \in \mathcal{B}_h$ , the dispersion curves which touch at the Dirac point  $(\mathbf{K}, E_\star)$  do not “fold over” and attain energies within  $c_1 \cdot \omega(\mathfrak{a}^\nu)$  of  $E_\star$  for quasimomenta bounded away from  $\mathbf{K}$ .

- (2) Dispersion curves of periodic Schrödinger operators on  $\mathbb{R}^1$  (Hill’s operators,  $H = -\partial_x^2 + Q(x)$ , where  $Q(x + 1) = Q(x)$ ) with “Dirac points” (see [7, 10]) always satisfy the natural 1D analogue of the spectral no-fold condition with  $\omega(\mathfrak{a}) = \mathfrak{a}$ . Dirac points occur at quasi-momentum  $k = \pm\pi$  and ODE arguments ensure that dispersion curves are monotone functions of  $k$  away from  $k = 0, \pm\pi$ .
- (3) In Section 8 we prove that  $H_{\varepsilon V} = -\Delta + \varepsilon V$ , where  $V$  is a honeycomb potential, satisfies the no-fold condition along the zigzag slice ( $\mathfrak{v}_1 = \mathfrak{v}_1$ ) with modulus  $\omega(\mathfrak{a}) = \mathfrak{a}^2$ , under the assumption that  $\varepsilon V_{1,1} > 0$  and  $\varepsilon$  is sufficiently small.

We now state a key result of this paper, giving sufficient conditions for the existence of  $\mathfrak{v}_1$ - edge states of  $H^{(\delta)}$ , for  $\mathfrak{v}_1 \in \Lambda_h$ .

**Theorem 7.3** *Consider the  $\mathfrak{v}_1$ - edge state eigenvalue problem, (7.1), where  $V(\mathbf{x})$ ,  $W(\mathbf{x})$  and  $\kappa(\zeta)$  satisfy assumptions (A1)–(A4). Then, there exist positive constants  $\delta_0, c_0$  and a branch of solutions of (7.1),*

$$|\delta| \in (0, \delta_0) \mapsto (E^\delta, \Psi^\delta) \in (E_\star - c_0 \delta_0, E_\star + c_0 \delta_0) \times H_{k_\parallel = \mathbf{K} \cdot \mathfrak{v}_1}^2(\Sigma),$$

such that the following holds:

- (1)  $\Psi^\delta$  is well-approximated by a slow modulation of a linear combination of degenerate Floquet-Bloch modes  $\Phi_+$  and  $\Phi_-$  ((6.6)), which is decaying transverse to the edge,  $\mathbb{Z}\mathfrak{v}_1$ :

$$\| \Psi^\delta(\cdot) - [\alpha_{\star,+}(\delta\mathfrak{K}_2 \cdot \cdot)\Phi_+(\cdot) + \alpha_{\star,-}(\delta\mathfrak{K}_2 \cdot \cdot)\Phi_-(\cdot)] \|_{H_{k_\parallel = \mathbf{K} \cdot \mathfrak{v}_1}^2} \lesssim \delta^{\frac{1}{2}}, \tag{7.4}$$

$$E^\delta = E_\star + E^{(2)}\delta^2 + o(\delta^2), \tag{7.5}$$

where  $E^{(2)}$  is obtained directly from (6.28), (6.27) and (6.25). The implied constant in (7.4) depends on  $V, W$  and  $\kappa$ , but is independent of  $\delta$ .

- (2) The amplitude vector,  $\alpha_\star(\zeta) = (\alpha_{\star,+}(\zeta), \alpha_{\star,-}(\zeta))$ , is an  $L^2(\mathbb{R}_\zeta)$ - normalized, topologically protected zero-energy eigenstate of the Dirac system (6.22):  $\mathcal{D}\alpha_\star = 0$  (see Proposition 6.3).

Perturbation theory for  $k_\parallel$  near  $\mathbf{K} \cdot \mathfrak{v}_1$  can be used to show the persistence of edge states for parallel quasi-momenta near  $\mathbf{K} \cdot \mathfrak{v}_1$ .

**Corollary 7.4** *Fix  $V, W, \kappa$  and  $\delta$  as in Theorem 7.3. Then there exists  $\eta_0 \ll \delta$  such that for all  $k_\parallel$  satisfying  $|k_\parallel - \mathbf{K} \cdot \mathfrak{v}_1| < \eta_0$ , there exists an  $H_{k_\parallel}^2(\Sigma)$ - eigenfunction with eigenvalue  $\mu(\delta, k_\parallel) = E^\delta + \mu^\delta (k_\parallel - \mathbf{K} \cdot \mathfrak{v}_1) + \mathcal{O}(|k_\parallel - \mathbf{K} \cdot \mathfrak{v}_1|^2)$ , where  $E^\delta$  is given in (7.5), and  $\mu^\delta$  is a constant, which is independent of  $k_\parallel$ .*

Zigzag edge states for  $k_{\parallel}$  in a neighborhood of  $k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1 = 2\pi/3$  ( $\mathbf{v}_1 = \mathbf{v}_1$ ) and, by symmetry, in a neighborhood of  $k_{\parallel} = 4\pi/3$  are indicated in Figure 6.

### 7.1 Corrector Equation

We seek a solution of the eigenvalue problem (7.1),  $\Psi^\delta$ , in the form

$$\Psi^\delta \equiv \psi^{(0)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) + \delta \psi^{(1)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) + \delta \eta^\delta(\mathbf{x}), \tag{7.6}$$

$$E^\delta \equiv E_\star + \delta^2 \mu^\delta. \tag{7.7}$$

Here,  $\psi^{(0)}$  and  $\psi_p^{(1)}$  are given by their respective multiple scale expressions (6.7) and (6.23):

$$\begin{aligned} \psi^{(0)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) &= \alpha_{\star,+}(\delta \mathfrak{R}_2 \cdot \mathbf{x}) \Phi_+(\mathbf{x}) + \alpha_{\star,-}(\delta \mathfrak{R}_2 \cdot \mathbf{x}) \Phi_-(\mathbf{x}), \\ \psi_p^{(1)}(\mathbf{x}, \delta \mathbf{x}) &= \left( R(E_\star) G^{(1)} \right) (\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}), \end{aligned}$$

and  $(\mu^\delta, \eta^\delta(\mathbf{x}))$  is the corrector, to be constructed. We may assume throughout that  $\delta \geq 0$ .

*Remark 7.5* We shall make frequent use of the regularity of  $\Phi_+(\mathbf{x})$ ,  $\Phi_-(\mathbf{x})$  and  $\alpha_\star(\zeta) \equiv (\alpha_{\star,+}(\zeta), \alpha_{\star,-}(\zeta))^T$ . In particular,  $V \in C^\infty(\mathbb{R}^2/\Lambda)$  and elliptic regularity theory imply that  $e^{-i\mathbf{K}\cdot\mathbf{x}}\Phi_\pm$  is  $C^\infty(\mathbb{R}^2/\Lambda)$ , and by Proposition 6.3,  $\alpha_\star(\zeta)$  and its derivatives with respect to  $\zeta$  are all exponentially decaying as  $|\zeta| \rightarrow \infty$ .

The following proposition lists useful bounds on  $\psi^{(0)}$  and  $\psi_p^{(1)}$ .

**Proposition 7.6** ( $H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^s(\Sigma_{\mathbf{x}})$  bounds on  $\psi^{(0)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x})$  and  $\psi_p^{(1)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x})$ ). *For all  $s = 1, 2, \dots$ , there exists  $\delta_0 > 0$ , such that if  $0 < |\delta| < \delta_0$ , then the leading order expansion terms  $\psi^{(0)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x})$  and  $\psi_p^{(1)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x})$  displayed in (6.7) and (6.23) satisfy the bounds:*

$$\begin{aligned} \left\| \psi^{(0)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) \right\|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^s} + \left\| \partial_\zeta^2 \psi^{(0)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta \mathfrak{R}_2 \cdot \mathbf{x}} \right\|_{L_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} &\approx |\delta|^{-1/2}, \\ \left\| \psi_p^{(1)}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) \right\|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^s} &\lesssim |\delta|^{-1/2}, \\ \left\| \partial_\zeta^2 \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta \mathfrak{R}_2 \cdot \mathbf{x}} \right\|_{L_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} + \left\| \partial_{\mathbf{x}} \partial_\zeta \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta \mathfrak{R}_2 \cdot \mathbf{x}} \right\|_{L_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} &\lesssim |\delta|^{-1/2}. \end{aligned}$$

It follows that  $\|\psi^{(0)}\|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} \approx \delta^{-1/2} \gg \|\delta \psi_p^{(1)}(\cdot, \delta \cdot)\|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} = \mathcal{O}(\delta^{1/2})$ .

The proof of Proposition 7.6 follows the approach taken in the proof of Lemma 6.1 in Appendix G of [10]. We omit the details but make two key technical remarks, that facilitate this proof.



*Bound on  $\|\Phi_b\|_{H^s}$ :* Recall  $\Phi_b(\mathbf{x}; \mathbf{k}) = e^{i\mathbf{k}\cdot\mathbf{x}} p_b(\mathbf{x}; \mathbf{k})$ , where  $\|\Phi_b\|_{L^2(\Omega)} = \|p_b\|_{L^2(\Omega)} = 1$ . Now  $p_b(\mathbf{x}; \mathbf{k})$  satisfies  $-\Delta p_b = 2i\mathbf{k} \cdot \nabla p_b - |\mathbf{k}|^2 p_b - V p_b + E_b(\mathbf{k}) p_b$ , where  $V$  is bounded and smooth. By 2D Weyl asymptotics  $|E_b(\mathbf{k})| \approx (1 + |b|)$ ,  $b \gg 1$  and therefore we have  $\|\Delta p_b\|_{H^{s-1}} \leq C_s(1 + b) \|p_b\|_{H^s}$ . Hence, by elliptic theory  $\|p_b\|_{H^{s+1}} \leq C_s(1 + b) \|p_b\|_{H^s}$  and induction on  $s \geq 0$  yields  $\|p_b\|_{H^s} \leq C_s(1 + b)^s$ .

*Rapid decay of  $\langle \Phi_b(\cdot; \mathbf{K}), f(\cdot) \rangle_{L^2(\Omega)}$ :* Using  $H^{(0)}\Phi_b(\mathbf{x}; \mathbf{K}) = E_b(\mathbf{K})\Phi_b(\mathbf{x}; \mathbf{K})$ , for sufficiently smooth  $f$  we have:  $\langle \Phi_b(\cdot; \mathbf{K}), f(\cdot) \rangle_{L^2(\Omega)} = (E_b(\mathbf{K}))^{-M} \langle \Phi_b(\cdot; \mathbf{K}), [H^{(0)}]^M f(\cdot) \rangle_{L^2(\Omega)}$ . Hence, for any  $M \geq 0$ ,  $|\langle \Phi_b(\cdot; \mathbf{K}), f(\cdot) \rangle_{L^2(\Omega)}| \leq C_M(1+b)^{-M}$ .

It remains to construct and bound the corrector  $(\mu, \eta(\mathbf{x}))$ . Substitution of the expansion (7.6) into the eigenvalue problem (7.1), yields an equation for  $\eta(\mathbf{x}) \in H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$ , which depends on  $\mu$  and the small parameter  $\delta$ :

$$\begin{aligned} & (-\Delta_{\mathbf{x}} + V(\mathbf{x}) - E_{\star}) \eta(\mathbf{x}) + \delta\kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x})W(\mathbf{x})\eta(\mathbf{x}) - \delta^2\mu \eta(\mathbf{x}) \\ &= \delta \left( 2\mathfrak{K}_2 \cdot \nabla_{\mathbf{x}} \partial_{\zeta} - \kappa(\delta\mathfrak{K}_2 \cdot \mathbf{x})W(\mathbf{x}) \right) \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta\mathfrak{K}_2 \cdot \mathbf{x}} + \delta\mu \psi^{(0)}(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) \\ &+ \delta|\mathfrak{K}_2|^2 \partial_{\zeta}^2 \psi^{(0)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta\mathfrak{K}_2 \cdot \mathbf{x}} + \delta^2\mu \psi_p^{(1)}(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) \\ &+ \delta^2|\mathfrak{K}_2|^2 \partial_{\zeta}^2 \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta\mathfrak{K}_2 \cdot \mathbf{x}}. \end{aligned} \tag{7.8}$$

To prove Theorem 7.3, we shall prove that (7.8) has a solution  $(\mu(\delta), \eta^{\delta})$ , with  $\eta^{\delta} \in H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}$  satisfying the bound

$$\|\delta\eta^{\delta}\|_{H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}} \leq C\delta^{1/2}.$$

### 7.2 Decomposition of Corrector, $\eta$ , into Near and Far Energy Components

Introduce the abbreviated notation, for  $|\lambda| \leq 1/2$ :

$$E_b(\lambda) = \begin{cases} E_b(\mathbf{K} + \lambda\mathfrak{K}_2) & b_{\star} \notin \{b_{\star}, b_{\star} + 1\}, \\ E_{-}(\lambda) & b = b_{\star}, \\ E_{+}(\lambda) & b = b_{\star} + 1, \end{cases} \tag{7.9}$$

and

$$\Phi_b(\mathbf{x}; \lambda) = \begin{cases} \Phi_b(\mathbf{x}; \mathbf{K} + \lambda\mathfrak{K}_2) & b_{\star} \notin \{b_{\star}, b_{\star} + 1\}, \\ \Phi_{-}(\mathbf{x}; \lambda) & b = b_{\star}, \\ \Phi_{+}(\mathbf{x}; \lambda) & b = b_{\star} + 1. \end{cases} \tag{7.10}$$

Define  $\tilde{f}_b(\lambda) = \langle \Phi_b(\cdot, \lambda), f(\cdot) \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}}$ . By Theorem 4.2, any  $\eta \in H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$  has the representation

$$\eta(\mathbf{x}) = \sum_{b \geq 1} \int_{|\lambda| \leq 1/2} \Phi_b(\mathbf{x}; \lambda) \tilde{\eta}_b(\lambda) d\lambda. \tag{7.11}$$

Our strategy is to next derive a system of equations governing  $\{\tilde{\eta}_b(\lambda)\}_{b \geq 1}$ , which is formally equivalent to system (7.8). We then prove this system has a solution, which is used to construct  $\eta(\mathbf{x})$ .

Take the inner product of (7.8) with  $\Phi_b(\mathbf{x}; \lambda)$ , for  $b \geq 1$ , to obtain

$$\begin{aligned} b \geq 1 : & (E_b(\lambda) - E_{\star}) \tilde{\eta}_b(\lambda) \\ & + \delta \langle \Phi_b(\cdot; \lambda), \kappa(\delta \mathfrak{K}_2 \cdot) W(\cdot) \eta(\cdot) \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}} \\ & = \delta \tilde{F}_b[\mu, \delta](\lambda) + \delta^2 \mu \tilde{\eta}_b(\lambda), \quad |\lambda| \leq 1/2. \end{aligned} \tag{7.12}$$

Here,  $\tilde{F}_b[\mu, \delta](\lambda)$ ,  $b \geq 1$ , is given by:

$$\tilde{F}_b[\mu, \delta](\lambda) \equiv \tilde{F}_b^{1,\delta}(\lambda) + \mu \tilde{F}_b^{2,\delta}(\lambda) + \delta \mu \tilde{F}_b^{3,\delta}(\lambda) + \tilde{F}_b^{4,\delta}(\lambda) + \delta \tilde{F}_b^{5,\delta}(\lambda), \tag{7.13}$$

where

$$\begin{aligned} \tilde{F}_b^{1,\delta}(\lambda) & \equiv \left\langle \Phi_b(\mathbf{x}, \lambda), (2\mathfrak{K}_2 \cdot \nabla_{\mathbf{x}} \partial_{\zeta} - \kappa(\delta \mathfrak{K}_2 \cdot \mathbf{x}) W(\mathbf{x})) \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta \mathfrak{K}_2 \mathbf{x}} \right\rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}}, \\ \tilde{F}_b^{2,\delta}(\lambda) & \equiv \left\langle \Phi_b(\mathbf{x}, \lambda), \psi^{(0)}(\mathbf{x}, \delta \mathfrak{K}_2 \cdot \mathbf{x}) \right\rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}}, \\ \tilde{F}_b^{3,\delta}(\lambda) & \equiv \left\langle \Phi_b(\mathbf{x}, \lambda), \psi_p^{(1)}(\mathbf{x}, \delta \mathfrak{K}_2 \cdot \mathbf{x}) \right\rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}}, \\ \tilde{F}_b^{4,\delta}(\lambda) & \equiv \left\langle \Phi_b(\mathbf{x}, \lambda), |\mathfrak{K}_2|^2 \partial_{\zeta}^2 \psi^{(0)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta \mathfrak{K}_2 \cdot \mathbf{x}} \right\rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}}, \\ \tilde{F}_b^{5,\delta}(\lambda) & \equiv \left\langle \Phi_b(\mathbf{x}, \lambda), |\mathfrak{K}_2|^2 \partial_{\zeta}^2 \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta \mathfrak{K}_2 \cdot \mathbf{x}} \right\rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}}. \end{aligned} \tag{7.14}$$

Recall the spectral no-fold condition ensuring that  $\delta/\omega(\delta^{\nu}) \rightarrow 0$  as  $\delta \rightarrow 0$ , where  $\nu > 0$ . We next decompose  $\eta(\mathbf{x})$  into its components with energies ‘‘near’’ and ‘‘far’’ from the Dirac point:

$$\begin{aligned} \eta(\mathbf{x}) & = \eta_{\text{near}}(\mathbf{x}) + \eta_{\text{far}}(\mathbf{x}), \quad \text{where} \\ \eta_{\text{near}}(\mathbf{x}) & \equiv \sum_{b=\pm} \int_{|\lambda| \leq 1/2} \Phi_b(\mathbf{x}; \lambda) \tilde{\eta}_{b,\text{near}}(\lambda) d\lambda, \\ \eta_{\text{far}}(\mathbf{x}) & \equiv \sum_{b \geq 1} \int_{|\lambda| \leq 1/2} \Phi_b(\mathbf{x}; \lambda) \tilde{\eta}_{b,\text{far}}(\lambda) d\lambda, \quad \text{and} \end{aligned} \tag{7.15}$$

$$\begin{aligned} \tilde{\eta}_{\pm, \text{near}}(\lambda) &\equiv \chi(|\lambda| \leq \delta^\nu) \tilde{\eta}_{\pm}(\lambda), \\ \tilde{\eta}_{b, \text{far}}(\lambda) &\equiv \chi\left(\left(\delta_{b,+} + \delta_{b,-}\right)\delta^\nu \leq |\lambda| \leq \frac{1}{2}\right) \tilde{\eta}_b(\lambda), \quad b \geq 1; \end{aligned} \tag{7.16}$$

$\delta_{b,+}$  and  $\delta_{b,-}$  are Kronecker delta symbols.

We rewrite system (7.12) as two coupled subsystems: a pair of equations, which governs the **near energy components**:

$$\begin{aligned} &(E_+(\lambda) - E_\star) \tilde{\eta}_{+, \text{near}}(\lambda) \\ &\quad + \delta\chi(|\lambda| \leq \delta^\nu) \langle \Phi_+(\cdot, \lambda), \kappa(\delta\mathfrak{K}_2 \cdot) W(\cdot) [\eta_{\text{near}}(\cdot) + \eta_{\text{far}}(\cdot)] \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)} \\ &= \delta\chi(|\lambda| \leq \delta^\nu) \tilde{F}_+[\mu, \delta](\lambda) + \delta^2\mu \tilde{\eta}_{+, \text{near}}(\lambda), \end{aligned} \tag{7.17}$$

$$\begin{aligned} &(E_-(\lambda) - E_\star) \tilde{\eta}_{-, \text{near}}(\lambda) \\ &\quad + \delta\chi(|\lambda| \leq \delta^\nu) \langle \Phi_-(\cdot, \lambda), \kappa(\delta\mathfrak{K}_2 \cdot) W(\cdot) [\eta_{\text{near}}(\cdot) + \eta_{\text{far}}(\cdot)] \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)} \\ &= \delta\chi(|\lambda| \leq \delta^\nu) \tilde{F}_-[\mu, \delta](\lambda) + \delta^2\mu \tilde{\eta}_{-, \text{near}}(\lambda), \end{aligned} \tag{7.18}$$

coupled to an infinite system governing the **far energy components**:

$$\begin{aligned} &(E_b(\lambda) - E_\star) \tilde{\eta}_{b, \text{far}}(\lambda) + \delta\chi\left(1/2 \geq |\lambda| \geq (\delta_{b,-} + \delta_{b,+})\delta^\nu\right) \\ &\quad \times \langle \Phi_b(\cdot, \lambda), \kappa(\delta\mathfrak{K}_2 \cdot) W(\cdot) [\eta_{\text{near}}(\cdot) + \eta_{\text{far}}(\cdot)] \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)} \\ &= \delta\chi\left(1/2 \geq |\lambda| \geq (\delta_{b,-} + \delta_{b,+})\delta^\nu\right) \tilde{F}_b[\mu, \delta](\lambda) + \delta^2\mu \tilde{\eta}_{b, \text{far}}(\lambda), \quad b \geq 1. \end{aligned} \tag{7.19}$$

We now systematically manipulate (7.17)–(7.19) into the form of a band-limited Dirac system; see Proposition 7.12. This latter equation is then solved in Proposition 7.15. Since all steps are reversible, this yields a solution  $(\mu^\delta, \{\tilde{\eta}_b^\delta(\lambda)\}_{b \geq 1})$  of (7.17)–(7.19). Finally,  $\eta^\delta \in H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$ , the solution of corrector equation (7.8), is reconstructed from the amplitudes  $\{\tilde{\eta}_b^\delta(\lambda)\}_{b \geq 1}$  using (7.11).

### 7.3 Construction of $\eta_{\text{far}} = \eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta]$ and Derivation of a Closed System for $\eta_{\text{near}}$

We solve (7.19) for  $\eta_{\text{far}}$  as a functional of  $\eta_{\text{near}}$ , and the parameters  $\mu$  and  $\delta$ . We then study the *closed* equation for  $\eta_{\text{near}}$  obtained by substitution of  $\eta_{\text{far}}$  into (7.17) and (7.18).

*It is in the construction of this map that we use assumption (A4), the spectral no-fold condition along the  $\mathfrak{K}_2$ - slice; Definition 7.1. We apply it in the form: There exists a modulus,  $\omega(\alpha)$ , and positive constants  $\nu, c_1$  and  $c_2$ , depending on  $V$ , such that for all  $\delta \neq 0$  and sufficiently small:*

$$\delta^{\nu} \leq |\lambda| \leq \frac{1}{2} \implies \left| E_{\pm}(\lambda) - E_{\star} \right| \geq c_1 \omega(\delta^{\nu}), \tag{7.20}$$

$$b \neq \pm : |\lambda| \leq 1/2 \implies \left| E_b(\lambda) - E_{\star} \right| \geq c_2 (1 + |b|). \tag{7.21}$$

The far energy system (7.19) may be written as a fixed point system for  $\tilde{\eta}_{\text{far}} = \{\tilde{\eta}_{b,\text{far}}(\lambda)\}_{b \geq 1}$ :

$$\tilde{\mathcal{E}}_b[\tilde{\eta}_{\text{far}}; \eta_{\text{near}}, \mu, \delta] = \tilde{\eta}_{b,\text{far}}, \quad b \geq 1, \tag{7.22}$$

where the mapping  $\tilde{\mathcal{E}}_b$  is given by

$$\begin{aligned} &\tilde{\mathcal{E}}_b[\phi; \psi, \mu, \delta](\lambda) \\ &\equiv \delta^2 \mu \frac{\tilde{\phi}_{b,\text{far}}(\lambda)}{E_b(\lambda) - E_{\star}} + \frac{\delta \chi \left( 1/2 \geq |\lambda| \geq (\delta_{b,-} + \delta_{b,+}) \delta^{\nu} \right)}{E_b(\lambda) - E_{\star}} \\ &\quad \times \left( - \langle \Phi_b(\cdot, \lambda), \kappa(\delta \mathfrak{R}_2 \cdot) W(\cdot) [\psi(\cdot) + \phi(\cdot)] \rangle_{L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}} + \tilde{F}_b[\mu, \delta](\lambda) \right), \end{aligned}$$

and

$$\begin{aligned} \phi(\mathbf{x}) &= \sum_{b \geq 1} \int_{|\lambda| \leq 1/2} \chi \left( |\lambda| \geq (\delta_{b,-} + \delta_{b,+}) \delta^{\nu} \right) \tilde{\phi}_b(\lambda) \Phi_b(\mathbf{x}; \lambda) d\lambda \\ &= \sum_{b \geq 1} \int_{|\lambda| \leq 1/2} \tilde{\phi}_{b,\text{far}}(\lambda) \Phi_b(\mathbf{x}; \lambda) d\lambda. \end{aligned}$$

Equivalently,

$$\mathcal{E}[\eta_{\text{far}}; \eta_{\text{near}}, \mu, \delta] = \eta_{\text{far}}. \tag{7.23}$$

For fixed  $\mu, \delta$  and band-limited  $\eta_{\text{near}}$ :

$$\tilde{\eta}_{\pm,\text{near}}(\lambda) = \chi \left( |\lambda| \leq \delta^{\nu} \right) \tilde{\eta}_{\pm,\text{near}}(\lambda), \tag{7.24}$$

we seek a solution  $\{\tilde{\eta}_{b,\text{far}}(\lambda)\}_{b \geq 1}$ , supported at energies bounded away from  $E_{\star}$ :

$$\tilde{\eta}_{b,\text{far}}(\lambda) = \chi \left( |\lambda| \geq (\delta_{b,-} + \delta_{b,+}) \delta^{\nu} \right) \tilde{\eta}_{b,\text{far}}(\lambda), \quad b \geq 1. \tag{7.25}$$

Introduce the Banach spaces of functions limited to ‘‘far’’ and ‘‘near’’ energy regimes:

$$\begin{aligned} L^2_{\text{near},\delta^{\nu}}(\Sigma) &\equiv \left\{ f \in L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}(\Sigma) : \tilde{f}_b(\lambda) \text{ satisfies (7.24)} \right\}, \\ L^2_{\text{far},\delta^{\nu}}(\Sigma) &\equiv \left\{ f \in L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}(\Sigma) : \tilde{f}_b(\lambda) \text{ satisfies (7.25)} \right\}, \end{aligned}$$

Near- and far- energy Sobolev spaces  $H_{\text{far}}^s(\Sigma)$  and  $H_{\text{near}}^s(\Sigma)$  are analogously defined. The corresponding open balls of radius  $\rho$  are given by:

$$B_{\text{near},\delta^v}(\rho) \equiv \left\{ f \in L_{\text{near},\delta^v}^2 : \|f\|_{L_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} < \rho \right\},$$

$$B_{\text{far},\delta^v}(\rho) \equiv \left\{ f \in L_{\text{far},\delta^v}^2 : \|f\|_{L_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} < \rho \right\}.$$

Using (A4) that  $H^{(0)} = -\Delta + V$  satisfies the no-fold condition for the  $\mathbf{v}_1$  – edge, we deduce:

**Proposition 7.7** (1) *For any fixed  $M > 0, R > 0$ , there exists a positive number,  $\delta_0 \leq 1$ , such that for all  $0 < \delta < \delta_0$ , equation (7.23), or equivalently, the system (7.22), has a unique solution*

$$(\eta_{\text{near}}, \mu, \delta) \in B_{\text{near},\delta^v}(R) \times \{|\mu| < M\} \times \{0 < \delta < \delta_0\}$$

$$\mapsto \eta_{\text{far}}(\cdot; \eta_{\text{near}}, \mu, \delta) = \mathcal{T}^{-1} \tilde{\eta}_{\text{far}} \in B_{\text{far},\delta^v}(\rho_\delta), \quad \rho_\delta = \mathcal{O}\left(\frac{\delta^{\frac{1}{2}}}{\omega(\delta^v)}\right).$$

(2) *The mapping  $(\eta_{\text{near}}, \mu, \delta) \mapsto \eta_{\text{far}}(\cdot; \eta_{\text{near}}, \mu, \delta) \in H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2$  is Lipschitz in  $(\eta_{\text{near}}, \mu)$  with:*

$$\begin{aligned} & \| \eta_{\text{far}}[\psi_1, \mu_1, \delta] - \eta_{\text{far}}[\psi_2, \mu_2, \delta] \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2(\Sigma)} \\ & \leq C' \frac{\delta}{\omega(\delta^v)} \left( \| \psi_1 - \psi_2 \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} + |\mu_1 - \mu_2| \right), \\ & \| \eta_{\text{far}}[\eta_{\text{near}}; \mu, \delta] \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} \leq C'' \left( \frac{\delta}{\omega(\delta^v)} \| \eta_{\text{near}} \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} + \frac{\delta^{\frac{1}{2}}}{\omega(\delta^v)} \right). \end{aligned} \tag{7.26}$$

*The constants  $C'$  and  $C''$  depend only on  $M, R$  and  $v$ .*

(3) *The mapping  $(\eta_{\text{near}}, \mu, \delta) \mapsto \eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta]$  satisfies:*

$$\eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta](\mathbf{x}) = [A\eta_{\text{near}}](\mathbf{x}; \mu, \delta) + \mu B(\mathbf{x}; \delta) + C(\mathbf{x}; \delta). \tag{7.27}$$

*For  $\eta_{\text{near}} \in B_{\text{near}}(R)$  we have:*

$$\begin{aligned} & \| [A\eta_{\text{near}}](\cdot, \mu_1, \delta) - [A\eta_{\text{near}}](\cdot, \mu_2, \delta) \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} \leq C'_{M,R} \frac{\delta}{\omega(\delta^v)} |\mu_1 - \mu_2|, \\ & \| [A\eta_{\text{near}}](\cdot; \mu, \delta) \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} \leq \frac{\delta}{\omega(\delta^v)} \| \eta_{\text{near}} \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2}, \\ & \| B(\cdot; \delta) \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} \leq \frac{\delta^{\frac{1}{2}}}{\omega(\delta^v)}, \quad \text{and} \quad \| C(\cdot; \delta) \|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} \leq \frac{\delta^{\frac{1}{2}}}{\omega(\delta^v)}. \end{aligned}$$

(4) We may extend  $\eta_{\text{far}}[\cdot; \eta_{\text{near}}, \mu, \delta]$  to be defined on the half-open interval  $\delta \in [0, \delta_0]$  by defining  $\eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta = 0] = 0$ . Then, by (7.26)  $\eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta]$  is continuous at  $\delta = 0$ .

**Remark 7.8** [Remarks on the proof of Proposition 7.7] The proof follows that of Corollary 6.4 in [10], with changes that we now discuss.

(a) The fixed point equation (7.22) for  $\psi_{\text{far}}$  is of the form:

$$\eta_{\text{far}} = \mathcal{Q}_\delta \eta_{\text{far}} + \frac{\delta \chi(|\lambda| \geq (\delta_{b,-} + \delta_{b,+})\delta^\nu)}{E_b(\lambda) - E_\star} \times \left( - \langle \Phi_b(\cdot, \lambda), \kappa(\delta \mathfrak{K}_2 \cdot) W(\cdot) \eta_{\text{near}}(\cdot) \rangle_{L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}} + \tilde{F}_b[\mu, \delta](\lambda) \right), \tag{7.28}$$

where  $\mathcal{Q}_\delta$  is bounded and linear on  $H^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}$  and defined by:

$$\begin{aligned} & [\widetilde{\mathcal{Q}_\delta \phi}]_b(\lambda) \\ & \equiv -\delta \frac{\chi(|\lambda| \geq (\delta_{b,b_\star} + \delta_{b,b_\star+1})\delta^\nu)}{E_b(\lambda) - E_\star} \langle \Phi_b(\cdot, \lambda), \kappa(\delta \mathfrak{K}_2 \cdot) W(\cdot) \phi(\cdot) \rangle_{L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}} \\ & \quad + \delta^2 \mu \frac{\tilde{\phi}_b(\lambda)}{E_b(\lambda) - E_\star}. \end{aligned} \tag{7.29}$$

To construct the mapping  $(\eta_{\text{near}}, \mu, \delta) \mapsto \eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta]$  and obtain the conclusions of Proposition 7.7 it is convenient to solve (7.28) via the contraction mapping principle. Thus we need to bound the operator norm of  $\mathcal{Q}_\delta$  and we find from (7.29) that  $\mathcal{Q}_\delta$  maps  $L^2_{\text{near}, \delta^\nu}$  to  $H^2_{\text{near}, \delta^\nu}$  with norm bounded by constant  $\times \epsilon(\delta)$ , where

$$\epsilon(\delta) \equiv \sup_{b=\pm} \sup_{|\delta|^\nu \leq |\lambda| \leq \frac{1}{2}} \frac{|\delta|}{|E_b(\lambda) - E_\star|} + \sup_{b \geq 1, b \neq \pm} (1 + |b|) \sup_{0 \leq |\lambda| \leq \frac{1}{2}} \frac{|\delta|}{|E_b(\lambda) - E_\star|}. \tag{7.30}$$

The spectral no-fold condition hypothesis (7.20)–(7.21) implies that

$$\epsilon(\delta) \lesssim \frac{|\delta|}{\omega(\delta^\nu) c_1(V)} + \frac{|\delta|}{c_2(V)}, \tag{7.31}$$

which tends to zero as  $\delta$  tends to zero. Hence, the contraction mapping principle can be applied on the ball  $B_{\text{far}, \delta^\nu}(\rho_\delta)$ ,  $\rho_\delta = \mathcal{O}(\delta^{\frac{1}{2}}/\omega(\delta^\nu))$ .

(b) We note that although  $\Sigma$  is a two-dimensional region, since  $\Sigma$  is unbounded in only one direction, estimates on  $H^2_{k_{\parallel}}(\Sigma)$  have the same scaling behavior in the parameter  $\delta$  as in the 1D study [10].

### 7.4 Analysis of the Closed System for $\eta_{\text{near}}$

Substitution of  $\eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta]$  into the system (7.17)–(7.18) yields a closed system for  $(\eta_{\text{near}}, \mu)$ , which depends on the parameter  $\delta \in [0, \delta_0)$ . In this section we show, by careful rescaling and expansion of terms, that the equation for  $\eta_{\text{near}}$  may be rewritten as a Dirac-type system. We then solve this system in Section 7.5. Recall the abbreviated notation:  $E_b(\lambda)$  and  $\Phi_b(\mathbf{x}; \lambda)$ , introduced in (7.9)–(7.10).

Since both the spectral support of  $\eta_{\text{near}}$  (parametrized by  $\mathbf{K} + \lambda \mathfrak{K}_2$ , with  $|\lambda| \leq \delta^\nu$ ), and size of the domain wall perturbation,  $\mathcal{O}(\delta)$ , tend to zero as  $\delta \rightarrow 0$ , it is natural to scale in such a way as to obtain an order one limit. We begin by introducing  $\xi$ , a scaling of the quasi-momentum parameter,  $\lambda$ , and  $\widehat{\eta}_{\pm, \text{near}}(\xi)$ , an expression for  $\widetilde{\eta}_{\pm, \text{near}}(\lambda)$  as a standard Fourier transform on  $\mathbb{R}$ :

$$\widehat{\eta}_{\pm, \text{near}}(\xi) \equiv \widetilde{\eta}_{\pm, \text{near}}(\lambda), \quad \text{where } \xi \equiv \frac{\lambda}{\delta}. \tag{7.32}$$

By Proposition 4.5:  $E_{\pm}(\lambda) - E_{\star} = \pm |\lambda_{\sharp}| |\mathfrak{K}_2| \delta \xi + E_{2, \pm}(\delta \xi) (\delta \xi)^2$ , where  $|E_{2, \pm}(\delta \xi)| \lesssim 1$ , for all  $\xi$ ; see (4.12). Substitution of this expansion and the rescaling (7.32) into (7.17)–(7.18), and then canceling a factor of  $\delta$  yields:

$$\begin{aligned} &+ |\lambda_{\sharp}| |\mathfrak{K}_2| \xi \widehat{\eta}_{+, \text{near}}(\xi) + \chi(|\xi| \leq \delta^{\nu-1}) \langle \Phi_+(\cdot, \delta \xi), \kappa(\delta \mathfrak{K}_2 \cdot) W(\cdot) \eta_{\text{near}}(\cdot) \rangle_{L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}} \\ &= \chi(|\xi| \leq \delta^{\nu-1}) \widetilde{F}_+[\mu, \delta](\lambda) + \delta \mu \widehat{\eta}_{+, \text{near}}(\xi) - \delta E_{2, +}(\delta \xi) \xi^2 \widehat{\eta}_{+, \text{near}}(\xi) \\ &\quad - \chi(|\xi| \leq \delta^{\nu-1}) \langle \Phi_+(\cdot, \delta \xi), \kappa(\delta \mathfrak{K}_2 \cdot) W(\cdot) \eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta](\cdot) \rangle_{L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}}, \end{aligned} \tag{7.33}$$

$$\begin{aligned} &- |\lambda_{\sharp}| |\mathfrak{K}_2| \xi \widehat{\eta}_{-, \text{near}}(\xi) + \chi(|\xi| \leq \delta^{\nu-1}) \langle \Phi_-(\cdot, \delta \xi), \kappa(\delta \mathfrak{K}_2 \cdot) W(\cdot) \eta_{\text{near}}(\cdot) \rangle_{L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}} \\ &= \chi(|\xi| \leq \delta^{\nu-1}) \widetilde{F}_-[\mu, \delta](\lambda) + \delta \mu \widehat{\eta}_{-, \text{near}}(\xi) - \delta E_{2, -}(\delta \xi) \xi^2 \widehat{\eta}_{-, \text{near}}(\xi) \\ &\quad - \chi(|\xi| \leq \delta^{\nu-1}) \langle \Phi_-(\cdot, \delta \xi), \kappa(\delta \mathfrak{K}_2 \cdot) W(\cdot) \eta_{\text{far}}[\eta_{\text{near}}, \mu, \delta](\cdot) \rangle_{L^2_{k_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}}. \end{aligned} \tag{7.34}$$

We next extract the dominant behavior, for  $\delta$  small, of the inner products involving  $\eta_{\text{near}}$  by first expanding  $\eta_{\text{near}}$  in terms of its spectral components near energy  $E_{\star} = E_{\pm}(\lambda = 0)$  plus a correction. To this end we apply Proposition 4.5 to expand  $p_{\pm}(\mathbf{x}, \lambda)$  for  $\lambda = \delta \xi$  small:

$$\begin{aligned} p_{\pm}(\mathbf{x}, \lambda) &= P_{\pm}(\mathbf{x}) + \varphi_{\pm}(\mathbf{x}, \delta \xi), \quad P_{\pm}(\mathbf{x}) \equiv \frac{1}{\sqrt{2}} \left[ \frac{\overline{\lambda_{\sharp}}}{|\lambda_{\sharp}|} \frac{\beta_2}{|\beta_2|} P_1(\mathbf{x}) \pm P_2(\mathbf{x}) \right] \quad \text{where} \\ |\varphi_{\pm}(\mathbf{x}, \delta \xi)| &\leq \sup_{\mathbf{x} \in \Sigma, |\omega| \leq \delta^\nu} |\varphi_{\pm}(\mathbf{x}, \omega)| \leq \delta^\nu, \quad |\xi| \leq \delta^{\nu-1}. \end{aligned} \tag{7.35}$$

Thus, using (7.15) and that  $\Phi_{\pm}(\mathbf{x}; \lambda) = e^{i(\mathbf{K} + \lambda \mathfrak{K}_2) \cdot \mathbf{x}} p_{\pm}(\mathbf{x}; \lambda)$  (see (4.11)), we obtain

$$\begin{aligned} \eta_{\text{near}}(\mathbf{x}) &= \int_{|\lambda| \leq \delta^\nu} \Phi_+(\mathbf{x}, \lambda) \widetilde{\eta}_{+, \text{near}}(\lambda) d\lambda + \int_{|\lambda| \leq \delta^\nu} \Phi_-(\mathbf{x}, \lambda) \widetilde{\eta}_{-, \text{near}}(\lambda) d\lambda \\ &= \int_{|\lambda| \leq \delta^\nu} e^{i\mathbf{K} \cdot \mathbf{x}} e^{i\lambda \mathfrak{K}_2 \cdot \mathbf{x}} p_+(\mathbf{x}, \lambda) \widehat{\eta}_{+, \text{near}}\left(\frac{\lambda}{\delta}\right) d\lambda \end{aligned}$$

$$\begin{aligned}
 & + \int_{|\lambda| \leq \delta^{\nu}} e^{i\mathbf{K} \cdot \mathbf{x}} e^{i\lambda \mathfrak{R}_2 \cdot \mathbf{x}} p_{-}(\mathbf{x}, \lambda) \widehat{\eta}_{-, \text{near}} \left( \frac{\lambda}{\delta} \right) d\lambda \\
 & = \delta e^{i\mathbf{K}\mathbf{x}} P_{+}(\mathbf{x}) \int_{|\xi| \leq \delta^{\nu-1}} e^{i\delta\xi \mathfrak{R}_2 \cdot \mathbf{x}} \widehat{\eta}_{+, \text{near}}(\xi) d\xi + \delta e^{i\mathbf{K} \cdot \mathbf{x}} \rho_{+}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) \\
 & + \delta e^{i\mathbf{K}\mathbf{x}} P_{-}(\mathbf{x}) \int_{|\xi| \leq \delta^{\nu-1}} e^{i\delta\xi \mathfrak{R}_2 \cdot \mathbf{x}} \widehat{\eta}_{-, \text{near}}(\xi) d\xi + \delta e^{i\mathbf{K} \cdot \mathbf{x}} \rho_{-}(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) \\
 & = \delta e^{i\mathbf{K} \cdot \mathbf{x}} \left[ P_{+}(\mathbf{x}) \eta_{+, \text{near}}(\delta \mathfrak{R}_2 \cdot \mathbf{x}) + P_{-}(\mathbf{x}) \eta_{-, \text{near}}(\delta \mathfrak{R}_2 \cdot \mathbf{x}) \right. \\
 & \left. + \sum_{b=\pm} \rho_b(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) \right], \tag{7.36}
 \end{aligned}$$

$$\text{where } \rho_{\pm}(\mathbf{x}, \zeta) = \int_{|\xi| \leq \delta^{\nu-1}} e^{i\xi\zeta} \varphi_{\pm}(\mathbf{x}, \delta\xi) \widehat{\eta}_{\pm, \text{near}}(\xi) d\xi. \tag{7.37}$$

We now expand the inner product in (7.33); the corresponding term in (7.34) is treated similarly. Substituting (7.36) into the inner product in (7.33) yields (using  $\Phi_{\pm}(\mathbf{x}; \mathbf{k}) = e^{i\mathbf{k} \cdot \mathbf{x}} p_{\pm}(\mathbf{x}; \mathbf{k})$ )

$$\begin{aligned}
 & \langle \Phi_{+}(\cdot, \delta\xi), \kappa(\delta \cdot) W(\cdot) \eta_{\text{near}}(\cdot) \rangle_{L^2_{\mathbf{k}_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}} \\
 & \equiv \langle \Phi_{+}(\cdot, \mathbf{K} + \delta\xi \mathfrak{R}_2), \kappa(\delta \cdot) W(\cdot) \eta_{\text{near}}(\cdot) \rangle_{L^2_{\mathbf{k}_{\parallel} = \mathbf{K} \cdot \mathbf{v}_1}} \tag{7.38}
 \end{aligned}$$

$$= \delta \left\langle e^{i\delta\xi \mathfrak{R}_2 \cdot} p_{+}(\cdot, \delta\xi), P_{+}(\cdot) W(\cdot) \kappa(\delta \mathfrak{R}_2 \cdot) \eta_{+, \text{near}}(\delta \mathfrak{R}_2 \cdot) \right\rangle_{L^2(\Sigma)} \tag{7.39}$$

$$+ \delta \left\langle e^{i\delta\xi \mathfrak{R}_2 \cdot} p_{+}(\cdot, \delta\xi), P_{-}(\cdot) W(\cdot) \kappa(\delta \mathfrak{R}_2 \cdot) \eta_{-, \text{near}}(\delta \mathfrak{R}_2 \cdot) \right\rangle_{L^2(\Sigma)} \tag{7.40}$$

$$+ \delta \sum_{b=\pm} \left\langle e^{i\delta\xi \mathfrak{R}_2 \cdot} p_{+}(\cdot, \delta\xi), W(\cdot) \kappa(\delta \mathfrak{R}_2 \cdot) \rho_b(\cdot, \delta \mathfrak{R}_2 \cdot) \right\rangle_{L^2(\Sigma)}. \tag{7.41}$$

The inner product terms in (7.39)–(7.41) are each of the form:

$$\mathcal{G}(\delta; \xi) \equiv \delta \int_{\Sigma} e^{-i\xi \delta \mathfrak{R}_2 \cdot \mathbf{x}} g(\mathbf{x}, \delta\xi) \Gamma(\mathbf{x}, \delta \mathfrak{R}_2 \cdot \mathbf{x}) d\mathbf{x}, \text{ where} \tag{7.42}$$

(IP1)  $g(\mathbf{x}, y)$  is a smooth function of  $(\mathbf{x}, y) \in \mathbb{R}^2 / \Lambda_h \times \mathbb{R}$  and

(IP2)  $\mathbf{x} \mapsto \Gamma(\mathbf{x}, \zeta)$  is  $\Lambda_h$ -periodic and  $H^2(\Omega)$  with values in  $L^2(\mathbb{R}_{\zeta})$ , i.e.

$$\Gamma(\mathbf{x} + \mathbf{v}, \zeta) = \Gamma(\mathbf{x}, \zeta), \text{ for all } \mathbf{v} \in \Lambda_h, \tag{7.43}$$

$$\sum_{j=0}^2 \sum_{|\mathbf{c}|=j} \int_{\Omega} \|\partial_{\mathbf{x}}^{\mathbf{c}} \Gamma(\mathbf{x}, \zeta)\|_{L^2(\mathbb{R}_{\zeta})}^2 d\mathbf{x} < \infty. \tag{7.44}$$

We denote this Hilbert space of functions by  $\mathbb{H}^2$  with norm-squared,  $\|\cdot\|_{\mathbb{H}^2}^2$ , given in (7.44). It is easy to check that conditions (7.43)–(7.44) are satisfied for the cases  $\Gamma = \Gamma(\zeta) = \kappa(\zeta) \eta_{\pm, \text{near}}(\zeta)$  and  $\Gamma = \Gamma(\mathbf{x}, \zeta) = \kappa(\zeta) \rho_{\pm}(\mathbf{x}, \zeta)$ , where  $\rho_{\pm}$  is defined in (7.37).



To expand expressions of the form  $G(\delta, \xi)$ , we use:

**Lemma 7.9** *Let  $g(\mathbf{x}, y)$  and  $\Gamma(\mathbf{x}, \zeta)$  satisfy conditions (IP1) and (IP2), respectively. Denote by  $\widehat{\Gamma}(\mathbf{x}, \omega)$  the Fourier transform of  $\Gamma(\mathbf{x}, \zeta)$  with respect to the  $\zeta$  – variable, given by*

$$\widehat{\Gamma}(\mathbf{x}, \omega) \equiv \lim_{N \uparrow \infty} \frac{1}{2\pi} \int_{|\zeta| \leq N} e^{-i\omega\zeta} \Gamma(\mathbf{x}, \zeta) d\zeta, \tag{7.45}$$

where the limit is taken in  $L^2(\Omega \times \mathbb{R}_\omega; d\mathbf{x}d\omega)$ . Then,

$$\mathcal{G}(\delta; \xi) = \sum_{n \in \mathbb{Z}} \int_{\Omega} e^{in\mathfrak{K}_2 \cdot \mathbf{x}} \widehat{\Gamma}\left(\mathbf{x}, \frac{n}{\delta} + \xi\right) g(\mathbf{x}, \delta\xi) d\mathbf{x}, \tag{7.46}$$

with equality holding in  $L^2_{\text{loc}}([-\xi_{\max}, \xi_{\max}]; d\xi)$ , for any fixed  $\xi_{\max} > 0$ .

We adapt the proof in [10] (Lemma 6.5) for the 1D setting. We require the following variant of the Poisson summation formula in  $L^2_{\text{loc}}$ .

**Theorem 7.10** *Let  $\Gamma(\mathbf{x}, \zeta)$  satisfy (IP2). Denote by  $\widehat{\Gamma}(\mathbf{x}, \omega)$  the Fourier transform of  $\Gamma(\mathbf{x}, \zeta)$  with respect to the variable,  $\zeta$ ; see (7.45). Fix an arbitrary  $y_{\max} > 0$ , and introduce the parameterization of the cylinder  $\Sigma: \mathbf{x} = \tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2$ ,  $0 \leq \tau_1 \leq 1$ ,  $\tau_2 \in \mathbb{R}$ . Then,*

$$\sum_{n \in \mathbb{Z}} e^{-iy(\tau_2+n)} \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \tau_2 + n) = 2\pi \sum_{n \in \mathbb{Z}} e^{2\pi i n \tau_2} \widehat{\Gamma}(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi n + y)$$

in  $L^2([0, 1]^2 \times [-y_{\max}, y_{\max}]; d\tau_1 d\tau_2 \cdot dy)$ .

The 1D analogue of Theorem 7.10 was proved in Appendix A of [10]. Since the proof is very similar, we omit it. We also require

**Lemma 7.11** *Let  $F(\mathbf{x}, y)$  and  $F_N(\mathbf{x}, y)$ ,  $N = 1, 2, \dots$ , belong to  $L^2(\Sigma \times [-y_{\max}, y_{\max}]; d\mathbf{x}dy)$ . Assume that*

$$\|F_N - F\|_{L^2(\Sigma \times [-y_{\max}, y_{\max}]; d\mathbf{x}dy)} \rightarrow 0, \text{ as } N \rightarrow \infty.$$

Let  $G \in L^2([-y_{\max}, y_{\max}]; dy)$ . Then, in the  $L^2(\Sigma; d\mathbf{x})$  sense, we have:

$$\begin{aligned} \lim_{N \rightarrow \infty} \int_{-y_{\max}}^{y_{\max}} F_N(\mathbf{x}, y) G(y) dy &= \int_{-y_{\max}}^{y_{\max}} \lim_{N \rightarrow \infty} F_N(\mathbf{x}, y) G(y) dy \\ &= \int_{-y_{\max}}^{y_{\max}} F(\mathbf{x}, y) G(y) dy. \end{aligned}$$

*Proof of Lemma 7.11* Square the difference, apply Cauchy-Schwarz and then integrate  $d\mathbf{x}$  over  $\Sigma$ . □

*Proof of Lemma 7.9* Recall the parameterization of the cylinder,  $\Sigma$ :

$$\mathbf{x} \in \Sigma : \quad \mathbf{x} = \tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \quad 0 \leq \tau_1 \leq 1, \quad \tau_2 \in \mathbb{R}, \quad \mathfrak{K}_1 \cdot \mathbf{x} = 2\pi \tau_1, \quad \mathfrak{K}_2 \cdot \mathbf{x} = 2\pi \tau_2, \\ dx_1 dx_2 = |\mathbf{v}_1 \wedge \mathbf{v}_2| d\tau_1 d\tau_2 \equiv |\Omega| d\tau_1 d\tau_2.$$

Using that  $g(\mathbf{x}, \delta\xi) = g(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \delta\xi)$  and  $\Gamma(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) = \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi \delta\tau_2)$  are both appropriately 1-periodic, we expand  $\mathcal{G}(\delta; \xi)$  defined in (7.42). By Lemma 7.11:

$$\begin{aligned} \mathcal{G}(\delta; \xi) &= \delta |\Omega| \int_0^1 d\tau_1 \int_{-\infty}^{\infty} e^{-2\pi i \delta \xi \tau_2} g(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \delta\xi) \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi \delta\tau_2) d\tau_2 \\ &= \delta |\Omega| \int_0^1 d\tau_1 \lim_{N \rightarrow \infty} \sum_{n=-N}^N \int_n^{n+1} e^{-2\pi i \delta \xi \tau_2} g(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \delta\xi) \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi \delta\tau_2) d\tau_2 \\ &= \delta |\Omega| \int_0^1 d\tau_1 \lim_{N \rightarrow \infty} \sum_{n=-N}^N \int_0^1 e^{-2\pi i \delta \xi (\tau_2+n)} g(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \delta\xi) \\ &\quad \times \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi \delta(\tau_2+n)) d\tau_2 \\ &= \delta |\Omega| \int_0^1 d\tau_1 \int_0^1 g(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \delta\xi) \left[ \sum_{n \in \mathbb{Z}} e^{-2\pi i \delta \xi (\tau_2+n)} \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi \delta(\tau_2+n)) \right] d\tau_2. \end{aligned}$$

By Theorem 7.10 with  $\Gamma = \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi \delta\tau_2)$  and  $y = 2\pi \delta\xi$ , we have

$$\sum_{n \in \mathbb{Z}} e^{-2\pi i \delta \xi (\tau_2+n)} \Gamma(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, 2\pi \delta\tau_2) = \frac{1}{\delta} \sum_{n \in \mathbb{Z}} e^{2\pi i n \tau_2} \widehat{\Gamma} \left( \tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \frac{n}{\delta} + \xi \right),$$

with equality holding in  $L^2([0, 1]^2 \times [-\xi_{\max}, \xi_{\max}]; d\tau_1 d\tau_2 \cdot d\xi)$ . Again using Lemma 7.11 we may interchange the sum and integral to obtain

$$\begin{aligned} \mathcal{G}(\delta; \xi) &= \frac{\delta}{\delta} |\Omega| \int_0^1 d\tau_1 \int_0^1 g(\tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \delta\xi) \sum_{n \in \mathbb{Z}} e^{2\pi i n \tau_2} \widehat{\Gamma} \left( \tau_1 \mathbf{v}_1 + \tau_2 \mathbf{v}_2, \frac{n}{\delta} + \xi \right) d\tau_2 \\ &= \sum_{n \in \mathbb{Z}} \int_{\Omega} e^{in\mathfrak{K}_2 \cdot \mathbf{x}} \widehat{\Gamma} \left( \mathbf{x}, \frac{n}{\delta} + \xi \right) g(\mathbf{x}, \delta\xi) d\mathbf{x}. \end{aligned} \tag{7.47}$$

This completes the proof of Lemma 7.9. □

We next apply Lemma 7.9 to each of the inner products (7.39)–(7.41).

Expansion of inner product (7.39):

Let  $g(\mathbf{x}, \delta\xi) = p_+(\mathbf{x}, \delta\xi) P_+(\mathbf{x}) W(\mathbf{x})$  and  $\Gamma(\mathbf{x}, \zeta) = \kappa(\zeta) \eta_{+, \text{near}}(\zeta)$ . By Lemma 7.9,

$$\begin{aligned} &\delta \left\langle e^{i\xi \delta \mathfrak{K}_2 \cdot} p_+(\cdot, \delta\xi), P_+(\cdot) W(\cdot) \kappa(\delta \mathfrak{K}_2 \cdot) \eta_{+, \text{near}}(\delta \mathfrak{K}_2 \cdot) \right\rangle_{L^2(\Sigma)} \\ &= \sum_{n \in \mathbb{Z}} \int_{\Omega} e^{in\mathfrak{K}_2 \cdot \mathbf{x}} \mathcal{F}_{\zeta}[\kappa \eta_{+, \text{near}}] \left( \frac{n}{\delta} + \xi \right) \overline{p_+(\mathbf{x}, \delta\xi) P_+(\mathbf{x}) W(\mathbf{x})} d\mathbf{x}. \end{aligned}$$

Since  $p_{\pm}(\mathbf{x}, \lambda = \delta\xi) = P_{\pm}(\mathbf{x}) + \varphi_{\pm}(\mathbf{x}, \delta\xi)$ , where  $\varphi_{\pm}(\mathbf{x}, \delta\xi)$  satisfies the bound (7.35), we have

$$\begin{aligned} & \delta \left\langle e^{i\xi\delta\mathfrak{R}_2\cdot} p_+(\cdot, \delta\xi), P_+(\cdot)W(\cdot)\kappa(\delta\mathfrak{R}_2\cdot)\eta_{+,near}(\delta\mathfrak{R}_2\cdot) \right\rangle_{L^2(\Sigma)} \\ & \equiv I_+^1(\xi; \eta_{+,near}) + I_+^2(\xi; \eta_{+,near}), \end{aligned}$$

where

$$\begin{aligned} I_+^1(\xi; \eta_{+,near}) &= \sum_{n \in \mathbb{Z}} \mathcal{F}_{\zeta}[\kappa\eta_{+,near}] \left(\frac{n}{\delta} + \xi\right) \int_{\Omega} e^{in\mathfrak{R}_2\cdot\mathbf{x}} |P_+(\mathbf{x})|^2 W(\mathbf{x})d\mathbf{x}, \\ I_+^2(\xi; \eta_{+,near}) &= \sum_{n \in \mathbb{Z}} \mathcal{F}_{\zeta}[\kappa\eta_{+,near}] \left(\frac{n}{\delta} + \xi\right) \int_{\Omega} e^{in\mathfrak{R}_2\cdot\mathbf{x}} \overline{\varphi_+(\mathbf{x}, \delta\xi)} P_+(\mathbf{x})W(\mathbf{x})d\mathbf{x}. \end{aligned} \tag{7.48}$$

From Proposition 6.2 and Assumption (W3) we have

$$\int_{\Omega} |P_+(\mathbf{x})|^2 W(\mathbf{x})d\mathbf{x} = 0 \quad \text{and} \quad \int_{\Omega} \overline{P_+(\mathbf{x})} P_-(\mathbf{x})W(\mathbf{x})d\mathbf{x} = \vartheta_{\#} \neq 0. \tag{7.49}$$

Therefore, the  $n = 0$  term in the summation of  $I_+^1(\xi; \eta_{+,near})$  in (7.48) is zero and we may write:

$$I_+^1(\xi; \eta_{+,near}) = \sum_{|n| \geq 1} \mathcal{F}_{\zeta}[\kappa\eta_{+,near}] \left(\frac{n}{\delta} + \xi\right) \int_{\Omega} e^{in\mathfrak{R}_2\cdot\mathbf{x}} |P_+(\mathbf{x})|^2 W(\mathbf{x})d\mathbf{x}.$$

*Expansion of the inner product (7.40):*

Similarly, with  $g(\mathbf{x}, \delta\xi) = \overline{p_+(\mathbf{x}, \delta\xi)} P_-(\mathbf{x})W(\mathbf{x})$  and  $\Gamma(\mathbf{x}, \zeta) = \kappa(\zeta)\eta_{-,near}(\zeta)$ , we have

$$\begin{aligned} & \delta \left\langle e^{i\xi\delta\mathfrak{R}_2\cdot} p_+(\cdot, \delta\xi), P_-(\cdot)W(\cdot)\kappa(\delta\mathfrak{R}_2\cdot)\eta_{-,near}(\delta\mathfrak{R}_2\cdot) \right\rangle_{L^2(\Sigma)} \\ & \equiv \tilde{I}_+^3(\xi; \eta_{-,near}) + I_+^4(\xi; \eta_{-,near}), \end{aligned}$$

where (noting, by (7.49), that the  $n = 0$  contribution is nonzero)

$$\begin{aligned} \tilde{I}_+^3(\xi; \eta_{-,near}) &= \vartheta_{\#} \widehat{\kappa\eta}_{+,near}(\xi) + I_+^3(\xi; \eta_{-,near}), \quad \text{where} \\ I_+^3(\xi; \eta_{-,near}) &\equiv \sum_{|n| \geq 1} \mathcal{F}_{\zeta}[\kappa\eta_{-,near}] \left(\frac{n}{\delta} + \xi\right) \int_{\Omega} e^{in\mathfrak{R}_2\cdot\mathbf{x}} \overline{P_+(\mathbf{x})} P_-(\mathbf{x})W(\mathbf{x})d\mathbf{x}, \quad \text{and} \\ I_+^4(\xi; \eta_{-,near}) &= \sum_{n \in \mathbb{Z}} \mathcal{F}_{\zeta}[\kappa\eta_{-,near}] \left(\frac{n}{\delta} + \xi\right) \int_{\Omega} e^{in\mathfrak{R}_2\cdot\mathbf{x}} \overline{\varphi_+(\mathbf{x}, \delta\xi)} P_-(\mathbf{x})W(\mathbf{x})d\mathbf{x}. \end{aligned}$$

Expansion of inner products (7.41):

Consider the  $b = +$  term in (7.41). Let  $g(\mathbf{x}, \delta\xi) = \overline{p_+(\mathbf{x}, \delta\xi)W(\mathbf{x})}$  and  $\Gamma(\mathbf{x}, \zeta) = \kappa(\zeta)\rho_+(\mathbf{x}, \zeta)$ . By Lemma 7.9 and the expansion of  $p_+(\mathbf{x}, \delta\xi)$  about  $P_+(\mathbf{x})$  in (7.35) we have:

$$\delta \left\langle e^{i\xi\delta\mathfrak{R}_2} p_+(\cdot, \delta\xi), W(\cdot)\kappa(\delta\mathfrak{R}_2)\rho_+(\cdot, \delta\mathfrak{R}_2) \right\rangle_{L^2(\Sigma)} \equiv I_+^5(\xi; \eta_{+,near}) + I_+^6(\xi; \eta_{+,near}),$$

where

$$I_+^5(\xi; \eta_{+,near}) = \sum_{n \in \mathbb{Z}} \int_{\Omega} \mathcal{F}_{\zeta}[\kappa\rho_+] \left( \mathbf{x}, \frac{n}{\delta} + \xi \right) e^{in\mathfrak{R}_2 \cdot \mathbf{x}} \overline{P_+(\mathbf{x})} W(\mathbf{x}) d\mathbf{x},$$

$$I_+^6(\xi; \eta_{+,near}) = \sum_{n \in \mathbb{Z}} \int_{\Omega} \mathcal{F}_{\zeta}[\kappa\rho_+] \left( \mathbf{x}, \frac{n}{\delta} + \xi \right) e^{in\mathfrak{R}_2 \cdot \mathbf{x}} \overline{\varphi_+(\mathbf{x}, \delta\xi)} W(\mathbf{x}) d\mathbf{x}.$$

For the  $b = -$  term in (7.41) we have

$$\delta \left\langle e^{i\xi\delta\mathfrak{R}_2} p_+(\cdot, \delta\xi), W(\cdot)\kappa(\delta\mathfrak{R}_2)\rho_-(\cdot, \delta\mathfrak{R}_2) \right\rangle_{L^2(\Sigma)} \equiv I_+^7(\xi; \eta_{-,near}) + I_+^8(\xi; \eta_{-,near}),$$

where

$$I_+^7(\xi; \eta_{-,near}) = \sum_{n \in \mathbb{Z}} \int_{\Omega} \mathcal{F}_{\zeta}[\kappa\rho_-] \left( \mathbf{x}, \frac{n}{\delta} + \xi \right) e^{in\mathfrak{R}_2 \cdot \mathbf{x}} \overline{P_+(\mathbf{x})} W(\mathbf{x}) d\mathbf{x},$$

$$I_+^8(\xi; \eta_{-,near}) = \sum_{n \in \mathbb{Z}} \int_{\Omega} \mathcal{F}_{\zeta}[\kappa\rho_-] \left( \mathbf{x}, \frac{n}{\delta} + \xi \right) e^{in\mathfrak{R}_2 \cdot \mathbf{x}} \overline{\varphi_+(\mathbf{x}, \delta\xi)} W(\mathbf{x}) d\mathbf{x}.$$

Assembling the above expansions, we find that the full inner product, (7.38), may be expressed as:

$$\langle \Phi_+(\cdot, \delta\xi), \kappa(\delta\mathfrak{R}_2)W(\cdot)\eta_{near}(\cdot) \rangle_{L^2(\Sigma)} = \vartheta_{\sharp}\widehat{\kappa}\widehat{\eta}_{near,-}(\xi) + \sum_{j=1}^8 I_+^j(\xi; \eta_{near}), \quad (7.50)$$

A similar calculation yields:

$$\langle \Phi_-(\cdot, \delta\xi), \kappa(\delta\mathfrak{R}_2)W(\cdot)\eta_{near}(\cdot) \rangle_{L^2(\Sigma)} = \vartheta_{\sharp}\widehat{\kappa}\widehat{\eta}_{near,+}(\xi) + \sum_{j=1}^8 I_-^j(\xi; \eta_{near}), \quad (7.51)$$

where the terms  $I_{\pm}^j(\xi; \eta_{near})$  are defined analogously to  $I_+^j(\xi; \eta_{near})$ . We now substitute our results (7.50)–(7.51), (7.13)–(7.14) and (7.27) into (7.33)–(7.34) to obtain the following:

**Proposition 7.12** *Let  $\widehat{\beta}(\xi) = (\widehat{\eta}_{+,near}(\xi), \widehat{\eta}_{-,near}(\xi))^T$ . Equations (7.33)–(7.34), the closed system governing the near energy components,  $\eta_{near}$ , of the corrector,  $\eta$ , is of the form:*

$$(\widehat{\mathcal{D}}^\delta + \widehat{\mathcal{L}}^\delta(\mu) - \delta\mu) \widehat{\beta}(\xi) = \mu \widehat{\mathcal{M}}(\xi; \delta) + \widehat{\mathcal{N}}(\xi; \delta). \tag{7.52}$$

Here,  $\mathcal{D}^\delta$  denotes the band-limited Dirac operator defined by

$$\widehat{\mathcal{D}}^\delta \widehat{\beta}(\xi) \equiv |\lambda_\sharp| |\mathfrak{R}_2| \sigma_3 \xi \widehat{\beta}(\xi) + \vartheta_\sharp \chi \left( |\xi| \leq \delta^{\nu-1} \right) \sigma_1 \kappa \widehat{\beta}(\xi). \tag{7.53}$$

The linear operator,  $\widehat{\mathcal{L}}^\delta(\mu)$ , acting on  $\widehat{\beta}$ , and the source terms  $\widehat{\mathcal{M}}(\xi; \delta)$  and  $\widehat{\mathcal{N}}(\xi; \delta)$  are defined by:

$$\begin{aligned} \widehat{\mathcal{L}}^\delta(\mu) \widehat{\beta}(\xi) &\equiv \chi \left( |\xi| \leq \delta^{\nu-1} \right) \sum_{j=1}^3 \widehat{\mathcal{L}}_j^\delta(\mu) \widehat{\beta}(\xi), \quad \text{where} \\ \widehat{\mathcal{L}}_1^\delta(\mu) \widehat{\beta}(\xi) &\equiv \delta \xi^2 \begin{pmatrix} E_{2,+}(\delta\xi) \widehat{\eta}_{+,near}(\xi) \\ E_{2,-}(\delta\xi) \widehat{\eta}_{-,near}(\xi) \end{pmatrix}, \quad \widehat{\mathcal{L}}_2^\delta(\mu) \widehat{\beta}(\xi) \equiv \sum_{j=1}^8 \begin{pmatrix} I_{\pm}^j(\xi; \widehat{\eta}_{\pm,near}(\xi)) \\ I_{\mp}^j(\xi; \widehat{\eta}_{\pm,near}(\xi)) \end{pmatrix}, \\ \widehat{\mathcal{L}}_3^\delta(\mu) \widehat{\beta}(\xi) &\equiv \begin{pmatrix} \langle \Phi_+(\cdot, \delta\xi), \kappa(\delta\mathfrak{R}_2 \cdot) W(\cdot) [A\eta_{near}](\cdot; \mu, \delta) \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}} \\ \langle \Phi_-(\cdot, \delta\xi), \kappa(\delta\mathfrak{R}_2 \cdot) W(\cdot) [A\eta_{near}](\cdot; \mu, \delta) \rangle_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}} \end{pmatrix}, \\ \widehat{\mathcal{M}}(\xi; \delta) &\equiv \chi \left( |\xi| \leq \delta^{\nu-1} \right) \sum_{j=1}^3 \widehat{\mathcal{M}}_j(\xi; \delta), \quad \text{where (inner products over } L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}) \tag{7.54} \\ \widehat{\mathcal{M}}_1(\xi; \delta) &\equiv \begin{pmatrix} \langle \Phi_+(\cdot, \delta\xi), \psi^{(0)}(\cdot, \delta \cdot) \rangle \\ \langle \Phi_-(\cdot, \delta\xi), \psi^{(0)}(\cdot, \delta \cdot) \rangle \end{pmatrix}, \quad \widehat{\mathcal{M}}_2(\xi; \delta) \equiv \delta \begin{pmatrix} \langle \Phi_+(\cdot, \delta\xi), \psi_p^{(1)}(\cdot, \delta \cdot) \rangle \\ \langle \Phi_-(\cdot, \delta\xi), \psi_p^{(1)}(\cdot, \delta \cdot) \rangle \end{pmatrix}, \\ \widehat{\mathcal{M}}_3(\xi; \delta) &\equiv - \begin{pmatrix} \langle \Phi_+(\cdot, \delta\xi), \kappa(\delta\mathfrak{R}_2 \cdot) W(\cdot) B(\cdot; \delta) \rangle \\ \langle \Phi_-(\cdot, \delta\xi), \kappa(\delta\mathfrak{R}_2 \cdot) W(\cdot) B(\cdot; \delta) \rangle \end{pmatrix}, \tag{7.55} \\ \widehat{\mathcal{N}}(\xi; \delta) &\equiv \chi \left( |\xi| \leq \delta^{\nu-1} \right) \sum_{j=1}^4 \widehat{\mathcal{N}}_j(\xi; \delta), \quad \text{where (inner products over } L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}) \\ \widehat{\mathcal{N}}_1(\xi; \delta) &\equiv \begin{pmatrix} \langle \Phi_+(\mathbf{x}, \delta\xi), (2\mathfrak{R}_2 \cdot \nabla_{\mathbf{x}} \partial_{\zeta} - \kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x}) W(\mathbf{x})) \psi_p^{(1)}(\mathbf{x}, \delta\mathfrak{R}_2 \cdot \mathbf{x}) \rangle \\ \langle \Phi_-(\mathbf{x}, \delta\xi), (2\mathfrak{R}_2 \cdot \nabla_{\mathbf{x}} \partial_{\zeta} - \kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x}) W(\mathbf{x})) \psi_p^{(1)}(\mathbf{x}, \delta\mathfrak{R}_2 \cdot \mathbf{x}) \rangle \end{pmatrix}, \\ \widehat{\mathcal{N}}_2(\xi; \delta) &\equiv \begin{pmatrix} \langle \Phi_+(\mathbf{x}, \delta\xi), |\mathfrak{R}_2|^2 \partial_{\zeta}^2 \psi^{(0)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta\mathfrak{R}_2 \cdot \mathbf{x}} \rangle \\ \langle \Phi_-(\mathbf{x}, \delta\xi), |\mathfrak{R}_2|^2 \partial_{\zeta}^2 \psi^{(0)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta\mathfrak{R}_2 \cdot \mathbf{x}} \rangle \end{pmatrix}, \\ \widehat{\mathcal{N}}_3(\xi; \delta) &\equiv \begin{pmatrix} \langle \Phi_+(\mathbf{x}, \delta\xi), |\mathfrak{R}_2|^2 \partial_{\zeta}^2 \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta\mathfrak{R}_2 \cdot \mathbf{x}} \rangle \\ \langle \Phi_-(\mathbf{x}, \delta\xi), |\mathfrak{R}_2|^2 \partial_{\zeta}^2 \psi_p^{(1)}(\mathbf{x}, \zeta) \Big|_{\zeta=\delta\mathfrak{R}_2 \cdot \mathbf{x}} \rangle \end{pmatrix}, \\ \widehat{\mathcal{N}}_4(\xi; \delta) &\equiv - \begin{pmatrix} \langle \Phi_+(\mathbf{x}, \delta\xi), \kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x}) W(\mathbf{x}) C(\mathbf{x}; \delta) \rangle \\ \langle \Phi_-(\mathbf{x}, \delta\xi), \kappa(\delta\mathfrak{R}_2 \cdot \mathbf{x}) W(\mathbf{x}) C(\mathbf{x}; \delta) \rangle \end{pmatrix}. \tag{7.56} \end{aligned}$$

We conclude this section with the assertion that from an appropriate solution  $(\widehat{\beta}^\delta(\xi), \mu(\delta))$  of the band-limited Dirac system (7.52) one can construct a bound state  $(\Psi^\delta, E^\delta)$  of the Schrödinger eigenvalue problem (7.1). We say  $f \in L^{2,1}(\mathbb{R})$  if  $\|f\|_{L^{2,1}(\mathbb{R})}^2 \equiv \int (1 + |\xi|^2)^{1/2} f(\xi) d\xi < \infty$ .

**Proposition 7.13** *Suppose, for  $0 < \delta < \delta_0$ , the band-limited Dirac system (7.52) has a solution  $(\widehat{\beta}^\delta(\xi), \mu(\delta))$ ,  $\widehat{\beta}^\delta = (\widehat{\beta}_+^\delta, \widehat{\beta}_-^\delta)^T$ , where  $\text{supp} \widehat{\beta}^\delta \subset \{|\xi| \leq \delta^{\nu-1}\}$ , satisfying:*

$$\begin{aligned} & \|\widehat{\beta}^\delta(\cdot; \mu, \delta)\|_{L^{2,1}(\mathbb{R})} \lesssim \delta^{-1}, \quad 0 < \delta < \delta_0 \quad (\text{to be verified in Proposition 7.15}), \\ & \mu(\delta) \text{ bounded and } \mu(\delta) - \mu_0 \rightarrow 0 \text{ as } \delta \rightarrow 0 \quad (\text{to be verified in Proposition 7.16}). \end{aligned}$$

Define

$$\widehat{\eta}_{\text{near},+}^\delta(\xi) = \widehat{\beta}_+^\delta(\xi), \quad \widehat{\eta}_{\text{near},-}^\delta(\xi) = \widehat{\beta}_-^\delta(\xi), \tag{7.57}$$

and construct  $\eta^\delta \equiv \eta_{\text{near}}^\delta + \eta_{\text{far}}^\delta$  as follows:

$$\begin{aligned} \eta_{\text{near}}^\delta(\mathbf{x}) &= \sum_{b=\pm} \int_{|\lambda| \leq \delta^\nu} \widehat{\eta}_{\text{near},b}^\delta \left( \frac{\lambda}{\delta} \right) \Phi_b(\mathbf{x}; \lambda) d\lambda, \\ \widetilde{\eta}_{\text{far},b}^\delta(\lambda) &= \widetilde{\eta}_{\text{far},b}[\eta_{\text{near}}, \mu, \delta](\lambda), \quad b \geq 1; \quad (\text{see Proposition 7.7}), \\ \eta_{\text{far}}^\delta(\mathbf{x}) &= \sum_{b=\pm} \int_{\delta^\nu \leq |\lambda| \leq 1/2} \widetilde{\eta}_{\text{far},b}^\delta(\lambda) \Phi_b(\mathbf{x}; \lambda) d\lambda + \sum_{b \neq \pm} \int_{|\lambda| \leq 1/2} \widetilde{\eta}_{\text{far},b}^\delta(\lambda) \Phi_b(\mathbf{x}; \lambda) d\lambda. \\ \eta^\delta(\mathbf{x}) &\equiv \eta_{\text{near}}^\delta(\mathbf{x}) + \eta_{\text{far}}^\delta(\mathbf{x}), \quad E^\delta \equiv E_\star + \delta^2 \mu(\delta), \quad 0 < \delta < \delta_0. \end{aligned} \tag{7.58}$$

Then, for all  $0 < |\delta| < \delta_0$ , the following holds:

- (a)  $\eta^\delta(\mathbf{x}) \in H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2(\Sigma)$ .
- (b)  $(\eta^\delta, \mu(\delta))$  solves the corrector equation (7.8).
- (c) Theorem 7.3 holds. The pair  $(\Psi^\delta, E^\delta)$ , defined by (see also (7.6)–(7.7))

$$\begin{aligned} \Psi^\delta(\mathbf{x}) &= \psi^{(0)}(\mathbf{x}, \mathbf{X}) + \delta \psi_p^{(1)}(\mathbf{x}, \mathbf{X}) + \delta \eta^\delta(\mathbf{x}), \quad \mathbf{X} = \delta \mathfrak{K}_2 \cdot \mathbf{x}, \\ E^\delta &= E_\star + \delta^2 \mu_0 + o(\delta^2), \end{aligned} \tag{7.59}$$

is a solution of the eigenvalue problem (7.1) with corrector estimates asserted in the statement of Theorem 7.3.

To prove Proposition 7.13 we use the following lemma.

**Lemma 7.14** *There exists a  $\delta_0 > 0$  such that, for all  $0 < \delta < \delta_0$ , the following holds: Assume  $\beta \in L^2(\mathbb{R})$  and let  $\eta_{\text{near}}^\delta(\mathbf{x})$  be defined by (7.57)–(7.58). Then,*

$$\|\eta_{\text{near}}\|_{H_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}^2} \lesssim \delta^{1/2} \|\beta\|_{L^2(\mathbb{R})}.$$

The proof of Lemma 7.14 parallels that of Lemma 6.9 in [10], and is not reproduced here.

*Proof of Proposition 7.13* From  $\widehat{\beta}$  we construct  $\eta_{\text{near}}^\delta$ , such that:  $\|\eta_{\text{near}}\|_{H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}} \lesssim \delta^{1/2} \|\beta\|_{L^2(\mathbb{R})}$  (Lemma 7.14). Next, part 2 of Proposition 7.7, (7.26), gives a bound on  $\eta_{\text{far}}$ :  $\|\eta_{\text{far}}[\eta_{\text{near}}; \mu, \delta]\|_{H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}} \leq C'' \left( \frac{\delta}{\omega(\delta^{\nu})} \|\eta_{\text{near}}\|_{L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}} + \frac{\delta^{\frac{1}{2}}}{\omega(\delta^{\nu})} \right)$ . These two bounds give the desired  $H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$  bound on  $\eta^\delta$ . Note that all steps in our derivation of the band-limited Dirac system (7.52) are reversible, in particular our application of the Poisson summation formula in  $L^2_{\text{loc}}$ . Therefore,  $(\Psi^\delta, E^\delta)$ , given by (7.59) is an  $H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}$  eigenpair of (7.1).  $\square$

We focus then on constructing and estimating the solution of the band-limited Dirac system (7.52).

### 7.5 Analysis of the Band-Limited Dirac System

The formal  $\delta \downarrow 0$  limit of the band-limited operator  $\widehat{\mathcal{D}}^\delta$ , displayed in (7.53), is a 1D Dirac operator  $\mathcal{D}$  defined via:

$$\widehat{\mathcal{D}} \widehat{\beta}(\xi) \equiv |\lambda_{\sharp}| |\mathfrak{K}_2| \sigma_3 \xi \widehat{\beta}(\xi) + v_{\sharp} \sigma_1 \widehat{\kappa} \widehat{\beta}(\xi). \tag{7.60}$$

Our goal is to solve the system (7.52). We therefore rewrite the linear operator in equation (7.52) as a perturbation of  $\widehat{\mathcal{D}}$  (7.60), and seek  $\widehat{\beta}$  as a solution to:

$$\widehat{\mathcal{D}} \widehat{\beta}(\xi) + (\widehat{\mathcal{D}}^\delta - \widehat{\mathcal{D}} + \widehat{\mathcal{L}}^\delta(\mu) - \delta\mu) \widehat{\beta}(\xi) = \mu \widehat{\mathcal{M}}(\xi; \delta) + \widehat{\mathcal{N}}(\xi; \delta). \tag{7.61}$$

We next solve (7.61) using a Lyapunov-Schmidt reduction strategy. By Proposition 6.3, the null space of  $\widehat{\mathcal{D}}$  is spanned by  $\widehat{\alpha}_*(\xi)$ , the Fourier transform of the zero energy eigenstate (6.29). Since  $\alpha_*(\zeta)$  is Schwartz class, so too is  $\widehat{\alpha}_*(\xi)$  and  $\widehat{\alpha}_*(\xi) \in H^s(\mathbb{R})$  for any  $s \geq 1$ .

For any  $f \in L^2(\mathbb{R})$ , introduce the orthogonal projection operators,

$$\widehat{P}_{\parallel} f = \langle \widehat{\alpha}_*, f \rangle_{L^2(\mathbb{R})} \widehat{\alpha}_*, \quad \text{and} \quad \widehat{P}_{\perp} f = (I - \widehat{P}_{\parallel}) f.$$

Since  $\widehat{P}_{\parallel} \widehat{\mathcal{D}} \widehat{\beta}(\xi) = 0$  and  $\widehat{P}_{\perp} \widehat{\mathcal{D}} \widehat{\beta}(\xi) = \widehat{\mathcal{D}} \widehat{\beta}(\xi)$ , equation (7.61) is equivalent to the system

$$\widehat{P}_{\parallel} \{ (\widehat{\mathcal{D}}^\delta - \widehat{\mathcal{D}} + \widehat{\mathcal{L}}^\delta(\mu) - \delta\mu) \widehat{\beta}(\xi) - \mu \widehat{\mathcal{M}}(\xi; \delta) - \widehat{\mathcal{N}}(\xi; \delta) \} = 0, \tag{7.62}$$

$$\widehat{\mathcal{D}} \widehat{\beta}(\xi) + \widehat{P}_{\perp} \{ (\widehat{\mathcal{D}}^\delta - \widehat{\mathcal{D}} + \widehat{\mathcal{L}}^\delta(\mu) - \delta\mu) \widehat{\beta}(\xi) \} = \widehat{P}_{\perp} \{ \mu \widehat{\mathcal{M}}(\xi; \delta) + \widehat{\mathcal{N}}(\xi; \delta) \}. \tag{7.63}$$

Our strategy will be to first solve (7.63) for  $\widehat{\beta} = \widehat{\beta}[\mu, \delta]$ , for  $\delta > 0$  and sufficiently small. We then substitute  $\widehat{\beta}[\mu, \delta]$  into (7.62) to obtain a closed scalar equation. This

equation is then solved for  $\mu = \mu(\delta)$  for  $\delta$  small. The first step in this strategy is accomplished in

**Proposition 7.15** *Fix  $M > 0$ . There exists  $\delta_0 > 0$  and a mapping  $(\mu, \delta) \in R_{M, \delta_0} \equiv \{|\mu| < M\} \times (0, \delta_0) \mapsto \widehat{\beta}(\cdot; \mu, \delta) \in L^{2,1}(\mathbb{R})$  which is Lipschitz in  $\mu$ , such that  $\widehat{\beta}(\cdot; \mu, \delta)$  solves (7.63) for  $(\mu, \delta) \in R_{M, \delta_0}$ . Furthermore, we have the bound*

$$\|\widehat{\beta}(\cdot; \mu, \delta)\|_{L^{2,1}(\mathbb{R})} \lesssim \delta^{-1}, \quad 0 < \delta < \delta_0.$$

The details of the proof of Proposition 7.15 are similar to those in proof of Proposition 6.10 in [10]; equation (7.63) is expressed as  $(I + C^\delta(\mu))\widehat{\beta}(\xi; \mu, \delta) = \widehat{\mathcal{D}}^{-1}\widehat{P}_\perp \{\mu\widehat{\mathcal{M}}(\xi; \delta) + \widehat{\mathcal{N}}(\xi; \delta)\}$  and the operator  $C^\delta(\mu)$  is proved to be bounded on  $L^{2,1}(\mathbb{R})$  and of norm less than one for all  $0 < \delta < \delta_0$ , with  $\delta_0$  sufficiently small. In bounding  $C^\delta(\mu)$  on  $L^{2,1}(\mathbb{R})$ , we require  $H^1(\mathbb{R})$  bounds for wave operators associated with the Dirac operator,  $\mathcal{D}$ . These can be derived from corresponding results for scalar Schrödinger operators, under the assumptions implied by  $\kappa(\zeta)$  being a domain wall function in the sense of Definition 5.1.

### 7.6 Final Reduction to an Equation for $\mu = \mu(\delta)$ and Its Solution

Substituting the solution  $\widehat{\beta}(\xi; \mu, \delta)$  (Proposition 7.15) into (7.62), yields the equation  $\mathcal{J}_+[\mu, \delta] = 0$ , relating  $\mu$  and  $\delta$ . Here,  $\mathcal{J}_+[\mu; \delta]$  is given by:

$$\begin{aligned} \mathcal{J}_+[\mu; \delta] \equiv & \mu \delta \langle \widehat{\alpha}_*(\cdot), \widehat{\mathcal{M}}(\cdot; \delta) \rangle_{L^2(\mathbb{R})} + \delta \langle \widehat{\alpha}_*(\cdot), \widehat{\mathcal{N}}(\cdot; \delta) \rangle_{L^2(\mathbb{R})} \\ & - \delta \langle \widehat{\alpha}_*(\cdot), (\widehat{\mathcal{D}}^\delta - \widehat{\mathcal{D}}) \widehat{\beta}(\cdot; \mu, \delta) \rangle_{L^2(\mathbb{R})} - \delta \langle \widehat{\alpha}_*(\cdot), \widehat{\mathcal{L}}^\delta(\mu) \widehat{\beta}(\cdot; \mu, \delta) \rangle_{L^2(\mathbb{R})} \\ & + \delta^2 \mu \langle \widehat{\alpha}_*(\cdot), \widehat{\beta}(\cdot; \mu, \delta) \rangle_{L^2(\mathbb{R})}. \end{aligned}$$

The mapping  $(\mu, \delta) \in \{|\mu| < M, \delta \in (0, \delta_0)\} \mapsto \mathcal{J}_+(\mu, \delta)$  is well defined and Lipschitz continuous with respect to  $\mu$ . In the following proposition, we note that  $\mathcal{J}_+[\mu, \delta]$  can be extended to a continuous function on the half-open interval  $[0, \delta_0)$ .

**Proposition 7.16** *Let  $\delta_0 > 0$  be as above. Define*

$$\mathcal{J}[\mu, \delta] \equiv \begin{cases} \mathcal{J}_+[\mu, \delta] & \text{for } 0 < \delta < \delta_0, \\ \mu - \mu_0 & \text{for } \delta = 0, \end{cases}$$

where  $\mu_0 \equiv -\langle \widehat{\alpha}_*, \mathcal{G}^{(2)} \rangle_{L^2(\mathbb{R})} = E^{(2)}$ , and  $\mathcal{G}^{(2)}$  is given in (6.27); see also (6.25) and (6.28). Fix  $M = \max\{2|\mu_0|, 1\}$ . Then,  $(\mu, \delta) \in \{|\mu| < M, 0 \leq \delta < \delta_0\} \mapsto \mathcal{J}(\mu, \delta)$  is well-defined and continuous.

*Proof* The proof parallels that of Proposition 6.16 of [10]. The key is to establish the following asymptotic relations, for all  $0 < \delta < \delta_0$  with  $\delta_0$  sufficiently small:

$$\lim_{\delta \rightarrow 0} \delta \langle \widehat{\alpha}_*(\cdot), \widehat{\mathcal{M}}(\cdot; \delta) \rangle_{L^2(\mathbb{R})} = 1; \tag{7.64}$$



$$\lim_{\delta \rightarrow 0} \delta \langle \widehat{\alpha}_*(\cdot), \widehat{\mathcal{N}}(\cdot; \delta) \rangle_{L^2(\mathbb{R})} = -\mu_0; \tag{7.65}$$

and the following bounds hold for some constant  $C_M$ :

$$\left| \delta \langle \widehat{\alpha}_*(\cdot), (\widehat{\mathcal{D}}^\delta - \widehat{\mathcal{D}}) \widehat{\beta}(\cdot; \mu, \delta) \rangle_{L^2(\mathbb{R})} \right| \leq C_M \delta^{1-\nu}; \tag{7.66}$$

$$\left| \delta \langle \widehat{\alpha}_*(\cdot), \widehat{\mathcal{L}}^\delta(\mu) \widehat{\beta}(\cdot; \mu, \delta) \rangle_{L^2(\mathbb{R})} \right| \leq C_M \delta^\nu; \tag{7.67}$$

$$\left| \delta^2 \mu \langle \widehat{\alpha}_*(\cdot), \widehat{\beta}(\cdot; \mu, \delta) \rangle_{L^2(\mathbb{R})} \right| \leq C_M \delta. \tag{7.68}$$

The detailed verification of (7.64)–(7.68) follows the approach taken in Appendix H of [10]. We make a few remarks on the calculations. Each of the expressions in (7.64)–(7.65) consists of inner products of the form:

$$\mathfrak{J}(\delta) \equiv \delta \left\langle \widehat{\alpha}_*(\xi), \chi \left( |\xi| \leq \delta^{\nu-1} \right) \left( \begin{array}{l} \langle \Phi_+(\mathbf{x}, \delta\xi), J(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) \rangle_{L^2_{k_{\parallel}=\mathbf{k} \cdot \mathbf{v}_1}} \\ \langle \Phi_-(\mathbf{x}, \delta\xi), J(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) \rangle_{L^2_{k_{\parallel}=\mathbf{k} \cdot \mathbf{v}_1}} \end{array} \right) \right\rangle_{L^2(\mathbb{R}_\xi)}. \tag{7.69}$$

Here,  $J(\mathbf{x}, \zeta) = e^{i\mathbf{K} \cdot \mathbf{x}} \mathcal{K}(\mathbf{x}, \zeta)$ , where  $\mathbf{x} \mapsto \mathcal{K}(\mathbf{x}, \zeta)$  is  $\Lambda_h$ -periodic and  $\zeta \mapsto \mathcal{K}(\mathbf{x}, \zeta)$  is smooth and rapidly decaying on  $\mathbb{R}$ . Consider, for example, the expression within:  $\langle \Phi_+(\mathbf{x}, \delta\xi), J(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) \rangle_{L^2_{k_{\parallel}=\mathbf{k} \cdot \mathbf{v}_1}}$ . This may be rewritten and expanded, using Lemma 7.9:

$$\begin{aligned} & \delta \int_{\Sigma} e^{-i\delta\xi \mathfrak{K}_2 \cdot \mathbf{x}} \overline{p_+(\mathbf{x}, \delta\xi)} \mathcal{K}(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) \, d\mathbf{x} \\ &= \sum_{n \in \mathbb{Z}} \int_{\Omega} e^{in\mathfrak{K}_2 \cdot \mathbf{x}} \overline{p_+(\mathbf{x}, \delta\xi)} \widehat{\mathcal{K}}\left(\mathbf{x}, \frac{n}{\delta} + \xi\right) \, d\mathbf{x} \\ &= \int_{\Omega} \overline{p_+(\mathbf{x}, \delta\xi)} \widehat{\mathcal{K}}(\mathbf{x}, \xi) \, d\mathbf{x} + \sum_{|n| \geq 1} \int_{\Omega} e^{in\mathfrak{K}_2 \cdot \mathbf{x}} \overline{p_+(\mathbf{x}, \delta\xi)} \widehat{\mathcal{K}}\left(\mathbf{x}, \frac{n}{\delta} + \xi\right) \, d\mathbf{x}. \end{aligned}$$

Since in (7.69)  $\xi$  is localized to the set where  $|\xi| \leq \delta^{\nu-1}$ ,  $\nu > 0$ , for  $|n| \geq 1$ , we have  $n/\delta + \xi \approx n/\delta$  and the decay of  $\zeta \mapsto \widehat{\mathcal{K}}(\mathbf{x}, \zeta)$  can be used to show that, as  $\delta$  tends to zero, the sum over  $|n| \geq 1$  tends to zero in  $L^2(d\xi)$ . It can also be shown, using the localization of  $\xi$ , that the  $n = 0$  contribution to the sum, tends to  $\langle P_+(\mathbf{x}), \widehat{\mathcal{K}}(\mathbf{x}, \xi) \rangle_{L^2(\Omega)}$ . Therefore, uniformly in  $|\xi| \leq \delta^{\nu-1}$ , we have

$$\lim_{\delta \rightarrow 0} \delta \langle \Phi_+(\mathbf{x}, \delta\xi), J(\mathbf{x}, \delta\mathfrak{K}_2 \cdot \mathbf{x}) \rangle_{L^2_{k_{\parallel}=\mathbf{k} \cdot \mathbf{v}_1}} = \langle P_+(\mathbf{x}), \widehat{\mathcal{K}}(\mathbf{x}, \xi) \rangle_{L^2(\Omega)}.$$

Therefore,

$$\begin{aligned} \lim_{\delta \rightarrow 0} \mathfrak{J}(\delta) &= \int_{\mathbb{R}} d\xi \left[ \overline{\widehat{\alpha}_{*,+}(\xi)} \langle P_+(\mathbf{x}), \widehat{\mathcal{K}}(\mathbf{x}, \xi) \rangle_{L^2(\Omega)} \right. \\ &\quad \left. + \overline{\widehat{\alpha}_{*,-}(\xi)} \langle P_-(\mathbf{x}), \widehat{\mathcal{K}}(\mathbf{x}, \xi) \rangle_{L^2(\Omega)} \right]. \tag{7.70} \end{aligned}$$

The principle contribution to the limit in (7.64) comes from the  $\widehat{\mathcal{M}}_1(\xi; \delta)$  term in (7.54). We apply (7.70) with the choice  $J = J_{\mathcal{M}}(\mathbf{x}, \zeta) = \psi^{(0)}(\mathbf{x}, \zeta)$  and

$$\mathcal{K}_{\mathcal{M}}(\mathbf{x}, \zeta) \equiv e^{-i\mathbf{K}\cdot\mathbf{x}} J_{\mathcal{M}}(\mathbf{x}, \zeta) = \alpha_{\star,+}(\zeta) P_+(\mathbf{x}) + \alpha_{\star,-}(\zeta) P_-(\mathbf{x}).$$

The principle contribution to the limit in (7.65) comes from the  $\widehat{\mathcal{N}}_1(\xi; \delta)$  and  $\widehat{\mathcal{N}}_2(\xi; \delta)$  terms in (7.56). We apply (7.70) with the choice

$$J = J_{\mathcal{N}}(\mathbf{x}, \zeta) = (2\mathfrak{K}_2 \cdot \nabla_{\mathbf{x}} \partial_{\zeta} - \kappa(\zeta)W(\mathbf{x})) \psi_p^{(1)}(\mathbf{x}, \zeta) + |\mathfrak{K}_2|^2 \partial_{\zeta}^2 \psi^{(0)}(\mathbf{x}, \zeta)$$

and  $\mathcal{K}_{\mathcal{N}}(\mathbf{x}, \zeta) \equiv e^{-i\mathbf{K}\cdot\mathbf{x}} J_{\mathcal{N}}(\mathbf{x}, \zeta)$ . The detailed computations are omitted since they are similar to those in [10].

By (7.64)–(7.68), it follows that  $\mathcal{J}_+(\mu; \delta) = \mu - \mu_0 + o(1)$  as  $\delta \rightarrow 0$  uniformly for  $|\mu| \leq M$ . Therefore,  $\mathcal{J}[\mu, \delta]$  is well-defined on  $\{(\mu, \delta) : |\mu| < M, 0 \leq \delta < \delta_0\}$ , continuous at  $\delta = 0$  and Proposition 7.16 is proved.

Summarizing, we have that given  $\widehat{\beta}(\cdot, \mu, \delta)$ , constructed in Proposition 7.15, to complete our construction of a solution to (7.62)–(7.63), it suffices to solve (7.62) for  $\mu = \mu(\delta)$ . Furthermore, we have just shown that (7.62) holds if and only if  $\mu = \mu(\delta)$  is a solution of  $\mathcal{J}[\mu; \delta] = 0$ . From Proposition 7.16 it follows that  $\mathcal{J}[\mu; \delta] = 0$  has a transverse zero,  $\mu = \mu(\delta)$ , for all  $\delta$  and sufficiently small. The details are presented in Proposition 6.17 of [10]:

**Proposition 7.17** *There exists  $\delta_0 > 0$ , and a function  $\delta \mapsto \mu(\delta)$ , defined for  $0 \leq \delta < \delta_0$  such that:  $|\mu(\delta)| \leq M$ ,  $\lim_{\delta \rightarrow 0} \mu(\delta) = \mu(0) = \mu_0 \equiv E^{(2)}$  and  $\mathcal{J}[\mu(\delta), \delta] = 0$  for all  $0 \leq \delta < \delta_0$ .*

We have constructed a solution pair  $(\widehat{\beta}^{\delta}(\xi), \mu(\delta))$ , with  $\widehat{\beta}^{\delta} \in L^{2,1}(\mathbb{R}; d\xi)$ , of the band-limited Dirac system (7.52). Now apply Proposition 7.13 and the proof of Theorem 7.3 is complete.  $\square$

## 8 Edge States for Weak Potentials and the No-Fold Condition for the Zigzag Slice

In Section 7 we fixed an arbitrary edge,  $\mathbf{v}_1 = a_1 \mathbf{v}_1 + a_2 \mathbf{v}_2$  and proved the existence of topologically protected  $\mathbf{v}_1$ – edge states under the spectral no-fold condition. In this section, we consider the special case of the zigzag edge, corresponding to the choice:  $\mathbf{v}_1 = \mathbf{v}_1$ . We prove that the spectral no-fold condition holds in the weak potential regime, provided  $\varepsilon V_{1,1} > 0$ ; this implies the existence of a topologically protected family zigzag edge states.

We proceed in this section to prove the following:

- (1) Theorem 8.2: The operator  $-\Delta + \varepsilon V$  satisfies the no-fold condition along the zigzag ( $\mathbf{k}_2$ ) slice at the Dirac point  $(\mathbf{K}, E_{\star}^{\varepsilon})$ ; see Definition 7.1.
- (2) Theorem 8.3:  $-\Delta + \varepsilon V(\mathbf{x}) + \delta W(\mathbf{x})$  acting in  $L^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$  has a spectral gap about the energy  $E = E_{\star}^{\varepsilon}$ .

- (3) Theorem 8.4: If  $\varepsilon V_{1,1} < 0$ , then the spectral no-fold condition for the zigzag slice does not hold.
- (4) Theorem 8.5: For  $0 < |\delta| \ll \varepsilon^2$  and  $\varepsilon$  sufficiently small, the zigzag edge state eigenvalue problem for  $H^{(\varepsilon,\delta)} = -\Delta + \varepsilon V(\mathbf{x}) + \delta\kappa(\delta\mathbf{k}_2 \cdot \mathbf{x})W(\mathbf{x})$  has topologically protected edge states.

We begin by stating our detailed assumptions on  $V(\mathbf{x})$  and  $W(\mathbf{x})$ . There exists  $\mathbf{x}_0 \in \mathbb{R}^2$  such that  $\tilde{V}(\mathbf{x}) = V(\mathbf{x} - \mathbf{x}_0)$  and  $\tilde{W}(\mathbf{x}) = W(\mathbf{x} - \mathbf{x}_0)$  satisfy the following:

**Assumptions (V)** (8.1)

- (V1)  $\Lambda_h$ - periodicity:  $\tilde{V}(\mathbf{x} + \mathbf{v}) = \tilde{V}(\mathbf{x})$  for all  $\mathbf{v} \in \Lambda_h$ .
- (V2) Inversion symmetry:  $\tilde{V}(\mathbf{x}) = \tilde{V}(-\mathbf{x})$ .
- (V3)  $2\pi/3$ -rotational invariance:  $\tilde{V}(R^*\mathbf{x}) = \tilde{V}(\mathbf{x})$ .
- (V4) Positivity of Fourier coefficient of  $\varepsilon V$ ,  $\varepsilon V_{1,1}$ :  $\varepsilon \tilde{V}_{1,1} > 0$ , where  $\tilde{V}_{1,1} = \frac{1}{|\Omega|} \int_{\Omega} e^{-i(\mathbf{k}_1 + \mathbf{k}_2) \cdot \mathbf{y}} \tilde{V}(\mathbf{y}) d\mathbf{y}$ ; see (3.7) and (2.3).

**Assumptions (W)** (8.2)

- (W1)  $\Lambda_h$ - periodicity:  $\tilde{W}(\mathbf{x} + \mathbf{v}) = \tilde{W}(\mathbf{x})$  for all  $\mathbf{v} \in \Lambda_h$ .
- (W2) Anti-symmetry:  $\tilde{W}(-\mathbf{x}) = -\tilde{W}(\mathbf{x})$ .
- (W3\*) Uniform nondegeneracy of  $\tilde{W}$ : Let  $\Phi_j^\varepsilon(\mathbf{x})$ ,  $j = 1, 2$  denote the  $L^2_{\mathbf{K},\tau}$ , respectively,  $L^2_{\mathbf{K},\bar{\tau}}$ , modes of the degenerate  $L^2_{\mathbf{K}}$ -eigenspace of  $H^{(\varepsilon,0)} = -\Delta + \varepsilon V$ . Then, there exists  $\theta_0 > 0$ , independent of  $\varepsilon$ , such that for all  $\varepsilon$  sufficiently small:

$$\left| \vartheta_{\sharp}^\varepsilon \right| \equiv \left| \left\langle \Phi_1^\varepsilon, \tilde{W} \Phi_1^\varepsilon \right\rangle_{L^2_{\mathbf{K}}} \right| \geq \theta_0 > 0. \tag{8.3}$$

N.B. Consistent with our earlier convention, in the following discussion, we shall drop the “tildes” on both  $V$  and  $W$ . It will be understood that we have chosen coordinates with  $\mathbf{x}_0 = 0$ .

*Remark 8.1* We claim that (W3\*) (see (8.3)) uniform non-degeneracy of  $W$  is equivalent to the assumption:

$$W_{0,1} + W_{1,0} - W_{1,1} \neq 0, \tag{W3*}$$

where  $\{W_{\mathbf{m}}\}_{\mathbf{m} \in \mathbb{Z}^2}$  denote the Fourier coefficients of  $W(\mathbf{x})$ . To see this, note by Proposition 3.1 of [11], that for sufficiently small  $\varepsilon$ ,

$$\Phi_1^\varepsilon(\mathbf{x}) = \frac{1}{\sqrt{3|\Omega|}} e^{i\mathbf{K} \cdot \mathbf{x}} \left[ 1 + \bar{\tau} e^{i\mathbf{k}_2 \cdot \mathbf{x}} + \tau e^{-i\mathbf{k}_1 \cdot \mathbf{x}} \right] + \mathcal{O}(\varepsilon);$$

see also (3.5). Evaluation of  $\vartheta_{\sharp}^{\varepsilon}$  gives

$$\begin{aligned} \vartheta_{\sharp}^{\varepsilon} &= \frac{1}{3} \int_{\Omega} \left| 1 + \bar{\tau} e^{i\mathbf{k}_2 \cdot \mathbf{x}} + \tau e^{-i\mathbf{k}_1 \cdot \mathbf{x}} \right|^2 W(\mathbf{x}) \, d\mathbf{x} + \mathcal{O}(\varepsilon) \\ &= \frac{1}{3} \left[ (W_{0,1} + W_{1,0}) (\tau - \bar{\tau}) + W_{1,1} (\tau^2 - \bar{\tau}^2) \right] + \mathcal{O}(\varepsilon) \\ &= i \frac{\sqrt{3}}{3} [W_{0,1} + W_{1,0} - W_{1,1}] + \mathcal{O}(\varepsilon), \end{aligned}$$

which is nonzero if (W3\*) holds and  $\varepsilon$  is sufficiently small.

Let  $(\mathbf{K}, E_{\star}^{\varepsilon})$  denote a Dirac point of  $H^{(\varepsilon,0)} = -\Delta + \varepsilon V(\mathbf{x})$ , guaranteed to exist by Theorem 3.5 for all  $0 < |\varepsilon| < \varepsilon_0$  and assume that  $V(\mathbf{x})$  and  $W(\mathbf{x})$  satisfy Assumptions (V), (W); see (8.1)–(8.2).

In our next result, we verify the spectral no-fold condition for the zigzag edge. This is central to applying Theorem 7.3 to prove our result (Theorem 8.5) on the existence of a family of zigzag edge states.

**Theorem 8.2** *There exists a positive constant,  $\varepsilon_2 \leq \varepsilon_0$ , such that for any  $0 < |\varepsilon| < \varepsilon_2$ ,  $H^{(\varepsilon,0)} = -\Delta + \varepsilon V$  satisfies the spectral no-fold condition at quasi-momentum  $\mathbf{K}$  along the zigzag slice; see Definition 7.1.*

*By Assumptions (V),  $E_{-}(\lambda) \leq E_{+}(\lambda) \leq E_b(\lambda)$ ,  $b \geq 3$ . For any  $\alpha$  sufficiently small:*

$$\begin{aligned} b = \pm : \quad \alpha \leq |\lambda| \leq \frac{1}{2} &\implies \left| E_b^{\varepsilon,0}(\lambda) - E_{\star}^{\varepsilon} \right| \geq \frac{q^4}{2} |V_{1,1}| \varepsilon |\lambda|^2 \geq c_1 |\varepsilon| \alpha^2, \\ b \geq 3 : \quad |\lambda| \leq 1/2 &\implies \left| E_b^{\varepsilon,0}(\lambda) - E_{\star}^{\varepsilon} \right| \geq c_2 |\varepsilon| (1 + |b|). \end{aligned}$$

Theorem 8.2 controls the zigzag slice of the band structure at  $\mathbf{K}$ , globally and outside a neighborhood of  $(\mathbf{K}, E_{\star}^{\varepsilon})$ . Since a small perturbation of  $V$  which breaks inversion symmetry opens a gap, locally about  $\mathbf{K}$  (see [11]), it can be shown that  $H^{(\varepsilon,\delta)}$  has a  $L^2_{k_{\parallel}=\mathbf{k} \cdot \mathbf{v}_1=2\pi/3}$ -spectral gap about  $E = E_{\star}^{\varepsilon}$ :

**Theorem 8.3** *Assume  $V(\mathbf{x})$  and  $W(\mathbf{x})$  satisfy Assumptions (V) and (W). Let  $\varepsilon_2$  be as in Theorem 8.2. Then, there exists  $c_b > 0$  such that for all  $0 < |\varepsilon| < \varepsilon_2$  and  $0 < \delta \leq c_b \varepsilon^2$ , the operator  $-\Delta + \varepsilon V(\mathbf{x}) + \delta W(\mathbf{x})$  has a non-trivial  $L^2_{k_{\parallel}=2\pi/3}$ -spectral gap about the energy  $E = E_{\star}^{\varepsilon}$ .*

In the case where (V4) does not hold and the Fourier coefficient of  $\varepsilon V$ ,  $\varepsilon V_{1,1}$ , is negative:  $\varepsilon \tilde{V}_{1,1} < 0$ , then we prove that the no-fold condition does not hold:

**Theorem 8.4** [Conditions for non-existence of a zigzag spectral gap] *Assume hypotheses (VI)–(V3) but, instead of hypothesis (V4), assume  $\varepsilon V_{1,1} < 0$ . Then, for any  $\varepsilon$  sufficiently small, the no-fold condition of Definition 7.1 does not hold for the zigzag slice.*

The proofs of Theorems 8.2 and 8.3 are presented below. Section 8.1 discusses a reduction to the lowest three spectral bands. The general strategy, based on an analysis

of a  $3 \times 3$  determinant, is given in Section 8.2. Theorem 8.4 is proved in Section 8.4 as a consequence of Proposition 8.15.

We prove the following theorem on zigzag edge states using results of Section 7.

**Theorem 8.5** *Let  $H^{(\varepsilon, \delta)} = -\Delta + \varepsilon V(\mathbf{x}) + \delta \kappa(\delta \mathbf{k}_2 \cdot \mathbf{x})W(\mathbf{x})$ , where  $V(\mathbf{x})$  and  $W(\mathbf{x})$  satisfy Assumptions (V) and (W), and  $\kappa(\mathbf{X})$  is a domain wall function in the sense of Definition 5.1. Let  $\varepsilon_2 > 0$  and  $c_b > 0$  be as in Theorem 8.2 and assume  $0 < |\varepsilon| < \varepsilon_2$  and  $0 < |\delta| \leq c_b \varepsilon^2$ . Then, there exist edge states,  $\Psi(\mathbf{x}; k_{\parallel}) \in L^2_{k_{\parallel}}(\Sigma)$ , with  $|k_{\parallel} - 2\pi/3|$  sufficiently small. Furthermore, continuous superposition in  $k_{\parallel}$  yields wave-packets which are concentrated along the zigzag edge.*

*Proof of Theorem 8.5* We claim that the theorem is an immediate consequence of the spectral no-fold condition for  $-\Delta + \varepsilon V$  for the zigzag edge, stated in Theorem 8.2. This follows by an application of Theorem 7.3 (and Corollary 7.4). Since the details of the proof of Theorem 7.3 are carried out for the case of  $H^{(\varepsilon, \delta)}$  with  $\varepsilon = 1$ , we wish to point out how the proof applies with  $\varepsilon$  and  $\delta$  varying as in the statement of Theorem 8.5.

The proof of Theorem 7.3 uses a Lyapunov-Schmidt reduction strategy where the eigenvalue problem is reduced to an equivalent eigenvalue problem (nonlinear in the eigenvalue parameter,  $E$ ) for the Floquet-Bloch spectral components of the bound states in a neighborhood of the Dirac point  $(\mathbf{K}, E^*)$ . Stated for the relevant case of the zigzag edge, this reduction step requires the invertibility of an operator  $(I - Q_{\delta})$  acting on  $H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$ , where  $Q_{\delta}$  is defined in terms of Floquet-Bloch components in (7.29) for  $\mathfrak{R}_2 = \mathbf{k}_2$ .

It suffices to show that the  $H^2_{k_{\parallel}=\mathbf{K}\cdot\mathbf{v}_1}(\Sigma)$  norm of  $Q_{\delta}$  is  $o(1)$  as  $\delta \downarrow 0$ . From (7.31) in Remark 7.8, the operator norm of  $Q_{\delta}$  is bounded by  $\epsilon(\delta)$ , given by:

$$\epsilon(\delta) \lesssim \frac{|\delta|}{\omega(\delta^{\nu})c_1(V)} + \frac{|\delta|}{(1 + |b|)c_2(V)} \leq \frac{|\delta|^1}{\omega(\delta^{\nu})c_1(V)} + \frac{|\delta|}{c_2(V)}.$$

By Theorem 8.2, the no-fold condition holds with modulus  $\omega(\mathbf{a}) = \mathbf{a}^2$  and constants

$$c_1(V) = \tilde{c}_1 \frac{q^4}{2} |V_{1,1}\varepsilon|, \quad c_2(V) = \tilde{c}_2 |\varepsilon|.$$

Therefore, with  $\mathbf{a} = \delta^{\nu}$ ,

$$\epsilon(\delta) \lesssim \frac{|\delta|^{1-2\nu}}{c_1(V)} + \frac{|\delta|}{c_2(V)} \lesssim \frac{2}{q^4 \tilde{c}_1 |V_{1,1}|} \cdot \frac{|\delta|^{1-2\nu}}{|\varepsilon|} + \frac{1}{\tilde{c}_2} \cdot \frac{|\delta|}{|\varepsilon|}.$$

By hypothesis,  $|\delta| \leq c_b \varepsilon^2$ . Hence,  $0 \leq \epsilon(\delta) \lesssim |\varepsilon|^{1-4\nu} + |\varepsilon| \rightarrow 0$  as  $\varepsilon \rightarrow 0$  if we choose  $\nu \in (0, 1/4)$ . This completes the proof of Theorem 8.5.  $\square$

To prove Theorems 8.2 - 8.4 we introduce a tool to localize the analysis about the lowest three bands. Throughout the analysis, without loss of generality, we take  $\varepsilon > 0$  and satisfy the cases  $\varepsilon V_{1,1} > 0$  and  $\varepsilon V_{1,1} < 0$  by varying the sign of  $V_{1,1}$ .

### 8.1 Reduction to the Lowest Three Bands

In this subsection we show, via a Lyapunov-Schmidt reduction argument, that the proofs of Theorems 8.2 and 8.3 can be reduced to the study of the lowest three spectral bands. To achieve this, we consider several parameter space regimes separately.

We start by considering  $\varepsilon = \delta = \lambda = 0$ . In this case,  $H^{(0,0,0)}(\mathbf{K}) = (\nabla + i\mathbf{K})^2$  has a triple eigenvalue,  $E_\star^0 = |\mathbf{K}|^2$ , with corresponding 3– dimensional  $L^2(\mathbb{R}^2/\Lambda_h)$ –eigenspace spanned by the eigenfunctions  $p_\sigma$ , for  $\sigma = 1, \tau, \bar{\tau}$ ; see Section 3.1.

Next, we turn on  $\varepsilon$ , keeping  $\delta = \lambda = 0$ . From Theorem 3.5, there exists  $\varepsilon_0 > 0$  such that for  $\varepsilon \in I_{\varepsilon_0} \equiv (-\varepsilon_0, \varepsilon_0) \setminus \{0\}$ , the operator  $H^{(\varepsilon,0,0)}(\mathbf{K}) = -(\nabla + i\mathbf{K})^2 + \varepsilon V(\mathbf{x})$  has a double  $L^2(\mathbb{R}^2/\Lambda_h)$  eigenvalue,  $E_\star^\varepsilon$ . Let  $E_\star^0 = |\mathbf{K}|^2$ . The maps  $\varepsilon \mapsto E_\star^\varepsilon$  and  $\varepsilon \mapsto \tilde{E}_\star^\varepsilon$  are real analytic for  $\varepsilon \in I_{\varepsilon_0}$  with expansions (3.10), (3.11):

$$\begin{aligned} E_\star^\varepsilon &= E_\star^0 + \varepsilon(V_{0,0} - V_{1,1}) + \mathcal{O}(\varepsilon^2), \\ \tilde{E}_\star^\varepsilon &= E_\star^0 + \varepsilon(V_{0,0} + 2V_{1,1}) + \mathcal{O}(\varepsilon^2). \end{aligned}$$

More generally, we may study the eigenvalue problem

$$(H^{(\varepsilon,\delta,\lambda)} - E)p = 0, \quad p \in L^2(\mathbb{R}^2/\Lambda_h), \quad \text{with } E = E_\star^\varepsilon + \mu, \tag{8.4}$$

and seek, via Lyapunov-Schmidt reduction, to localize (8.4) about the three lowest zigzag slices. Written out, the eigenvalue problem has the form:

$$\left[ -(\nabla + i[\mathbf{K} + \lambda\mathbf{k}_2])^2 - E_\star^\varepsilon - \mu + \varepsilon V + \delta W \right] p(\mathbf{x}) = 0, \quad p \in L^2(\mathbb{R}^2/\Lambda_h). \tag{8.5}$$

Since  $\varepsilon$  and  $\delta$  will be chosen to be small, we shall expand  $p(\mathbf{x})$  relative to the natural basis of the  $L^2(\mathbb{R}^2/\Lambda_h)$ –eigenspace of the free operator,  $H^{(0,0,0)} = -(\nabla + i\mathbf{K})^2$ , displayed explicitly in (3.5). Let  $P^\parallel$  denote the projection onto  $\text{span}\{p_\sigma : \sigma = 1, \tau, \bar{\tau}\}$  and  $P^\perp = I - P^\parallel$ .

We seek a solution of (8.5) in the form  $p(\mathbf{x}) = p_\parallel(\mathbf{x}) + p_\perp(\mathbf{x})$ , where

$$p_\parallel \in \text{span}\{p_\sigma : \sigma = 1, \tau, \bar{\tau}\}, \quad p_\perp \in \left[ \text{span}\{p_\sigma : \sigma = 1, \tau, \bar{\tau}\} \right]^\perp.$$

Then, we have that (8.5) is equivalent to the coupled system of equations:

$$\begin{aligned} &\left[ -(\nabla + i[\mathbf{K} + \lambda\mathbf{k}_2])^2 - E_\star^\varepsilon - \mu \right] p_\parallel \\ &\quad + \left[ \varepsilon P^\parallel V + \delta P^\parallel W \right] p_\parallel + \left[ \varepsilon P^\parallel V + \delta P^\parallel W \right] p_\perp = 0, \end{aligned} \tag{8.6}$$

$$\begin{aligned} &\left[ -(\nabla + i[\mathbf{K} + \lambda\mathbf{k}_2])^2 - E_\star^\varepsilon - \mu \right] p_\perp \\ &\quad + \left[ \varepsilon P^\perp V + \delta P^\perp W \right] p_\perp + \left[ \varepsilon P^\perp V + \delta P^\perp W \right] p_\parallel = 0. \end{aligned} \tag{8.7}$$

**Proposition 8.6** *There exists a constant  $c > 0$  such that if  $|\varepsilon| + |\mu| < c$  then*

$$H^{(\varepsilon,0,\lambda)} - \mu \equiv \left[ -(\nabla + i[\mathbf{K} + \lambda\mathbf{k}_2])^2 - E_\star^\varepsilon - \mu \right] \text{ is invertible on } P^\perp L^2(\mathbb{R}^2/\Lambda_h).$$

*Proof of Proposition 8.6* This follows from the lower bound:

$$0 < g_0 \equiv \inf_{|\lambda| \leq 1/2} \inf_{\mathbf{m} \notin \{(0,0), (0,1), (-1,0)\}} \left| |\mathbf{K} + \mathbf{m}\mathbf{k} + \lambda\mathbf{k}_2|^2 - |\mathbf{K}|^2 \right|,$$

where  $\mathbf{m}\mathbf{k} = m_1\mathbf{k}_1 + m_2\mathbf{k}_2$ . □

By Proposition 8.6, for all  $\varepsilon$  and  $\mu$  sufficiently small equation (8.7) is equivalent to:

$$\begin{aligned} & \left[ I + \left[ H^{(\varepsilon,0,\lambda)} - \mu \right]^{-1} \left[ \varepsilon P^\perp V + \delta P^\perp W \right] \right] p_\perp \\ & = - \left[ H^{(\varepsilon,0,\lambda)} - \mu \right]^{-1} \left[ \varepsilon P^\perp V + \delta P^\perp W \right] p_\parallel. \end{aligned}$$

Suppose now  $|\varepsilon| + |\delta| + |\mu| < d_1$ , where  $0 < d_1 \leq c$  is chosen sufficiently small. Then we have

$$\begin{aligned} p_\perp & = - \left[ I + \left[ H^{(\varepsilon,0,\lambda)} - \mu \right]^{-1} \left[ \varepsilon P^\perp V + \delta P^\perp W \right] \right]^{-1} \\ & \quad \times \left[ H^{(\varepsilon,0,\lambda)} - \mu \right]^{-1} \left[ \varepsilon P^\perp V + \delta P^\perp W \right] p_\parallel = \mathcal{P}(\varepsilon, \delta, \lambda, \mu) p_\parallel. \end{aligned} \tag{8.8}$$

Equation (8.8) defines a bounded linear mapping on  $P^\parallel L^2(\mathbb{R}^2/\Lambda_h)$  with operator norm  $\lesssim 1$ :

$$p_\parallel \mapsto p_\perp[\varepsilon, \delta, \lambda; p_\parallel] = \mathcal{P}(\varepsilon, \delta, \lambda, \mu) p_\parallel : \text{Ran} \left( P^\parallel \right) \rightarrow \text{Ran} \left( P^\perp \right),$$

which is analytic in  $\varepsilon, \delta, \lambda$  and  $\mu$  for  $|\varepsilon| + |\delta| + |\mu| < d_1$  and  $|\lambda| < 1/2$ . Consequently, equation (8.6) becomes a closed equation for  $p_\parallel$  which we write as:

$$\mathcal{M}(\varepsilon, \delta, \lambda, \mu) p = 0,$$

where

$$\begin{aligned} \mathcal{M}(\varepsilon, \delta, \lambda, \mu) & \equiv P^\parallel \left[ -(\nabla + i[\mathbf{K} + \lambda\mathbf{k}_2])^2 - E_\star^\varepsilon - \mu + \varepsilon V + \delta W \right. \\ & \quad \left. + (\varepsilon V + \delta W) \mathcal{P}(\varepsilon, \delta, \lambda, \mu) \right] P^\parallel \end{aligned} \tag{8.9}$$

$$\begin{aligned} & = P^\parallel \left[ -(\nabla + i[\mathbf{K} + \lambda\mathbf{k}_2])^2 - E_\star^\varepsilon - \mu + \varepsilon V + \delta W \right. \\ & \quad \left. + (\varepsilon V + \delta W) P^\perp \left[ H^{(\varepsilon,0,\lambda)} - \mu + \varepsilon V + \delta W \right]^{-1} P^\perp (\varepsilon V + \delta W) \right] P^\parallel. \end{aligned} \tag{8.10}$$

The operator  $\mathcal{M}(\varepsilon, \delta, \lambda, \mu)$  acts on the three-dimensional space  $P^\parallel L^2(\mathbb{R}^2/\Lambda_h) = \text{span}\{p_\sigma : \sigma = 1, \tau, \bar{\tau}\}$ . Moreover, from the expression (8.10) it is clear that for  $\varepsilon, \delta, \lambda, \mu$  complex,  $\mathcal{M}(\varepsilon, \delta, \lambda, \mu)$  is self-adjoint. We shall study it via its matrix representation relative to the basis  $\{p_\sigma : \sigma = 1, \tau, \bar{\tau}\}$ :

$$M_{\sigma, \bar{\sigma}}(\varepsilon, \delta, \lambda, \mu) \equiv \langle p_\sigma, \mathcal{M}(\varepsilon, \delta, \lambda, \mu)p_{\bar{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)}, \quad \sigma = 1, \tau, \bar{\tau}. \quad (8.11)$$

Clearly,  $M(\varepsilon, \delta, \lambda, \mu)$  is Hermitian for  $\varepsilon, \delta, \lambda, \mu$  real:  $M_{\sigma, \bar{\sigma}}(\varepsilon, \delta, \lambda, \mu) = \overline{M_{\bar{\sigma}, \sigma}(\varepsilon, \delta, \lambda, \mu)}$ .

Summarizing the above discussion we have the following:

- Proposition 8.7** (1) *The entries of the  $3 \times 3$  matrix  $M(\varepsilon, \delta, \lambda, \mu)$  are analytic functions of complex  $\varepsilon, \delta, \lambda$  and  $\mu$  for  $|\varepsilon| + |\delta| + |\mu| < d_1$  and  $|\lambda| < 1/2$ .*  
 (2) *For  $|\varepsilon| + |\delta| + |\mu| < d_1$  and  $|\lambda| < 1/2$ , we have that  $E = E_\star^\varepsilon + \mu$  is an  $L^2(\mathbb{R}^2/\Lambda_h)$ -eigenvalue of  $H^{(\varepsilon, \delta, \lambda)}$  if and only if  $\det M(\varepsilon, \delta, \lambda, \mu) = 0$ .*

We now study the roots of  $\det M(\varepsilon, \delta, \lambda, \mu) = 0$  (eigenvalues of  $H^{(\varepsilon, \delta, \lambda)}$ ) for  $\varepsilon$  and  $\delta$  small. First let  $\varepsilon = \delta = 0$ . By the formulae (8.42) and (8.46), derived and also applied in Section 8.3, we have:

$$\begin{aligned} M(0, 0, \lambda, \mu) &= \left( \langle p_\sigma, \mathcal{M}(0, 0, \lambda, \mu)p_{\bar{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)} \right)_{\sigma, \bar{\sigma}=1, \tau, \bar{\tau}}, \\ &= \left( \left\langle p_\sigma, \left( -(\nabla + i(\mathbf{K} + \lambda \mathbf{k}_2))^2 \right), p_{\bar{\sigma}} \right\rangle_{L^2(\mathbb{R}^2/\Lambda_h)} \right. \\ &\quad \left. - (E_\star^0 + \mu)\delta_{\sigma, \bar{\sigma}} \right)_{\sigma, \bar{\sigma}=1, \tau, \bar{\tau}}, \\ &= \begin{pmatrix} \lambda^2 q^2 - \mu & \alpha \lambda & \bar{\alpha} \lambda \\ \bar{\alpha} \lambda & \lambda^2 q^2 - \mu & \alpha \lambda \\ \alpha \lambda & \bar{\alpha} \lambda & \lambda^2 q^2 - \mu \end{pmatrix}, \quad \alpha = \frac{q^2}{\sqrt{3}} i \tau. \end{aligned}$$

Thus,  $M(0, 0, \lambda, \mu)$  is singular if  $\mu$  is a root of the polynomial:

$$\begin{aligned} \det M(0, 0, \lambda, \mu) &= -\mu^3 + \mu^2(3q^2\lambda^2) + \mu(3\lambda^2|\alpha|^2 - 3\lambda^4q^4) + \lambda^6q^6 - 3\lambda^4q^2|\alpha|^2 + 2\lambda^3\Re(\alpha^3) \\ &= -\mu^3 + \mu^2(3\lambda^2q^2) + \mu(\lambda^2q^4 - 3\lambda^4q^4) + \lambda^6q^6 + \lambda^4q^6, \end{aligned}$$

where we have used that  $|\alpha|^2 = \frac{q^4}{3}$  and  $\Re(\alpha^3) = 0$ . The roots,  $\mu_j^{(0)}(\lambda)$ ,  $j = 1, 2, 3$ , defined by the ordering  $\mu_1^{(0)}(\lambda) \leq \mu_2^{(0)}(\lambda) \leq \mu_3^{(0)}(\lambda)$ , listed with multiplicity, are given by:

$$\mathbf{0} \leq \lambda \leq \frac{\mathbf{1}}{2} : \mu_1^{(0)}(\lambda) = q^2\lambda(\lambda - 1), \mu_2^{(0)}(\lambda) = q^2\lambda^2, \mu_3^{(0)}(\lambda) = q^2\lambda(\lambda + 1), \quad (8.12)$$

$$-\frac{\mathbf{1}}{2} \leq \lambda \leq \mathbf{0} : \mu_1^{(0)}(\lambda) = q^2\lambda(\lambda + 1), \mu_2^{(0)}(\lambda) = q^2\lambda^2, \mu_3^{(0)}(\lambda) = q^2\lambda(\lambda - 1). \quad (8.13)$$



The roots  $\mu_j^{(0)}(\lambda)$ ,  $j = 1, 2, 3$ , are eigenvalues of  $-(\nabla + i[\mathbf{K} + \lambda\mathbf{k}_2])^2 - E_\star^0$ . They are uniformly bounded away from all other  $L^2(\mathbb{R}^2/\Lambda_h)$ - spectrum. This distance is given by

$$g_0 \equiv \inf_{|\lambda| \leq 1/2} \inf_{\mathbf{m} \notin \{(0,0), (0,1), (-1,0)\}} \left| |\mathbf{K} + \mathbf{m}\mathbf{k} + \lambda\mathbf{k}_2|^2 - |\mathbf{K}|^2 \right| > 0, \quad (E_\star^0 = |\mathbf{K}|^2),$$

where  $\mathbf{m}\mathbf{k} = m_1\mathbf{k}_1 + m_2\mathbf{k}_2$ .

Note that  $\det M(0, 0, 0, \mu) = -\mu^3$  has a root of multiplicity three:  $\mu = 0$ . By Proposition 8.7 and analyticity of  $\det M(\varepsilon, \delta, \lambda, \mu)$ , we have that for  $\varepsilon, \delta$  and  $\lambda$  in a small neighborhood of the origin in  $\mathbb{C}^3$ , there are three solutions of  $\det M(\varepsilon, \delta, \lambda, \mu) = 0$ . We label them  $\mu_j(\varepsilon, \delta, \lambda)$ ,  $j = 1, 2, 3$ . By self-adjointness of  $M(\varepsilon, \delta, \lambda, \mu)$ , these roots are real for real values of  $\varepsilon$  and  $\delta$ . Correspondingly, for small and real  $\varepsilon, \delta$  and  $\lambda$  there are three real  $L^2_{k_{\parallel}=2\pi/3}$ - eigenvalues of  $H^{(\varepsilon, \delta, \lambda)}$ , denoted

$$E_j^{(\varepsilon, \delta)}(\lambda) \equiv E_j^{(\varepsilon, \delta)}(\mathbf{K} + \lambda\mathbf{k}_2) \equiv E_\star^\varepsilon + \mu_j(\varepsilon, \delta, \lambda), \quad j = 1, 2, 3.$$

The ordering of the  $E_j$  implies

$$\mu_1(\varepsilon, \delta, \lambda) \leq \mu_2(\varepsilon, \delta, \lambda) \leq \mu_3(\varepsilon, \delta, \lambda).$$

A mild extension of Proposition 4.5 yields

**Proposition 8.8** *For each  $|\lambda| \leq 1/2$ , there exist orthonormal  $L^2_{\mathbf{K}+\lambda\mathbf{k}_2}$ - eigenpairs  $(\Phi_\pm(\mathbf{x}; \lambda), E_\pm(\lambda))$  and  $(\tilde{\Phi}(\mathbf{x}; \lambda), \tilde{E}(\lambda))$ , real analytic in  $\lambda$ , such that*

$$\text{span} \{ \Phi_-(\mathbf{x}; \lambda), \Phi_+(\mathbf{x}; \lambda), \tilde{\Phi}(\mathbf{x}; \lambda) \} = \text{span} \{ \Phi_j(\mathbf{x}; \mathbf{K} + \lambda\mathbf{k}_2) : j = 1, 2, 3 \}.$$

For fixed  $\varepsilon$  small and  $\lambda$  tending to 0 we have:

$$(1) \quad E_\pm^{\varepsilon, \delta=0}(\lambda) = E_\star^\varepsilon \pm |\lambda_\#^\varepsilon| |z_2| \lambda + \lambda^2 e_\pm(\lambda, \varepsilon), \tag{8.14}$$

$$\tilde{E}^{\varepsilon, \delta=0}(\lambda) = \tilde{E}_\star^\varepsilon + \lambda^2 \tilde{e}(\lambda, \varepsilon), \tag{8.15}$$

where  $e_\pm(\lambda, \varepsilon)$ ,  $\tilde{e}(\lambda, \varepsilon) = \mathcal{O}(1)$  as  $\lambda, \varepsilon \rightarrow 0$ , and  $z_2 = k_2^{(1)} + ik_2^{(2)}$ . These functions can be represented in a convergent power series in  $\varepsilon$  and  $\lambda$  in a fixed  $\mathbb{C}^2$  neighborhood of the origin. Furthermore,  $e_\pm(\lambda, \varepsilon)$ ,  $\tilde{e}(\lambda, \varepsilon)$  are real-valued for real  $\lambda$  and  $\varepsilon$ .

(2) *Therefore, for all small  $\varepsilon$  and  $\lambda$ , the three roots of  $\det M(\varepsilon, \delta = 0, \lambda, \mu)$  may be labeled:*

$$\mu_+(\lambda, \varepsilon) = |\lambda_\#^\varepsilon| |z_2| \lambda + \lambda^2 e_+(\lambda, \varepsilon) \tag{8.16}$$

$$\mu_-(\lambda, \varepsilon) = -|\lambda_\#^\varepsilon| |z_2| \lambda + \lambda^2 e_-(\lambda, \varepsilon) \tag{8.17}$$

$$\tilde{\mu}(\lambda, \varepsilon) = \tilde{E}_\star^\varepsilon - E_\star^\varepsilon + \lambda^2 \tilde{e}(\lambda, \varepsilon), \quad \text{where } \tilde{E}_\star^\varepsilon - E_\star^\varepsilon = 3\varepsilon V_{1,1} + \mathcal{O}(\varepsilon^2). \tag{8.18}$$

*Proof of Proposition 8.8* Part 1 can be proved as follows. The expansion (8.14) and analyticity follow by perturbation theory as in Proposition 4.5; see also [13, 20]. The expansion (8.18) also follows by perturbation theory of the simple eigenvalue  $\tilde{E}_\star^\varepsilon$  for  $\lambda = 0$ . It is easy to see that

$$\tilde{E}^{\varepsilon, \delta=0}(\lambda) = \tilde{E}_\star^\varepsilon + \lambda \times \left( -2i\mathbf{k}_2 \cdot \langle \tilde{\Phi}^\varepsilon, \nabla_{\mathbf{x}} \tilde{\Phi}^\varepsilon \rangle_{L^2_{\mathbf{k}}} \right) + \lambda^2 \tilde{e}(\varepsilon, \lambda). \tag{8.19}$$

We claim that  $\langle \tilde{\Phi}^\varepsilon, \nabla_{\mathbf{x}} \tilde{\Phi}^\varepsilon \rangle_{L^2_{\mathbf{k}}} = 0$ . This follows since  $\tilde{\Phi}^\varepsilon \in L^2_{\mathbf{k}, 1}$  as in the proof of Proposition 4.1 of [11]. This proves the expansion (8.15).  $\square$

Finally we discuss a useful symmetry of  $\det M(\varepsilon, \delta, \lambda, \mu = 0)$ .

**Proposition 8.9** *Assume  $V$  satisfies Assumptions (V) and  $W$  satisfies Assumptions (W). Recall  $M(\varepsilon, \delta, \lambda, 0)$ , defined in (8.9)–(8.11). Then,  $\det M(\varepsilon, \delta, \lambda, 0)$  is real-valued for real  $\varepsilon, \delta, \lambda$  and analytic in a small neighborhood of the origin in  $\mathbb{C}^3$ . Furthermore,*

$$\det M(\varepsilon, \delta, \lambda, 0) = \det M(\varepsilon, -\delta, \lambda, 0) \tag{8.20}$$

and therefore  $\det M(\varepsilon, \delta, \lambda, 0)$  is a real analytic in  $\varepsilon, \delta^2$  and  $\lambda$ , and we write

$$D(\varepsilon, \delta^2, \lambda) \equiv \det M(\varepsilon, \delta, \lambda, 0)$$

*Proof of Proposition 8.9* Let  $\mathcal{I}[f](\mathbf{x}) = f(-\mathbf{x})$  and  $\mathcal{C}[f](\mathbf{x}) = \overline{f(\mathbf{x})}$ . Using that  $\varepsilon, \delta$  and  $\lambda$  are real,  $V(\mathbf{x})$  is even and  $W(\mathbf{x})$  is odd, one can check directly that

$$\mathcal{C} \circ \mathcal{I} \circ H^{\varepsilon, -\delta, \lambda} = H^{\varepsilon, \delta, \lambda} \circ \mathcal{I} \circ \mathcal{C} \tag{8.21}$$

Furthermore, note that

$$(\mathcal{C} \circ \mathcal{I})p_1 = p_1, \quad (\mathcal{C} \circ \mathcal{I})p_\tau = p_{\bar{\tau}}, \quad (\mathcal{C} \circ \mathcal{I})p_{\bar{\tau}} = p_\tau. \tag{8.22}$$

It follows that

$$\mathcal{C} \circ \mathcal{I} \circ P^\parallel = P^\parallel \circ \mathcal{C} \circ \mathcal{I}. \tag{8.23}$$

Using the symmetry relations (8.21)–(8.23) to rewrite  $M(\varepsilon, -\delta, \lambda, 0)$  in terms of  $H^{\varepsilon, \delta, \lambda}$ , we find that  $M(\varepsilon, -\delta, \lambda, 0)$  can be transformed into  $M(\varepsilon, \delta, \lambda, 0)$  by interchanging its second and third rows, and then interchanging its second and third columns. Therefore,  $\det M(\varepsilon, \delta, \lambda, 0) = \det M(\varepsilon, -\delta, \lambda, 0)$  and the proof of Proposition 8.9 is complete.  $\square$

### 8.2 Strategy for Analysis of $\det M(\varepsilon, \delta, \lambda, \mu)$ in the Case $\varepsilon V_{1,1} > 0$

We first observe that for a positive constant,  $d_1$ , if  $|\varepsilon| + |\delta| < d_1$  then

$$|E_j^{(\varepsilon, \delta)}(\lambda) - E_\star^\varepsilon| \geq c_4(1 + |j|), \quad j \geq 4. \tag{8.24}$$

Indeed, by the discussion following Proposition 8.7, we have that there exists  $d_2 > 0$  such that for  $j \geq 4$ ,  $|\mu_j(\varepsilon, \delta, \lambda)| \equiv |E_j^{(\varepsilon, \delta)}(\lambda) - E_\star^\varepsilon| \geq d_2$ ; the lower bound (8.24) now follows from the Weyl asymptotics for eigenvalues of second order elliptic operators in two space dimensions.

Hence, we restrict our attention to  $E_j^{(\varepsilon, \delta)}(\lambda) = E_\star^\varepsilon + \mu_j(\varepsilon, \delta)$ ,  $j = 1, 2, 3$ , which we study by a detailed analysis of  $\det M(\varepsilon, \delta, \lambda, \mu = 0)$ . The analysis consists of verifying two steps, which we now outline.

**Step 1:** Fix  $c_b > 0$  and arbitrary. We will prove that there exists  $C_b > 0$ , such that the following holds. There exists  $\varepsilon_1 > 0$  and constant  $c_3$ , depending on  $V$  and  $W$ , such that for all  $0 < |\varepsilon| < \varepsilon_1$  and  $0 \leq |\delta| \leq c_b \varepsilon^2$ :

$$C_b \sqrt{\varepsilon} \leq |\lambda| \leq \frac{1}{2} \implies |E_j^{(\varepsilon, \delta)}(\lambda) - E_\star^\varepsilon| \geq c_3 \varepsilon, \quad j = 1, 2, 3. \tag{8.25}$$

Furthermore, by (8.25) and (8.24), it follows that

$$C_b \sqrt{\varepsilon} \leq |\lambda| \leq \frac{1}{2} \implies L^2(\mathbb{R}/\Lambda_h) - \text{spec}(H^{(\varepsilon, \delta, \lambda)}) \cap [E_\star^\varepsilon - c\varepsilon, E_\star^\varepsilon + c\varepsilon] \text{ is empty.} \tag{8.26}$$

**Step 2:** Let  $c_b$  and  $C_b$  be as in Step 1. We will prove that there exists  $0 < \varepsilon_2 \leq \varepsilon_1$ , such that if  $(\lambda, \delta)$  are in the set:

$$|\lambda| \leq C_b \varepsilon^{\frac{1}{2}} \text{ and } 0 \leq |\delta| \leq c_b \varepsilon^2, \text{ where } 0 < |\varepsilon| < \varepsilon_2, \text{ then} \tag{8.27}$$

$$\det M(\varepsilon, \lambda, \delta, 0) = \left(q^2 \lambda^2 + \varepsilon V_{1,1}\right) \left(q^4 \lambda^2 + \delta^2 |W_{0,1} + W_{1,0} - W_{1,1}|^2\right) \times (1 + o(1)). \tag{8.28}$$

A simple lower bound on the three eigenvalues  $|\mu_j(\varepsilon, \lambda)| = |E_j^\varepsilon(\lambda) - E_\star^\varepsilon|$  is then obtained as follows. By (8.27), for some positive constants:  $C_1$  and  $C_2$ , we have

$$\begin{aligned} & C_1(\lambda^2 + \varepsilon) \cdot (\lambda^2 + \delta^2) \\ & \leq |\det M(\varepsilon, \lambda, \delta, 0)| \\ & = |\det M(\varepsilon, \lambda, \delta, 0) - \det M(\varepsilon, \lambda, \delta, \mu_j(\lambda, \varepsilon, \delta))| \\ & \leq C_2 |0 - \mu_j(\varepsilon, \delta, \lambda)| = C_2 |\mu_j(\varepsilon, \delta, \lambda)|, \end{aligned}$$

for  $j = 1, 2, 3$ . Therefore, with  $C_3 = C_1/C_2$ ,

$$|E_j^{\varepsilon, \delta}(\lambda) - E_\star^\varepsilon| = |\mu_j(\varepsilon, \delta, \lambda)| \geq C_3 \varepsilon (\lambda^2 + \delta^2) \geq C_3 \varepsilon \delta^2, \quad j = 1, 2, 3. \tag{8.29}$$

It follows from (8.29) and (8.24) that

$$\text{the } L^2(\mathbb{R}^2/\Lambda_h) - \text{spec}(H^{(\varepsilon,\delta,\lambda)}) \cap [E_\star^\varepsilon - \eta, E_\star^\varepsilon + \eta] \text{ is empty}$$

with  $\eta = \frac{1}{2}C_3 \varepsilon \delta^2$ , whenever  $\varepsilon, (\lambda, \delta)$  satisfy the constraints (8.27).

Theorem 8.2 and Theorem 8.3 are immediate consequences of (8.26) (Step 1) and (8.29) (Step 2) and the representation:

$$H^{(\varepsilon,\delta)} \Big|_{L^2(\Sigma_{k_{\parallel}=2\pi/3})} = \oplus \int_{|\lambda| \leq \frac{1}{2}} H^{(\varepsilon,\delta,\lambda)} \Big|_{L^2(\mathbb{R}^2/\Lambda_h)} d\lambda.$$

Hence, we now turn to their proofs. We first carry out Step 1 by a simple perturbation analysis about the free Hamiltonian,  $H^{(0,0,\lambda)}$ . We then turn to Step 2, which is much more involved.

**Verification of (8.25) from Step 1.** Let  $C_b$  denote a positive constant, which we will specify shortly, and consider the range  $C_b\sqrt{\varepsilon} \leq \lambda \leq 1/2$ . Using the expressions for  $\mu_j^{(0)}(\lambda)$ ,  $j = 1, 2, 3$ , in (8.12) we have that if  $\varepsilon \leq \varepsilon'(C_b) \equiv (4C_b^2)^{-1}$ , then  $|E_1^{(0)}(\lambda) - E_\star^0| = q^2|\lambda| |1 - \lambda| \geq C_b q^2 \sqrt{\varepsilon}/2$ ,  $|E_2^{(0)}(\lambda) - E_\star^0| = q^2|\lambda|^2 \geq C_b^2 q^2 \varepsilon$ , and  $|E_3^{(0)}(\lambda) - E_\star^0| = q^2|\lambda| |1 + \lambda| \geq C_b^2 q^2 \sqrt{\varepsilon}/2$ . Note that the eigenvalues  $(\varepsilon, \delta, \lambda) \mapsto E^{\varepsilon,\delta}(\lambda)$  are Lipschitz continuous functions; see Chapter XII of [34] or Appendix A of [12]. Therefore, we have

$$|E_2^{(\varepsilon,\delta)}(\lambda) - E_\star^\varepsilon| \geq C_b^2 q^2 \varepsilon - |\varepsilon| \|V\|_\infty - |\delta| \|W\|_\infty \geq \frac{1}{2} C_b^2 q^2 \varepsilon,$$

for some  $C_b$  positive, finite and sufficiently large. With this choice of  $C_b$ , we also have

$$\begin{aligned} |E_1^{(\varepsilon,\delta)}(\lambda) - E_\star^\varepsilon| &\geq C_b q^2 \sqrt{\varepsilon}/2 - |\varepsilon| \|V\|_\infty - |\delta| \|W\|_\infty, \\ |E_3^{(\varepsilon,\delta)}(\lambda) - E_\star^\varepsilon| &\geq C_b q^2 \sqrt{\varepsilon}/2 - |\varepsilon| \|V\|_\infty - |\delta| \|W\|_\infty. \end{aligned}$$

Therefore, there exists  $\varepsilon_1 > 0$ , such that for all  $0 < |\varepsilon| < \varepsilon_1$  we have

$$|E_1^{(\varepsilon,\delta)}(\lambda) - E_\star^\varepsilon| + |E_3^{(\varepsilon,\delta)}(\lambda) - E_\star^\varepsilon| \geq C_b q^2 \sqrt{\varepsilon}/4.$$

This completes the proof of the assertions in Step 1.

### 8.3 Expansion of $M(\varepsilon, \delta, \lambda, 0)$ and Its Determinant for $\varepsilon V_{1,1} \neq 0$

The key to verifying Step 2 and proving Theorem 8.2 is the following:

**Proposition 8.10** *Let  $C_b$  be as chosen in Step 1; see (8.26). Then, there exist constants  $\varepsilon_2 > 0$  and  $c > 0$  such that for all  $0 \leq \varepsilon < \varepsilon_2$ , if*

$$0 \leq |\lambda| \leq C_b \varepsilon^{1/2} \text{ and } 0 \leq |\delta| \leq c \varepsilon^2, \text{ then} \tag{8.30}$$

$$-\det M(\varepsilon, \delta, \lambda, 0) = \pi(\varepsilon, \delta^2, \lambda) + o\left((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2)\right), \tag{8.31}$$

where

$$\pi(\varepsilon, \delta^2, \lambda) \equiv \left(q^2\lambda^2 + \varepsilon V_{1,1}\right) \left(q^4\lambda^2 + \delta^2 |W_{0,1} + W_{1,0} - W_{1,1}|^2\right). \tag{8.32}$$

Here,  $W_{\mathbf{m}}, \mathbf{m} \in \mathbb{Z}^2$ , denote Fourier coefficients of  $W(\mathbf{x})$  and, by (8.30), the correction term in (8.31) divided by  $(\lambda^2 + \varepsilon)(\lambda^2 + \delta^2)$  tends to zero as  $\varepsilon$  tends to zero. Thus,

$$\varepsilon V_{1,1} > 0 \implies -\det M(\varepsilon, \delta, \lambda, 0) = \pi(\varepsilon, \delta^2, \lambda) (1 + o(1)) \text{ in the region (8.30).}$$

We now embark on an expansion of  $\det M(\varepsilon, \delta, \lambda, 0)$  and the proof of Proposition 8.10.  $M(\varepsilon, \delta, \lambda, 0)$ , see (8.9)–(8.11), may be written as the sum of matrices:

$$M(\varepsilon, \delta, \lambda, 0) = \left[ M^0 + M^V + M^W + M^P \right] (\varepsilon, \delta, \lambda, 0), \tag{8.33}$$

where the  $\sigma, \bar{\sigma} = 1, \tau, \bar{\tau}$  entries are given by:

$$\begin{aligned} M_{\sigma, \bar{\sigma}}^0(\varepsilon, \delta, \lambda, 0) &= \left\langle p_\sigma, \left( -(\nabla + i[\mathbf{K} + \lambda \mathbf{k}_2])^2 - E_\star^\varepsilon \right) p_{\bar{\sigma}} \right\rangle_{L^2(\mathbb{R}^2/\Lambda_h)}, \\ M_{\sigma, \bar{\sigma}}^V(\varepsilon) &= \varepsilon \langle p_\sigma, V p_{\bar{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)}, \\ M_{\sigma, \bar{\sigma}}^W(\delta) &= \delta \langle p_\sigma, W p_{\bar{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)}, \\ M_{\sigma, \bar{\sigma}}^P(\varepsilon, \delta, \lambda, 0) &= \langle p_\sigma, (\varepsilon V + \delta W) \mathcal{P}(\varepsilon, \delta, \lambda, 0) p_{\bar{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)}. \end{aligned} \tag{8.34}$$

For  $\varepsilon$  and  $\delta$  small,

$$M_{\sigma, \bar{\sigma}}^0(\varepsilon, \delta, \lambda, 0) = M_{\sigma, \bar{\sigma}}^{0, approx}(\varepsilon, \lambda) + \mathcal{O}(\varepsilon^2), \tag{8.35}$$

where (inner products over  $L^2(\mathbb{R}^2/\Lambda_h)$ )

$$\begin{aligned} M_{\sigma, \bar{\sigma}}^{0, approx}(\varepsilon, \lambda) &= \left\langle p_\sigma, \left( -(\nabla + i[\mathbf{K} + \lambda \mathbf{k}_2])^2 - [E_\star^0 + \varepsilon(V_{0,0} - V_{1,1})] \right) p_{\bar{\sigma}} \right\rangle, \text{ and} \\ M_{\sigma, \bar{\sigma}}^P(\varepsilon, \delta, \lambda, 0) &= \left\langle (\varepsilon V + \delta W) p_\sigma, P^\perp \left( -(\nabla + i[\mathbf{K} + \lambda \mathbf{k}_2])^2 - E_\star^\varepsilon + \varepsilon V + \delta W \right)^{-1} P^\perp (\varepsilon V + \delta W) p_{\bar{\sigma}} \right\rangle \\ &= \left\langle (\varepsilon V + \delta W) p_\sigma, P^\perp \left( -(\nabla + i[\mathbf{K} + \lambda \mathbf{k}_2])^2 - E_\star^\varepsilon \right)^{-1} P^\perp (\varepsilon V + \delta W) p_{\bar{\sigma}} \right\rangle \\ &\quad + \mathcal{O}(\delta^3 + \delta^2\varepsilon + \delta\varepsilon^2 + \varepsilon^3) = \mathcal{O}(\varepsilon^2 + \varepsilon\delta + \delta^2). \end{aligned} \tag{8.37}$$

We next explain that to calculate the determinant of  $M(\varepsilon, \delta, \lambda, 0)$  to the desired order in the region (8.27), it suffices to calculate the determinant of the approximate matrix:

$$M^{approx}(\varepsilon, \delta, \lambda) \equiv M^{0, approx}(\varepsilon, \lambda) + M^V(\varepsilon) + M^W(\delta). \tag{8.38}$$

That is, we show that the omitted terms in  $M(\varepsilon, \delta, \lambda, 0) - M^{approx}(\varepsilon, \delta, \lambda, 0)$  contribute negligibly to the determinant of  $M(\varepsilon, \delta, \lambda, 0)$ , when compared with the polynomial,  $\pi(\varepsilon, \delta^2, \lambda)$ , in (8.32), provided  $\lambda$  and  $\delta$  are in the region (8.27):

$$|\lambda| \leq C_b \varepsilon^{\frac{1}{2}} \text{ and } |\delta| \leq c_b \varepsilon^2, \tag{8.39}$$

where  $C_b$  and  $c_b$  are appropriately chosen constants.

Recall that  $D(\varepsilon, \delta^2 = 0, \lambda = 0) = \det M(\varepsilon, 0, 0, 0) = 0$  for all  $\varepsilon$ , since  $\mu = 0$  corresponds to  $E = E_x^\varepsilon$ , which is an eigenvalue of  $H^{(\varepsilon, \delta=0, \lambda=0)} = -\Delta + \varepsilon V$ . Thus,  $D(\varepsilon, \delta^2, \lambda) = \det M(\varepsilon, \delta, \lambda, 0)$  is a convergent power series in  $\varepsilon, \delta^2$  and  $\lambda$  with no “pure  $\varepsilon$ ” terms. On the other hand, the entries of the matrix  $M(\varepsilon, \delta, \lambda, 0)$  are convergent power series in  $\varepsilon, \delta$  and  $\lambda$ .

**Proposition 8.11** *For  $(\lambda, \delta)$  in the region (8.39) we have*

$$|\lambda| \delta^2 = o\left((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2)\right).$$

*Therefore we may drop the  $\mathcal{O}(\lambda\delta^2)$  terms, a further simplification.*

*Proof of Proposition 8.11* Consider separately the two regimes: (a)  $|\lambda| \leq \varepsilon^{1.1}$  and (b)  $|\lambda| \geq \varepsilon^{1.1}$ . For  $|\lambda| \leq \varepsilon^{1.1}$ , we have  $|\lambda|\delta^2 \leq \varepsilon^{1.1}\delta^2 = \varepsilon^{0.1}\varepsilon\delta^2 \leq \varepsilon^{0.1}(\lambda^2 + \varepsilon) \cdot (\lambda^2 + \delta^2)$ . And for  $|\lambda| \geq \varepsilon^{1.1}$ , note that  $(\lambda^2 + \varepsilon) \cdot (\lambda^2 + \delta^2) \geq \varepsilon\lambda^2 \geq \varepsilon \cdot \varepsilon^{2.2} = \varepsilon^{3.2}$ . On the other hand,  $|\lambda|\delta^2 \leq \frac{1}{2}\delta^2 \lesssim \varepsilon^4 \leq \varepsilon^{-8} \cdot (\lambda^2 + \varepsilon) \cdot (\lambda^2 + \delta^2)$ . This completes the proof of Proposition 8.11.  $\square$

Let us now attach “weight” 1 to the variable  $\varepsilon$  and “weight” 1/2 to the variables  $\delta$  and  $\lambda$ . A monomial of the form  $\varepsilon^a \lambda^b \delta^c$  carries the weight  $a + b/2 + c/2$ , where  $a, b, c \in \mathbb{N}$ . In Proposition 8.12 we show that all terms in the power series of  $\det M(\varepsilon, \lambda, \delta)$  which are of weight strictly larger than two introduce negligible corrections to  $\det M^{approx}(\varepsilon, \lambda, \delta)$  for  $\lambda$  and  $\delta$  in the region (8.27).

Recalling that there are no pure  $\varepsilon$  terms, we see that a monomial in the power series of  $D(\varepsilon, \delta^2, \lambda)$  of weight larger than 2 must have one of the following two forms ( $a, b, c \in \mathbb{N}$ ):

- (I)  $\lambda \times \varepsilon^a \lambda^b (\delta^2)^c$ , with  $a + b/2 + c > 3/2 \implies 2a + b + 2c \geq 4$
- (II)  $\delta^2 \times \varepsilon^a \lambda^b (\delta^2)^c$ , with  $a + b/2 + c > 1 \implies 2a + b + 2c \geq 3$ .

**Proposition 8.12** *Terms of form (I) and form (II) that may appear in  $D(\varepsilon, \delta^2, \lambda)$  are  $o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  as  $\varepsilon \rightarrow 0$ , for  $(\lambda, \delta)$  in the region (8.39):  $|\lambda| \leq C_b \varepsilon^{\frac{1}{2}}$  and  $|\delta| \lesssim \varepsilon^2$ . We may therefore neglect all terms in the power series of  $D(\varepsilon, \delta^2, \lambda)$  which are of weight strictly larger than 2 for  $(\lambda, \delta)$  in the region (8.39).*

We prove Proposition 8.12 by estimating all terms of the form (I) or (II), and we begin with the following lemma, which is a consequence of part 2 of Proposition 8.8:

**Lemma 8.13** *Let  $\mu_-(\varepsilon, \lambda)$ ,  $\mu_+(\varepsilon, \lambda)$  and  $\tilde{\mu}(\varepsilon, \lambda)$  denote the three roots of  $\det M(\varepsilon, \delta = 0, \lambda, \mu)$ , defined and analytic in  $(\varepsilon, \lambda)$  in a  $\mathbb{C}^2$  neighborhood of the origin and displayed in (8.16)–(8.18). Then,*

$$\det M(\varepsilon, \delta = 0, \lambda, \mu) = (\mu - \mu_-(\varepsilon, \lambda)) \times (\mu - \mu_+(\varepsilon, \lambda)) \times (\mu - \tilde{\mu}(\varepsilon, \lambda)) \times \Omega(\varepsilon, \lambda, \mu),$$

where  $\Omega(\varepsilon, \lambda, \mu)$  is bounded. In particular, for all  $\varepsilon$  such that  $0 < |\varepsilon| < \varepsilon_0$  there exists a constant  $C_\varepsilon$  such that

$$|\det M(\varepsilon, \delta = 0, \lambda, 0)| \leq C_\varepsilon |\lambda|^2. \tag{8.40}$$

*Proof* For fixed  $\varepsilon$  and  $\lambda$ , the mapping  $\mu \mapsto \det M(\varepsilon, \delta = 0, \lambda, \mu)$  is analytic for  $|\mu| < \mu_0$  with zeros at  $\mu_\pm(\varepsilon, \lambda)$ ,  $\tilde{\mu}(\varepsilon, \lambda)$ ; see Proposition 8.8. Fix  $\varepsilon'$  and  $\lambda'$  small such that if  $|\varepsilon| < \varepsilon'$  and  $|\lambda| < \lambda'$ , the roots all satisfy  $|\mu_+(\varepsilon, \lambda)|, |\mu_-(\varepsilon, \lambda)|, |\tilde{\mu}(\varepsilon, \lambda)| < \mu_0/2$ . We claim that for such  $\varepsilon$  and  $\delta$ ,

$$\Omega(\varepsilon, \lambda, \mu) \equiv \frac{\det M(\varepsilon, \delta = 0, \lambda, \mu)}{(\mu - \mu_-(\varepsilon, \lambda)) \times (\mu - \mu_+(\varepsilon, \lambda)) \times (\mu - \tilde{\mu}(\varepsilon, \lambda))}$$

is uniformly bounded for all  $|\mu| \leq \mu_0$ ,  $|\varepsilon| \leq \varepsilon'$  and  $|\lambda| \leq \lambda'$ . Indeed, since the roots are bounded in magnitude by  $\mu_0/2$ , we have  $\max_{|\mu|=\mu_0} |\Omega(\varepsilon, \lambda, \mu)| \leq (2/\mu_0)^3 \max_{|\mu|=\mu_0} |\det M(\varepsilon, \delta = 0, \lambda, \mu)|$ . Applying the maximum principle we have

$$\max_{|\mu| \leq \mu_0} |\Omega(\varepsilon, \lambda, \mu)| \leq (2/\mu_0)^3 \max_{|\mu|=\mu_0} |\det M(\varepsilon, \delta = 0, \lambda, \mu)| \leq (2/\mu_0)^3 C(\mu_0, \varepsilon', \lambda'),$$

where  $C(\mu_0, \varepsilon', \lambda')$  is a constant. The bound (8.40) now follows from the expansions of the roots. □

*Proof of Proposition 8.12: (I) Terms of the form  $\lambda \times \varepsilon^a \lambda^b (\delta^2)^c$ , with  $2a + b + 2c \geq 4$ ,  $a, b, c \in \mathbb{N}$ :*

(i) Suppose first that  $c = 0$ . Then, we consider  $\lambda \times \varepsilon^a \lambda^b$  with  $2a + b \geq 4$ . By Lemma 8.13 we must have  $b \geq 1$ . Thus,  $\lambda \times \varepsilon^a \lambda^b = \lambda^2 \varepsilon^a \lambda^{b-1}$ . If  $a \geq 2$ , then  $\lambda \times \varepsilon^a \lambda^b = \lambda^2 \varepsilon^2 \varepsilon^{a-2} \lambda^{b-1} \lesssim (\lambda^2 + \delta^2) \times (\lambda^2 + \varepsilon)^2 = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region (8.39). Otherwise,  $a = 0$  or  $a = 1$ . If  $a = 0$ , then  $b \geq 4$  and  $\lambda \times \varepsilon^a \lambda^b = \lambda \cdot \lambda^2 \times \lambda^2 \cdot \lambda^{b-4} \lesssim \lambda \cdot (\lambda^2 + \varepsilon) \times (\lambda^2 + \delta^2) = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region (8.27). Now suppose  $a = 1$ . Then,  $b \geq 2$  and we have  $\lambda \times \varepsilon^a \lambda^b = \lambda \cdot \lambda^2 \times \varepsilon \cdot \lambda^{b-2} \lesssim \lambda \cdot (\lambda^2 + \delta^2) \times (\lambda^2 + \varepsilon) = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region (8.39).

(ii) Suppose now that  $c \geq 1$ . If  $b = 0$ , then  $\lambda \times \varepsilon^a \lambda^b (\delta^2)^c = \lambda \delta^2 \varepsilon^a (\delta^2)^{c-1}$  with  $2a + 2c \geq 4$ , which is  $o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region by Proposition 8.11. Finally, if  $b \geq 1$ , then  $\lambda \times \varepsilon^a \lambda^b (\delta^2)^c = \lambda \delta^2 \cdot \varepsilon^a \lambda^b (\delta^2)^{c-1} = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region (8.39).

**(II) Terms of the form**  $\delta^2 \times \varepsilon^a \lambda^b (\delta^2)^c$ , with  $2a + b + 2c \geq 3$ ,  $a, b, c \in \mathbb{N}$ :

(i) Suppose first that  $a = 0$ . Then,  $\delta^2 \times \varepsilon^a \lambda^b (\delta^2)^c = \delta^2 \times \lambda^b (\delta^2)^c$ ,  $b + 2c \geq 3$ . If  $b \geq 1$ , then we rewrite this as  $\delta^2 \lambda \times \lambda^{b-1} (\delta^2)^c = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region (8.39), by Proposition 8.11. And if  $b = 0$ , then  $\delta^2 \times \varepsilon^a \lambda^b (\delta^2)^c = (\delta^2)^{c+1}$ , with  $c \geq 2$ , which is  $\lesssim \delta^2 \delta^2 (\delta^2)^{c-1} \lesssim \delta^2 \varepsilon \cdot \varepsilon^3 (\delta^2)^{c-1} \lesssim (\lambda^2 + \delta^2)(\lambda^2 + \varepsilon) \cdot \varepsilon^3 (\delta^2)^{c-1} = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region (8.39).

(ii) If now  $a \geq 1$ , then  $\delta^2 \times \varepsilon^a \lambda^b (\delta^2)^c = \delta^2 \varepsilon \cdot \varepsilon^{a-1} \lambda^b (\delta^2)^c \leq (\lambda^2 + \delta^2) \cdot (\lambda^2 + \varepsilon) \cdot \varepsilon^{a-1} \lambda^b (\delta^2)^c = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  for  $(\lambda, \delta)$  in the region (8.39). This completes the proof of Proposition 8.12.

Now each entry in the  $3 \times 3$  matrix,  $M(\varepsilon, \delta, \lambda, 0)$  is a sum of terms of weight  $\geq 1/2$ ; this is a consequence of the expansion (8.33), (8.34), (8.35), (8.8) and the explicit expansion of  $M^{approx}$  displayed in (8.47). If we change any one entry by a term of weight  $\geq 3/2$ , then the effect on the  $3 \times 3$  determinant  $D(\varepsilon, \delta^2, \lambda)$  will be a sum of terms of weight  $\geq 3/2 + 1/2 + 1/2 > 2$ . By Propositions 8.11 and 8.12, such terms are  $o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  in the region (8.39). Therefore, we may compute each entry of  $M(\varepsilon, \delta, \lambda, 0)$ , retaining only terms of weight strictly smaller than  $3/2$  and discarding the rest. The resulting determinant will differ from  $D(\varepsilon, \delta^2, \lambda)$  by terms which are  $o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  in the region (8.39).

We next study the power series of the  $3 \times 3$  matrix,  $M(\varepsilon, \delta, \lambda, 0)$ , keeping in mind that the relevant monomials are those of weight  $\geq 1/2$  but strictly less than  $3/2$ . The complete list of such monomials is:  $\varepsilon, \delta, \lambda, \lambda^2, \delta^2$  and  $\lambda\delta$ .

Before proceeding further we show that in fact that a monomial of type  $\delta^2$  can be neglected. Indeed, the weight  $\leq 2$  contributions of such a monomial to  $D(\varepsilon, \lambda, \delta^2, 0) = \det M(\varepsilon, \delta, \lambda, 0)$  will be a sum of monomials of the type: (i)  $\delta^2 \times \delta \cdot \delta$ , (ii)  $\delta^2 \times \lambda \cdot \lambda$  and (iii)  $\delta^2 \times \lambda \cdot \delta$ . Terms of type (ii) and (iii) are clearly  $o(\lambda\delta^2) = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  as  $\varepsilon \rightarrow 0$  for  $(\lambda, \delta)$  in the region (8.39), by Proposition 8.11. For the type (i) term we have, for  $(\lambda, \delta)$  in the region (8.39),  $\delta^2 \times \delta \cdot \delta \lesssim \delta^2 \varepsilon \varepsilon \delta \lesssim (\lambda^2 + \delta^2) \cdot (\lambda^2 + \varepsilon) \varepsilon \delta = o((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2))$  as  $\varepsilon \rightarrow 0$ . Hence, we may strike  $\delta^2$  from our list. In particular, we may neglect the contribution from the matrix  $\mathcal{M}^P$ ; see (8.37).

**Relevant monomials in the expansion of  $M(\varepsilon, \delta, \lambda, 0)$ :** We shall call the monomials:  $\varepsilon, \delta, \lambda, \lambda^2$  and  $\lambda\delta$  relevant. All others are called irrelevant.

Stepping back, we have shown above that  $M = M^0 + M^V + M^W + M^P$  ((8.33)), where  $M^0 = M^{0,approx} + \mathcal{O}(\varepsilon^2)$  ((8.35)) and  $M^P = \mathcal{O}(\varepsilon^2 + \varepsilon\delta + \delta^2)$  ((8.37)). We have further shown that the relevant monomial contributions for calculation of  $\det M(\varepsilon, \delta, \lambda, 0)$  are all contained in  $M^{approx}(\varepsilon, \delta, \lambda, 0) \equiv M^{0,approx}(\varepsilon, \lambda) + M^V(\varepsilon) + M^W(\delta)$ . We consider each of these matrices individually, and explicitly extract the relevant terms in each; see Proposition 8.14 below.

**Expansion of  $M^{0,approx}$ :** The entries of  $M^{0,approx}$  are

$$\begin{aligned} &M_{\sigma, \tilde{\sigma}}^{0,approx}(\varepsilon, \delta, \lambda, 0) \\ &\equiv \left\langle p_\sigma, \left( -(\nabla + i[\mathbf{K} + \lambda \mathbf{k}_2])^2 - [E_\star^0 + \varepsilon(V_{0,0} - V_{1,1})] \right) p_{\tilde{\sigma}} \right\rangle_{L^2(\mathbb{R}^2/\Lambda_h)} \\ &= \left\langle p_\sigma, -(\nabla + i[\mathbf{K} + \lambda \mathbf{k}_2])^2 p_{\tilde{\sigma}} \right\rangle_{L^2(\mathbb{R}^2/\Lambda_h)} - [E_\star^0 + \varepsilon(V_{0,0} - V_{1,1})] \delta_{\sigma, \tilde{\sigma}}, \end{aligned} \tag{8.41}$$



where we have used that  $\langle p_\sigma, p_{\bar{\sigma}} \rangle = \delta_{\sigma, \bar{\sigma}}$ . The first term in (8.41) may be written, using (3.5)–(3.6),  $E_\star^0 = |\mathbf{K}|^2$  and  $|\mathbf{k}_2|^2 = q^2$  as:

$$\begin{aligned} & \left\langle p_\sigma, -(\nabla + i[\mathbf{K} + \lambda \mathbf{k}_2])^2 p_{\bar{\sigma}} \right\rangle_{L^2(\mathbb{R}^2/\Lambda_h)} \\ &= \left\langle p_\sigma, -(\nabla + i\mathbf{K})^2 p_{\bar{\sigma}} \right\rangle - 2i\lambda \mathbf{k}_2 \cdot \langle p_\sigma, (\nabla + i\mathbf{K}) p_{\bar{\sigma}} \rangle + \left\langle p_\sigma, \lambda^2 q^2 p_{\bar{\sigma}} \right\rangle \\ &= \left( E_\star^0 + \lambda^2 q^2 \right) \delta_{\sigma, \bar{\sigma}} + \lambda J_{\sigma, \bar{\sigma}}. \end{aligned} \tag{8.42}$$

Consider now the matrix

$$\begin{aligned} J_{\sigma, \bar{\sigma}} &= -2i\mathbf{k}_2 \cdot \langle \Phi_\sigma, \nabla \Phi_{\bar{\sigma}} \rangle_{L^2_{\mathbf{K}}} = -2i\mathbf{k}_2 \cdot \int_{\Omega} \overline{\Phi_\sigma} \nabla \Phi_{\bar{\sigma}} dx \\ &= 2\mathbf{k}_2 \cdot \frac{1}{3} \left( I + \sigma \bar{\sigma} R + \bar{\sigma} \sigma R^2 \right) \mathbf{K}. \end{aligned} \tag{8.43}$$

We pause to collect some properties that will enable the evaluation of  $J_{\sigma, \bar{\sigma}}$ ; see also [11]. Recall that  $R$  has eigenpairs:  $(\tau, \zeta)$  and  $(\bar{\tau}, \bar{\zeta})$ , where  $\zeta = \frac{1}{\sqrt{2}}(1, i)^T$ . Then,  $\bar{\tau}R$  has eigenpairs:  $[1, \zeta]$  and  $[\tau, \bar{\zeta}]$ . Furthermore,  $\tau R$  has eigenpairs  $[1, \bar{\zeta}]$  and  $[\bar{\tau}, \zeta]$ , and

$$\begin{aligned} \frac{1}{3} \left[ I + \bar{\tau}R + (\bar{\tau}R)^2 \right] \zeta &= \zeta, \quad \left[ I + \bar{\tau}R + (\bar{\tau}R)^2 \right] \bar{\zeta} = 0, \\ \frac{1}{3} \left[ I + \tau R + (\tau R)^2 \right] \bar{\zeta} &= \bar{\zeta}, \quad \left[ I + \tau R + (\tau R)^2 \right] \zeta = 0. \end{aligned}$$

Hence,  $\frac{1}{3} [I + \bar{\tau}R + (\bar{\tau}R)^2]$  and  $\frac{1}{3} [I + \tau R + (\tau R)^2]$  are, respectively, projections onto  $\text{span}\{\zeta\}$  and  $\text{span}\{\bar{\zeta}\}$ . For any  $\mathbf{w} \in \mathbb{C}^2$ , we have  $\mathbf{w} = \langle \zeta, \mathbf{w} \rangle_{\mathbb{C}^2} \zeta + \langle \bar{\zeta}, \mathbf{w} \rangle_{\mathbb{C}^2} \bar{\zeta}$ , where  $\langle \mathbf{x}, \mathbf{y} \rangle_{\mathbb{C}^2} = \bar{\mathbf{x}} \cdot \mathbf{y}$ . Therefore

$$\frac{1}{3} \left[ I + \bar{\tau}R + (\bar{\tau}R)^2 \right] \mathbf{w} = \langle \zeta, \mathbf{w} \rangle \zeta, \quad \frac{1}{3} \left[ I + \tau R + (\tau R)^2 \right] \mathbf{w} = \langle \bar{\zeta}, \mathbf{w} \rangle \bar{\zeta}. \tag{8.44}$$

Also,  $(I - R)(I + R + R^2) = I - R^3 = 0$  and therefore

$$I + R + R^2 = 0. \tag{8.45}$$

We next calculate  $J_{\sigma, \bar{\sigma}}$  using (8.44)–(8.45). Note that  $J$  is Hermitian, and by (8.45) its diagonal elements  $J_{\sigma, \sigma}$  all vanish:  $J_{\sigma, \bar{\sigma}} = \overline{J_{\bar{\sigma}, \sigma}}$ ,  $J_{\sigma, \sigma} = 0$ ,  $\sigma = 1, \tau, \bar{\tau}$ . It suffices therefore to compute the three entries  $J_{1, \tau}$ ,  $J_{1, \bar{\tau}}$  and  $J_{\tau, \bar{\tau}}$ :

$$\begin{aligned} J_{1, \tau} &= 2 \frac{1}{3} \left[ I + \bar{\tau}R + (\bar{\tau}R)^2 \right] \mathbf{K} \cdot \mathbf{k}_2 = 2 (\bar{\zeta} \cdot \mathbf{K}) (\zeta \cdot \mathbf{k}_2) \equiv \alpha, \\ J_{1, \bar{\tau}} &= 2 \frac{1}{3} \left[ I + \tau R + (\tau R)^2 \right] \mathbf{K} \cdot \mathbf{k}_2 = 2 (\zeta \cdot \mathbf{K}) (\bar{\zeta} \cdot \mathbf{k}_2) = \bar{\alpha}, \\ J_{\tau, \bar{\tau}} &= 2 \frac{1}{3} \left[ I + \bar{\tau}R + (\bar{\tau}R)^2 \right] \mathbf{K} \cdot \mathbf{k}_2 = 2 (\bar{\zeta} \cdot \mathbf{K}) (\zeta \cdot \mathbf{k}_2) = \alpha. \end{aligned}$$

Thus,

$$J = (J_{\sigma, \tilde{\sigma}}) = \begin{pmatrix} 0 & \alpha \bar{\alpha} \\ \bar{\alpha} & 0 \\ \alpha & \bar{\alpha} \\ \alpha & \bar{\alpha} \\ 0 & 0 \end{pmatrix}, \quad \text{where } \alpha = 2(\bar{\zeta} \cdot \mathbf{K})(\zeta \cdot \mathbf{k}_2). \tag{8.46}$$

It follows that

$$M_{\sigma, \tilde{\sigma}}^{0, approx}(\varepsilon, \delta, \lambda, 0) = \left(-\varepsilon(V_{0,0} - V_{1,1}) + \lambda^2 q^2\right) \delta_{\sigma, \tilde{\sigma}} + \lambda J_{\sigma, \tilde{\sigma}}. \tag{8.47}$$

**Expansion of  $M^V(\varepsilon)$ :**  $M_{\sigma, \tilde{\sigma}}^V(\varepsilon) = \varepsilon \langle p_\sigma, V p_{\tilde{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)} = \varepsilon \mathcal{V}_{\sigma, \tilde{\sigma}}$ , where

$$\begin{aligned} \mathcal{V}_{\sigma, \tilde{\sigma}} &= \langle p_\sigma, V p_{\tilde{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)} \\ &= \frac{1}{3} \left[ (1 + \sigma \bar{\sigma} + \bar{\sigma} \tilde{\sigma}) V_{0,0} + \sigma V_{0,1} + \bar{\sigma} V_{0,-1} + \tilde{\sigma} V_{1,0} \right. \\ &\quad \left. + \bar{\sigma} V_{-1,0} + \sigma \tilde{\sigma} V_{1,1} + \bar{\sigma} \tilde{\sigma} V_{-1,-1} \right]. \end{aligned}$$

Since  $V$  is real-valued and even, it follows that  $V_{-\mathbf{m}} = V_{\mathbf{m}}$ . Furthermore,  $V$  is also  $R$ -invariant and therefore  $V_{0,1} = V_{1,0} = V_{1,1}$ . Hence

$$\mathcal{V}_{\sigma, \tilde{\sigma}} = \frac{1}{3} (1 + \sigma \bar{\sigma} + \bar{\sigma} \tilde{\sigma}) V_{0,0} + \frac{1}{3} (\sigma + \bar{\sigma} + \tilde{\sigma} + \bar{\sigma} + \sigma \tilde{\sigma} + \bar{\sigma} \tilde{\sigma}) V_{1,1}.$$

$\mathcal{V}$  is clearly symmetric and using that  $1 + \tau + \tau^2 = 1 + \tau + \bar{\tau} = 0$ , we obtain  $M^V(\varepsilon) = \varepsilon \mathcal{V}$ , where

$$\mathcal{V} = \begin{pmatrix} V_{0,0} + 2 V_{1,1} & 0 & 0 \\ 0 & V_{0,0} - V_{1,1} & 0 \\ 0 & 0 & V_{0,0} - V_{1,1} \end{pmatrix}.$$

**Expansion of  $M^W(\delta)$ :**  $M_{\sigma, \tilde{\sigma}}^W(\varepsilon) = \delta \langle p_\sigma, W p_{\tilde{\sigma}} \rangle_{L^2(\mathbb{R}^2/\Lambda_h)} = \delta \mathcal{W}_{\sigma, \tilde{\sigma}}$ , where

$$\mathcal{W}_{\sigma, \tilde{\sigma}} = \frac{1}{3} \left[ \sigma W_{0,1} + \bar{\sigma} W_{0,-1} + \bar{\sigma} W_{-1,0} + \tilde{\sigma} W_{1,0} + \sigma \tilde{\sigma} W_{1,1} + \bar{\sigma} \tilde{\sigma} W_{-1,-1} \right]. \tag{8.48}$$

Since  $W$  is real and odd, we have that  $W_{-\mathbf{m}} = -W_{\mathbf{m}}$  and  $W_{\mathbf{m}}$  is purely imaginary. Therefore,

$$\mathcal{W}_{\sigma, \tilde{\sigma}} = \frac{1}{3} \left[ (\sigma - \bar{\sigma}) W_{0,1} + (\tilde{\sigma} - \bar{\sigma}) W_{1,0} + (\sigma \tilde{\sigma} - \bar{\sigma} \tilde{\sigma}) W_{1,1} \right], \quad \sigma, \tilde{\sigma} = 1, \tau, \bar{\tau}.$$

It follows that  $M^W(\delta) = \delta \mathcal{W}$ , where

$$\mathcal{W} = w_{01} \begin{pmatrix} 0 & \tau & -\bar{\tau} \\ \bar{\tau} & -1 & 0 \\ -\tau & 0 & 1 \end{pmatrix} + w_{10} \begin{pmatrix} 0 & \bar{\tau} & -\tau \\ \tau & -1 & 0 \\ -\bar{\tau} & 0 & 1 \end{pmatrix} + w_{11} \begin{pmatrix} 0 & -1 & 1 \\ -1 & 1 & 0 \\ 1 & 0 & -1 \end{pmatrix},$$

and  $w_{ij} \equiv -i W_{i,j}/\sqrt{3} \in \mathbb{R}$ .

Now assembling all relevant terms (weights  $\geq 1/2$  and less than  $3/2$ ) we obtain

**Proposition 8.14** For  $\sigma, \tilde{\sigma} = 1, \tau, \bar{\tau}$ ,

$$\begin{aligned} M_{\sigma, \tilde{\sigma}}(\varepsilon, \delta, \lambda, 0) &\approx M_{\sigma, \tilde{\sigma}}^{approx}(\varepsilon, \delta, \lambda, 0) \\ &\approx \left( -\varepsilon(V_{0,0} - V_{1,1}) + \lambda^2 q^2 \right) \delta_{\sigma, \tilde{\sigma}} + \lambda J_{\sigma, \tilde{\sigma}} + \varepsilon \mathcal{V}_{\sigma, \tilde{\sigma}} + \delta \mathcal{W}_{\sigma, \tilde{\sigma}}. \end{aligned}$$

Here,  $A_{\sigma, \tilde{\sigma}} \approx B_{\sigma, \tilde{\sigma}}$ , means that their difference is a matrix with entries having weight  $\geq 3/2$ . Hence, the contribution of such terms to the determinant consists of terms of weight strictly larger than 2, for  $(\lambda, \delta)$  in the region (8.39). Hence, these terms can be neglected, by Proposition 8.12.

So the calculation of  $\det M(\varepsilon, \delta, \lambda, 0)$  boils down to the calculation of  $\det M^{approx}(\varepsilon, \delta, \lambda, 0)$ .

**Calculation of  $\det M^{approx}(\varepsilon, \delta, \lambda, 0)$ :** Assembling the above computations, we have that

$$M^{approx} = \begin{pmatrix} \lambda^2 q^2 + 3\varepsilon V_{1,1} & \alpha\lambda - \delta\tilde{w} & \bar{\alpha}\lambda + \delta\tilde{w} \\ \bar{\alpha}\lambda - \delta\tilde{w} & \lambda^2 q^2 - \delta(w_{01} + w_{10} - w_{11}) & \alpha\lambda \\ \alpha\lambda + \delta\tilde{w} & \bar{\alpha}\lambda & \lambda^2 q^2 + \delta(w_{01} + w_{10} - w_{11}) \end{pmatrix},$$

where  $\tilde{w} = w_{11} - w_{01}\tau - w_{10}\bar{\tau}$  and  $\alpha = 2(\bar{\zeta} \cdot \mathbf{K})$  ( $\zeta \cdot \mathbf{k}_2$ ). Note that:

$$\alpha = \frac{q^2}{\sqrt{3}} i\tau, \quad \Re(\alpha) = -\frac{q^2}{2}, \quad \Re(\alpha^3) = 0. \tag{8.49}$$

Calculating the determinant of  $M^{approx}$ , and using (8.49) and that  $w_{ij} = -iW_{i,j}/\sqrt{3}$  yields:

$$\begin{aligned} \det M^{approx}(\varepsilon, \delta, \lambda, 0) &= - \left( q^2 \lambda^2 + \varepsilon V_{1,1} \right) \left( q^4 \lambda^2 + 3\delta^2 (w_{01}^2 + w_{10}^2 + w_{11}^2) \right) \\ &\quad + 6\varepsilon V_{1,1} \delta^2 (w_{11} w_{01} + w_{10} w_{11} - w_{01} w_{10}) + \mathcal{O}(\lambda \delta^2) + \mathcal{O}(\varepsilon \lambda^4) + \mathcal{O}(\lambda^6) \\ &= - \left( q^2 \lambda^2 + \varepsilon V_{1,1} \right) \left( q^4 \lambda^2 + 3\delta^2 (w_{01} + w_{10} - w_{11})^2 \right) \\ &\quad + \mathcal{O}(\lambda^2 \delta^2) + \mathcal{O}(\lambda \delta^2) + \mathcal{O}(\varepsilon \lambda^4) + \mathcal{O}(\lambda^6), \\ &= - \left( q^2 \lambda^2 + \varepsilon V_{1,1} \right) \left( q^4 \lambda^2 + \delta^2 |W_{0,1} + W_{1,0} - W_{1,1}|^2 \right) \end{aligned}$$

$$\begin{aligned}
 & + \mathcal{O}(\lambda^2\delta^2) + \mathcal{O}(\lambda\delta^2) + \mathcal{O}(\varepsilon\lambda^4) + \mathcal{O}(\lambda^6) \\
 & = -\pi(\varepsilon, \delta^2, \lambda) + o\left((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2)\right), \tag{8.50}
 \end{aligned}$$

for  $(\lambda, \delta)$  in the region (8.39). This completes the proof of Proposition 8.10.  $\square$

### 8.4 If $\varepsilon V_{1,1} < 0$ , the Zigzag Slice does not Satisfy the No-Fold Condition

Recall that to satisfy the case  $\varepsilon V_{1,1} < 0$  we assume, without loss of generality, that  $\varepsilon > 0$  and  $V_{1,1} < 0$ . Theorem 8.4 follows from:

**Proposition 8.15** *Assume*

$$0 < |\varepsilon| < \varepsilon_2, \text{ and } 0 \leq \delta \leq c_b \varepsilon^2. \tag{8.51}$$

There exists  $\theta_0 > 0$  and  $\lambda_\varepsilon > 0$  satisfying  $\varepsilon < \lambda_\varepsilon < \theta_0\sqrt{\varepsilon}$  such that for all  $\varepsilon$  sufficiently small,

$$\det M(\varepsilon, \delta, \lambda_\varepsilon, \mu = 0) = 0.$$

Thus,  $E_\star^\varepsilon$  is an interior point of the  $L^2_{k_\parallel}(\Sigma)$ -spectrum of  $H^{(\varepsilon,\delta)}$ .

It follows that for  $\varepsilon V_{1,1} < 0$ , the operator  $H^{(\varepsilon,\delta)}$  does not have a spectral gap about  $E = E_\star^\varepsilon$  along the zigzag slice. Referring to the middle panel of Figure 7, we see that, for  $\delta \neq 0$  and small, a local in  $\lambda$  gap opens, for  $\lambda$  small, about the energy  $E = E_\star^\varepsilon$ . But since the no-fold property is not satisfied (by Proposition 8.15), this is not a true (global in  $\lambda \in [-1/2, 1/2]$ ) spectral gap.

*Proof of Proposition 8.15* Let  $C_b$  denote the constant in Proposition 8.10. Note that  $C_b$  was chosen to be sufficiently large in the proof of Proposition 8.10 and can be arranged to be taken so that  $C_b > \theta_0$ , where  $\theta_0$  is defined by  $\theta_0^2 = 2|V_{1,1}|/q^2$ . Also, choose a constant  $\zeta_0$  such that  $\zeta_0^2 = |V_{1,1}|/2q^2$ . Note  $\zeta_0 < \theta_0$ ; below we shall see why we make these choices. For  $(\lambda, \delta)$  in the region (8.51) we have:

$$\begin{aligned}
 -\det M(\varepsilon, \delta, \lambda, 0) & = \pi(\varepsilon, \delta^2, \lambda) + o\left((\lambda^2 + \varepsilon)(\lambda^2 + \delta^2)\right) = \pi(\varepsilon, \delta^2, \lambda) + o\left(\varepsilon^2\right), \\
 & \tag{8.52}
 \end{aligned}$$

where

$$\pi(\varepsilon, \delta^2, \lambda) \equiv \left(q^2\lambda^2 + \varepsilon V_{1,1}\right) \left(q^4\lambda^2 + \delta^2 |W_{0,1} + W_{1,0} - W_{1,1}|^2\right).$$

We now show that there exists  $\lambda^{\varepsilon,\delta} \in (\zeta_0\sqrt{\varepsilon}, \theta_0\sqrt{\varepsilon})$  such that  $\pi(\varepsilon, \delta^2, \lambda^{\varepsilon,\delta}) = 0$ . Note first that  $\varepsilon V_{1,1} < 0$ ,  $\varepsilon^2 \ll \varepsilon$  and the choice of  $\zeta_0$  implies, upon evaluation of  $\pi(\varepsilon, \delta^2, \lambda)$  at  $\lambda = \zeta_0\sqrt{\varepsilon}$ , that:

$$\pi(\varepsilon, \delta^2, \zeta_0\sqrt{\varepsilon}) = \left(q^2\zeta_0^2\varepsilon + \varepsilon V_{1,1}\right) \left(q^4\zeta_0^2\varepsilon + \delta^2 |W_{0,1} + W_{1,0} - W_{1,1}|^2\right) < 0$$

and by (8.52)  $-\det M(\varepsilon, \delta, \zeta_0\sqrt{\varepsilon}, 0) < 0$ . On the other hand, the choice of  $\theta_0$  implies, upon evaluation at  $\lambda = \theta_0\sqrt{\varepsilon}$  that:

$$\pi(\varepsilon, \delta^2, \theta_0\sqrt{\varepsilon}) = \left(q^2\theta_0^2\varepsilon + \varepsilon V_{1,1}\right) \left(q^4\theta_0^2\varepsilon + \delta^2 |W_{0,1} + W_{1,0} - W_{1,1}|^2\right) > 0$$

and hence, by (8.52)  $-\det M(\varepsilon, \delta, \theta_0\sqrt{\varepsilon}, 0) > 0$ . Now  $\det M(\varepsilon, \delta^2, \lambda, 0)$  is, for all  $0 < \varepsilon < \varepsilon_1$ , a continuous function of  $\lambda$ . Hence, there exists  $\lambda^{\varepsilon,\delta} \in (\zeta_0\sqrt{\varepsilon}, \theta_0\sqrt{\varepsilon})$  such that  $\det M(\varepsilon, \delta, \lambda^{\varepsilon,\delta}, \mu = 0) = 0$ . Hence,  $E^{\varepsilon,\delta}(\lambda^{\varepsilon,\delta}) = E_\star^\varepsilon \in L_{k_{||}=2\pi/3}^2 - \text{spec}(H^{(\varepsilon,\delta)})$ . This completes the proof of Proposition 8.15.  $\square$

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### Appendix A. Evaluation of $\varepsilon V_{1,1}$ for Two Examples

Recall the bases  $\{\mathbf{v}_1, \mathbf{v}_2\}$  of  $\Lambda_h = \mathbb{Z}\mathbf{v}_1 \oplus \mathbb{Z}\mathbf{v}_2$  and  $\{\mathbf{k}_1, \mathbf{k}_2\}$  of  $\Lambda_h^* = \mathbb{Z}\mathbf{k}_1 \oplus \mathbb{Z}\mathbf{k}_2$ , introduced in Section 2.3. More generally, introduce a lattice spacing parameter,  $a > 0$ , and define the scaled lattices:  $\Lambda_h^{(a)}$  and  $(\Lambda_h^{(a)})^*$  with bases:  $\mathbf{v}_1^a = a(\frac{\sqrt{3}}{2}, \frac{1}{2})^T$ ,  $\mathbf{v}_2^a = a(\frac{\sqrt{3}}{2}, -\frac{1}{2})^T$  and  $\mathbf{k}_1^a = \frac{q}{a}(\frac{1}{2}, \frac{\sqrt{3}}{2})^T$ ,  $\mathbf{k}_2^a = \frac{q}{a}(\frac{1}{2}, -\frac{\sqrt{3}}{2})^T$ , where  $q \equiv \frac{4\pi}{\sqrt{3}}$  and  $\mathbf{k}_j^{(a)} \cdot \mathbf{v}_j^{(a)} = 2\pi \delta_{ij}$ . Now introduce the base points:  $\mathbf{A}^{(a)} = (0, 0)$  and  $\mathbf{B}^{(a)} = a(\frac{1}{\sqrt{3}}, 0)$  and the honeycomb structure with general lattice spacing parameter,  $a > 0$ :  $\mathbf{H}^{(a)} = (\mathbf{A}^{(a)} + \Lambda_h^{(a)}) \cup (\mathbf{B}^{(a)} + \Lambda_h^{(a)})$ . To be consistent with previous notation, we write:  $\mathbf{A}^{(1)} = \mathbf{A} = (0, 0)$ ,  $\mathbf{B}^{(1)} = \mathbf{B} = (\frac{1}{\sqrt{3}}, 0)$ ,  $\Lambda_h^{(1)} = \Lambda$ ,  $(\Lambda_h^{(1)})^* = (\Lambda_h)^*$ ,  $\mathbf{H}^{(1)} = \mathbf{H}$ .

Let  $g_0(\mathbf{x})$  denote a smooth, real-valued, radially symmetric ( $g_0(\mathbf{x}) = g_0(|\mathbf{x}|)$ ) and rapidly decaying function on  $\mathbb{R}^2$ . Below we shall use the 2D Poisson Summation formula:

$$\sum_{\mathbf{n} \in \mathbb{Z}^2} f(\mathbf{x} + \mathbf{nv}) = \frac{(2\pi)^2}{|\Omega_h|} \sum_{\mathbf{m} \in \mathbb{Z}^2} \widehat{f}(\mathbf{mk}) e^{i\mathbf{mk} \cdot \mathbf{x}}.$$

We next present two examples: sums of translates of  $g_0$  over the scaled triangular lattice,  $\Lambda_h^{(a)}$ , and honeycomb structure,  $\mathbf{H}^{(a)}$ . In both cases,  $V_{1,1}^{(a)}$  is expressible in terms of  $\widehat{g}_0\left(\frac{4\pi}{\sqrt{3}a}\right)$ . Therefore, if  $\widehat{g}_0(\xi)$  changes sign, then the sign of  $V_{1,1}^{(a)}$  can be changed by varying the lattice constant,  $a$ .

#### A.1. Example 1: Evaluation of $\varepsilon V_{1,1}$ for $V$ Equal to a Sum of Translates Over the Scaled Triangular Lattice, $\Lambda_h^{(a)}$

Define  $V(\mathbf{x}; a) = \sum_{\mathbf{v} \in \Lambda_h^{(a)}} g_0(\mathbf{x} + \mathbf{v})$ . The potential  $V(\mathbf{x}; a)$  is a honeycomb potential; it is  $\Lambda_h^{(a)}$ -periodic, inversion symmetric and  $\mathcal{R}$ -invariant with respect to the origin of coordinates  $\mathbf{x}_0 = 0$ .

**Claim 8.16**  $V_{1,1}^{(a)} = \frac{(2\pi)^2}{|\Omega_h|} \widehat{g}_0\left(\frac{\mathbf{k}_1 + \mathbf{k}_2}{a}\right) = \frac{(2\pi)^2}{|\Omega_h|} \widehat{g}_0\left(\frac{4\pi}{\sqrt{3}} \frac{1}{a}\right)$ .

*Proof of Claim 8.16* The Poisson summation gives

$$V(\mathbf{x}; a) = \frac{(2\pi)^2}{|\Omega_h|} \sum_{\mathbf{m} \in \mathbb{Z}^2} \widehat{g}_0(\mathbf{m}\mathbf{k}^{(a)}) e^{i(\mathbf{m}\mathbf{k}^{(a)}) \cdot \mathbf{x}}.$$

Recall also that  $\mathbf{m}\mathbf{k}^{(a)} = m_1 \mathbf{k}_1^{(a)} + m_2 \mathbf{k}_2^{(a)} = \frac{1}{a}(m_1 \mathbf{k}_1 + m_2 \mathbf{k}_2)$ . Claim 1 now follows from:

$$V(\mathbf{x}; a) = \frac{(2\pi)^2}{|\Omega_h|} \sum_{\mathbf{m} \in \mathbb{Z}^2} \widehat{g}_0\left(\frac{m_1 \mathbf{k}_1 + m_2 \mathbf{k}_2}{a}\right) e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot \mathbf{x}} = \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}}^{(a)} e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot \mathbf{x}}.$$

□

**A.2. Evaluation of  $\varepsilon V_{1,1}$  for  $V$  Equal to a Sum of Translates over the Scaled Honeycomb Structure  $\mathbf{H}^{(a)}$**

As earlier, take  $\mathbf{A}^{(a)} = (0, 0)^T$  and  $\mathbf{B}^{(a)} = a(\frac{1}{\sqrt{3}}, 0)^T$ . The point at the center of hexagon, immediately northeast of  $\mathbf{A}^{(a)}$  is  $\tau_0^{(a)} = \frac{a}{2}(\frac{1}{\sqrt{3}}, 1)^T$ . Define

$$V(\mathbf{x}; a) = \sum_{\mathbf{v} \in \Lambda_h^{(a)}} g_0(\mathbf{x} - \mathbf{A}^{(a)} + \tau_0^{(a)} + \mathbf{v}) + \sum_{\mathbf{v} \in \Lambda_h^{(a)}} g_0(\mathbf{x} - \mathbf{B}^{(a)} + \tau_0^{(a)} + \mathbf{v}).$$

$V(\mathbf{x}; a)$  is a honeycomb potential; it is  $\Lambda_h$ -periodic, inversion symmetric and  $\mathcal{R}$ -invariant with respect to the origin coordinates,  $\mathbf{x}_0 = 0$ , located at the center of a hexagon.

**Claim 8.17**  $V_{1,1}^{(a)} = -\frac{(2\pi)^2}{|\Omega_h|} \times \widehat{g}_0\left(\frac{4\pi}{\sqrt{3}} \frac{1}{a}\right)$ .

*Proof of Claim 8.17* Poisson summation yields

$$\begin{aligned} &V(\mathbf{x}; a) \\ &= \frac{(2\pi)^2}{|\Omega_h|} \sum_{\mathbf{m} \in \mathbb{Z}^2} \left[ \widehat{g}_0\left(\cdot - \mathbf{A}^{(a)} + \tau_0^{(a)}\right)(\mathbf{m}\mathbf{k}^{(a)}) + \widehat{g}_0\left(\cdot - \mathbf{B}^{(a)} + \tau_0^{(a)}\right)(\mathbf{m}\mathbf{k}^{(a)}) \right] e^{i(\mathbf{m}\mathbf{k}^{(a)}) \cdot \mathbf{x}}. \end{aligned}$$

Now,  $\widehat{g}_0\left(\cdot - \mathbf{A}^{(a)} + \tau_0^{(a)}\right)(\xi) = \exp\left(i\xi \cdot \tau_0^{(a)}\right) \widehat{g}_0(\xi)$  and  $\widehat{g}_0\left(\cdot - \mathbf{B}^{(a)} + \tau_0^{(a)}\right)(\xi) = \exp\left(i\xi \cdot (-\mathbf{B}^{(a)} + \tau_0^{(a)})\right) \widehat{g}_0(\xi)$ , and therefore

$$V(\mathbf{x}; a) = \frac{(2\pi)^2}{|\Omega_h|} \sum_{\mathbf{m} \in \mathbb{Z}^2} \left[ e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot \tau_0^{(a)}} + e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot (-\mathbf{B}^{(a)} + \tau_0^{(a)})} \right] \widehat{g}_0(\mathbf{m}\mathbf{k}^{(a)}) e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot \mathbf{x}}.$$

Noting that  $\mathbf{m}\mathbf{k}^{(a)} \cdot \boldsymbol{\tau}_0^{(a)} = \mathbf{m}\mathbf{k} \cdot \boldsymbol{\tau}_0$  and  $\mathbf{m}\mathbf{k}^{(a)} \cdot (-\mathbf{B}^{(a)} + \boldsymbol{\tau}_0^{(a)}) = \mathbf{m}\mathbf{k} \cdot (-\mathbf{B} + \boldsymbol{\tau}_0)$  (independent of the lattice constant,  $a$ ), we have

$$\begin{aligned}\mathbf{m}\mathbf{k}^{(a)} \cdot \boldsymbol{\tau}_0^{(a)} &= (m_1\mathbf{k}_1 + m_2\mathbf{k}_2) \cdot \boldsymbol{\tau}_0 = \frac{2\pi}{3}(2m_1 - m_2), \quad \text{and} \\ \mathbf{m}\mathbf{k}^{(a)} \cdot (-\mathbf{B}^{(a)} + \boldsymbol{\tau}_0^{(a)}) &= (m_1\mathbf{k}_1 + m_2\mathbf{k}_2) \cdot (-\mathbf{B} + \boldsymbol{\tau}_0) = -\frac{2\pi}{3}(2m_1 - m_2).\end{aligned}$$

Recall again that  $\mathbf{m}\mathbf{k}^{(a)} = m_1\mathbf{k}_1^{(a)} + m_2\mathbf{k}_2^{(a)} = \frac{1}{a}(m_1\mathbf{k}_1 + m_2\mathbf{k}_2)$ . Hence,

$$\begin{aligned}V(\mathbf{x}; a) &= \frac{(2\pi)^2}{|\Omega_h|} \sum_{\mathbf{m} \in \mathbb{Z}^2} \left[ e^{\frac{2\pi i}{3}(2m_1 - m_2)} + e^{-\frac{2\pi i}{3}(2m_1 - m_2)} \right] \widehat{g}_0 \left( \frac{m_1\mathbf{k}_1 + m_2\mathbf{k}_2}{a} \right) e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot \mathbf{x}} \\ &= \frac{(2\pi)^2}{|\Omega_h|} \sum_{\mathbf{m} \in \mathbb{Z}^2} 2 \cos \left( \frac{2\pi}{3}(2m_1 - m_2) \right) \widehat{g}_0 \left( \frac{m_1\mathbf{k}_1 + m_2\mathbf{k}_2}{a} \right) e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot \mathbf{x}} \\ &= \sum_{\mathbf{m} \in \mathbb{Z}^2} V_{\mathbf{m}}^{(a)} e^{i\mathbf{m}\mathbf{k}^{(a)} \cdot \mathbf{x}}.\end{aligned}$$

Therefore,  $V_{1,1}^{(a)} = \frac{(2\pi)^2}{|\Omega_h|} 2 \cos \left( \frac{2\pi}{3} \right) \times \widehat{g}_0 \left( \frac{\mathbf{k}_1 + \mathbf{k}_2}{a} \right) = -\frac{(2\pi)^2}{|\Omega_h|} \times \widehat{g}_0 \left( \frac{4\pi}{\sqrt{3}} \frac{1}{a} \right)$ .  $\square$

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