

Interface Modes in Honeycomb Topological Photonic Structures with Broken Reflection Symmetry*

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Abstract

In this work, we present a mathematical theory for Dirac points and interface modes in honeycomb topological photonic structures consisting of impenetrable obstacles. Starting from a honeycomb lattice of obstacles attaining 120° -rotation symmetry and horizontal reflection symmetry, we apply the boundary integral equation method to show the existence of Dirac points for the first two bands at the vertices of the Brillouin zone. We then study interface modes in a joint honeycomb photonic structure, which consists of two periodic lattices obtained by perturbing the honeycomb one with Dirac points differently. The perturbations break the reflection symmetry of the system, as a result, they annihilate the Dirac points and generate two structures with different topological phases, which mimics the quantum valley Hall effect in topological insulators. We investigate the interface modes that decay exponentially away from the interface of the joint structure in several configurations with different interface geometries, including the zigzag interface, the armchair interface, and the rational interfaces. Using the layer potential technique and asymptotic analysis, we first characterize the band-gap opening for the two perturbed periodic structures and derive the asymptotic expansions of the Bloch modes near the band gap surfaces. By formulating the eigenvalue problem for each joint honeycomb structure using boundary integral equations over the interface and analyzing the characteristic values of the associated boundary integral operators, we prove the existence of interface modes when the perturbation is small.

Keywords: Interface modes, Honeycomb structure, Helmholtz equations, Dirac points, Topological photonics

MSC:35P15, 35Q60, 35J05, 45M05

1 Introduction and outline

1.1 Background and motivation

Photonic and phononic materials with band gaps can be used to localize and confine waves, which have wide applications in the transportation and manipulation of wave energy [45, 50]. In a gapped

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photonic or phononic crystal, a localized wave mode with frequency in the band gap can be created by introducing a local perturbation in the periodic structure, such as a point or line defect [45]. Such a wave mode is called a defect mode and it is confined near the defect. Mathematically, a defect mode and its frequency correspond to an eigenpair of a locally perturbed periodic operator for the acoustic wave equation or Maxwell’s equations. The existence of point defect modes and line defect modes was proved in [4, 5, 13, 14, 37, 36, 46, 69] for several different configurations of periodic acoustic and electromagnetic media, including the periodic dielectric media, high contrast media, and bubbly media, etc. Besides the deterministic approaches, random media also allows for wave localization. One well-known strategy is the Anderson localization, wherein a periodic medium is randomly perturbed in the whole spatial domain [31, 32, 35, 67].

The recent development in topological insulators (cf. [42, 12, 63]) opens up new avenues for wave localization and confinement in photonic and phononic materials. The concept of topological phases for classical waves was proposed in the seminal work [23], when it was realized that topological band structures are a ubiquitous property of waves for periodic media, regardless of the classical or quantum nature of the waves. Therefore, the concepts in topological insulators can be parallelly extended to periodic wave media, and remarkably, extensive research work has been sparked in pursuit of topological acoustic, electromagnetic, and mechanical insulators to manipulate the classical wave in the same way as solids modulating electrons [48, 57, 59, 61, 75]. Briefly speaking, there are mainly two strategies to realize topological structures for classical waves. The first strategy mimics the quantum Hall effect in topological insulators using active components to break the time-reversal symmetry of the system [49, 73]. The second strategy relies on an analog of the quantum spin Hall effect or quantum valley Hall effect, and it uses passive components to break the spatial symmetry of the system [58, 74].

Wave localization in topological structures is achieved by gluing together two periodic media with distinct topological invariants. The topological phase transition at the interface of two media gives rise to the so-called interface modes, which propagate parallel to the interface but localize in the direction transverse to the interface. Recently there has been intensive mathematical research investigating the interface modes in topological insulators from different perspectives. In particular, the existence of interface modes was proved in [20, 26, 27, 54] for the Schrödinger operator and several other elliptic operators, wherein the interfaces are modeled by smooth domain walls. In addition, the spectra of interface modes are closely related to the topological nature of the bulk media. In general, the net number of interface modes is equal to the difference of the bulk topological invariants across the interface, which is known as the *bulk-edge correspondence* [42, 61]. We refer to [9, 10, 22, 21, 43] for the studies of the bulk-edge correspondence in discrete electron models and [17, 19] for the bulk-edge correspondence in several elliptic PDE models.

In this work, we study the interface modes in a joint honeycomb photonic structure, where two periodic lattices separated by an interface are obtained by perturbing a honeycomb lattice with Dirac points differently. Such perturbations break the reflection symmetry of the system, as a result, they annihilate the Dirac points and generate two structures with different topological phases. This mimics the quantum valley Hall effect in topological insulators [58, 74]. A one-dimensional joint structure with a similar setup was investigated [56, 70] using the transfer matrix method and the oscillatory theory for Sturm-Liouville operators. In contrast to the studies of interface modes in [20, 26, 27, 54], where two bulk media are “connected” adiabatically over a length scale that is much larger than the period of the structure to form a joint photonic structure and the interface is modeled by a smooth domain wall extending to the whole spatial domain, we consider more realistic models where two periodic media are connected directly such that the medium coefficient

attains a jump across the interface. Therefore, we have to address the new challenges in the spectral analysis brought by the discontinuities of coefficients in the PDE model. Beyond that, we consider the model with more general shapes of the interface that separates two bulk media. The goal of this work is to develop a mathematical framework based on a combination of layer potential theory, asymptotic analysis, and the generalized Rouché theorem to examine the existence of the interface modes in such settings. The mathematical framework can be extended to study localized modes in other contexts.

1.2 Outline

1.2.1 The honeycomb lattice and Dirac points

We start from a honeycomb lattice consisting of a two-dimensional array of impenetrable obstacles and examine the existence of Dirac points in the band structure of the lattice. A schematic plot of the periodic structure and its band structure is shown in Figure 1.1. The honeycomb lattice is a natural choice for the photonic structure, as it attains the desired symmetry to create Dirac points over the vertices of the Brillouin zone [11, 24].

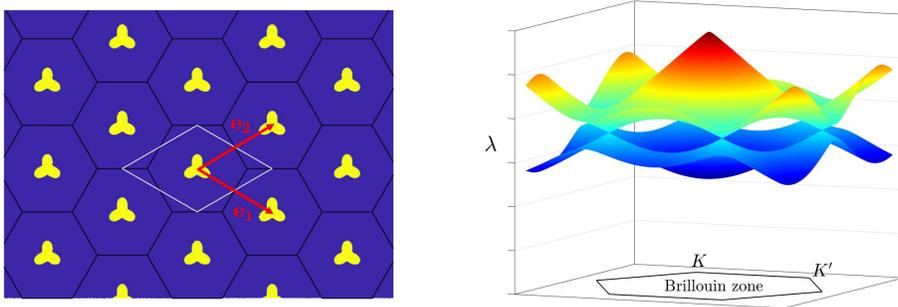


Figure 1.1: An infinite array of impenetrable obstacles are arranged over the honeycomb lattice (left) and its band structure (right). The obstacle in each periodic cell attains 120° -rotation symmetry and horizontal reflection symmetry.

Dirac points refer to conical intersections of two dispersion surfaces in the band structure. They are the degenerate points in the spectrum where the topological phases of the material may change. More specifically, at a Dirac point $(\mathbf{p}^*, \lambda^*)$, the eigenspace of the associated partial differential operator spans a two-dimensional space. In addition, the two dispersion surfaces forming the Dirac point attain the following expansion

$$\lambda^\pm(\mathbf{p}) = \lambda^* \pm \alpha |\mathbf{p} - \mathbf{p}^*| + O(|\mathbf{p} - \mathbf{p}^*|^2), \quad (1.1)$$

wherein $\alpha \neq 0$ denotes the slope of the linear dispersion relation near the Dirac point. Due to the surging interest in topological insulators, Dirac points were investigated for a broad class of PDE operators recently, especially for the Schrödinger operator over the honeycomb lattice, the Helmholtz operator with high-contrast medium and resonant bubbles, etc [3, 15, 24, 11, 29, 53, 54]. In general, Dirac points exist at the vertices of the Brillouin zone when the medium coefficients in the honeycomb lattice attain suitable symmetry, such as inversion and 120° -rotation symmetry,

horizontal reflection and 120° -rotation symmetry, etc. The degeneracy at a Dirac point can be deduced from the representation of the relevant symmetry group, and the conical shape of the dispersion relation is obtained from its invariance under the rotation symmetry [11].

In this work, we apply the boundary integral equation method to show the existence of Dirac points for the first two bands at the vertices of the Brillouin zone, assuming that the shape of each obstacle in the lattice attains 120° -rotation symmetry and horizontal reflection symmetry as shown in Figure 1.1. The existence of Dirac points for obstacles with other symmetries can be examined similarly using this method.

1.2.2 The perturbed honeycomb lattices: spectral gap and topological phase

We then break the spatial reflection symmetry of the honeycomb lattice by rotating the obstacles in opposite directions to obtain two photonic structures in Figure 1.2, which will create spectral gaps at the Dirac point as shown in Figure 1.3 so that wave propagation is prohibited for frequencies located in the gap interval. We carry out the asymptotic analysis for the spectrum of each perturbed periodic operator using the layer potential technique and prove that a spectral gap is opened at the Dirac point when the perturbation is small. Furthermore, we prove that the eigenspaces at the band edges are swapped for the two perturbed periodic operators, which demonstrates the topological phase transition of the medium at the Dirac point. The topological phase difference between the two lattices can also be manifested through the Berry phase, which describes the phase evolution of eigenfunctions in the momentum space [8]. As demonstrated in Figure 1.4, the Berry curvatures associated with the first bands of the two perturbed lattices attain opposite values.

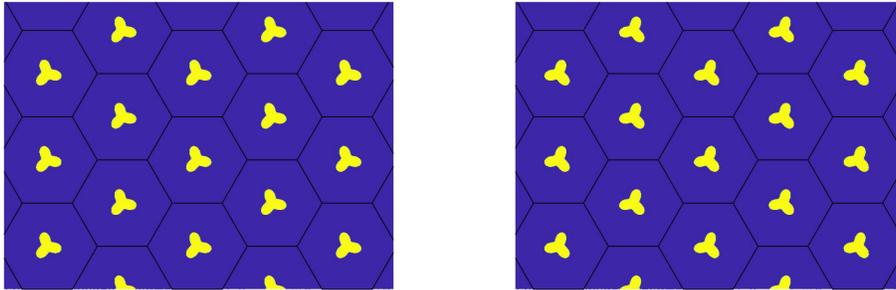


Figure 1.2: The two perturbed honeycomb lattices by rotating the obstacles counter-clockwisely and clockwisely, respectively.

1.2.3 Interface modes in the joint honeycomb lattice

Finally, we investigate the interface modes for the joint photonic structure formed by gluing the two perturbed honeycomb lattices together. The interface modes propagate parallel to the interface of the two media but decay along the direction perpendicular to the interface (cf. Figure 1.5). We consider the PDE operators for several configurations of joint photonic structures attaining different interface geometries, including the zigzag interface, the armchair interface, and the rational interfaces. The configurations of the joint structure with the zigzag and armchair interface are shown in Figure 1.6. We prove the existence of interface modes for the joint structures for each scenario, with

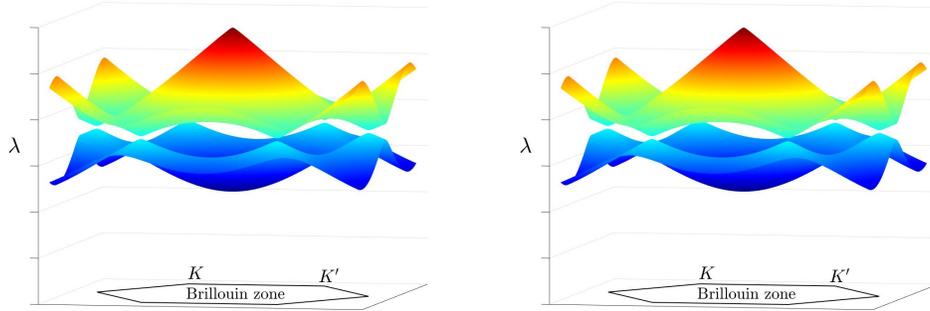


Figure 1.3: The band structure of the two perturbed honeycomb lattices in Figure 1.2.

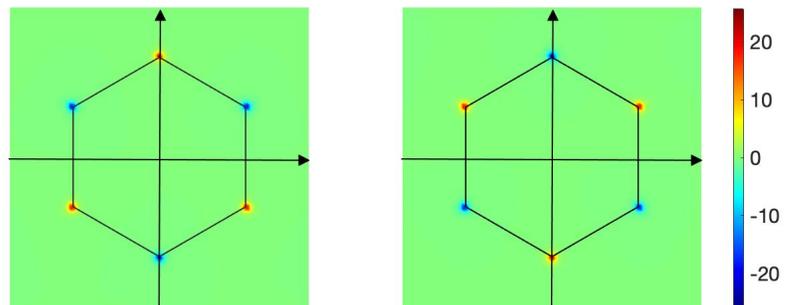


Figure 1.4: The Berry curvature in the momentum space for the two perturbed honeycomb lattices in Figure 1.2.

the corresponding eigenfrequencies located in the common band gap of the two perturbed media enclosing the Dirac point. To address the sharp discontinuity of the medium coefficient across the interface, we set up a matching condition for the wave field at the interface using integral equations and investigate the characteristic values using the generalized Rouché Theorem in Gohberg-Sigal theory [40, 2]. The method was applied to study the interface modes bifurcated from Dirac points in the topological waveguide structure recently [64] and can be employed to study interface modes in photonic structures with piecewise constant media in a general context.

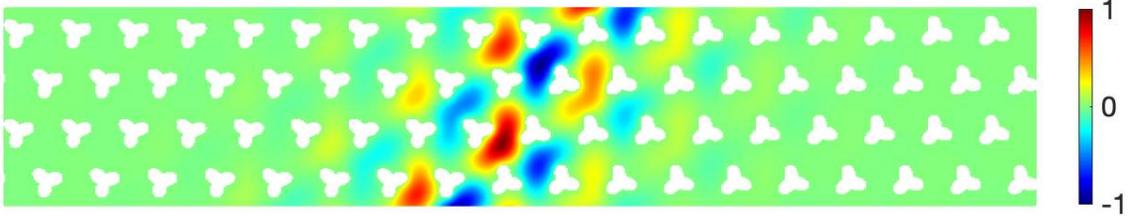


Figure 1.5: Interface mode propagating along the interface of two perturbed honeycomb lattices.

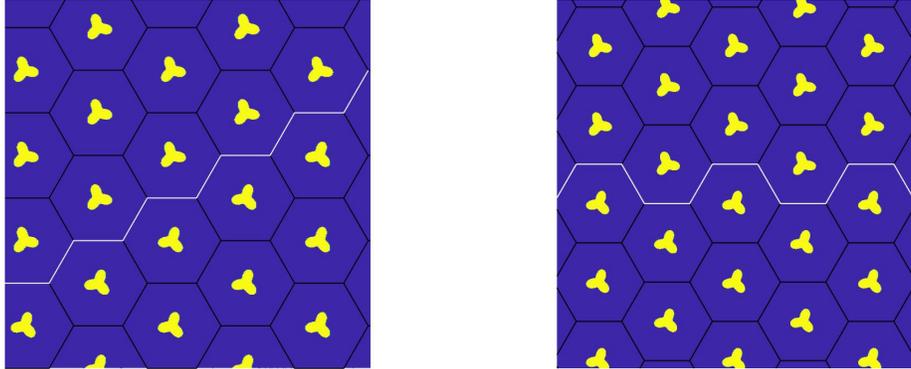


Figure 1.6: Join photonic structures with a zigzag interface (left) and armchair interface (right).

1.3 Notations

Honeycomb lattice

Λ, Λ^* : the honeycomb lattice and its dual lattice.

K, K' : high symmetry points in the Brillouin zone.

$\tilde{\Lambda}^* := K + \Lambda^*$.

\mathcal{C}_z : the fundamental cell of the honeycomb lattice for the zigzag interface.

$\mathbf{e}_1, \mathbf{e}_2$: generating vectors of the honeycomb lattice Λ with the fundamental cell \mathcal{C}_z .

$\Gamma_l, \Gamma_r, \Gamma_t, \Gamma_b$, the left, right, top and bottom sides of \mathcal{C}_z . See Figure 2.1.

ν_1, ν_2 : unit normal to Γ_l and Γ_b . See Figure 2.1.

β_1, β_2 : generating vectors of the dual lattice Λ^* with $\beta_i \cdot \mathbf{e}_j = \delta_{ij}$.

\mathcal{C}_a : the fundamental cell of the honeycomb lattice for the armchair interface.

$\mathbf{e}_1^a, \mathbf{e}_2^a$: generating vectors of the honeycomb lattice with the fundamental cell \mathcal{C}_a .

β_1^a, β_2^a : generating vectors of the dual lattice with $\mathbf{e}_i^a \cdot \mathbf{e}_j^a = \delta_{ij}$.

D_* : the reference inclusion with required symmetries.

$D(\eta) := \eta D_*$.

$D := D(\eta_0)$ with a sufficiently small η_0 .

D^ε : the domain obtained by rotating D by an angle of ε counterclockwise.

Layer potentials defined over the inclusion boundary

$S_0[\phi](\mathbf{x})$: single layer potential with Green function for free space Laplacian on ∂D_* , see (3.19).

$\mathcal{S}(\eta, \lambda, \mathbf{p})$: single layer potential with quasiperiodic Green function for Helmholtz equation on ∂D_* , see (3.4).

$T(\varepsilon, \lambda, \mathbf{p})$: single layer potential with quasiperiodic Green function for Helmholtz equation on ∂D , where ε represents the orientation, see (4.1).

Infinite strips for joint honeycomb structures

$\Omega^J := \cup_{m \in \mathbb{Z}} (\mathcal{C}_z + m\mathbf{e}_1)$: the infinite strip for the joint honeycomb structure with a zigzag interface.

$D^{J,\varepsilon} := (\cup_{m \geq 0} (D^\varepsilon + m\mathbf{e}_1)) \cup (\cup_{m < 0} (D^{-\varepsilon} + m\mathbf{e}_1))$: the domain of inclusions located in Ω^J for the joint honeycomb with the zigzag interface.

$\Omega_a^{J,\varepsilon} := \Omega^J \setminus \overline{D^{J,\varepsilon}}$.

Γ : the zigzag interface for the joint honeycomb structure.

$\Gamma_\pm := \{\pm \frac{1}{2}\mathbf{e}_2 + \ell\mathbf{e}_1, \ell \in \mathbb{R}\}$: the top and bottom boundaries of the domain Ω^J .

$\Omega_a^J := \cup_{m \in \mathbb{Z}} (\mathcal{C}_a + m\mathbf{e}_1^a)$: the infinite strip for the joint honeycomb structure with an armchair interface.

$D_a^{J,\varepsilon} := (\cup_{m \geq 0} (D^\varepsilon + m\mathbf{e}_1^a)) \cup (\cup_{m < 0} (D^{-\varepsilon} + m\mathbf{e}_1^a))$: the domain of inclusions located in Ω_a^J for the joint honeycomb with the armchair interface.

$\Omega_a^{J,\varepsilon} := \Omega_a^J \setminus \overline{D_a^{J,\varepsilon}}$.

Γ^a : the armchair interface restricted on Ω_a^J .

$\Gamma_\pm^a := \{\pm \frac{1}{2}\mathbf{e}_2^a + \ell\mathbf{e}_1^a, \ell \in \mathbb{R}\}$: the top and bottom boundaries of Ω_a^J .

$k_{\parallel}^* = K \cdot \mathbf{e}_2 = \frac{4\pi}{3}$, $k_{\parallel}^{*'} = K' \cdot \mathbf{e}_2 = -\frac{4\pi}{3}$, $k_{\parallel}^{*,a} = K \cdot \mathbf{e}_2^a = 2\pi$.

Energies and modes

$w_i, i = 1, 2$: Bloch modes with quasimomentum K at the Dirac point energy λ_* . See Theorem 2.1.

$\lambda_{n,\varepsilon}(\mathbf{p}(\ell))$: dispersion energies that are numbered from small to large.

$u_{n,\varepsilon}(\mathbf{x}; \mathbf{p})$: Bloch modes at energy $\lambda_{n,\varepsilon}(\mathbf{p}(\ell))$.

$\mu_{n,\varepsilon}(\mathbf{p}(\ell))$: dispersion energies that are smooth along $\mathbf{p}(\ell)$.

$v_{n,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))$: Bloch modes at energy $\mu_{n,\varepsilon}(\mathbf{p}(\ell))$ that are smooth along $\mathbf{p}(\ell)$.

λ_n, u_n, μ_n and v_n : abbreviations of $\lambda_{n,0}, u_{n,0}, \mu_{n,0}$ and $v_{n,0}$. See Section 5.1.

$\vec{v}_i := \begin{pmatrix} v_i|_{\Gamma} \\ \partial_n v_i|_{\Gamma} \end{pmatrix}, \quad i = 1, 2, \text{ see (7.2)}$

$\mathbf{u}_1 := \vec{v}_1 + i\vec{v}_2, \mathbf{u}_2 := \vec{v}_1 - i\vec{v}_2..$

Green functions

$G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})$: quasi-periodic Green function for the Helmholtz equation in \mathbb{R}^2 ; see (3.1).
 $G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda)$: Green function for the Helmholtz equation in $\mathbb{R}^2 \setminus \cup_{n_1, n_2 \in \mathbb{Z}} (D^\varepsilon + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2)$ that is quasiperiodic in \mathbf{e}_2 , see (5.25).

Layer potentials over the interface of the joint honeycomb lattice

$\mathcal{S}^\varepsilon, \mathcal{D}^\varepsilon, \mathcal{K}^{*,\varepsilon}, \mathcal{K}^\varepsilon, \mathcal{N}^\varepsilon$: layer potentials over interface Γ , with the kernel $G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda)$.
 $\mathbb{T}^\varepsilon, \mathbb{T}_s^\varepsilon, \mathbb{T}_t^\varepsilon, \mathbb{T}_n^\varepsilon$: matrix operators with layer potentials over Γ with the kernel $G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda)$.
 $\Omega^0, \tilde{\mathcal{S}}^0(\lambda_*) , \tilde{\mathcal{D}}^0(\lambda_*) , \tilde{\mathcal{K}}^0(\lambda_*) , \tilde{\mathcal{K}}^{*,0}(\lambda_*)$ and $\tilde{\mathcal{N}}^0(\lambda_*)$: layer potentials over Γ , with kernel $\tilde{G}^0(\mathbf{x}, \mathbf{y}; \lambda)$.
 $\tilde{\mathbb{T}}^0(\lambda_*)$: matrix operator with layer potentials over Γ with kernel $\tilde{G}^0(\mathbf{x}, \mathbf{y}; \lambda)$.

Function spaces

(2.15)

$$\begin{aligned} \mathcal{H}^{J,\varepsilon} := \{ & u \in H^1(\Omega^{J,\varepsilon}) : \Delta u \in L^2(\Omega^{J,\varepsilon}), \quad u = 0 \text{ on } \partial D^{J,\varepsilon}, \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_- \}, \end{aligned}$$

(2.19)

$$\begin{aligned} \mathcal{H}_a^{J,\varepsilon} := \{ & u \in H^1(\Omega_a^{J,\varepsilon}) : \Delta u \in L^2(\Omega_a^{J,\varepsilon}), \quad u = 0 \text{ on } \partial D_a^{J,\varepsilon}, \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^{*,a}} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-^a, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^{*,a}} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-^a \}. \end{aligned}$$

(3.8)

$$\mathcal{H}_i^s(\partial D) := \{ \phi \in H^s(\partial D); R\phi(\mathbf{x}) := \phi(R^{-1}\mathbf{x}) = \tau^i \phi(\mathbf{x}) \}, \quad i = 0, 1, 2.$$

(5.1)

$$\begin{aligned} \mathcal{H}_{\text{loc}}^\varepsilon := \{ & u \in H_{\text{loc}}^1(\Omega^\varepsilon) : \Delta u \in L_{\text{loc}}^2(\Omega^\varepsilon), \quad u = 0 \text{ on } \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1), \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-, \quad \partial_{\nu_1} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} \partial_{\nu_1} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_- \}. \end{aligned}$$

(5.3)

$$\begin{aligned} \mathcal{H}^\varepsilon(\ell) := \{ & u \in H^1(\mathcal{C}_z \setminus D) : \Delta u \in L^2(\mathcal{C}_z \setminus D^\varepsilon), \quad u = 0 \text{ on } \partial D^\varepsilon, \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b \\ & u(\mathbf{x} + \mathbf{e}_1) = e^{i(K+\ell\beta_1) \cdot \mathbf{e}_1} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_1, \quad \partial_{\nu_1} u(\mathbf{x} + \mathbf{e}_1) = e^{i(K+\ell\beta_1) \cdot \mathbf{e}_1} \partial_{\nu_1} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_1 \}. \end{aligned}$$

(5.7)

$$\begin{aligned} H^1(\Delta, \mathcal{C}_z \setminus D^\varepsilon) := \{ & u \in H^1(\mathcal{C}_z \setminus D^\varepsilon) : \Delta u \in L^2(\mathcal{C}_z \setminus D^\varepsilon), \quad u = 0 \text{ on } \partial D^\varepsilon, \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b \}. \end{aligned}$$

(5.17)

$$\mathcal{H}^s(\Gamma) := \left\{ u(\mathbf{x}_0 + t\mathbf{e}_2) = \sum_{n \in \mathbb{Z}} a_n e^{ik_{\parallel}^* t} e^{i2\pi n t} : \|u\|_{\mathcal{H}^s(\Gamma)}^2 := \sum_{n \in \mathbb{Z}} |a_n|^2 (1 + |n|^2)^{s/2} \right\}.$$

2 Main results

The first main result of this work is the existence and asymptotic analysis of Dirac points for a family of honeycomb lattices of impenetrable obstacles with Dirichlet boundary conditions. We assume that the shape of each obstacle in the honeycomb lattice attains 120° -rotation symmetry and horizontal reflection symmetry. The second main result is the existence and the number of interface modes for a joint photonic structure formed by gluing two lattices perturbed from the honeycomb lattice attaining Dirac points along an interface. Our results cover the case of a zigzag interface, an armchair interface, and a rational interface. These interface modes are quasi-periodic along the direction of the interface but decay in the direction transverse the interface direction. We also derive the dispersion relation of the interface modes with respect to the quasi-momentum along the interface.

2.1 The honeycomb lattice of impenetrable obstacles

As illustrated in Figure 1.1, an infinite array of impenetrable obstacles are arranged periodically over the honeycomb lattice

$$\Lambda := \mathbb{Z}\mathbf{e}_1 \oplus \mathbb{Z}\mathbf{e}_2 := \{\ell_1\mathbf{e}_1 + \ell_2\mathbf{e}_2 : \ell_1, \ell_2 \in \mathbb{Z}\},$$

wherein the lattice vectors

$$\mathbf{e}_1 = a\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)^T, \quad \mathbf{e}_2 = a\left(\frac{\sqrt{3}}{2}, \frac{1}{2}\right)^T.$$

In what follows, without loss of generality, we assume that the lattice constant $a = 1$. Let

$$\mathcal{C}_z := \{\ell_1\mathbf{e}_1 + \ell_2\mathbf{e}_2 : \ell_1, \ell_2 \in [-1/2, 1/2)\} \quad (2.1)$$

be the fundamental cell of the lattice. Let $D_* \subset \subset \mathcal{C}_z$ be a connected smooth domain that is invariant under the $\frac{2\pi}{3}$ -rotation transform R and the horizontal reflection transform F given by

$$R\mathbf{x} := \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \mathbf{x}, \quad F(x_1, x_2) = (-x_1, x_2). \quad (2.2)$$

Denote the scaled inclusion $D(\eta) := \{\mathbf{x} = \eta\mathbf{x}', \mathbf{x}' \in \partial D_*\}$ for $\eta \in (0, 1)$.

Let

$$\Lambda^* = \{2\pi\ell_1\boldsymbol{\beta}_1 + 2\pi\ell_2\boldsymbol{\beta}_2 : \ell_1, \ell_2 \in \mathbb{Z}\},$$

be the reciprocal lattice, where the reciprocal lattice vectors

$$\boldsymbol{\beta}_1 = \left(\frac{1}{\sqrt{3}}, -1\right)^T, \quad \boldsymbol{\beta}_2 = \left(\frac{1}{\sqrt{3}}, 1\right)^T \quad (2.3)$$

satisfy $\mathbf{e}_i \cdot \boldsymbol{\beta}_j = \delta_{ij}$, $i, j = 1, 2$. The hexagon-shaped fundamental cell in Λ^* , or the Brillouin zone, is denoted by \mathcal{B}_z as shown in Figure 2.1 (right). The high symmetry points located at the vertices of the Brillouin zone are given by

$$K := 2\pi\left(\frac{1}{\sqrt{3}}, \frac{1}{3}\right) = 2\pi\left(\frac{1}{3}\boldsymbol{\beta}_1 + \frac{2}{3}\boldsymbol{\beta}_2\right), \quad K' := -K, \quad RK, \quad R^2K, \quad RK' \text{ and } R^2K'.$$

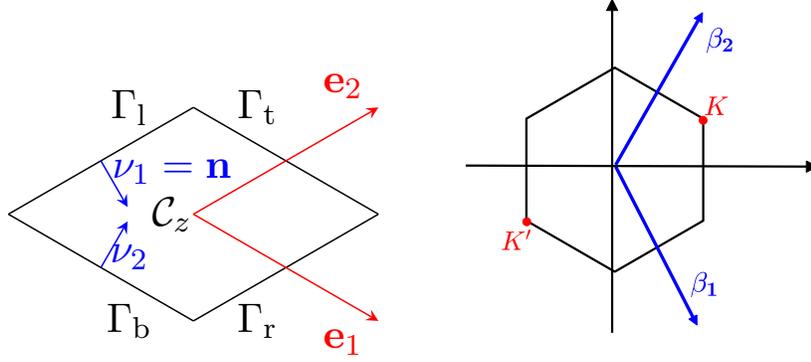


Figure 2.1: The fundamental cell \mathcal{C}_z (left) and the Brillouin zone (right).

2.2 Dirac points for the honeycomb lattice

Following the Floquet-Bloch theory [51], for each $\mathbf{p} \in \mathcal{B}_z$, we consider the following eigenvalue problem:

$$\begin{aligned} -\Delta u(\mathbf{x}; \mathbf{p}) - \lambda u(\mathbf{x}; \mathbf{p}) &= 0, & \mathbf{x} \in \mathcal{C}_z \setminus D(\eta) + \Lambda, \\ u(\mathbf{x}; \mathbf{p}) &= 0, & \mathbf{x} \in \partial D(\eta) + \Lambda, \\ u(\mathbf{x} + \mathbf{e}; \mathbf{p}) &= e^{i\mathbf{p} \cdot \mathbf{e}} u(\mathbf{x}; \mathbf{p}), & \text{for } \mathbf{e} \in \Lambda. \end{aligned} \quad (2.4)$$

For each \mathbf{p} , the eigenvalues can be ordered by $\lambda_1(\mathbf{p}) \leq \lambda_2(\mathbf{p}) \leq \dots \leq \lambda_n(\mathbf{p}) \leq \dots$. As \mathbf{p} varies in the Brillouin zone \mathcal{B}_z , one obtains the band structure of the honeycomb lattice.

We define the η^2 -vicinity of $|K|$:

$$U_\eta := \left\{ \lambda \in \mathbb{C} : \frac{(2\pi)^2}{3|\mathcal{C}_z|} \mathfrak{a} \eta^2 \leq |\lambda - |K|^2| \leq \frac{(2\pi)^2}{|\mathcal{C}_z|} \mathfrak{a} \eta^2 \right\}. \quad (2.5)$$

where $\mathfrak{a} \neq 0$ is a complex number defined by (3.22). The main results regarding the Dirac points at $\mathbf{p} = K$ and K' are stated below.

Theorem 2.1. *If Assumption 3.2 holds, then for η sufficiently small but nonzero, there exists a Dirac point at (K, λ_*) in the band structure of the honeycomb lattice $D(\eta) + \Lambda$ with $\lambda_* \in U_\eta$. The dispersion surface near (K, λ_*) takes the form*

$$(\lambda - \lambda_*)^2 = m_*^2 |\mathbf{p} - K|^2 + O(|\mathbf{p} - K|^3), \quad m_* \in \mathbb{R}, \quad m_* \geq 0, \quad (2.6)$$

where the slope of the Dirac cone is

$$m_* = \frac{2}{3}(1 + O(\eta)). \quad (2.7)$$

In addition, the basis of the eigenspace at the Dirac point (K, λ_*) can be chosen as w_1 and w_2 that satisfy

$$Rw_1(\mathbf{x}) := w_1(R^{-1}\mathbf{x}) = \tau w_1(\mathbf{x}), \quad Rw_2(\mathbf{x}) := w_2(R^{-1}\mathbf{x}) = \bar{\tau} w_2(\mathbf{x}), \quad w_2(\mathbf{x}) = Fw_1(\mathbf{x}) := w_1(F\mathbf{x}), \quad (2.8)$$

in which $\tau = e^{i\frac{2\pi}{3}}$.

Remark 2.2. Recall that R and F defined in (2.2) denote the $\frac{2\pi}{3}$ -rotation operation and the horizontal reflection operation acting on vectors in \mathbb{R}^2 . Here and henceforth, for convenience of notation, we also use R and F to denote the rotation and reflection operators acting on functions. The meaning of the notations should be clear in the context, depending on whether they are applied to vectors or functions.

Remark 2.3. In this work, we only prove the existence of Dirac points for the first two bands and when $\eta \ll 1$. It can be shown that Dirac points also exist for higher bands and for η not small. This is not the focus of this work and will be reported separately elsewhere.

Corollary 2.4. For $\eta \ll 1$, (K', λ_*) is also a Dirac point with the corresponding eigenspace spanned by

$$w'_1(\mathbf{x}) := \bar{w}_2(\mathbf{x}), \quad w'_2(\mathbf{x}) := \bar{w}_1(\mathbf{x}), \quad (2.9)$$

which attain the following symmetry relations:

$$Rw'_1(\mathbf{x}) := w'_1(R^{-1}\mathbf{x}) = \tau w'_1(\mathbf{x}), \quad Rw'_2(\mathbf{x}) := w'_2(R^{-1}\mathbf{x}) = \bar{\tau} w'_2(\mathbf{x}), \quad w'_2(\mathbf{x}) = w'_1(F\mathbf{x}). \quad (2.10)$$

2.3 Band-gap opening at Dirac points

The existence of Dirac points as established in the previous subsection is due to the $\frac{2\pi}{3}$ -rotation symmetry and the horizontal reflection symmetry of the lattice structure. Under suitable perturbations that break one of these symmetries, the Dirac points will disappear and a bandgap can be opened therein. We show that this is indeed the case when the obstacles in the honeycomb lattice are rotated to their centers with an angle of $\pm\varepsilon$ (cf. Figure 1.2) so that the horizontal reflection symmetry of the lattice structure is broken.

In subsequent analysis, we fix $D = D(\eta_0)$ by fixing a small enough $\eta_0 > 0$ such that Theorem 2.1 holds for $D(\eta_0)$. Denote by $D^{\pm\varepsilon}$ the domain obtained by rotating D by an angle of $\pm\varepsilon$ counterclockwise. We consider the following eigenvalue problem for each $\mathbf{p} \in \mathcal{B}_z$:

$$\begin{aligned} -\Delta u_{\pm\varepsilon}(\mathbf{x}; \mathbf{p}) - \lambda u_{\pm\varepsilon}(\mathbf{x}; \mathbf{p}) &= 0, & \mathbf{x} \in \mathcal{C}_z \setminus D^{\pm\varepsilon} + \Lambda, \\ u_{\pm\varepsilon}(\mathbf{x}; \mathbf{p}) &= 0, & \mathbf{x} \in \partial D^{\pm\varepsilon} + \Lambda, \\ u_{\pm\varepsilon}(\mathbf{x} + \mathbf{e}; \mathbf{p}) &= e^{i\mathbf{p} \cdot \mathbf{e}} u_{\pm\varepsilon}(\mathbf{x}; \mathbf{p}), & \text{for } \mathbf{e} \in \Lambda. \end{aligned} \quad (2.11)$$

Theorem 2.5. Let the constants t_* and γ_* be defined as in (4.8) and assume $t_* > 0$. Then the following dispersion relations hold for \mathbf{p} near K and λ near λ_* :

$$\begin{aligned} \lambda_{1, \pm\varepsilon}(\mathbf{p}) &= \lambda_* - \frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + m_*^2 |\gamma_*|^2 |\mathbf{p} - K|^2} (1 + O(\varepsilon, |\mathbf{p} - K|)), \\ \lambda_{2, \pm\varepsilon}(\mathbf{p}) &= \lambda_* + \frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + m_*^2 |\gamma_*|^2 |\mathbf{p} - K|^2} (1 + O(\varepsilon, |\mathbf{p} - K|)). \end{aligned} \quad (2.12)$$

In addition, the corresponding Bloch modes at $\mathbf{p} = K$ attain the following expansions:

$$\begin{aligned} u_{1, \varepsilon}(\mathbf{x}; K) &= w_1 + O(\varepsilon), & u_{2, \varepsilon}(\mathbf{x}; K) &= w_2 + O(\varepsilon) \\ u_{1, -\varepsilon}(\mathbf{x}; K) &= w_2 + O(\varepsilon), & u_{2, -\varepsilon}(\mathbf{x}; K) &= w_1 + O(\varepsilon), \end{aligned} \quad (2.13)$$

in which w_1 and w_2 are defined in Theorem 2.1.

Theorem (2.5) can be concluded from Proposition 4.3 with $\ell = 0$. From the symmetry of the lattice, similar expansions hold for \mathbf{p} near K' and λ near λ_* . In view of (2.12), when $\varepsilon \neq 0$, there holds $\lambda_{1,\pm\varepsilon}(\mathbf{p}) < \lambda_{2,\pm\varepsilon}(\mathbf{p})$ for \mathbf{p} near K , thus a spectral gap is opened. The expansion (2.13) demonstrates the swap of the eigenspace at $\mathbf{p} = K$ when the obstacles are rotated with the opposite rotation parameter $\pm\varepsilon$.

Remark 2.6. *The assumption that $t_* \neq 0$ can be verified numerically for the structure considered in this work.*

2.4 Interface modes for the joint photonic structure along a zigzag interface

We investigate interface modes for the joint photonic structure with the zigzag interface shown in Figure 2.2. The obstacles are rotated with an angle of $-\varepsilon$ and ε about the origin respectively for the semi-infinite honeycomb lattice on the left and right side of the interface.

Note that the direction of the interface is parallel to \mathbf{e}_2 . Employing the Floquet theory along \mathbf{e}_2 , we can restrict our studies to the infinite strip $\Omega^J := \cup_{m \in \mathbb{Z}} (\mathcal{C}_z + m\mathbf{e}_1)$, which is a fundamental period of the joint photonic structure along the interface direction. Inside the strip Ω^J , the region occupied by the inclusions is denoted by

$$D^{J,\varepsilon} := (\cup_{m \geq 0} (D^\varepsilon + m\mathbf{e}_1)) \cup (\cup_{m < 0} (D^{-\varepsilon} + m\mathbf{e}_1)),$$

and the region exterior to the inclusions is denoted by $\Omega^{J,\varepsilon} := \Omega^J \setminus \overline{D^{J,\varepsilon}}$. We also denote the lower boundary of the infinite strip Ω^J by $\Gamma_- := \{-\frac{1}{2}\mathbf{e}_2 + \ell\mathbf{e}_1, \ell \in \mathbb{R}\}$, then the upper boundary of the strip is $\Gamma_+ = \mathbf{e}_2 + \Gamma_-$. The normal direction on Γ_\pm is $\nu_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$.

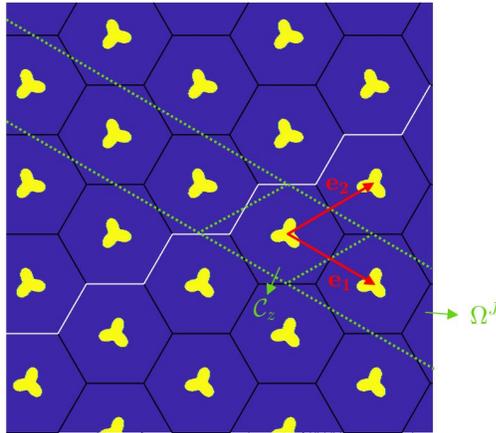


Figure 2.2: Joined photonic structure with a zigzag interface.

An interface mode $u \in L^2(\Omega^{J,\varepsilon})$ for the joint photonic structure solves the following spectral

problem:

$$\begin{aligned}
-\Delta u - \lambda u &= 0, & \text{in } \Omega^{J,\varepsilon}, \\
u &= 0, & \text{on } \partial D^{J,\varepsilon}, \\
u(\mathbf{x} + \mathbf{e}_2) &= e^{ik_{\parallel}} u(\mathbf{x}), & \mathbf{x} \in \Gamma_{-} \\
\partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) &= e^{ik_{\parallel}} \partial_{\nu_2} u(\mathbf{x}), & \mathbf{x} \in \Gamma_{-}.
\end{aligned} \tag{2.14}$$

In the above, $k_{\parallel} \in (0, 2\pi)$ is the quasi-momentum of the interface modes along the interface, and ∂_{ν_2} is normal derivative to Γ_{-} .

We first focus on interface modes with the quasi-momentum $k_{\parallel}^* = K \cdot \mathbf{e}_2 = \frac{4\pi}{3}$ by projecting the Bloch wave vector K onto the direction of the interface \mathbf{e}_2 . Namely, we investigate the interface modes bifurcated from the Dirac point (K, λ^*) . The interface modes with other quasi-momenta will be discussed in Section 2.6. To this end, we introduce the following function space

$$\begin{aligned}
\mathcal{H}^{J,\varepsilon} := \{ & u \in H^1(\Omega^{J,\varepsilon}) : \Delta u \in L^2(\Omega^{J,\varepsilon}), \quad u = 0 \text{ on } \partial D^{J,\varepsilon}, \\
& u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_{-}, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^*} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_{-} \}.
\end{aligned} \tag{2.15}$$

Then an interface mode $u \in L^2(\Omega^{J,\varepsilon})$ satisfies

$$-\Delta u - \lambda u = 0 \quad \text{in } \Omega^{J,\varepsilon} \text{ and } u \in \mathcal{H}^{J,\varepsilon}. \tag{2.16}$$

Assumption 2.7 (The no-fold condition along the direction β). *Let $\beta \in \mathbb{R}^2$ be a fixed Bloch wave vector and λ_* be the energy of the Dirac point at K and K' introduced in Theorem 2.1. For $\mathbf{p} \in \{K + \ell\beta, \ell \in \mathbb{R}\}$, the band energy of (2.4) takes the value λ_* only when $\mathbf{p} \in (K + \Lambda^*) \cup (K' + \Lambda^*)$.*

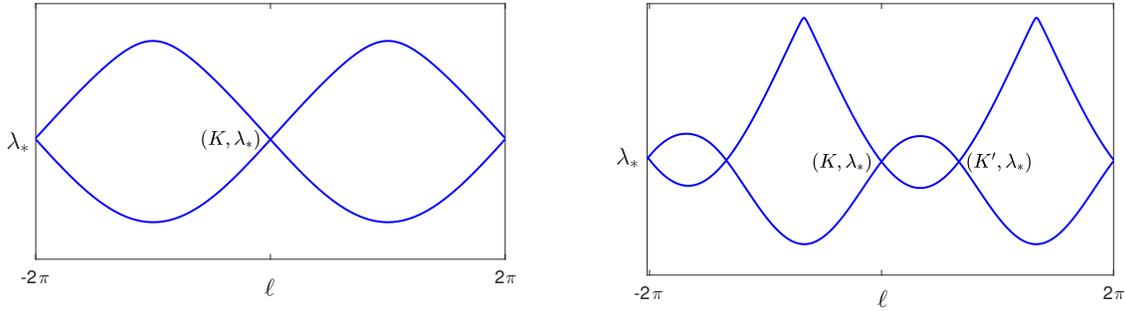


Figure 2.3: The band structure of the spectral problem (2.4) for $\mathbf{p} \in \{K + \ell\beta, \ell \in [-2\pi, 2\pi]\}$. Left: $\beta = \beta_1 := (\frac{1}{\sqrt{3}}, -1)^T$; Right: $\beta = \beta_1^a := (0, -2)^T$.

Remark 2.8. *The above no-fold condition holds for the configuration of the periodic structures considered in this work. Indeed, the first two bands of the spectral problem (2.4) touch at the Dirac point (K, λ_*) . Moreover, the energy λ_* is the maximum of the eigenvalues for the first band and the minimum of the eigenvalues for the second band. This can be rigorously proved when the inclusion size η is small by using the layer potential technique and asymptotic analysis. The general case, when η is not necessarily small, is beyond the scope of this work. Instead, we demonstrate numerically the no-fold conditions in Figure 2.3 that are used in Theorems 2.9 and 2.12, wherein $\beta = \beta_1$ and β_1^a respectively.*

Theorem 2.9. *Let Assumption 2.7 hold along the reciprocal lattice vector β_1 . Let t_* and γ_* be the two constants defined in (4.8) and assume that $t_* \neq 0$. Let \mathfrak{d} be an arbitrary constant in $(0, 1)$. For sufficiently small positive ε , there exists a unique interface mode $u \in L^2(\Omega^{J,\varepsilon})$ satisfying (2.16) with the corresponding eigenvalue $\lambda \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$. In addition, the interface mode u decays exponentially as $|\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty$.*

Define the quasi-momentum $k_{\parallel}^{*'} = K' \cdot \mathbf{e}_2 = -\frac{4\pi}{3}$. By the time-reversal symmetry of the differential operator, the following corollary is a direct consequence of Theorem 2.9.

Corollary 2.10. *Under the same assumptions as in Theorem 2.9, for sufficiently small positive ε , there exists a unique interface mode $u \in L^2(\Omega^{J,\varepsilon})$ satisfying (2.14) with $k_{\parallel}^{*'} = -\frac{4\pi}{3}$ and the eigenvalue $\lambda \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$. Furthermore, u decays exponentially as $|\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty$.*

Remark 2.11. *Numerical experiment demonstrates that the interface mode persists for ε not small. This will be analyzed rigorously in the future work.*

2.5 Interface modes along an armchair interface

We consider interface modes for the joint photonic structure with an armchair interface as shown in Figure 2.4. The inclusions above the interface are rotated to their centers with an angle of $-\varepsilon$, while the ones below are rotated with an angle of ε . Note that the direction of the interface is along the x_1 axis, we rewrite the honeycomb lattice equivalently as

$$\Lambda := \mathbb{Z}\mathbf{e}_1^a \oplus \mathbb{Z}\mathbf{e}_2^a := \{\ell_1\mathbf{e}_1^a + \ell_2\mathbf{e}_2^a : \ell_1, \ell_2 \in \mathbb{Z}\},$$

in which the lattice vectors are given by

$$\mathbf{e}_1^a = \mathbf{e}_1 = \left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right)^T, \quad \mathbf{e}_2^a := \mathbf{e}_1 + \mathbf{e}_2 = (\sqrt{3}, 0)^T. \quad (2.17)$$

Correspondingly, the fundamental periodic cell is

$$\mathcal{C}_a := \{\ell_1\mathbf{e}_1^a + \ell_2\mathbf{e}_2^a : \ell_1, \ell_2 \in [-1/2, 1/2)\}, \quad (2.18)$$

and the reciprocal lattice vectors are

$$\beta_1^a = (0, -2)^T, \quad \beta_2^a = \left(\frac{1}{\sqrt{3}}, 1\right)^T.$$

We assume that the inclusions D and $D^{\pm\varepsilon}$ are strictly included in the cell \mathcal{C}_a . Similar to the zigzag interface, we introduce the infinite-strip domain $\Omega_a^J := \cup_{m \in \mathbb{Z}} (\mathcal{C}_a + m\mathbf{e}_1^a)$ as the fundamental period for the joint photonic structure, which consists of the inclusions $D_a^{J,\varepsilon} := (\cup_{m \geq 0} (D^\varepsilon + m\mathbf{e}_1^a)) \cup (\cup_{m < 0} (D^{-\varepsilon} + m\mathbf{e}_1^a))$ and their complement $\Omega_a^{J,\varepsilon} := \Omega_a^J \setminus D_a^{J,\varepsilon}$.

We now investigate the interface modes bifurcated from the Dirac point (K, λ^*) that propagate along the interface direction \mathbf{e}_2^a with the quasi-momentum $k_{\parallel}^{*,a} = K \cdot \mathbf{e}_2^a = 2\pi$. Correspondingly, we define the function space

$$\begin{aligned} \mathcal{H}_a^{J,\varepsilon} := \{ & u \in H^1(\Omega_a^{J,\varepsilon}) : \Delta u \in L^2(\Omega_a^{J,\varepsilon}), \quad u = 0 \text{ on } \partial D_a^{J,\varepsilon}, \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^{*,a}} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-^a, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_{\parallel}^{*,a}} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-^a \}. \end{aligned} \quad (2.19)$$

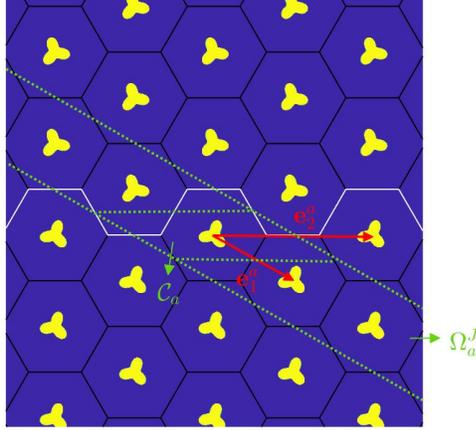


Figure 2.4: Join photonic structure with an armchair interface.

Here $\Gamma_a^- := \{-\frac{1}{2}\mathbf{e}_2^a + \ell\mathbf{e}_1^a, \ell \in \mathbb{R}\}$ is the lower boundary of the strip Ω_a^J . Then an interface mode with the quasimomentum $k_{\parallel}^{*,a} = 2\pi$ and energy λ solves

$$-\Delta u - \lambda u = 0 \quad \text{in } \Omega_a^{J,\varepsilon} \text{ for } u \in \mathcal{H}_a^{J,\varepsilon}. \quad (2.20)$$

Note that the quasi-momenta \mathbf{p} satisfying $\mathbf{p} \cdot \mathbf{e}_2^a = K \cdot \mathbf{e}_2^a$ lies on the line $\mathbf{p}(\ell) = K + \ell\beta_1^a$ for $\ell \in \mathbb{R}$. We have the following results similar to Theorem 2.9 for the spectral problem (2.20).

Theorem 2.12. *Let Assumption 2.7 hold along the reciprocal lattice vector β_1^a . Let t_* and γ_* be the two constants defined in (4.8) and assume that $t_* \neq 0$. Let \mathfrak{d} be an arbitrary constant in $(0, 1)$. For sufficiently small positive ε , there exist exactly two interface modes with $k_{\parallel}^{*,a} = 2\pi$, with the corresponding eigenvalues $\lambda_{\pm} \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}|\varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}|\varepsilon)$. In addition, both interface modes decay exponentially as $|\mathbf{x} \cdot \mathbf{e}_1^a| \rightarrow \infty$.*

2.6 Dispersion relations of the interface modes

We consider interface modes with quasi-momentum k_{\parallel} near k_{\parallel}^* or $k_{\parallel}^{*,a}$. In particular, we derive the leading order of the dispersion relation $\lambda(k_{\parallel})$ for the interface modes along a zigzag or armchair interface for k_{\parallel} near k_{\parallel}^* or $k_{\parallel}^{*,a}$. The dispersion curve $\lambda(k_{\parallel})$ over the whole Bloch interval $[0, 2\pi]$ for both configurations are shown in Figure 2.5.

Theorem 2.13. *Let the assumptions in Theorem 2.9 hold and \mathfrak{d} be an arbitrary constant in $(0, 1)$. If $\varepsilon > 0$ is sufficiently small and $|k_{\parallel} - k_{\parallel}^*| < \mathfrak{d}\varepsilon|\frac{\gamma_*}{t_*m_*}|$, the eigenvalue of the interface mode of the spectral problem (2.14) is given by $\lambda - \lambda_* = \text{sgn}(t_*) \cdot m_*(k_{\parallel} - k_{\parallel}^*) \cdot (1 + o(1))$.*

Theorem 2.14. *Let the assumptions in Theorem 2.12 hold and \mathfrak{d} be an arbitrary constant in $(0, 1)$. If $\varepsilon > 0$ is sufficiently small and $|k_{\parallel} - k_{\parallel}^{*,a}| < \sqrt{3}\mathfrak{d}\varepsilon|\frac{\gamma_*}{t_*m_*}|$, the eigenvalues of the two interface modes along the armchair interface are $\lambda_{\pm} - \lambda_* = \pm\frac{1}{\sqrt{3}}m_*(k_{\parallel} - k_{\parallel}^{*,a}) \cdot (1 + o(1))$.*

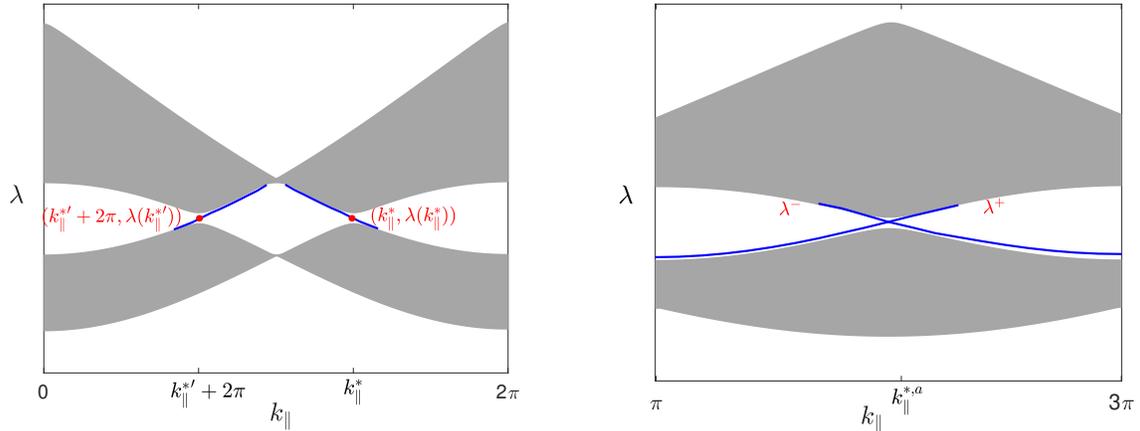


Figure 2.5: The dispersion relations for the interface modes along the zigzag (left) and armchair interface (right).

2.7 Interface modes along rational interfaces

We extend the previous studies to interface modes along a rational interface separating two honeycomb photonic structures. A rational interface is a line with a direction

$$a\mathbf{e}_1 + b\mathbf{e}_2, \quad (2.21)$$

where a and b are relatively prime integers. When a and b are relatively prime, there exist $c, d \in \mathbb{Z}$, such that $bc - ad = 1$ and

$$\begin{pmatrix} c & a \\ d & b \end{pmatrix}^{-1} = \begin{pmatrix} b & -a \\ -d & c \end{pmatrix}.$$

Therefore, the vectors

$$\mathbf{e}_1^r = c\mathbf{e}_1 + d\mathbf{e}_2, \quad \mathbf{e}_2^r = a\mathbf{e}_1 + b\mathbf{e}_2 \quad (2.22)$$

generate the honeycomb lattice. Correspondingly, the reciprocal vectors

$$(\boldsymbol{\beta}_1^r \quad \boldsymbol{\beta}_2^r) = (\boldsymbol{\beta}_1 \quad \boldsymbol{\beta}_2) \left(\begin{pmatrix} c & a \\ d & b \end{pmatrix}^{-1} \right)^T = (\boldsymbol{\beta}_1 \quad \boldsymbol{\beta}_2) \begin{pmatrix} b & -d \\ -a & c \end{pmatrix} \quad (2.23)$$

generate the dual lattice.

We call an interface direction $\mathbf{e}_2^r := a\mathbf{e}_1 + b\mathbf{e}_2$ of the zigzag type if the dual slice $\{\mathbf{p}(\ell) = K + \ell\boldsymbol{\beta}_1^r, \ell \in \mathbb{R}\}$ intersects with $K + \Lambda^*$ but not with $K' + \Lambda^*$, and is of armchair if the slice intersects with both $K + \Lambda^*$ and $K' + \Lambda^*$. A straightforward calculation shows that $K + \ell\boldsymbol{\beta}_1^r \in K' + \Lambda^*$ if and only if $a - b = 3k$ for some $k \in \mathbb{Z}$.

Definition 2.15. *The direction $\mathbf{e}_2^r := a\mathbf{e}_1 + b\mathbf{e}_2$ is called a rational if a and b are relatively prime integers. The rational interface is of zigzag type if $a - b \neq 3k$ for all $k \in \mathbb{Z}$, and is of armchair type if $a - b = 3k$ for some $k \in \mathbb{Z}$.*

Let the inclusion D and all of its rotations be compactly supported in the cell $\mathcal{C}_r := \{\ell_1 \mathbf{e}_1^r + \ell_2 \mathbf{e}_2^r : \ell_1, \ell_2 \in [-1/2, 1/2]\}$. We prove that the analog of Theorem 2.9 - Theorem 2.14 holds in the case of rational interfaces for the zigzag and armchair types. More specifically,

Denote

$$\mathfrak{f}^r = B - \frac{A}{|A|^2} \operatorname{Re}(A\bar{B}), \quad (2.24)$$

wherein

$$A = b - a\bar{\tau}, \quad B = -d + c\bar{\tau}. \quad (2.25)$$

Then if the rational interface \mathbf{e}_2^r is of zigzag type, we have the following theorem.

Theorem 2.16. *Let \mathbf{e}_2^r be a rational edge of zigzag type and let Assumption 2.7 hold along the reciprocal lattice vector β_1^r . Let t_* and γ_* be the two constants defined in (4.8) and assume that $t_* \neq 0$. Let \mathfrak{d} be an arbitrary constant in $(0, 1)$. If $\varepsilon > 0$ is sufficiently small, then*

- (i) *There exists a unique interface mode along the interface, with the quasi-momentum $k_{\parallel}^* = K \cdot \mathbf{e}_2^r$ and the eigenvalue $\lambda \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$.*
- (ii) *For $|k_{\parallel} - k_{\parallel}^*| < \mathfrak{d}\varepsilon|\frac{\gamma_*}{t_*}|/(|\mathfrak{f}^r|\frac{\sqrt{3}}{2}m_*)$, the dispersion relation for the interface mode adopts the expansion $\lambda - \lambda_* = \operatorname{sgn}(t_*) \cdot |\mathfrak{f}^r| \cdot \frac{\sqrt{3}}{2}m_* \cdot (k_{\parallel} - k_{\parallel}^*) \cdot (1 + o(1))$.*

If the rational interface \mathbf{e}_2^r is of armchair type, we have the following theorem.

Theorem 2.17. *Let \mathbf{e}_2^r be a rational edge of armchair type and let Assumption 2.7 hold along the reciprocal lattice vector β_1^r . Let t_* and γ_* be the two constants defined in (4.8) and assume that $t_* \neq 0$. Let \mathfrak{d} be an arbitrary constant in $(0, 1)$. If $\varepsilon > 0$ is sufficiently small, then*

- (i) *There exist exactly two interface modes along the interface, with the quasi-momentum $k_{\parallel}^{*,r} = K \cdot \mathbf{e}_2^r$ and the eigenvalues $\lambda_{\pm} \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$.*
- (ii) *For $|k_{\parallel} - k_{\parallel}^{*,r}| < \mathfrak{d}\varepsilon|\frac{\gamma_*}{t_*}|/(|\mathfrak{f}^r|\frac{\sqrt{3}}{2}m_*)$, the dispersion relations for the interface modes adopt the expansions $\lambda - \lambda_* = \pm|\mathfrak{f}^r| \cdot \frac{\sqrt{3}}{2}m_* \cdot (k_{\parallel} - k_{\parallel}^{*,r}) \cdot (1 + o(1))$.*

2.8 Extension of results to other settings

We note that the method and framework developed in this paper can be extended to other settings:

- (1) There are multiple inclusions in one periodic cell;
- (2) The inclusions are penetrable such that the medium coefficient is piecewise constant;
- (3) The topological phase transition is induced by perturbations that break either the inversion symmetry or the time-reversal symmetry.

3 Dirac points for the honeycomb lattice

In this section, we prove Theorem 2.1 regarding the Dirac points by the layer potential technique.

3.1 Integral equation formulation

In this subsection, we formulate the spectral problem for the honeycomb structure by using boundary integral equations. For each $\mathbf{p} \in \mathcal{B}_z$, let $G^f(\mathbf{x}, \mathbf{y}; \mathbf{p}, \lambda)$ be the quasi-periodic Green function over the honeycomb lattice that solves

$$(-\Delta - \lambda)G^f(\mathbf{x}, \mathbf{y}; \mathbf{p}, \lambda) = \sum_{\mathbf{e} \in \Lambda} e^{i\mathbf{p} \cdot \mathbf{e}} \delta(\mathbf{x} - \mathbf{y} - \mathbf{e}) \quad \text{for } \mathbf{x}, \mathbf{y} \in \mathbb{R}^2. \quad (3.1)$$

Define the single-layer potential

$$u(\mathbf{x}; \mathbf{p}) := \int_{\partial D(\eta)} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p}) \tilde{\phi}(\mathbf{y}) ds_{\mathbf{y}},$$

wherein the density function $\tilde{\phi} \in H^{-1/2}(\partial D(\eta))$. Then it can be shown that u solves the eigenvalue problem (2.4) if and only if $\tilde{\phi} \in H^{-1/2}(\partial D(\eta))$ solves the following boundary integral equation:

$$\int_{\partial D(\eta)} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p}) \tilde{\phi}(\mathbf{y}) ds_{\mathbf{y}} = 0, \quad \mathbf{x} \in \partial D(\eta). \quad (3.2)$$

Define $\phi(\mathbf{x}) := \tilde{\phi}(\eta\mathbf{x})$. Then a point (\mathbf{p}, λ) belongs to the dispersion surface of the honeycomb lattice if and only if the triple $(\lambda, \mathbf{p}, \phi) \in \mathbb{R} \times \mathcal{B}_z \times H^{-1/2}(\partial D_*)$ solves the integral equation

$$\mathcal{S}(\eta, \lambda, \mathbf{p})[\phi] = 0, \quad (3.3)$$

where the single-layer integral operator

$$\mathcal{S}(\eta, \lambda, \mathbf{p})[\phi](\mathbf{x}) := \int_{\partial D_*} G^f(\eta\mathbf{x}, \eta\mathbf{y}; \lambda, \mathbf{p}) \phi(\mathbf{y}) ds_{\mathbf{y}} \quad \mathbf{x} \in \partial D_*. \quad (3.4)$$

In the rest of this section, we investigate the characteristic values of the integral operator $\mathcal{S}(\eta, \lambda, \mathbf{p})$ when $\mathbf{p} = K$.

3.2 Symmetry of the integral operator

In this subsection, we establish symmetry properties of the integral operator $\mathcal{S}(\eta, \lambda, \mathbf{p})$. Note that the Green function satisfying (3.1) can be represented by the lattice sum (cf. [2])

$$G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p}) = \frac{i}{4} \sum_{\mathbf{e} \in \Lambda} e^{i\mathbf{p} \cdot \mathbf{e}} H_0^{(1)}(\omega|\mathbf{x} - \mathbf{y} - \mathbf{e}|), \quad (3.5)$$

where $H_0^{(1)}$ is the zero-order Hankel function of the first kind. More precisely,

$$\frac{i}{4} H_0^{(1)}(\omega; \mathbf{x}) = -\frac{1}{2\pi} \left(\ln|\mathbf{x}| + \ln\omega + \gamma_0 + \ln(\omega|\mathbf{x}|) \sum_{p \geq 1} b_{p,1}(\omega|\mathbf{x}|)^{2p} + \sum_{p \geq 1} b_{p,2}(\omega|\mathbf{x}|)^{2p} \right), \quad (3.6)$$

where

$$b_{p,1} = \frac{(-1)^p}{2^{2p}(p!)^2}, \quad b_{p,2} = \left(\gamma_0 - \sum_{s=1}^p \frac{1}{s} \right) b_{p,1}, \quad \gamma_0 = E_0 - \ln 2 - \frac{i\pi}{2},$$

and $E_0 = \lim_{N \rightarrow \infty} \left(\sum_{p=1}^N \frac{1}{p} - \ln N \right)$ is the Euler constant. The Green function also attains the following spectral decomposition (cf. [2]):

$$G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p}) = -\frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{q} \in \Lambda^*} \frac{e^{i(\mathbf{p}+\mathbf{q}) \cdot (\mathbf{x}-\mathbf{y})}}{\lambda - |\mathbf{p} + \mathbf{q}|^2}, \quad (3.7)$$

wherein $|\mathcal{C}_z| = \frac{\sqrt{3}}{2}$ represents the area of the fundamental cell \mathcal{C}_z .

Recall that $H^s(\partial D_*)$ is the Sobolev space of order s defined on ∂D_* . Note that the transformation $R\phi(\mathbf{x}) := \phi(R^{-1}\mathbf{x})$ is unitary and it attains three eigenvalues 1, τ and τ^2 , where $\tau = e^{i\frac{2\pi}{3}}$. Define

$$H_i^s(\partial D_*) := \{ \phi \in H^s(\partial D_*) : R\phi(\mathbf{x}) := \phi(R^{-1}\mathbf{x}) = \tau^i \phi(\mathbf{x}) \}, \quad i = 0, 1, 2. \quad (3.8)$$

These subspaces are pairwise orthogonal under the $L^2(\partial D_*)$ inner product and there holds

$$H^s(\partial D_*) = H_0^s(\partial D_*) \oplus H_1^s(\partial D_*) \oplus H_2^s(\partial D_*).$$

In addition, using the relation $RF = FR^2$, we have $FH_1^s(\partial D) = H_2^s(\partial D)$.

Define

$$\tilde{\Lambda}^* := K + \Lambda^*. \quad (3.9)$$

A straightforward calculation shows that

$$R\tilde{\Lambda}^* = \tilde{\Lambda}^*, \quad F\tilde{\Lambda}^* = \tilde{\Lambda}^*. \quad (3.10)$$

Here we have used

$$R\beta_1 = -\beta_1 - \beta_2, \quad R\beta_2 = \beta_1, \quad F\beta_1 = -\beta_2, \quad F\beta_2 = -\beta_1, \quad (3.11)$$

and

$$K = 2\pi\left(\frac{2}{3}\beta_1 + \frac{1}{3}\beta_2\right), \quad RK = K - \beta_2, \quad FK = K - \beta_1 - \beta_2. \quad (3.12)$$

Lemma 3.1. *Let $\mathbf{p} = K$, then the following holds for the integral operator $\mathcal{S}(\eta, \lambda, K)$:*

(i) *The operator $\mathcal{S}(\eta, \lambda, K)$ commutes with R and F . That is,*

$$R\mathcal{S}(\eta, \lambda, K) = \mathcal{S}(\eta, \lambda, K)R \quad \text{and} \quad F\mathcal{S}(\eta, \lambda, K) = \mathcal{S}(\eta, \lambda, K)F.$$

(ii) *The operator $\mathcal{S}(\eta, \lambda, K)$ is bounded from $H_i^{-1/2}(\partial D_*)$ to $H_i^{1/2}(\partial D_*)$ ($i = 0, 1, 2$) for all η and λ .*

(iii) *The triple $(\mathbf{p}, \lambda, \phi) \in H_1^{-1/2}(\partial D_*)$ solves (3.3) if and only if the triple point $(\mathbf{p}, \lambda, \phi(F(\cdot))) \in H_2^{-1/2}(\partial D_*)$ solves (3.3).*

Proof. For Statement (i), in light of (3.7) and (3.10), we have

$$\mathcal{S}(\eta, \lambda, K)[R\phi](\mathbf{x}) = -\frac{1}{|\mathcal{C}_z|} \int_{\partial D_*} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (\mathbf{x}-\mathbf{y})} \phi(R^{-1}\mathbf{y}) ds_{\mathbf{y}},$$

and

$$\begin{aligned} R\mathcal{S}(\eta, \lambda, K)[\phi](\mathbf{x}) &= -\frac{1}{|\mathcal{C}_z|} \int_{\partial D_*} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (R^{-1}\mathbf{x} - \mathbf{y})} \phi(\mathbf{y}) ds_{\mathbf{y}} \\ &= -\frac{1}{|\mathcal{C}_z|} \int_{\partial D_*} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{\lambda - |\mathbf{m}|^2} e^{iR\mathbf{m} \cdot (\mathbf{x} - \mathbf{y}')} \phi(R^{-1}\mathbf{y}') ds_{\mathbf{y}'} = \mathcal{S}(\eta, \lambda, K)[R\phi](\mathbf{x}). \end{aligned}$$

In the above, we have used $R(\partial D_*) = \partial D_*$, $|R\mathbf{m}| = |\mathbf{m}|$ and $R\tilde{\Lambda}^* = \tilde{\Lambda}^*$. The relation

$$\mathcal{S}(\eta, \lambda, K)[F\phi](\mathbf{x}) = F\mathcal{S}(\eta, \lambda, K)[\phi](\mathbf{x})$$

can be shown similarly using the relation $F\tilde{\Lambda}^* = \tilde{\Lambda}^*$.

Statement (ii) follows from the standard layer potential theory; see for instance [2].

Statement (iii) is a consequence of the relation $RF = FR^2$, which implies $\phi(\mathbf{x}) \in H_1^{-1/2}(\partial D_*)$ if and only if $\phi(F\mathbf{x}) \in H_2^{-1/2}(\partial D_*)$. \square

3.3 Dirac points in the lowest two bands

In this subsection, we establish the existence of Dirac points in the lowest two bands. In view of (3.5) and (3.7), when $\mathbf{p} = K$, the Green function $G^f(\mathbf{x}, \mathbf{y}; \lambda, K)$ attains singularities around $|\mathbf{x} - \mathbf{y}| = 0$ and $\lambda = |\mathbf{m}|^2$ for each $\mathbf{m} \in \tilde{\Lambda}^*$. The singularity for the former arises naturally when the source point \mathbf{y} and the target point \mathbf{x} overlap, while the latter occurs at special frequencies $\lambda = |\mathbf{m}|^2$ when the spectral decomposition (3.7) is not well-defined.

As to be shown below, the Dirac point at K with the lowest energy λ appears when $\lambda \approx |\mathbf{m}_1|^2$, where $\mathbf{m}_1 \in \tilde{\Lambda}^*$ attains the smallest norm among all lattice points in $\tilde{\Lambda}^*$. A straightforward calculation shows that

$$|\mathbf{m}_1| = |K|, \quad \{\mathbf{m} \in \tilde{\Lambda}^*, |\mathbf{m}| = |\mathbf{m}_1|\} = K + \{\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3\},$$

in which

$$\mathbf{q}_1 = (0, 0)^T, \quad \mathbf{q}_2 = 2\pi\left(-\frac{2}{\sqrt{3}}, 0\right)^T, \quad \mathbf{q}_3 = 2\pi\left(-\frac{1}{\sqrt{3}}, -1\right)^T.$$

We now perform asymptotic expansion of the operator $\mathcal{S}(\eta, \lambda, K)$ for $\lambda \approx |\mathbf{m}_1|^2 = |K|^2$. To this end, we derive the expansion for Green's function $G^f(\eta\mathbf{x}, \eta\mathbf{y}; \lambda, K)$ when η is small. For simplicity we consider $G^f(\eta\mathbf{x}, 0; \lambda, K)$ instead, since $G^f(\eta\mathbf{x}, \eta\mathbf{y}; \lambda, K) = G^f(\eta(\mathbf{x} - \mathbf{y}), 0; \lambda, K)$. From the above discussions, the Green function $G^f(\eta\mathbf{x}, 0; \lambda, K)$ attains singularities when $\mathbf{x} = 0$ or $\lambda = |\mathbf{m}|^2$ for some $\mathbf{m} \in \tilde{\Lambda}^*$, and those terms contributing to the singularities are the leading-order terms in the expansion of $G^f(\eta\mathbf{x}, 0; \lambda, K)$.

From the lattice sum (3.5), the singularity at $\mathbf{x} = 0$ arises from the term $\frac{i}{4}H_0^{(1)}(\eta\mathbf{x}; \lambda)$ with $\mathbf{e} = (0, 0)^T$. Using the expansion

$$\frac{i}{4}H_0^{(1)}(\eta\mathbf{x}; \lambda) = -\frac{1}{2\pi} \left(\ln|\mathbf{x}| + \ln\eta + \ln\sqrt{\lambda} + \gamma_0 + \left(\ln(\sqrt{\lambda}|\mathbf{x}|) + \ln\eta \right) \sum_{p \geq 1} b_{p,1}(\sqrt{\lambda}\eta|\mathbf{x}|)^{2p} + \sum_{p \geq 1} b_{p,2}(\sqrt{\lambda}\eta|\mathbf{x}|)^{2p} \right),$$

we define the leading-order term by $L_1(\eta\mathbf{x}; \lambda)$ and the remainder by $R_1(\eta\mathbf{x}; \lambda)$ as follows:

$$\begin{aligned} L_1(\eta\mathbf{x}; \lambda) &:= -\frac{1}{2\pi} \left(\ln|\mathbf{x}| + \ln\eta + \ln\sqrt{\lambda} + \gamma_0 \right), \\ R_1(\eta\mathbf{x}; \lambda) &:= -\frac{1}{2\pi} \left(\left(\ln(\sqrt{\lambda}|\mathbf{x}|) + \ln\eta \right) \sum_{p \geq 1} b_{p,1}(\sqrt{\lambda}\eta|\mathbf{x}|)^{2p} + \sum_{p \geq 1} b_{p,2}(\sqrt{\lambda}\eta|\mathbf{x}|)^{2p} \right). \end{aligned} \tag{3.13}$$

From the spectral decomposition (3.7), the singularity at $\lambda \approx |\mathbf{m}_1|^2$ arises from the terms

$$\begin{aligned} -\frac{1}{|\mathcal{C}_z|} \sum_{K+\mathbf{q} \in [\mathbf{m}_1]} \frac{e^{i(\mathbf{p}+\mathbf{q}) \cdot \mathbf{x}}}{\lambda - |\mathbf{p} + \mathbf{q}|^2} &= -\frac{1}{|\mathcal{C}_z|} \sum_{K+\mathbf{q} \in [\mathbf{m}_1]} \frac{e^{i(\mathbf{p}+\mathbf{q}) \cdot \mathbf{x}}}{\lambda - |\mathbf{p} + \mathbf{q}|^2} \\ &= -\frac{1}{|\mathcal{C}_z|} \frac{1}{\lambda - |\mathbf{m}_1|^2} \left(3 - \frac{1}{3}(2\pi)^2(\eta|\mathbf{x}|)^2 + \sum_{j \geq 3, k=1,2,3} \frac{(i(K + \mathbf{q}_k) \cdot \eta \mathbf{x})^j}{j!} \right). \end{aligned}$$

We consider λ in the η^2 -neighborhood of $|\mathbf{m}_1|^2$, namely, $\lambda \in U_\eta$ where U_η is defined in (2.5). Correspondingly, we define the leading-order term by $L_2(\eta \mathbf{x}; \lambda)$ and the remainder by $R_2(\eta \mathbf{x}; \lambda)$ as follows:

$$\begin{aligned} L_2(\eta \mathbf{x}; \lambda, K) &:= -\frac{1}{|\mathcal{C}_z|} \frac{1}{\lambda - |\mathbf{m}_1|^2} \left(3 - \frac{1}{3}(2\pi)^2(\eta|\mathbf{x}|)^2 \right), \\ R_2(\eta \mathbf{x}; \lambda, K) &:= -\frac{1}{|\mathcal{C}_z|} \frac{1}{\lambda - |\mathbf{m}_1|^2} \left(\sum_{j \geq 3, k=1,2,3} \frac{(i(K + \mathbf{q}_k) \cdot \eta \mathbf{x})^j}{j!} \right). \end{aligned} \quad (3.14)$$

Finally, the smooth term in the Green's function is denoted by

$$R_0(\eta \mathbf{x}; \lambda) := G^f(\eta \mathbf{x}, 0; \lambda, K) - \frac{i}{4} H_0^{(1)}(\eta \mathbf{x}; \lambda) + \frac{1}{|\mathcal{C}_z|} \sum_{K+\mathbf{q} \in [\mathbf{m}_1]} \frac{e^{i(K+\mathbf{q}) \cdot \mathbf{x}}}{\lambda - |K + \mathbf{q}|^2}. \quad (3.15)$$

Using the above expansions for the Green's function, we obtain the decomposition for the integral operator $\mathcal{S}(\eta, \lambda, K)$:

$$\mathcal{S}(\eta, \lambda, K) = \mathcal{L}(\eta, \lambda, K) + \mathcal{R}(\eta, \lambda, K), \quad (3.16)$$

where the leading-order integral operator is

$$\mathcal{L}(\eta, \lambda, K)\phi(\mathbf{x}) := \int (L_1(\eta(\mathbf{x} - \mathbf{y}); \lambda) + L_2(\eta(\mathbf{x} - \mathbf{y}); \lambda, K))\phi(\mathbf{y}) ds_{\mathbf{y}}, \quad (3.17)$$

and the remainder operator is

$$\mathcal{R}(\eta, \lambda, K)\phi(\mathbf{x}) := \int (R_1(\eta(\mathbf{x} - \mathbf{y}); \lambda) + R_2(\eta(\mathbf{x} - \mathbf{y}); \lambda, K) + R_0(\eta(\mathbf{x} - \mathbf{y}); \lambda, K))\phi(\mathbf{y}) ds_{\mathbf{y}}. \quad (3.18)$$

Let $\mathcal{S}_0 : H^{-1/2}(\partial D_*) \rightarrow H^{1/2}(\partial D_*)$ be the single layer potential associated with the Laplace operator in free space defined by

$$\mathcal{S}_0[\phi](\mathbf{x}) := \int_{\partial D_*} -\frac{1}{2\pi} \ln(|\mathbf{x} - \mathbf{y}|)\phi(\mathbf{y}) ds_{\mathbf{y}}. \quad (3.19)$$

Assumption 3.2. *The operator $\mathcal{S}_0 : H^{-1/2}(\partial D_*) \rightarrow H^{1/2}(\partial D_*)$ is invertible.*

Remark 3.3. *According to [62, 71], the above assumption holds generically for a given geometry of the inclusion D_* . Therefore, we assume that Assumption 3.2 holds throughout the paper.*

Remark 3.4. *The operator \mathcal{S}_0 defined in (3.19), and the operators $\mathcal{L}(\eta, \lambda_0, K)$ and $\mathcal{R}(\eta, \lambda_0, K)$ commute with R and F .*

Lemma 3.5. When $\phi \in H_1^{-1/2}(\partial D_*)$,

$$\int_{\partial D_*} \phi(\mathbf{y}) ds_{\mathbf{y}} = 0, \quad (3.20a)$$

$$\int_{\partial D_*} |\mathbf{y}|^2 \phi(\mathbf{y}) ds_{\mathbf{y}} = 0, \quad (3.20b)$$

$$\int_{\partial D_*} \mathbf{y} \phi(\mathbf{y}) ds_{\mathbf{y}} \in \text{span}\{(1, i)\}, \quad (3.20c)$$

and

$$\int_{\partial D_*} L_2(\eta(\mathbf{x} - \mathbf{y}); \lambda, K) \phi(\mathbf{y}) ds_{\mathbf{y}} \in \text{span}\{x_1 + ix_2\}. \quad (3.21)$$

Proof. Using $R\phi(\mathbf{y}) = \phi(R^{-1}\mathbf{y}) = \tau\phi(\mathbf{y})$, we have

$$\begin{aligned} \int_{\partial D_*} \phi(\mathbf{y}) ds_{\mathbf{y}} &= \int_{\partial D_*} \phi(R^{-1}\mathbf{y}') ds_{\mathbf{y}'} = \int_{\partial D_*} \tau\phi(\mathbf{y}') ds_{\mathbf{y}'}, \\ \int_{\partial D_*} |\mathbf{y}|^2 \phi(\mathbf{y}) ds_{\mathbf{y}} &= \int_{\partial D_*} |R^{-1}\mathbf{y}'|^2 \phi(R^{-1}\mathbf{y}') ds_{\mathbf{y}'} = \int_{\partial D_*} |\mathbf{y}'|^2 \tau\phi(\mathbf{y}') ds_{\mathbf{y}'}. \end{aligned}$$

Since $\tau \neq 1$, we obtain (3.20a) and (3.20b). Similarly,

$$\int_{\partial D_*} \mathbf{y} \phi(\mathbf{y}) ds_{\mathbf{y}} = \int_{\partial D_*} R^{-1}\mathbf{y}' \phi(R^{-1}\mathbf{y}') ds_{\mathbf{y}'} = \int_{\partial D_*} R^{-1}\mathbf{y}' \tau\phi(\mathbf{y}') ds_{\mathbf{y}'}$$

Denoting $(a, b) := \int_{\partial D_*} \mathbf{y} \phi(\mathbf{y}) ds_{\mathbf{y}}$, the above relation reads $(a, b) = \tau R^{-1}(a, b)$, which implies (3.20c). Finally, (3.21) follows from (3.20a) - (3.20c). \square

Lemma 3.6. There exists a unique function $\phi_* \in H^{-1/2}(\partial D_*)$ such that $\mathcal{S}_0[\phi_*](\mathbf{x}) = x_1 + ix_2$. Moreover, $\int_{\partial D_*} \mathbf{y} \phi_*(\mathbf{y}) ds_{\mathbf{y}} = \mathbf{a}(1, i)$ for some $\mathbf{a} \in \mathbb{C} \setminus \{0\}$.

Proof. Noting that $x_1 + ix_2 \in H_1^{-1/2}(\partial D_*)$, we deduce that $\phi_* \in H_1^{-1/2}(\partial D_*)$ exists and is unique. Combining with Lemma 3.5, we have

$$\mathbf{a} := \frac{\int_{\partial D_*} \mathbf{x} \cdot \mathbf{y} \phi_*(\mathbf{y}) ds_{\mathbf{y}}}{x_1 + ix_2} \in \mathbb{C}. \quad (3.22)$$

To show $\mathbf{a} \neq 0$, we notice that

$$2\mathbf{a} = (1, -i) \cdot \int_{\partial D_*} \mathbf{y} \phi_*(\mathbf{y}) ds_{\mathbf{y}} = \langle f, \mathcal{S}_0^{-1}f \rangle_{H^{1/2}(\partial D_*), H^{-1/2}(\partial D_*)} \neq 0, \quad (3.23)$$

where $f(\mathbf{x}) = x_1 + ix_2$. The inequality follows since $\langle \cdot, \mathcal{S}_0^{-1}\cdot \rangle$ is an equivalent inner product on $H^{1/2}(\partial D_*) \times H^{-1/2}(\partial D_*)$. \square

Lemma 3.7. When η is sufficiently small, the following statements hold for the operator $\mathcal{L}(\eta, \lambda, K) : H_1^{-1/2}(\partial D_*) \rightarrow H_1^{1/2}(\partial D_*)$:

(i) $\mathcal{L}(\eta, \lambda, K)$ is analytic in λ in a neighborhood of U_η .

(ii) $\mathcal{L}(\eta, \lambda, K)$ is a Fredholm operator of index zero for $\lambda \in U_\eta$.

(iii) The only characteristic value of $\mathcal{L}(\eta, \lambda, K)$ located in U_η is given by

$$\lambda_0 := |\mathbf{m}_1|^2 + \frac{1}{|\mathcal{C}_z|} \frac{2}{3} (2\pi)^2 \mathbf{a} \eta^2.$$

Moreover,

$$\text{Ker}(\mathcal{L}(\eta, \lambda_0, K)) = \text{span}\{\phi_*\},$$

wherein ϕ_* is defined in (3.6).

(iv) The multiplicity of λ_0 is 1.

(v) For $\lambda \in \partial U_\eta$, $\mathcal{L}^{-1}(\eta, \lambda, K)$ exists and the norm $\|\mathcal{L}^{-1}(\eta, \lambda, K)\|$ is bounded by a constant independent of η .

Proof. (i) is obvious from the definition of the operator in (3.13), (3.14) and (3.17).

(ii) From Lemma 3.5, $\mathcal{L}(\eta, \lambda, K)$ is the sum of $\mathcal{S}_0 : H_1^{-1/2}(\partial D_*) \rightarrow H_1^{1/2}(\partial D_*)$, which is Fredholm of index zero [60], and a finite-rank operator whose range is in $\text{span}\{x_1 + ix_2\}$.

(iii). Using Lemma 3.5, we see that $\mathcal{L}(\eta, \lambda, K)[\phi](\mathbf{x}) = 0$ implies $\mathcal{S}_0\phi = -L_2(\eta, \lambda, K)[\phi](\mathbf{x}) \in \text{span}\{x_1 + ix_2\}$, thus $\phi \in \text{span}\{\phi_*\}$. In addition, a straightforward calculation shows that

$$\mathcal{L}(\eta, \lambda, \mathbf{p})[\phi_*] = (x_1 + ix_2) \left(1 - \frac{1}{|\mathcal{C}_z|} \frac{1}{\lambda - |\mathbf{m}_1|^2} \frac{2}{3} (2\pi)^2 \eta^2 \mathbf{a} \right).$$

Since $\mathbf{a} \neq 0$, $\mathcal{L}(\eta, \lambda, \mathbf{p})[\phi_*] = 0$ if and only if

$$\lambda = \lambda_0 := \frac{1}{|\mathcal{C}_z|} \frac{2}{3} (2\pi)^2 \mathbf{a} \eta^2 + |\mathbf{m}_1|^2. \quad (3.24)$$

(iv). Following the definitions in Appendix A, we assume that $\phi' \in H_1^{-1/2}(\partial D_*)$ satisfies

$$\frac{d}{d\lambda} \mathcal{L}(\eta, \lambda_0, K)[\phi_*] + \mathcal{L}(\eta, \lambda_0, K)[\phi'] = 0.$$

It can be shown that $\frac{d}{d\lambda} \mathcal{L}(\eta, \lambda_0, K)[\phi_*] \in \text{span}\{x_1 + ix_2\}$. Using $L_2(\eta, \lambda, K)[\phi'](\mathbf{x}) \in \text{span}\{x_1 + ix_2\}$, we obtain $\mathcal{S}_0\phi' \in \text{span}\{x_1 + ix_2\}$, which implies that $\phi' \propto \phi_*$. On the other hand, it follows from (iii) that $\mathcal{L}(\eta, \lambda_0, K)[\phi_*] = 0$. Hence ϕ' does not exist, ϕ_* is of rank 1, and the multiplicity of λ_0 is 1.

(v). For $\lambda \in \partial U_\eta$, $\mathcal{L}^{-1}(\eta, \lambda, K)$ exists because $\mathcal{L}(\eta, \lambda, K)$ is Fredholm and has no characteristic values on ∂U_η . When $|\lambda - |K|^2| = \frac{1}{|\mathcal{C}_z|} \frac{1}{3} (2\pi)^2 \mathbf{a} \eta^2$, there holds

$$\mathcal{L}(\eta, \lambda, K)\phi = \mathcal{S}_0\phi + e^{i\theta} \frac{2}{\mathbf{a}} \mathbf{x} \cdot \int_{\partial D_*} \mathbf{y} \phi(\mathbf{y}) ds_{\mathbf{y}}, \quad (3.25)$$

where $\theta \in \mathbb{R}$. When $|\lambda - |K|^2| = \frac{1}{|\mathcal{C}_z|} (2\pi)^2 \mathbf{a} \eta^2$, there holds

$$\mathcal{L}(\eta, \lambda, K)\phi = \mathcal{S}_0\phi e^{i\theta} \frac{2}{3\mathbf{a}} \mathbf{x} \cdot \int_{\partial D_*} \mathbf{y} \phi(\mathbf{y}) ds_{\mathbf{y}}, \quad (3.26)$$

where $\theta \in \mathbb{R}$. The operators above do not depend on η . Thus the norm of $\mathcal{L}^{-1}(\eta, \lambda, K)$ for $\lambda \in \partial U_\eta$ is bounded by a constant that does not depend on η . \square

Lemma 3.8. *When η is sufficiently small, the following statements hold for the operator $\mathcal{L}(\eta, \lambda, K) : H_0^{-1/2}(\partial D_*) \rightarrow H_0^{1/2}(\partial D_*)$:*

(i) $\mathcal{L}(\eta, \lambda, K)$ is analytic in λ in a neighborhood of U_η .

(ii) For $\lambda \in \overline{U_\eta}$, $\mathcal{L}^{-1}(\eta, \lambda, K)$ exists and the norm $\|\mathcal{L}^{-1}(\eta, \lambda, K)\|_{H_0^{-1/2}(\partial D_*) \rightarrow H_0^{1/2}(\partial D_*)}$ is bounded by a positive constant independent of η .

(iii) $\mathcal{L}(\eta, \lambda, K)$ is a Fredholm operator of index zero for $\lambda \in U_\eta$.

Proof. (i) follows similar lines as in Lemma 3.7. For (ii), let $f \in H_0^{-1/2}(\partial D_*)$ be the unique function that satisfies $\mathcal{S}_0 f = 1$. Since $\langle \phi, \mathcal{S}_0 \phi \rangle_{\partial D_*}$ is equivalent to $\|\phi\|_{H^{-1/2}(\partial D_*)}^2$, we know

$$\int_{\partial D_*} f(\mathbf{x}) ds_{\mathbf{x}} = C_1 > 0, \quad (3.27)$$

where C_1 is a constant. Thus for every $\phi \in H_0^{-1/2}(\partial D_*)$, we have the decomposition

$$\phi = \frac{\bar{\phi}}{C_1} f + g, \quad (3.28)$$

where $\bar{\phi} = \int_{\partial D_*} \phi(\mathbf{x}) ds_{\mathbf{x}}$, and $\int_{\partial D_*} g(\mathbf{x}) ds_{\mathbf{x}} = 0$.

Since $L(\eta, \lambda, K)$ is symmetric and $\langle \phi, \mathcal{S}_0^{-1} \phi \rangle_{\partial D_*}$ is equivalent to $\|\phi\|_{H^{1/2}(\partial D_*)}^2$, we calculate

$$\left| \frac{\langle \phi, \mathcal{L}(\eta, \lambda, K) \phi \rangle_{\partial D_*}}{\langle \mathcal{S}_0^{-1} \mathcal{L}(\eta, \lambda, K) \phi, \mathcal{L}(\eta, \lambda, K) \phi \rangle_{\partial D_*}} \right| = \left| \frac{-\frac{\ln \eta}{2\pi} |\bar{\phi}|^2 (1 + o(1)) + \langle g, \mathcal{S}_0 g \rangle_{\partial D_*} (1 + o(1))}{C_1 \left(\frac{\ln \eta}{2\pi}\right)^2 |\bar{\phi}|^2 (1 + o(1)) + \langle g, \mathcal{S}_0 g \rangle_{\partial D_*} (1 + o(1))} \right|. \quad (3.29)$$

Thus when η is sufficiently small, $\|\mathcal{L}^{-1}(\eta, \lambda, K)\|_{H_0^{-1/2}(\partial D_*) \rightarrow H_0^{1/2}(\partial D_*)} \leq \frac{1}{\min\{C_1, 1\}}$ for $\lambda \in \overline{U_\eta}$. This finishes the proof of (ii).

(iii) is a direct corollary of (ii). \square

Lemma 3.9. *There exists $\eta_0 > 0$ such that for all $\eta \in (0, \eta_0)$ and $\lambda \in \overline{U_\eta}$,*

$$\|\mathcal{R}(\eta, \lambda, K)\|_{H^{-1/2}(\partial D_*) \rightarrow H^{1/2}(\partial D_*)} \leq C\eta \quad (3.30)$$

for some constant C independent of η .

Proof. There exists $\eta_0 > 0$ and a constant C such that for all $\eta \in (0, \eta_0)$ and $\lambda \in \overline{U_\eta}$, the following holds

$$|\partial_{\mathbf{x}}^{\alpha_1} \partial_{\mathbf{y}}^{\alpha_2} R_1(\eta(\mathbf{x} - \mathbf{y}); \lambda)| < C\eta, \quad (3.31a)$$

$$|\partial_{\mathbf{x}}^{\alpha_1} \partial_{\mathbf{y}}^{\alpha_2} R_2(\eta(\mathbf{x} - \mathbf{y}); \lambda, \mathbf{p})| < C\eta, \quad (3.31b)$$

$$|\partial_{\mathbf{x}}^{\alpha_1} \partial_{\mathbf{y}}^{\alpha_2} R_0(\eta(\mathbf{x} - \mathbf{y}); \lambda, \mathbf{p})| < C\eta \quad (3.31c)$$

for all multi-indices $|\alpha_1 + \alpha_2| \leq 2$, $\mathbf{x}, \mathbf{y} \in \partial D_*$ and $\lambda \in U_\eta$. The relations (3.31a) and (3.31b) can be shown by a direct calculation, and (3.31c) was shown in [55]. An elementary calculation on the Fourier coefficients concludes the proof. \square

Theorem 3.10. *When η is sufficiently small, the following statements hold:*

(i) The operator $\mathcal{S}(\eta, \lambda, K) : H_i^{-1/2}(\partial D_*) \rightarrow H_i^{1/2}(\partial D_*)$, $i = 1, 2$, attains exactly one characteristic value $\lambda_* \in U_\eta$ of multiplicity 1. More precisely, there exists exactly one pair $(\lambda_i, \rho_i) \in U_\eta \times H_i^{-1/2}(\partial D_*)$ such that $\mathcal{S}(\eta, \lambda_i, K)\rho_i = 0$, $i = 1, 2$. In addition, $\lambda_1 = \lambda_2 =: \lambda_* \in \mathbb{R}$ and $\rho_2(\mathbf{x}) = \rho_1(F\mathbf{x})$.

(ii) The operator $\mathcal{S}(\eta, \lambda, K) : H_0^{-1/2}(\partial D_*) \rightarrow H_0^{1/2}(\partial D_*)$ has no characteristic value in U_η .

(iii) The function ρ_1 can be chosen such that

$$\rho_1 = \phi_* + O(\eta). \quad (3.32)$$

In addition, the function $\rho_2(\mathbf{x}) := \rho_1(F\mathbf{x})$ spans the one-dimensional kernel space for $\mathcal{S}(\eta, \lambda_*, K)$ restricted to the subspace $H_2^{-1/2}(\partial D_*)$.

Proof. For (i), we first find the multiplicity of the characteristic values for $\mathcal{S}(\eta, \lambda, K) : H_i^{-1/2}(\partial D_*) \rightarrow H_i^{1/2}(\partial D_*)$, $i = 1, 2$. To this end, we apply Theorem A.1 by setting $z = \lambda$, $X = H_i^{-1/2}(\partial D_*)$, $Y = H_i^{1/2}(\partial D_*)$, $V = U_\eta$, $A(z) = \mathcal{L}(\eta, \lambda, K)$ and $B(z) = \mathcal{R}(\eta, \lambda, K)$. Recall from Lemma 3.7 and Lemma 3.9 that $A(z)$ and $B(z)$ are analytic on a neighborhood of \bar{U}_η , $A(z)$ is Fredholm of index zero on a neighborhood of \bar{U}_η , and the multiplicity of $A(z)$ in U_η is 1. When η is sufficiently small, it follows that $\|A^{-1}(z)B(z)\|$ is small on ∂U_η by the uniform boundedness of $A^{-1}(z)$ in ∂U_η over η and the smallness of $B(z)$ in \bar{V} as $\eta \rightarrow 0$. Thus the characteristic value of $\mathcal{S}(\eta, \lambda, K) : H_i^{-1/2}(\partial D_*) \rightarrow H_i^{1/2}(\partial D_*)$ attains multiplicity 1 in V for $i = 1, 2$. Since the null multiplicity 1 corresponds to exactly one eigenpair, we deduce that there exists exactly one pair $(\lambda_i, \rho_i) \in U_\eta \times H_i^{-1/2}(\partial D_*)$ such that $\mathcal{S}(\eta, \lambda_i, K)\rho_i = 0$, $i = 1, 2$. The statement for $\lambda_1 = \lambda_2$ and $\rho_2(\mathbf{x}) = \rho_1(F\mathbf{x})$ follows from $\phi \in H_1^{-1/2}$ solves $\mathcal{S}(\eta, \lambda, K)\phi(\mathbf{x}) = 0$ if and only if $\phi(F(\mathbf{x})) \in H_2^{-1/2}$ solves $\mathcal{S}(\eta, \lambda, K)\phi(F\mathbf{x}) = 0$. Finally λ_i are real because $\overline{G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})} = G^f(\mathbf{y}, \mathbf{x}; \lambda, \mathbf{p})$, as can be seen from (3.7).

For (ii), the argument is similar to that in (i), except that we identify $X = H_0^{-1/2}(\partial D_*)$, $Y = H_0^{1/2}(\partial D_*)$. By Lemma 3.8 and Lemma 3.9 and Theorem A.1, we verify the statement.

For (iii), the correspondence between ρ_1 and ρ_2 follows similarly from Lemma 3.1. Finally, we show that (3.32) holds. Let $T_0 : H_1^{-1/2}(\partial D_*) \rightarrow H_1^{1/2}(\partial D_*)$ be defined by

$$T_0\phi(\mathbf{x}) := \mathcal{L}(\eta, \lambda_0, K)\phi(\mathbf{x}) = \mathcal{S}_0\phi(\mathbf{x}) - \frac{1}{\mathbf{a}} \int_{\partial D_*} \mathbf{x} \cdot \mathbf{y} \phi(\mathbf{y}) ds_{\mathbf{y}}, \quad (3.33)$$

where we have used Lemma 3.5. Note that $\text{Ker}(T_0) = \text{span}\{\phi_*\}$. We define $f(\mathbf{x}) := x_1 + ix_2$, then it follows that

$$\langle \phi_*, f \rangle_{\partial D_*} = \langle \mathcal{S}_0^{-1}f, f \rangle_{\partial D_*} \neq 0.$$

The inequality follows from the choice of the size of the inclusion stated after (3.19), which implies that the $\langle \mathcal{S}_0^{-1}\cdot, \cdot \rangle_{\partial D_*}$ pairing on $H_1^{-1/2}(\partial D_*)$ is an inner product [62]. Since $T_0 : H_1^{-1/2}(\partial D_*) \rightarrow H_1^{1/2}(\partial D_*)$ is a Fredholm operator, the range of T_0 is perpendicular to $\text{Ker}(T_0)$ given by

$$\text{Ran } T_0 = \{\psi \in H_1^{1/2}(\partial D_*) : \langle \phi_*, \psi \rangle_{\partial D_*} = 0\}.$$

Define

$$Q\psi := \psi - \frac{\langle \phi_*, \psi \rangle_{\partial D_*}}{\langle \phi_*, f \rangle_{\partial D_*}} f. \quad (3.34)$$

Then Q is a projection and

$$QH_1^{1/2}(\partial D_*) = \text{Ran } T_0.$$

Let the density $\rho_1 \in H^{-1/2}(\partial D_*)$ be a solution to $\mathcal{S}(\eta, \lambda_*, K)\rho_1 = 0$, where $\rho_1 = \phi_* + \phi^{(1)}$ for some $\phi^{(1)} \in (\text{Ker}(T_0))^\perp$. Applying Q to the following equation

$$\begin{aligned} 0 &= \mathcal{S}(\eta, \lambda_*, K)\rho_1 = (\mathcal{L}(\eta, \lambda_*, K) + \mathcal{R}(\eta, \lambda_*, K))\rho_1 \\ &= (T_0 + \mathcal{L}(\eta, \lambda_*, K) - \mathcal{L}(\eta, \lambda_0, K) + \mathcal{R}(\eta, \lambda_*, K))\rho_1, \end{aligned}$$

we obtain

$$0 = Q(T_0 + \mathcal{L}(\eta, \lambda_*, K) - \mathcal{L}(\eta, \lambda_0, K) + \mathcal{R}(\eta, \lambda_*, K))\rho_1 = Q(T_0 + \mathcal{R}(\eta, \lambda_*, K))\rho_1. \quad (3.35)$$

In the above, we have used the fact that

$$\text{Ran}(\mathcal{L}(\eta, \lambda_*, K) - \mathcal{L}(\eta, \lambda_0, K)) \subset \text{span}\{x_1 + ix_2\}, \quad Q(x_1 + ix_2) = 0.$$

Thus (3.35) implies that

$$Q(T_0 + \mathcal{R}(\eta, \lambda_*, K))\phi^{(1)} = -Q(T_0 + \mathcal{R}(\eta, \lambda_*, K))\phi_* = -Q\mathcal{R}(\eta, \lambda_*, K)\phi_*. \quad (3.36)$$

Let A be the inverse of $T_0 : (\text{Ker}(T_0))^\perp \rightarrow \text{Ran}(T_0)$, where the function space is perpendicular with respect to the $H^{1/2}(\partial D_*)$ inner product. We obtain

$$(I + AQ\mathcal{R}(\eta, \lambda_*, K))\phi^{(1)} = -AQ\mathcal{R}(\eta, \lambda_*, K)\phi_*.$$

Using the boundedness of A and Q , which do not depend on η , and (3.30), we obtain

$$\phi^{(1)} = -(I + AQ\mathcal{R}(\eta, \lambda_*, K))^{-1}AQ\mathcal{R}(\eta, \lambda_*, K)\phi_*.$$

Therefore, $\|\phi^{(1)}\|_{H^{-1/2}(\partial D_*)} = O(\eta)$. □

Note that the eigenmodes w_i in Theorem 2.1 is expanded by the single layer potential

$$w_i(\mathbf{x}) = \int_{\partial D_*} G^f(\mathbf{x}, \eta\mathbf{y}; \lambda_*, K)\rho_i(\mathbf{y}) ds_{\mathbf{y}}, \quad \mathbf{x} \in \mathcal{C}_z \setminus D(\eta),$$

where ρ_i is defined in Theorem 3.10.

3.4 Slope of the Dirac cone

In this subsection, we establish the conical singularity of the dispersion surfaces near the point (K, λ_*) for the band structure. In particular, we derive the slope value m_* for the Dirac cone.

Theorem 3.11. *When η is sufficiently small, the two dispersion surfaces around (λ_*, K) takes the form*

$$(\lambda - \lambda_*)^2 = m_*^2|\mathbf{p} - K|^2 + O(|\mathbf{p} - K|^3), \quad m_* \in \mathbb{R}, \quad m_* \geq 0. \quad (3.37)$$

The coefficient m_* represents the slope of the Dirac cone, and is given by

$$m_* = \frac{2}{3}(1 + O(\eta)). \quad (3.38)$$

Proof. To prove (3.37), we apply directly Proposition 4.3 that will be proved in Section 9, instead of presenting a similar proof here. Proposition 4.3 covers more general scenarios and can be applied to derive (3.37). In more details, we set $\varepsilon = 0$ in Proposition 4.3 and notice that the Bloch wave vector \mathbf{p} near K can be expanded as $\mathbf{p} = K + \ell\boldsymbol{\beta}_1 + \mu\boldsymbol{\beta}_2$, then the conical shape of the dispersion relation (3.37) follows by observing that $|\mathbf{p} - K|^2 = |\ell + \mu\bar{\tau}|^2|\boldsymbol{\beta}_1|^2$. Thus $m_* = \frac{1}{|\boldsymbol{\beta}_1|}|\frac{\theta_*}{\gamma_*}|$, where θ_* and γ_* are defined in (4.8).

Next we compute the slope $m_* := \frac{1}{|\boldsymbol{\beta}_1|}|\frac{\theta_*}{\gamma_*}|$. Note that the ratio $\frac{\theta_*}{\gamma_*}$ is independent of a scaling of ρ_i 's. We can thus use ρ_i 's defined in Theorem 3.10(iii) for the calculation. Since

$$\partial_\lambda G^f(\mathbf{y}, \mathbf{x}; \lambda, K) = \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})},$$

we have

$$\begin{aligned} & \langle \rho_1, \partial_\lambda \mathcal{S}(\eta, \lambda_*, K) \rho_1 \rangle_{\partial D_*} \\ &= \frac{1}{|\mathcal{C}_z|} \int_{(\partial D_*)^2} \left(\frac{1}{(\lambda - |\mathbf{m}_1|^2)^2} \left(3 - \frac{1}{3}(2\pi)^2(\eta|\mathbf{x} - \mathbf{y}|)^2 + O(\eta^3) \right) + O(1) \right) \overline{\rho_1(\mathbf{x})} \rho_1(\mathbf{y}) ds_{\mathbf{y}} ds_{\mathbf{x}} \quad (3.39) \\ &= \frac{1}{|\mathcal{C}_z|} 2\mathbf{a}^2 \frac{\eta^2}{(\lambda - |\mathbf{m}_1|^2)^2} \frac{2}{3} (2\pi)^2 (1 + O(\eta)). \end{aligned}$$

In addition,

$$\begin{aligned} (1, 0)^T \cdot \nabla_{\mathbf{p}} G^f(\mathbf{y}, \mathbf{x}; \lambda, K) &= -\frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} \mathbf{m} \cdot (1, 0)^T \\ &\quad - \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} (\mathbf{x} - \mathbf{y}) \cdot (1, 0)^T. \end{aligned}$$

Therefore,

$$\begin{aligned} & \langle \rho_2, (1, 0)^T \cdot \nabla_{\mathbf{p}} G^f(\mathbf{y}, \mathbf{x}; \lambda, K) \rho_1 \rangle_{\partial D_*} \\ &= -\frac{1}{|\mathcal{C}_z|} \iint_{\partial D_* \times \partial D_*} \left(\frac{2}{(\lambda - |\mathbf{m}_1|^2)^2} \left(-\eta^2 \frac{2}{9} (x_1 - y_1)(x_2 - y_2) + O(\eta^3) \right) + \frac{i}{\lambda - |\mathbf{m}_1|^2} O(\eta) + O(1) \right) \overline{\rho_2(\mathbf{x})} \rho_1(\mathbf{y}) ds_{\mathbf{y}} ds_{\mathbf{x}} \\ &= \frac{1}{|\mathcal{C}_z|} 2i\mathbf{a}^2 \frac{\eta^2}{(\lambda - |\mathbf{m}_1|^2)^2} \frac{4}{9} (2\pi)^2 (1 + O(\eta)). \quad (3.40) \end{aligned}$$

Here we have used the fact that $\rho_1 = \phi_* + O(\eta)$ and $\rho_2(\mathbf{x}) = \rho_1(F\mathbf{x})$ in Theorem 3.10. Applying Proposition 4.3 with $\varepsilon = 0$ again, we obtain $m_* = \frac{1}{|\boldsymbol{\beta}_1|}|\frac{\theta_*}{\gamma_*}| = \frac{2}{3}(1 + O(\eta))$. \square

Theorems 3.10 and 3.11 combined give the existence and asymptotic analysis of the Dirac point when the Bloch wave vector $\mathbf{p} = K$ as stated in Theorem 2.1. The Dirac point at K' follows similarly since

$$G^f(\mathbf{x}, \mathbf{y}; \lambda, K') = \overline{G^f(\mathbf{x}, \mathbf{y}; \lambda, K)}. \quad (3.41)$$

4 Band-gap opening at the Dirac point for the perturbed lattices

In this section, we consider the bandgap opening near the Dirac points for the perturbed honeycomb lattices. More precisely, we consider the spectral problem (2.11), in which the obstacle in each period

is rotated by an angle of $\pm\varepsilon$ for $\varepsilon \in \mathbb{R}$. Here and henceforth, we denote $D = D(\eta_0)$ for a fixed $\eta_0 > 0$ for the ease of notation. We define the operator $T(\varepsilon, \lambda, \mathbf{p}) : H^{-1/2}(\partial D) \rightarrow H^{1/2}(\partial D)$ as

$$T(\varepsilon, \lambda, \mathbf{p})[\phi](\mathbf{x}) := \int_{\partial D} G^f(R^\varepsilon \mathbf{x}, R^\varepsilon \mathbf{y}; \lambda, \mathbf{p}) \phi(\mathbf{y}) ds_{\mathbf{y}}, \quad \mathbf{x} \in \partial D. \quad (4.1)$$

Note that the ε in $T(\varepsilon, \lambda, \mathbf{p})$ represents the rotation angle, while the η in $\mathcal{S}(\eta, \lambda, \mathbf{p})$ defined in (3.3) represents the size of the obstacle. The dependence of $T(\varepsilon, \lambda, \mathbf{p})$ on η is suppressed since η is fixed at η_0 . Similar to the discussion in Section 3.1, (λ, \mathbf{p}) belongs to the dispersion surface of the honeycomb lattice if and only if the triple $(\lambda, \mathbf{p}, \phi) \in \mathbb{R} \times \mathcal{B}_z \times H^{-1/2}(\partial D)$ solves the integral equation

$$T(\varepsilon, \lambda, \mathbf{p})[\phi](\mathbf{x}) = 0, \quad \mathbf{x} \in \partial D. \quad (4.2)$$

The corresponding eigenmode is given by

$$u^\varepsilon(\mathbf{x}) := \int_{\partial D} G^f(\mathbf{x}, R^\varepsilon \mathbf{y}; \lambda, \mathbf{p}) \phi(\mathbf{y}) ds_{\mathbf{y}}, \quad \mathbf{x} \in \mathcal{C}_z \setminus D^\varepsilon. \quad (4.3)$$

We extend $u^\varepsilon(\mathbf{x})$ to \mathcal{C}_z by letting

$$\tilde{u}^\varepsilon(\mathbf{x}) := \begin{cases} u^\varepsilon(\mathbf{x}), & \mathbf{x} \in \mathcal{C}_z \setminus D^\varepsilon, \\ 0, & \mathbf{x} \in D^\varepsilon. \end{cases} \quad (4.4)$$

It is clear that $\|\tilde{u}^\varepsilon\|_{L^2(\mathcal{C}_z)} = \|u^\varepsilon\|_{L^2(\mathcal{C}_z \setminus D^\varepsilon)}$ and $\|\tilde{u}^\varepsilon\|_{H^1(\mathcal{C}_z)} = \|u^\varepsilon\|_{H^1(\mathcal{C}_z \setminus D^\varepsilon)}$. In what follows, for convenience we will abuse the notations and denote both u^ε and \tilde{u}^ε by u^ε .

4.1 Band structure and Bloch modes for the perturbed honeycomb structures

In this subsection, we compute the band structure of the perturbed honeycombs around K by a perturbation argument. Recall that at the Dirac point (λ_*, K) , there holds (see Proposition 3.10)

$$\text{Ker } T(0, \lambda_*, K) = \text{span} \{\rho_1, \rho_2\}, \quad (4.5)$$

where $R\rho_1(\mathbf{x}) := \rho_1(R^{-1}\mathbf{x}) = \tau\rho_1(\mathbf{x})$, $R\rho_2(\mathbf{x}) := \rho_2(R^{-1}\mathbf{x}) = \bar{\tau}\rho_2(\mathbf{x})$, and $\rho_2(\mathbf{x}) = \rho_1(F\mathbf{x})$. From now on, we normalize ρ_n such that

$$\|w_n\|_{L^2(\mathcal{C}_z \setminus D)} = 1, \quad (4.6)$$

where w_n is the single-layer potential defined as

$$w_n(\mathbf{x}) := \int_{\partial D} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p}) \rho_n(\mathbf{y}) ds_{\mathbf{y}}, \quad \mathbf{x} \in \Omega^0, \quad n = 1, 2. \quad (4.7)$$

We first characterize the partial derivatives of the integral operator $T(\varepsilon, \lambda, \mathbf{p})$ with respect to ε , λ , and \mathbf{p} respectively.

Proposition 4.1. *Let $\boldsymbol{\rho} = (\rho_1, \rho_2)$, where ρ_i are normalized such that (4.6) holds. Then the partial derivatives of $\langle \boldsymbol{\rho}, T(\varepsilon, \lambda, \mathbf{p}) \boldsymbol{\rho} \rangle_{\partial D}$ at $\varepsilon = 0$, $\lambda = \lambda_*$ and $\mathbf{p} = K$ take the following forms:*

$$\begin{aligned} \langle \boldsymbol{\rho}, \partial_\lambda T(0, \lambda_*, K) \boldsymbol{\rho} \rangle_{\partial D}|_{\lambda=\lambda_*} &= \begin{pmatrix} \gamma_* & 0 \\ 0 & \gamma_* \end{pmatrix}, \\ \langle \boldsymbol{\rho}, \boldsymbol{\beta}_1 \cdot \nabla_{\mathbf{p}} T(0, \lambda_*, \mathbf{p}) \boldsymbol{\rho} \rangle_{\partial D}|_{\mathbf{p}=K} &= \begin{pmatrix} 0 & \overline{\theta_*} \\ \theta_* & 0 \end{pmatrix}, \\ \langle \boldsymbol{\rho}, \boldsymbol{\beta}_2 \cdot \nabla_{\mathbf{p}} T(0, \lambda_*, \mathbf{p}) \boldsymbol{\rho} \rangle_{\partial D}|_{\mathbf{p}=K} &= \begin{pmatrix} 0 & \tau \overline{\theta_*} \\ \overline{\tau} \theta_* & 0 \end{pmatrix}, \\ \langle \boldsymbol{\rho}, \partial_\varepsilon T(\varepsilon, \lambda_*, K) \boldsymbol{\rho} \rangle_{\partial D}|_{\varepsilon=0} &= \begin{pmatrix} t_* & 0 \\ 0 & -t_* \end{pmatrix}, \end{aligned} \tag{4.8}$$

where $t_*, \gamma_* \in \mathbb{R}$, $\theta_* \in \mathbb{C}$.

In the above, for $(\phi_1, \phi_2) \in (H^{-1/2}(\partial D))^2$ and $(\psi_1, \psi_2) \in (H^{1/2}(\partial D))^2$, we denote

$$\langle (\phi_1, \phi_2), (\psi_1, \psi_2) \rangle_{\partial D} := \langle \phi_1, \psi_1 \rangle_{\partial D} + \langle \phi_2, \psi_2 \rangle_{\partial D},$$

where the symbol $\langle \cdot, \cdot \rangle_{\partial D}$ on the right hand side represents the regular $H^{-1/2}(\partial D)$ - $H^{1/2}(\partial D)$ pairing. The proof of Proposition 4.1 is given in Appendix B.

Remark 4.2. *In (3.39) and (3.40), we calculated the values of γ_* and θ_* and showed that $\gamma_* \neq 0$ and $\theta_* \neq 0$. For simplicity, in all calculations throughout the paper, we assume $\gamma_* > 0$ and $t_* > 0$. The cases when $\gamma_* < 0$ or $t_* < 0$ can be treated similarly. Therefore, the main results in Section 2 hold regardless of the signs of γ_* and t_* .*

Proposition 4.3. *Assume that $t_* > 0$ and parameterize the quasimomenta near K by $\mathbf{p}(\ell, \mu) := K + \ell \boldsymbol{\beta}_1 + \mu \boldsymbol{\beta}_2$. Let $\ell \in \mathbb{R}$, $\mu \in \mathbb{R}$ and $\varepsilon \geq 0$ be sufficiently small.*

(i) *The dispersion relations for the spectral problem (2.11) attain the following expansions:*

$$\begin{aligned} \lambda_{1, \pm \varepsilon}(\mathbf{p}(\ell, \mu)) &= \lambda_* - \frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 |\ell + \mu \overline{\tau}|^2} (1 + O(\varepsilon, \ell, \mu)), \\ \lambda_{2, \pm \varepsilon}(\mathbf{p}(\ell, \mu)) &= \lambda_* + \frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 |\ell + \mu \overline{\tau}|^2} (1 + O(\varepsilon, \ell, \mu)). \end{aligned} \tag{4.9}$$

(ii) *The corresponding density functions for the integral equation (4.2) attain the expansions*

$$\begin{aligned} \phi_{1, \varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) &= w_1 + L(\varepsilon, \ell, \mu) w_2 + O(\varepsilon, \ell, \mu), \\ \phi_{2, \varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) &= -\overline{L}(\varepsilon, \ell, \mu) w_1 + w_2 + O(\varepsilon, \ell, \mu), \end{aligned} \tag{4.10}$$

$$\begin{aligned} \phi_{1, -\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) &= \overline{L}(\varepsilon, \ell, \mu) w_1 + w_2 + O(\varepsilon, \ell, \mu), \\ \phi_{2, -\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) &= w_1 - L(\varepsilon, \ell, \mu) w_2 + O(\varepsilon, \ell, \mu). \end{aligned} \tag{4.11}$$

In the above,

$$L(\varepsilon, \ell, \mu) := \frac{\theta_*(\ell + \mu \overline{\tau})}{\varepsilon t_* + \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 |\ell + \mu \overline{\tau}|^2}}. \tag{4.12}$$

(iii) The corresponding Bloch modes with unit $L^2(\mathcal{C}_z \setminus D^\pm)$ norm take the form

$$u_{1,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) = (w_1 + L(\varepsilon, \ell, \mu)w_2 + O(\varepsilon, \ell, \mu)) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell, \mu)|^2 + O(\varepsilon, \ell, \mu)}}, \quad (4.13)$$

$$u_{2,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) = \left(-\overline{L(\varepsilon, \ell, \mu)}w_1 + w_2 + O(\varepsilon, \ell, \mu) \right) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell, \mu)|^2 + O(\varepsilon, \ell, \mu)}},$$

$$u_{1,-\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) = \left(\overline{L(\varepsilon, \ell, \mu)}w_1 + w_2 + O(\varepsilon, \ell, \mu) \right) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell, \mu)|^2 + O(\varepsilon, \ell, \mu)}}, \quad (4.14)$$

$$u_{2,-\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) = (w_1 - L(\varepsilon, \ell, \mu)w_2 + O(\varepsilon, \ell, \mu)) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell, \mu)|^2 + O(\varepsilon, \ell, \mu)}}.$$

Note that for all ε, ℓ and μ , the eigenvalues above satisfy $\lambda_{1,\pm\varepsilon}(\mathbf{p}(\ell, \mu)) < \lambda_{2,\pm\varepsilon}(\mathbf{p}(\ell, \mu))$. Hence, a band gap is opened near the Dirac point for the spectral problem (2.11). Another observation is that

$$|\mathbf{p} - K|^2 = |\ell\boldsymbol{\beta}_1 + \mu\boldsymbol{\beta}_2|^2 = \frac{4}{3}(\ell^2 + \mu^2 - \ell\mu) = \frac{4}{3}|\ell + \mu\bar{\tau}|^2.$$

This is used to relate Theorem 2.5 to Proposition 4.3.

Proof. Let V be a sufficiently small neighborhood of λ_* . We first show that for ε and $|\mathbf{p} - K|$ sufficiently small, the characteristic value of $T(\varepsilon, \lambda, \mathbf{p})$ in V has multiplicity two.

Note that for ε and $|\mathbf{p} - K|$ being sufficiently small, $T(\varepsilon, \lambda, \mathbf{p})$ is an analytic family of operators in the variable λ . When V is sufficiently small, from Section 3.3, it is known that $\lambda = \lambda_*$ is the only characteristic value of $T(0, \lambda, K)$ within V . Indeed, the multiplicity of the characteristic λ_* of $T(0, \lambda, K)$ is two. This follows from (4.5) and (4.8). That is, $\text{Ker } T(0, \lambda_*, K) = \text{span}\{\rho_1, \rho_2\}$ and

$$\langle \phi, \partial_\lambda T(0, \lambda, K)\phi \rangle_{\partial D} \neq 0 \quad \forall \phi \in \text{Ker } T(0, \lambda_*, K). \quad (4.15)$$

Thus $\partial_\lambda T(0, \lambda, K)|_{\lambda=\lambda_*} \psi \notin \text{Ran}(T(0, \lambda_*, K))$. We conclude, ϕ is of rank one and the multiplicity of $T(0, \lambda_*, K)$ is two. Since $T(\varepsilon, \lambda, \mathbf{p})$ is a Fredholm operator [60] and it is continuous with respect to ε and \mathbf{p} , by Theorem A.1, we deduce that $T(\varepsilon, \lambda, \mathbf{p})$ has multiplicity two in V .

Next, we use the perturbation argument to show that for ε and $|\mathbf{p} - K|$ being sufficiently small, $T(\varepsilon, \lambda, \mathbf{p})$ attains two characteristic values in V , with multiplicity one each. This argument also gives rise to the asymptotic expansion of the characteristic values and the density functions.

Let $\varepsilon, \ell, \mu \ll 1$. We solve for (λ, ϕ) pairs in $V \times H^{-1/2}(\partial D)$ such that $T(\varepsilon, \lambda, \mathbf{p})\phi = 0$. Let us express

$$\mathbf{p}(\ell, \mu) = K + \mathbf{p}^{(1)}, \quad \lambda = \lambda_* + \lambda^{(1)}, \quad T(\varepsilon, \lambda, \mathbf{p}(\ell, \mu)) = T^{(0)} + T^{(1)}, \quad \phi = \phi^{(0)} + \phi^{(1)}. \quad (4.16)$$

Here $|\mathbf{p}^{(1)}| = |\ell\boldsymbol{\beta}_1 + \mu\boldsymbol{\beta}_2| \ll 1$, $\lambda^{(1)} \ll 1$, $T^{(0)} = T(0, \lambda_*, K)$, $T^{(1)} = T(\varepsilon, \lambda, \mathbf{p}) - T^{(0)}$, $\phi^{(0)} \in \text{Ker}(T^{(0)})$, and $\phi^{(1)} \in (\text{Ker}(T^{(0)}))^\perp$, where the perpendicular sign is with respect to the inner product of $H^{-1/2}(\partial D)$. Using $T^{(0)}\phi^{(0)} = 0$, the integral equation $T(\varepsilon, \lambda, \mathbf{p})\phi = 0$ boils down to

$$T^{(0)}\phi^{(1)} + T^{(1)}(\phi^{(0)} + \phi^{(1)}) = 0. \quad (4.17)$$

Note that $T^{(0)} : H^{-1/2}(\partial D) \rightarrow H^{1/2}(\partial D)$ is a Fredholm operator and the range of T_0 is the space perpendicular to $\text{Ker}(T^{(0)})$ in the dual sense. That is,

$$\text{Ran } T^{(0)} = \{\psi \in H^{1/2}(\partial D) : \langle \rho_i, \psi \rangle_{\partial D} = 0, i = 1, 2\}. \quad (4.18)$$

Define

$$Q\psi := \psi - \sum_{i=1,2} \frac{\langle \rho_i, \psi \rangle_{\partial D}}{\langle \rho_i, f_i \rangle_{\partial D}} f_i, \quad (4.19)$$

where $f_i = S\rho_i$. It is straightforward to check that $QH^{1/2}(\partial D) = \text{Ran}(T^{(0)})$ and Q is a projection. Thus (4.17) is equivalent to

$$\langle \psi, T^{(0)}\phi^{(1)} + T^{(1)}(\phi^{(0)} + \phi^{(1)}) \rangle_{\partial D} = 0 \quad \forall \psi \in \text{Ker}T^{(0)}, \quad (4.20)$$

and

$$T^{(0)}\phi^{(1)} + QT^{(1)}(\phi^{(0)} + \phi^{(1)}) = 0. \quad (4.21)$$

Here we have used $QT^{(0)} = T^{(0)}$.

Let A be the inverse of $T^{(0)}|_{(\text{Ker}(T^{(0)}))^\perp} : (\text{Ker}(T^{(0)}))^\perp \rightarrow \text{Ran}(T^{(0)})$. It follows from (4.21) and $\phi^{(1)} \in (\text{Ker}(T^{(0)}))^\perp$ that

$$(I + AQT^{(1)})\phi^{(1)} + AQT^{(1)}\phi^{(0)} = 0.$$

Here we have used the fact that $AT^{(0)}\phi^{(1)} = \phi^{(1)}$ since $\phi^{(1)} \in \text{Ran}(T^{(0)})$. Since $T^{(1)} = O(|\varepsilon|, |\ell|, |\mu|, |\lambda^{(1)}|)$, when ε , ℓ and $\lambda^{(1)}$ are sufficiently small, $(I + AQT^{(1)})$ is invertible with an inverse norm bounded by $\frac{1}{2}$. Thus, there holds

$$\phi^{(1)} = -(I + AQT^{(1)})^{-1}AQT^{(1)}\phi^{(0)}, \quad (4.22)$$

where $(I + AQT^{(1)})^{-1}$ is the inverse of $I + AQT^{(1)} : (\text{Ker}(T^{(0)}))^\perp \rightarrow \text{Ran}(T^{(0)})$. We obtain

$$(I + AQT^{(1)})^{-1}AQT^{(1)} = O(|\varepsilon|, |\ell|, |\mu||\lambda^{(1)}|).$$

Using the expansions

$$\phi^{(0)} = a\rho_1 + b\rho_2 \text{ for some constants } a, b \in \mathbb{C}, \quad (4.23)$$

and

$$T^{(1)} = \varepsilon\partial_\varepsilon T(0, \lambda_*, K) + (\ell\beta_1 + \mu\beta_2) \cdot \nabla_{\mathbf{p}} T(0, \lambda_*, K) + \lambda^{(1)}\partial_\lambda T(0, \lambda, K) + O(|\varepsilon|^2, |\ell|^2, |\mu|^2, |\lambda^{(1)}|^2),$$

and applying Proposition 4.1, (4.20) becomes

$$\mathcal{M}(\varepsilon, \ell, \mu, \lambda^{(1)}) \begin{pmatrix} a \\ b \end{pmatrix} = 0, \quad (4.24)$$

where

$$\mathcal{M}(\varepsilon, \ell, \mu, \lambda^{(1)}) = \begin{pmatrix} t_*\varepsilon + \gamma_*\lambda^{(1)} & \ell\bar{\theta}_* + \mu\bar{\tau}\bar{\theta}_* \\ \ell\theta_* + \mu\bar{\tau}\theta_* & -t_*\varepsilon + \gamma_*\lambda^{(1)} \end{pmatrix} + O(|\varepsilon|^2, |\ell|^2, |\mu|^2, |\lambda^{(1)}|^2). \quad (4.25)$$

With the ansatz

$$\lambda^{(1)} = \frac{x}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 |\ell + \mu\bar{\tau}|^2}, \quad (4.26)$$

the inverse function theorem implies that when ε , ℓ , μ and $\phi^{(1)}$ are sufficiently small, there exist $x = 1 + O(\varepsilon, \ell, \mu)$ and $x = -1 + O(\varepsilon, \ell, \mu)$ such that $\lambda^{(1)}$ satisfies $\det(\mathcal{M}(\varepsilon, \ell, \mu, \lambda^{(1)})) = 0$. For each of these two values of $\lambda^{(1)}$, by solving (4.23), we obtain $\phi^{(1)}$ from (4.22) and (4.23).

The expansion of normalized eigenmodes follows from Lemma 4.5 below. \square

Before presenting Lemma 4.5, we introduce the following auxiliary lemma whose proof is elementary.

Lemma 4.4. *Let X and Y be two Banach spaces. Consider two operators $A_\varepsilon, A_0 : X \rightarrow Y$ and two functions $f_\varepsilon, f_0 \in Y$. Suppose A_ε^{-1} and A_0^{-1} exist. Then*

$$\|A_\varepsilon^{-1}f_\varepsilon - A_0^{-1}f_0\|_X \leq \|A_\varepsilon^{-1}\|_{Y \rightarrow X} \|A_0 - A_\varepsilon\|_{X \rightarrow Y} \|A_0^{-1}\|_{Y \rightarrow X} \|f_\varepsilon\|_Y + \|A_0^{-1}\|_{Y \rightarrow X} \|f_\varepsilon - f_0\|_Y. \quad (4.27)$$

Lemma 4.5. *Let*

$$\tilde{u}_{1,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) := \int_{\partial D} G^f(\mathbf{x}, R^\varepsilon \mathbf{y}; \lambda, \mathbf{p}(\ell, \mu)) \phi_{1,\varepsilon}(\mathbf{y}) ds_{\mathbf{y}}, \quad \mathbf{x} \in \mathcal{C}_z \setminus D^\varepsilon. \quad (4.28)$$

There holds

$$\|\tilde{u}_{1,\varepsilon}(\cdot; \mathbf{p}(\ell, \mu)) - (w_1 + L(\varepsilon, \ell, \mu)w_2)\|_{H^1(\mathcal{C}_z)} = O(\varepsilon, \ell), \quad n = 1, 2. \quad (4.29)$$

Here w_i are defined in (4.7) and $L(\varepsilon, \ell, \mu)$ is defined in (4.12).

Proof. The function $\tilde{u}_{n,\varepsilon}(\mathbf{x}, \mathbf{p}(\ell, \mu))$ attains the quasi-momentum $\mathbf{p}(\ell, \mu)$ and it solves the differential equation

$$(-\Delta - \lambda_{1,\varepsilon}(\mathbf{p}(\ell, \mu)))\tilde{u}_{1,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \mu)) = \delta(\mathbf{x} \in \partial D^\varepsilon) \phi_{1,\varepsilon}(R^{-\varepsilon} \mathbf{x}) \quad \text{in } \mathcal{C}_z, \quad (4.30)$$

The function $w_1 + L(\varepsilon, \ell, \mu)w_2$ attains the quasi-momentum K and it solves

$$(-\Delta - \lambda_*)(w_1 + L(\varepsilon, \ell, \mu)w_2) = \delta(\mathbf{x} \in \partial D)(\rho_1(\mathbf{x}) + L(\varepsilon, \ell, \mu)\rho_2(\mathbf{x})) \quad \text{in } \mathcal{C}_z. \quad (4.31)$$

Let us fix a pair of small ℓ and μ . Define the operators

$$A_\varepsilon := -\Delta - \lambda_{1,\varepsilon}(\mathbf{p}(\ell, \mu)) \quad \text{and} \quad f_\varepsilon := \delta(\mathbf{x} \in \partial D^\varepsilon) \phi_{1,\varepsilon}(R^{-\varepsilon} \mathbf{x}), \quad \text{for } \varepsilon \neq 0$$

and

$$A_0 := -\Delta - \lambda_* \quad \text{and} \quad f_0 := \delta(\mathbf{x} \in \partial D)(\rho_1(\mathbf{x}) + L(\varepsilon, \ell, \mu)\rho_2(\mathbf{x})).$$

Then $\tilde{u}_{1,\varepsilon} - (w_1 + L(\varepsilon, \ell, \mu)w_2) = A_\varepsilon^{-1}f_\varepsilon - A_0^{-1}f_0$. It is straightforward to verify that

$$\begin{aligned} |\mathbf{p}(\ell, \mu) - K| &= O(\ell, \mu), \quad |\lambda_{1,\varepsilon}(\mathbf{p}(\ell, \mu)) - \lambda_*| = O(\varepsilon, \ell, \mu), \\ \|\delta(\mathbf{x} \in \partial D^\varepsilon) \phi_{1,\varepsilon}(R^{-\varepsilon} \mathbf{x}) - \delta(\mathbf{x} \in \partial D)(\rho_1(\mathbf{x}) + L(\varepsilon, \ell, \mu)\rho_2(\mathbf{x}))\|_{H^{-1}(\mathcal{C}_z)} &= O(\varepsilon, \ell, \mu). \end{aligned} \quad (4.32)$$

By Theorem 2.1, for ε sufficiently small, $\lambda_{1,\varepsilon}$ are uniformly away from $\{|\mathbf{m}|^2\}_{\mathbf{m} \in \tilde{\Lambda}^*}$. Thus the inverses of A_ε and A_0 exist and are uniformly bounded. Applying Lemma 4.4, we finish the proof. \square

5 Floquet theory and the Green functions in a periodic strip with a zigzag cross section

In this section and the subsequent two sections, we investigate the existence of interface modes for the joint photonic structure along a zigzag interface that solve (2.14) for $k_{\parallel} = k_{\parallel}^* := \frac{4\pi}{3}$. The purpose of this section is to introduce the Floquet theory and Green functions in the following infinite strip

$$\Omega^\varepsilon := \Omega^J \setminus \cup_{m \in \mathbb{Z}} (D^\varepsilon + m\mathbf{e}_1), \quad \varepsilon \in \mathbb{R}.$$

We note that when $\varepsilon = 0$, Ω^0 represents the unperturbed strip. We define the following function spaces that are quasi-periodic along \mathbf{e}_2 :

$$\begin{aligned} \mathcal{H}_{\text{loc}}^\varepsilon := \{ & u \in H_{\text{loc}}^1(\Omega^\varepsilon) : \Delta u \in L_{\text{loc}}^2(\Omega^\varepsilon), \quad u = 0 \text{ on } \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1), \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik^* \|\cdot\|} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-, \quad \partial_{\nu_1} u(\mathbf{x} + \mathbf{e}_2) = e^{ik^* \|\cdot\|} \partial_{\nu_1} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-\}. \end{aligned} \quad (5.1)$$

Then the analysis boils down to the spectrum of the operator Δ in $\mathcal{H}_{\text{loc}}^\varepsilon$, that is, eigenpairs $(\lambda, u) \in \mathbb{R} \times \mathcal{H}_{\text{loc}}^\varepsilon$ satisfying

$$\begin{aligned} -\Delta u - \lambda u &= 0 && \text{on } \Omega^\varepsilon, \\ u &= 0 && \text{on } \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1). \end{aligned} \quad (5.2)$$

5.1 Floquet theory in a periodic strip with a zigzag cross section

In this subsection, we decompose the operator Δ on $\mathcal{H}_{\text{loc}}^\varepsilon$ using the Floquet theory along the direction \mathbf{e}_1 . Let $\mathbf{p}(\ell) := K + \ell\beta_1$. For each $\ell \in \mathbb{R}$, we denote $-\Delta^\varepsilon(\ell)$ the restriction of $-\Delta$ on the space $\mathcal{H}^\varepsilon(\ell)$ with the quasi-momentum $(K + \ell\beta_1) \cdot \mathbf{e}_1$ along the direction \mathbf{e}_1 , i.e.

$$\begin{aligned} \mathcal{H}^\varepsilon(\ell) := \{ & u \in H^1(\mathcal{C}_z \setminus D) : \Delta u \in L^2(\mathcal{C}_z \setminus D^\varepsilon), \quad u = 0 \text{ on } \partial D^\varepsilon, \\ & u(\mathbf{x} + \mathbf{e}_2) = e^{ik^* \|\cdot\|} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik^* \|\cdot\|} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b \\ & u(\mathbf{x} + \mathbf{e}_1) = e^{i(K + \ell\beta_1) \cdot \mathbf{e}_1} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_1, \quad \partial_{\nu_1} u(\mathbf{x} + \mathbf{e}_1) = e^{i(K + \ell\beta_1) \cdot \mathbf{e}_1} \partial_{\nu_1} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_1 \}. \end{aligned} \quad (5.3)$$

Here Γ_b and Γ_1 are the bottom and left boundaries of \mathcal{C}_z shown in Figure 2.1, the directional derivative ∂_{ν_2} is normal to Γ_t and Γ_b in the direction $\nu_2 = (\frac{1}{2}, \frac{\sqrt{3}}{2})$ and the directional derivative ∂_{ν_1} is normal to Γ_1 and Γ_r in the direction $\nu_1 = (\frac{1}{2}, -\frac{\sqrt{3}}{2})$. Equivalently, we solve for the (λ, u) pair for each $\ell \in \mathbb{R}$ that satisfies

$$\begin{cases} -\Delta u - \lambda u = 0 & \text{in } \mathcal{C}_z \setminus D^\varepsilon, \\ u = 0 & \text{on } \partial D^\varepsilon, \\ u(\mathbf{x} + \mathbf{e}_2) = e^{ik^* \|\cdot\|} u(\mathbf{x}) & \text{for } \mathbf{x} \in \Gamma_b, \\ \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik^* \|\cdot\|} \partial_{\nu_2} u(\mathbf{x}) & \text{for } \mathbf{x} \in \Gamma_b, \\ u(\mathbf{x} + \mathbf{e}_1) = e^{i(K + \ell\beta_1) \cdot \mathbf{e}_1} u(\mathbf{x}) & \text{for } \mathbf{x} \in \Gamma_1, \\ \partial_{\nu_1} u(\mathbf{x} + \mathbf{e}_1) = e^{i(K + \ell\beta_1) \cdot \mathbf{e}_1} \partial_{\nu_1} u(\mathbf{x}) & \text{for } \mathbf{x} \in \Gamma_1. \end{cases} \quad (5.4)$$

For each fixed $\ell \in \mathbb{R}$, $-\Delta^\varepsilon(\ell)$ is a self-adjoint positive operator with compact resolvent, thus its spectrum is real, discrete, and accumulates at ∞ . The eigenvalues of $-\Delta^\varepsilon(\ell)$ are labeled as $\lambda_n(\ell)$ in an increasing order

$$0 \leq \lambda_{1,\varepsilon}(\ell) \leq \lambda_{2,\varepsilon}(\ell) \leq \dots \leq \lambda_{n,\varepsilon}(\ell) \leq \dots \quad (5.5)$$

Note that $\lambda_{n,\varepsilon}(\ell)$ are 2π -periodic, continuous and piecewise differentiable functions in ℓ . The corresponding eigenmodes $u_{n,\varepsilon}(\mathbf{x}, \mathbf{p}(\ell))$ are chosen to be orthonormal with respect to the L^2 inner product in $\mathcal{C}_z \setminus D^\varepsilon$. $\lambda_{n,\varepsilon}(\ell)$ may not be differentiable at points ℓ where $\lambda_{n,\varepsilon}(\ell)$ is not a simple eigenvalue, which only occurs at a finite number of ℓ values within a period for each n .

The spectrum of $-\Delta^\varepsilon(\ell)$ can alternatively be labeled as smooth branches as follows. The smooth labeling enables a representation of the Green function using the Bloch modes to be introduced in Section 5.2. To be more precise, there exists a sequence of complex neighborhoods $D_{n,\varepsilon}$ of

\mathbb{R} , a sequence of analytic functions $\mu_{n,\varepsilon}(\ell) : D_{n,\varepsilon} \rightarrow \mathbb{C}$, and a sequence of analytic functions $v_{n,\varepsilon}(\mathbf{x}, \mathbf{p}(\ell)) : D_{n,\varepsilon} \rightarrow H^1(\Delta, \mathcal{C}_z \setminus D^\varepsilon)$ such that

$$\begin{aligned} v_{n,\varepsilon}(\cdot, \mathbf{p}(\ell)) &\in \mathcal{H}^\varepsilon(\ell), \quad -\Delta v_{n,\varepsilon}(\cdot, \mathbf{p}(\ell)) = \mu_{n,\varepsilon}(\ell) v_{n,\varepsilon}(\cdot, \mathbf{p}(\ell)), \quad \ell \in \mathbb{R}, \\ (v_{n,\varepsilon}(\cdot, \mathbf{p}(\ell)), v_{m,\varepsilon}(\cdot, \mathbf{p}(\ell)))_{L^2(\mathcal{C}_z \setminus D^\varepsilon)} &= \delta_{m,n}, \quad \ell \in \mathbb{R}. \end{aligned} \quad (5.6)$$

In the above,

$$\begin{aligned} H^1(\Delta, \mathcal{C}_z \setminus D^\varepsilon) &:= \{u \in H^1(\mathcal{C}_z \setminus D^\varepsilon) : \Delta u \in L^2(\mathcal{C}_z \setminus D^\varepsilon), \quad u = 0 \text{ on } \partial D^\varepsilon, \\ &\quad u(\mathbf{x} + \mathbf{e}_2) = e^{ik_* \|\cdot\|} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_* \|\cdot\|} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_b\}. \end{aligned} \quad (5.7)$$

Moreover,

$$\forall \ell \in \mathbb{R}, \quad \{\mu_{n,\varepsilon}(\ell), n \geq 1\} = \{\lambda_{n,\varepsilon}(\ell), n \geq 1\}, \quad (5.8)$$

and the eigenmodes $u_{n,\varepsilon}(\cdot, \ell)$ are chosen such that

$$\forall \ell \in \mathbb{R}, \quad \{v_{n,\varepsilon}(\cdot, \mathbf{p}(\ell)), n \geq 1\} = \{\alpha_{n,\varepsilon} u_{n,\varepsilon}(\cdot, \mathbf{p}(\ell)), n \geq 1\}, \quad (5.9)$$

where $\alpha_{n,\varepsilon}$ is an ℓ -dependent phase factor. We extended the eigenmodes $u_{n,\varepsilon}$ and $v_{n,\varepsilon}$ to the whole strip Ω^ε as quasi-periodic functions by letting

$$\begin{aligned} u_{n,\varepsilon}(\mathbf{x} + m\mathbf{e}_1, K + \ell\beta_1) &= e^{i(K + \ell\beta_1) \cdot m\mathbf{e}_1} u_{n,\varepsilon}(\mathbf{x}, K + \ell\beta_1), \quad \mathbf{x} \in \mathcal{C}_z \setminus D, \quad m \in \mathbb{Z}, \\ v_{n,\varepsilon}(\mathbf{x} + m\mathbf{e}_1, K + \ell\beta_1) &= e^{i(K + \ell\beta_1) \cdot m\mathbf{e}_1} v_{n,\varepsilon}(\mathbf{x}, K + \ell\beta_1), \quad \mathbf{x} \in \mathcal{C}_z \setminus D, \quad m \in \mathbb{Z}. \end{aligned} \quad (5.10)$$

When $\varepsilon = 0$, for convenience we will abbreviate $D_{n,0}$, $\lambda_{n,0}$, $u_{n,0}$, $\mu_{n,0}$ and $v_{n,0}$ as D_n , λ_n , u_n , μ_n and v_n , respectively.

5.2 The band structure for the periodic strip Ω^ε with a zigzag cross section near λ^*

In this subsection, we derive the band structure for the periodic strip Ω^ε with a zigzag cross section near λ^* . Note that the eigenvalues that solve (5.4) near the Dirac point (λ_*, K) can be obtained from Proposition 4.3 by letting $\mu = 0$. Denoting $L(\varepsilon, \ell) = L(\varepsilon, \ell, 0)$, where $L(\varepsilon, \ell, \mu)$ is defined in (4.12), we have

Lemma 5.1. *Assume $t_* > 0$. For sufficiently small $\ell \in \mathbb{R}$ and $\varepsilon \geq 0$, the eigenvalues for (5.4) are given by*

$$\begin{aligned} \lambda_{1,\pm\varepsilon}(\mathbf{p}(\ell)) &= \lambda_* - \frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} (1 + O(\varepsilon, \ell)), \\ \lambda_{2,\pm\varepsilon}(\mathbf{p}(\ell)) &= \lambda_* + \frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} (1 + O(\varepsilon, \ell)). \end{aligned} \quad (5.11)$$

The L^2 -normalized Bloch modes for the first two bands on the $\pm\varepsilon$ -strips take the following forms

$$\begin{aligned} u_{1,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) &= (w_1 + L(\varepsilon, \ell)w_2 + O(\varepsilon, \ell)) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell)|^2 + O(\varepsilon, \ell)}}, \\ u_{2,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) &= \left(-\overline{L(\varepsilon, \ell)}w_1 + w_2 + O(\varepsilon, \ell) \right) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell)|^2 + O(\varepsilon, \ell)}}, \end{aligned} \quad (5.12)$$

$$\begin{aligned}
u_{1,-\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) &= \left(\overline{L(\varepsilon, \ell)} w_1 + w_2 + O(\varepsilon, \ell) \right) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell)|^2 + O(\varepsilon, \ell)}}, \\
u_{2,-\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) &= (w_1 - L(\varepsilon, \ell) w_2 + O(\varepsilon, \ell)) \frac{1}{\sqrt{1 + |L(\varepsilon, \ell)|^2 + O(\varepsilon, \ell)}}.
\end{aligned} \tag{5.13}$$

Remark 5.2. By Lemma 5.1, when Assumption 2.7 holds in β_1 , for an arbitrary fixed constant $\mathfrak{d} \in (0, 1)$, when $\varepsilon > 0$ is sufficiently small, $-\Delta^{\pm\varepsilon}$ on $\Omega^{\pm\varepsilon}$ attain a common spectral band gap $(\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$.

Remark 5.3. When $\varepsilon > 0$ in Lemma 5.1, observe that $\lambda_{n,\pm\varepsilon}(\mathbf{p}(\ell))$, $n = 1, 2$, are smooth in ℓ . Thus $\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) = \lambda_{n,\pm\varepsilon}(\mathbf{p}(\ell))$ and $v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) = u_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))$.

Setting $\varepsilon = 0$ in Lemma 5.1, we observe that λ_n , $n = 1, 2$, are not smooth at $\ell = 0$. Thus $\mu_n(\mathbf{p}(\ell))$ are obtained by matching different branches of λ_n as shown in the following lemma and illustrated in Figure 5.1.

Lemma 5.4. For sufficiently small $\ell \in \mathbb{R}$,

$$\begin{aligned}
\mu_1(\mathbf{p}(\ell)) &= \lambda_* + \left| \frac{\theta_*}{\gamma_*} \right| \ell (1 + O(\ell)) \quad (\text{increasing in } \ell), \\
\mu_2(\mathbf{p}(\ell)) &= \lambda_* - \left| \frac{\theta_*}{\gamma_*} \right| \ell (1 + O(\ell)) \quad (\text{decreasing in } \ell).
\end{aligned} \tag{5.14}$$

The corresponding Bloch modes can be chosen as

$$\begin{aligned}
v_1(\mathbf{x}; \mathbf{p}(\ell)) &= \left(\frac{\overline{\theta_*}}{|\theta_*|} w_1 - w_2 + O(\ell) \right) \frac{1}{\sqrt{2 + O(\ell)}}, \\
v_2(\mathbf{x}; \mathbf{p}(\ell)) &= \left(\frac{\overline{\theta_*}}{|\theta_*|} w_1 + w_2 + O(\ell) \right) \frac{1}{\sqrt{2 + O(\ell)}}.
\end{aligned} \tag{5.15}$$

Let $v_i := v_i(\mathbf{x}; K)$. It follows that

$$\begin{cases} v_1 = \frac{1}{\sqrt{2}} \left(\frac{\overline{\theta_*}}{|\theta_*|} w_1 - w_2 \right) \\ v_2 = \frac{1}{\sqrt{2}} \left(\frac{\overline{\theta_*}}{|\theta_*|} w_1 + w_2 \right) \end{cases}, \quad \begin{cases} w_1 = \frac{1}{\sqrt{2}} \frac{\theta_*}{|\theta_*|} (v_1 + v_2) \\ w_2 = \frac{1}{\sqrt{2}} (-v_1 + v_2) \end{cases}. \tag{5.16}$$

Remark 5.5. For $n = 1, 2$, there exist ℓ -dependent phase factors α_n such that $\|u_n(\cdot, \mathbf{p}(\ell)) - \alpha_n u_{n,\varepsilon}(\cdot, \mathbf{p}(\ell))\|_{H^1(\mathcal{C}_z)} = O(\varepsilon)$ uniformly for $\ell > 0$ that are sufficiently small; and there exist ℓ -dependent phase factors β_n such that $\|u_n(\cdot, \mathbf{p}(\ell)) - \beta_n u_{n,\varepsilon}(\cdot, \mathbf{p}(\ell))\|_{H^1(\mathcal{C}_z)} = O(\varepsilon)$ uniformly for $\ell < 0$ that are sufficiently small. The same holds when $u_{n,\varepsilon}$ is replaced by $u_{n,-\varepsilon}$.

5.3 The q -sesquilinear form

Define the quasi-periodic Sobolev space on Γ , $\mathcal{H}^s(\Gamma)$, for $s \in \mathbb{R}$ by

$$\mathcal{H}^s(\Gamma) := \left\{ u(\mathbf{x}_0 + t\mathbf{e}_2) = \sum_{n \in \mathbb{Z}} a_n e^{ik_*^* t} e^{i2\pi n t} : \|u\|_{\mathcal{H}^s(\Gamma)}^2 := \sum_{n \in \mathbb{Z}} |a_n|^2 (1 + |n|^2)^s \right\}, \tag{5.17}$$

Here $\mathbf{x}_0 = -\frac{1}{2}\mathbf{e}_1 - \frac{1}{2}\mathbf{e}_2$ is the lower left corner of \mathcal{C}_z .

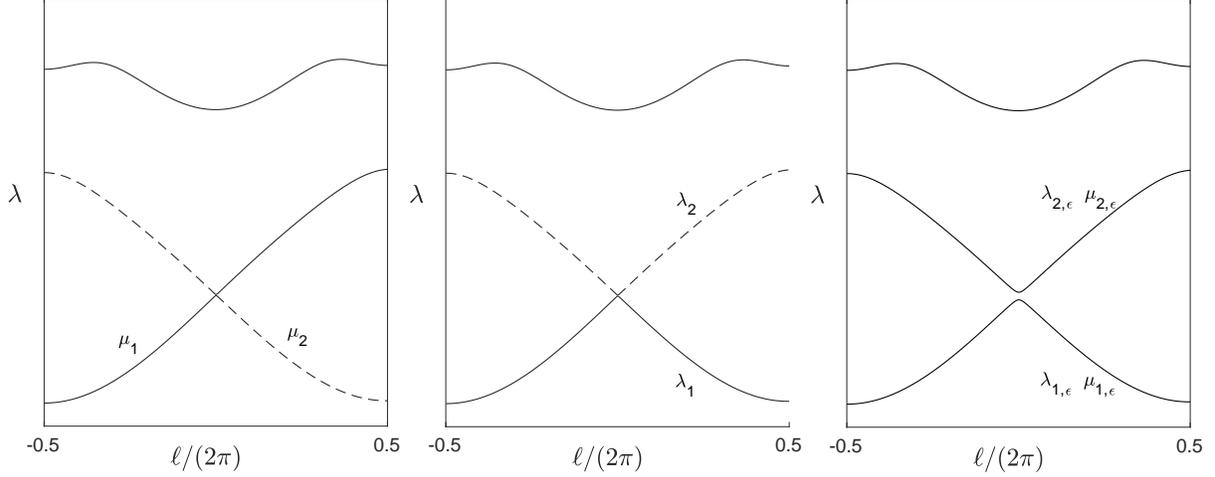


Figure 5.1: The labelings of the band eigenvalues: $\mu_{n,\varepsilon}$ are smooth branches, while $\lambda_{n,\varepsilon}$ are piecewise smooth. When $\varepsilon \neq 0$, $\mu_{n,\varepsilon} = \lambda_{n,\varepsilon}$ for $n = 1, 2$.

Define the q -sesquilinear form on Γ for functions a, b in some neighborhood of Γ with traces in $\mathcal{H}^{1/2}(\Gamma)$ and normal derivatives in $\mathcal{H}^{-1/2}(\Gamma)$:

$$q(a, b) := \overline{\langle \partial_n a, b \rangle_\Gamma} - \langle \partial_n b, a \rangle_\Gamma, \quad (5.18)$$

where ∂_n represents the normal derivative on Γ in the direction $\mathbf{n} = \nu_1 = (\frac{1}{2}, -\frac{\sqrt{3}}{2})$, $\langle \phi, \psi \rangle_\Gamma$ represents the $\mathcal{H}^{-1/2}(\Gamma)$ - $\mathcal{H}^{1/2}(\Gamma)$ pairing (basically $\int_\Gamma \bar{\phi} \psi ds$). The q -sesquilinear form orthogonalized the modes with the same quasimomentum and same energy. That is, if $\mu_n(\mathbf{p}(\ell_0)) = \mu_m(\mathbf{p}(\ell_0))$, then

$$q(v_n(\cdot, \mathbf{p}(\ell_0)), v_m(\cdot, \mathbf{p}(\ell_0))) = 0, \quad m, n \in \{1, 2\}, \quad m \neq n. \quad (5.19)$$

$$q(v_n(\cdot, \mathbf{p}(\ell_0)), v_n(\cdot, \mathbf{p}(\ell_0))) = i \frac{d\mu_n(\mathbf{p}(\ell))}{d\ell} \Big|_{\ell=\ell_0}, \quad n = 1, 2. \quad (5.20)$$

On the unperturbed strip Ω^0 , by Lemma 5.4, $\mu_1(\mathbf{p}(0)) = \mu_2(\mathbf{p}(0)) = \lambda_*$ and $\mathbf{p}(0) = K$, we know

$$q(v_n(\cdot, K), v_m(\cdot, K)) = 0, \quad m, n \in \{1, 2\}, \quad m \neq n. \quad (5.21)$$

$$q(v_n(\cdot, K), v_n(\cdot, K)) = i \frac{d\mu_n(\mathbf{p}(\ell))}{d\ell} \Big|_{\ell=0}, \quad n = 1, 2. \quad (5.22)$$

In addition, $\frac{d\mu_2(\mathbf{p}(\ell))}{d\ell} \Big|_{\ell=0} = -\frac{d\mu_1(\mathbf{p}(\ell))}{d\ell} \Big|_{\ell=0}$. We denote

$$\alpha_* := \left| \frac{d\mu_n(\mathbf{p}(\ell))}{d\ell} \Big|_{\ell=0} \right|, \quad n = 1, 2. \quad (5.23)$$

Remark 5.6. By Lemma 5.4, the derivative α_* defined in (5.23) is given by $\alpha_* = \left| \frac{\theta_*}{\gamma_*} \right|$.

5.4 The Green functions in the periodic strip Ω^ε with a zigzag cross section

In this subsection, we introduce the Green functions in Ω^ε with the quasi-periodic conditions using the limiting absorption principle and spectral representation in Section 5.1. This result extends that in [38].

Consider solving the following problem in Ω^ε :

$$\begin{cases} -\Delta u - (\lambda + i\sigma)u = f & \text{in } \Omega^\varepsilon, \\ u = 0 & \text{on } \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1), \\ u(\mathbf{x} + \mathbf{e}_2) = e^{ik_\parallel^*} u(\mathbf{x}) & \text{for } \mathbf{x} \in \Gamma_-, \\ \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_\parallel^*} \partial_{\nu_2} u(\mathbf{x}) & \text{for } \mathbf{x} \in \Gamma_-, \end{cases} \quad (5.24)$$

where $f \in L^2(\Omega^\varepsilon)$, and σ is a positive constant that converges to 0. The corresponding Green function $G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda)$ satisfies

$$\begin{cases} (-\Delta_{\mathbf{x}} - \lambda)G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda) = \delta(\mathbf{x} - \mathbf{y}) & \mathbf{x} \in \Omega^\varepsilon, \\ G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda) = 0 & \mathbf{x} \in \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1), \\ G^\varepsilon(\mathbf{x} + \mathbf{e}_2, \mathbf{y}; \lambda) = e^{ik_\parallel^*} G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda) & \text{for } \mathbf{x} \in \Gamma_-, \\ \partial_{\nu_2} G^\varepsilon(\mathbf{x} + \mathbf{e}_2, \mathbf{y}; \lambda) = e^{ik_\parallel^*} \partial_{\nu_2} G^\varepsilon(\mathbf{x}, \mathbf{y}; \lambda) & \text{for } \mathbf{x} \in \Gamma_-. \end{cases} \quad (5.25)$$

In addition, the radiation conditions are imposed using the limiting absorption principle.

We will need the Green functions on Ω^0 at the energy λ_* . Recall that λ_* is only an eigenvalue of (5.4) when $\varepsilon = 0$ and $\mathbf{p} = K$, where λ_* is an eigenvalue of (5.4) of multiplicity two. We have

$$\begin{aligned} G^0(\mathbf{x}, \mathbf{y}; \lambda_*) &= \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell + \sum_{n=1,2} \frac{1}{2\pi} \text{p.v.} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell \\ &\quad + \frac{i}{2\alpha_*} \overline{v_1(\mathbf{y}; K)} v_1(\mathbf{x}; K) + \frac{i}{2\alpha_*} \overline{v_2(\mathbf{y}; K)} v_2(\mathbf{x}; K), \quad \mathbf{x}, \mathbf{y} \in \Omega^0, \end{aligned} \quad (5.26)$$

where μ_n and v_n are the eigenvalues and eigenfunctions that are analytic in ℓ as introduced in (5.6). For convenience, we denote the integral portion of the Green function by

$$\tilde{G}^0(\mathbf{x}, \mathbf{y}; \lambda_*) := \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell + \sum_{n=1,2} \frac{1}{2\pi} \text{p.v.} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell. \quad (5.27)$$

When $\mathbf{x} \cdot \mathbf{e}_1 \rightarrow +\infty$, the terms in $G^0(\mathbf{x}, \mathbf{y}; \lambda_*)$ can be regrouped as

$$G^0(\mathbf{x}, \mathbf{y}; \lambda_*) = G^{0,+}(\mathbf{x}, \mathbf{y}; \lambda_*) + \frac{i}{\alpha_*} \overline{v_1(\mathbf{y}; K)} v_1(\mathbf{x}; K), \quad (5.28)$$

where $G^{0,+}(\mathbf{x}, \mathbf{y}; \lambda_*)$ decays exponentially as $\mathbf{x} \cdot \mathbf{e}_1 \rightarrow +\infty$, and is given by

$$G^{0,+}(\mathbf{x}, \mathbf{y}; \lambda_*) := \tilde{G}^0(\mathbf{x}, \mathbf{y}; \lambda_*) - \frac{i}{2\alpha_*} \overline{v_1(\mathbf{y}; K)} v_1(\mathbf{x}; K) + \frac{i}{2\alpha_*} \overline{v_2(\mathbf{y}; K)} v_2(\mathbf{x}; K). \quad (5.29)$$

When $\mathbf{x} \cdot \mathbf{e}_1 \rightarrow -\infty$, the terms in $G^0(\mathbf{x}, \mathbf{y}; \lambda_*)$ can be regrouped as

$$G^0(\mathbf{x}, \mathbf{y}; \lambda_*) = G^{0,-}(\mathbf{x}, \mathbf{y}; \lambda_*) + \frac{i}{\alpha_*} \overline{v_2(\mathbf{y}; K)} v_2(\mathbf{x}; K), \quad (5.30)$$

where $G^{0,-}(\mathbf{x}, \mathbf{y}; \lambda_*)$ decays exponentially as $\mathbf{x} \cdot \mathbf{e}_1 \rightarrow -\infty$, and is given by

$$G^{0,-}(\mathbf{x}, \mathbf{y}; \lambda_*) := \tilde{G}^0(\mathbf{x}, \mathbf{y}; \lambda_*) + \frac{i}{2\alpha_*} \overline{v_1(\mathbf{y}; K)} v_1(\mathbf{x}; K) - \frac{i}{2\alpha_*} \overline{v_2(\mathbf{y}; K)} v_2(\mathbf{x}; K). \quad (5.31)$$

Denote the Green functions in $\Omega^{\pm\varepsilon}$ by $G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)$. For $\lambda \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$, by [38], there holds

$$G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda) = \sum_{n \geq 1} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{v_{n,\pm\varepsilon}(\mathbf{y}; \mathbf{p}(\ell))} v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda} d\ell, \quad \mathbf{x}, \mathbf{y} \in \Omega^0. \quad (5.32)$$

Moreover, $G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)$ decays exponentially as $|\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty$.

Remark 5.7. Note that the q -sesquilinear form and the Green functions are independent of phase factors of the Floquet modes u_n , v_n , $u_{n,\pm\varepsilon}$ and $v_{n,\pm\varepsilon}$.

6 Integral equations for the interface modes along a zigzag interface

In this section, we establish the integral equations for the interface modes at a zigzag interface separating two honeycomb lattices using the layer potentials [16, 60]. This is achieved by matching the Dirichlet and Neumann traces of the wave fields along the interface. Let Γ be the interface two lattices as shown in Figure 2.2 and $\mathbf{n} = (\frac{1}{2}, -\frac{\sqrt{3}}{2})$ be the unit normal vector of Γ pointing to the right. Let $\varepsilon > 0$ and $\lambda \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$, for $(\psi, \phi) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, we define the single and double layer potentials:

$$\begin{aligned} \mathcal{S}^{\pm\varepsilon}(\lambda)\phi(\mathbf{x}) &:= \int_{\Gamma} G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)\phi(\mathbf{y}) ds_{\mathbf{y}}, \quad \mathbf{x} \notin \Gamma, \\ \mathcal{D}^{\pm\varepsilon}(\lambda)\psi(\mathbf{x}) &:= \int_{\Gamma} \partial_{n_{\mathbf{y}}} G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)\psi(\mathbf{y}) ds_{\mathbf{y}} \quad \mathbf{x} \notin \Gamma, \end{aligned} \quad (6.1)$$

where $G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)$ are the Green functions on the $\pm\varepsilon$ -strip defined in (5.32). The single layer potential $\mathcal{S}^{\pm\varepsilon}(\lambda)\phi(\mathbf{x})$ can be continuously extended to Γ and it defines an bounded integer operator from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$, which we still denote by $\mathcal{S}^{\pm\varepsilon}$. Given $(\psi, \phi) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, we also define the integral operators

$$\begin{aligned} \mathcal{K}^{\pm\varepsilon}(\lambda)\psi(\mathbf{x}) &:= \int_{\Gamma} \partial_{n_{\mathbf{y}}} G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)\psi(\mathbf{y}) ds_{\mathbf{y}} \quad \mathbf{x} \in \Gamma, \\ \mathcal{K}^{*,\pm\varepsilon}(\lambda)\phi(\mathbf{x}) &:= \int_{\Gamma} \partial_{n_{\mathbf{x}}} G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)\phi(\mathbf{y}) ds_{\mathbf{y}} \quad \mathbf{x} \in \Gamma. \end{aligned} \quad (6.2)$$

It can be shown that $\mathcal{K}^{\pm\varepsilon} : \mathcal{H}^{1/2}(\Gamma) \rightarrow \mathcal{H}^{1/2}(\Gamma)$ and $\mathcal{K}^* : \mathcal{H}^{-1/2}(\Gamma) \rightarrow \mathcal{H}^{-1/2}(\Gamma)$ are bounded.

By taking the limit of the layer potentials as $\mathbf{x} \rightarrow \Gamma$, the following jump relationship holds [16]:

$$\begin{aligned} [\mathcal{S}^{\varepsilon}\psi(\lambda)]_{\pm} &= \mathcal{S}^{\varepsilon}(\lambda)\psi, \\ [\partial_n \mathcal{S}^{\varepsilon}(\lambda)\psi]_{\pm} &= \mp \frac{1}{2}\psi + \mathcal{K}^{*,\varepsilon}(\lambda)\psi, \\ [\mathcal{D}^{\varepsilon}\phi(\lambda)]_{\pm} &= \pm \frac{1}{2}\phi + \mathcal{K}^{\varepsilon}(\lambda)\phi, \\ [\partial_n \mathcal{D}^{\varepsilon}(\lambda)\phi]_{\pm} &=: \mathcal{N}^{\varepsilon}\phi. \end{aligned} \quad (6.3)$$

In the above, the subscript $-$ and $+$ represent the limit of the layer potentials as $\mathbf{x} \rightarrow \Gamma$ from the left and right side respectively. ∂_n represents the normal derivative, and $\mathcal{N}^{\pm\varepsilon} : H^{1/2}(\Gamma) \rightarrow H^{-1/2}(\Gamma)$ are well-defined bounded operators. In addition, it is clear that the jump relations (6.3) hold when ε is replaced by $-\varepsilon$.

Assume that $u(\mathbf{x})$ is an interface mode of (2.14) with the eigenvalue λ . Let $u|_\Gamma \in \mathcal{H}^{1/2}(\Gamma)$ and $\partial_n u|_\Gamma \in \mathcal{H}^{-1/2}(\Gamma)$ be the traces of u and the normal derivatives of u on Γ . Then by the Green's formula, it can be shown that u attains the following representation in the infinite strip $\Omega^{J,\varepsilon}$:

$$u(\mathbf{x}) = \begin{cases} [\mathcal{D}^\varepsilon(\lambda)u|_\Gamma](\mathbf{x}) - [\mathcal{S}^\varepsilon(\lambda)\partial_n u|_\Gamma](\mathbf{x}) & \text{for } \mathbf{x} \text{ on the right of } \Gamma, \\ -[\mathcal{D}^{-\varepsilon}(\lambda)u|_\Gamma](\mathbf{x}) + [\mathcal{S}^{-\varepsilon}\partial_n u|_\Gamma(\lambda)](\mathbf{x}) & \text{for } \mathbf{x} \text{ on the left of } \Gamma. \end{cases} \quad (6.4)$$

Here we used the fact that $u \in \mathcal{H}^{J,\varepsilon}$, especially the decay of u when $|\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty$ when applying the Green's formula. Taking the limit from either side of Γ , we obtain the following two systems of integral equations:

$$\begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix} = \begin{pmatrix} \mathcal{K}^\varepsilon(\lambda) + \frac{1}{2}\mathcal{I} & -\mathcal{S}^\varepsilon(\lambda) \\ \mathcal{N}^\varepsilon(\lambda) & -\mathcal{K}^{*,\varepsilon}(\lambda) + \frac{1}{2}\mathcal{I} \end{pmatrix} \begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix}, \quad (6.5)$$

and

$$\begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix} = \begin{pmatrix} -\mathcal{K}^{-\varepsilon}(\lambda) + \frac{1}{2}\mathcal{I} & \mathcal{S}^{-\varepsilon}(\lambda) \\ -\mathcal{N}^{-\varepsilon}(\lambda) & \mathcal{K}^{*,-\varepsilon}(\lambda) + \frac{1}{2}\mathcal{I} \end{pmatrix} \begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix}. \quad (6.6)$$

The above is equivalent to the following two systems

$$\begin{pmatrix} -(\mathcal{K}^\varepsilon(\lambda) + \mathcal{K}^{-\varepsilon}(\lambda)) & \mathcal{S}^\varepsilon(\lambda) + \mathcal{S}^{-\varepsilon}(\lambda) \\ -(\mathcal{N}^\varepsilon(\lambda) + \mathcal{N}^{-\varepsilon}(\lambda)) & \mathcal{K}^{*,\varepsilon}(\lambda) + \mathcal{K}^{*,-\varepsilon}(\lambda) \end{pmatrix} \begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix} = 0,$$

and

$$\begin{pmatrix} -\mathcal{K}^\varepsilon(\lambda) + \mathcal{K}^{-\varepsilon}(\lambda) + \mathcal{I} & \mathcal{S}^\varepsilon(\lambda) - \mathcal{S}^{-\varepsilon}(\lambda) \\ -\mathcal{N}^\varepsilon(\lambda) + \mathcal{N}^{-\varepsilon}(\lambda) & \mathcal{K}^{*,\varepsilon}(\lambda) - \mathcal{K}^{*,-\varepsilon}(\lambda) + \mathcal{I} \end{pmatrix} \begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix} = 0. \quad (6.7)$$

It is obvious that u is nontrivial only when $(u|_\Gamma, \partial_n u|_\Gamma)$ is nontrivial.

Conversely, assume $\lambda \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$. Let $(\psi, \phi) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, which is not necessarily the Cauchy data of an interface mode on the interface Γ . We define $u(\mathbf{x})$ in the infinite strip $\Omega^{J,\varepsilon}$ as a combination of single and double layer potentials:

$$u(\mathbf{x}) = \begin{cases} [\mathcal{D}^\varepsilon(\lambda)\psi](\mathbf{x}) - [\mathcal{S}^\varepsilon(\lambda)\phi](\mathbf{x}) & \text{on the right of } \Gamma, \\ -[\mathcal{D}^{-\varepsilon}(\lambda)\psi](\mathbf{x}) + [\mathcal{S}^{-\varepsilon}(\lambda)\phi](\mathbf{x}) & \text{on the left of } \Gamma. \end{cases} \quad (6.8)$$

Since the Green functions $G^{\pm\varepsilon}(\mathbf{x}, \mathbf{y}; \lambda)$ decay as $|\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty$ for λ located in the gap, u defined above is an interface mode if and only if it is nontrivial and its value and normal derivatives are continuous across the interface Γ . Using (6.3), taking the limit of the layer potentials and their normal derivatives as $\mathbf{x} \rightarrow \Gamma$, we obtain the system of integral equations:

$$\begin{pmatrix} \mathcal{K}^\varepsilon(\lambda) + \frac{1}{2}\mathcal{I} & -\mathcal{S}^\varepsilon(\lambda) \\ \mathcal{N}^\varepsilon(\lambda) & -\mathcal{K}^{*,\varepsilon}(\lambda) + \frac{1}{2}\mathcal{I} \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} = \begin{pmatrix} -\mathcal{K}^{-\varepsilon}(\lambda) + \frac{1}{2}\mathcal{I} & \mathcal{S}^{-\varepsilon}(\lambda) \\ -\mathcal{N}^{-\varepsilon}(\lambda) & \mathcal{K}^{*,-\varepsilon}(\lambda) + \frac{1}{2}\mathcal{I} \end{pmatrix} \begin{pmatrix} \psi \\ \phi \end{pmatrix} \neq 0. \quad (6.9)$$

This is equivalent to

$$\begin{pmatrix} -(\mathcal{K}^\varepsilon(\lambda) + \mathcal{K}^{-\varepsilon}(\lambda)) & \mathcal{S}^\varepsilon(\lambda) + \mathcal{S}^{-\varepsilon}(\lambda) \\ -(\mathcal{N}^\varepsilon(\lambda) + \mathcal{N}^{-\varepsilon}(\lambda)) & \mathcal{K}^{*,\varepsilon}(\lambda) + \mathcal{K}^{*,-\varepsilon}(\lambda) \end{pmatrix} (\lambda) \begin{pmatrix} \psi \\ \phi \end{pmatrix} = 0, \quad (6.10)$$

and

$$\begin{pmatrix} \mathcal{K}^\varepsilon(\lambda) - \mathcal{K}^{-\varepsilon}(\lambda) + \mathcal{I} & -\mathcal{S}^\varepsilon(\lambda) + \mathcal{S}^{-\varepsilon}(\lambda) \\ \mathcal{N}^\varepsilon(\lambda) - \mathcal{N}^{-\varepsilon}(\lambda) & -\mathcal{K}^{*,\varepsilon}(\lambda) + \mathcal{K}^{*,-\varepsilon}(\lambda) + \mathcal{I} \end{pmatrix}(\lambda) \begin{pmatrix} \psi \\ \phi \end{pmatrix} \neq 0. \quad (6.11)$$

Define the integral operators on $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$

$$\mathbb{T}^\varepsilon(\lambda) := \begin{pmatrix} -\mathcal{K}^\varepsilon(\lambda) & \mathcal{S}^\varepsilon(\lambda) \\ -\mathcal{N}^\varepsilon(\lambda) & \mathcal{K}^{*,\varepsilon}(\lambda) \end{pmatrix}, \quad (6.12)$$

and

$$\mathbb{T}_s^\varepsilon(\lambda) := \mathbb{T}^\varepsilon + \mathbb{T}^{-\varepsilon}, \quad \mathbb{T}_t^\varepsilon(\lambda) := -\mathbb{T}^\varepsilon + \mathbb{T}^{-\varepsilon} + \mathbb{I}, \quad \mathbb{T}_n^\varepsilon(\lambda) := \mathbb{T}^\varepsilon - \mathbb{T}^{-\varepsilon} + \mathbb{I}, \quad (6.13)$$

where \mathbb{I} is the identity operator. Based on the above discussion, we obtain the following lemma for the characterization of interface modes.

Lemma 6.1. *Let $\lambda \in (\lambda_* - \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$.*

(i) *There exists an interface mode u satisfying (2.16) if and only if there exists $(\psi, \phi) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ such that*

$$\mathbb{T}_s^\varepsilon(\lambda) \begin{pmatrix} \psi \\ \phi \end{pmatrix} = 0, \quad \mathbb{T}_t^\varepsilon(\lambda) \begin{pmatrix} \psi \\ \phi \end{pmatrix} \neq 0. \quad (6.14)$$

Furthermore, each solution to (6.14) yields an interface mode expressed by (6.8).

(ii) *If u is an interface mode satisfying (2.16), then $0 \neq (u|_\Gamma, \partial_n u|_\Gamma) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ satisfies*

$$\mathbb{T}_s^\varepsilon(\lambda) \begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix} = 0, \quad \mathbb{T}_n^\varepsilon(\lambda) \begin{pmatrix} u|_\Gamma \\ \partial_n u|_\Gamma \end{pmatrix} = 0. \quad (6.15)$$

Remark 6.2. *First, suppose that $(\lambda, \psi_i, \phi_i)$ $i = 1, \dots, N$ satisfy (6.14) for some positive integer N . Let u_i be defined by (6.8) correspondingly. When $\{(\psi_i, \phi_i)\}_{i=1, \dots, N}$ are linearly independent, $\{u_i\}_{i=1, \dots, N}$ may be linearly dependent.*

Second, the converse of Lemma 6.1 part (ii) does not hold. That is, a triple (λ, ψ, ϕ) satisfying (6.15) may not produce an interface mode through (6.8).

Third, the subscript for \mathbb{T}_s^ε represents “sufficient”, that for \mathbb{T}_t^ε represents “nontrivial”, and that for \mathbb{T}_n^ε represents “necessary”.

We introduce some notations similar to (6.1)-(6.3) and (6.12). Specifically, for $\varepsilon = 0$, in the infinite strip Ω^0 , we define $\mathcal{S}^0(\lambda_*)$, $\mathcal{D}^0(\lambda_*)$, $\mathcal{K}^0(\lambda_*)$, $\mathcal{K}^{*,0}(\lambda_*)$ and $\mathcal{N}^0(\lambda_*)$ parallel to (6.1)-(6.3) where the Green functions are replaced by $G^0(\mathbf{x}, \mathbf{y}, \lambda_*)$ defined in (5.26), and $\tilde{\mathcal{S}}^0(\lambda_*)$, $\tilde{\mathcal{D}}^0(\lambda_*)$, $\tilde{\mathcal{K}}^0(\lambda_*)$, $\tilde{\mathcal{K}}^{*,0}(\lambda_*)$ and $\tilde{\mathcal{N}}^0(\lambda_*)$, where the Green functions are replaced by $\tilde{G}^0(\mathbf{x}, \mathbf{y}, \lambda_*)$ defined in (5.27). We also define $\mathcal{S}^{0,\pm}(\lambda_*)$, $\mathcal{D}^{0,\pm}(\lambda_*)$, $\mathcal{K}^{0,\pm}(\lambda_*)$, $\mathcal{K}^{*,0,\pm}(\lambda_*)$ and $\mathcal{N}^{0,\pm}(\lambda_*)$, where the Green functions are replaced by $G^{0,\pm}(\mathbf{x}, \mathbf{y}, \lambda_*)$ defined in (5.29) and (5.31). These layer potentials have the jump relations when ε is replaced by 0 and λ is replaced by λ_* in (6.3).

Finally, define the integral operators on $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$

$$\mathbb{T}^0(\lambda_*) := \begin{pmatrix} -\mathcal{K}^0(\lambda_*) & \mathcal{S}^0(\lambda_*) \\ -\mathcal{N}^0(\lambda_*) & \mathcal{K}^{0,*}(\lambda_*) \end{pmatrix} \quad \text{and} \quad \tilde{\mathbb{T}}^0(\lambda_*) := \begin{pmatrix} -\tilde{\mathcal{K}}^0(\lambda_*) & \tilde{\mathcal{S}}^0(\lambda_*) \\ -\tilde{\mathcal{N}}^0(\lambda_*) & \tilde{\mathcal{K}}^{0,*}(\lambda_*) \end{pmatrix}. \quad (6.16)$$

7 The proof of Theorem 2.9

In this section, we investigate interface modes along a zigzag interface using the integral equation formulation in Lemma 6.1. We will first derive the limit of the integral operators, and then apply the generalized Rouché theorem in Gohberg-Sigal theory to investigate the characteristic values of the integral operators.

7.1 The limiting operators for \mathbb{T}^ε , \mathbb{T}_s^ε , \mathbb{T}_t^ε , and \mathbb{T}_n^ε

We derive asymptotic expansions for the integral operators \mathbb{T}^ε , \mathbb{T}_s^ε , \mathbb{T}_t^ε , and \mathbb{T}_n^ε in this subsection. To this end, we first introduce several notations. For $\vec{\phi} = (\psi, \phi) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, let

$$c_i(\vec{\phi}) := \overline{\langle \phi, v_i \rangle_\Gamma} - \langle \partial_n v_i, \psi \rangle_\Gamma, \quad (7.1)$$

where v_i are defined in Remark 5.5. We also denote

$$\vec{v}_i := \begin{pmatrix} v_i|_\Gamma \\ \partial_n v_i|_\Gamma \end{pmatrix}, \quad i = 1, 2, \quad (7.2)$$

and define the operators

$$\mathbb{P}\vec{\phi} := c_1(\vec{\phi})\vec{v}_1 + c_2(\vec{\phi})\vec{v}_2, \quad (7.3)$$

$$\mathbb{Q}\vec{\phi} := c_2(\vec{\phi})\vec{v}_1 + c_1(\vec{\phi})\vec{v}_2. \quad (7.4)$$

Let $\beta(h)$ and $\xi(h)$ be two functions given by

$$\begin{aligned} \beta(h) &:= \frac{1}{2} \left| \frac{\gamma_*}{\theta_*} \right| \frac{h}{\sqrt{(\frac{t_*}{\gamma_*})^2 - h^2}} = \frac{1}{2\alpha_*} \frac{h}{\sqrt{\beta_*^2 - h^2}}, \\ \xi(h) &:= \frac{t_*}{2|\theta_*|} \frac{1}{\sqrt{(\frac{t_*}{\gamma_*})^2 - h^2}} = \frac{\beta_*}{2\alpha_*} \frac{1}{\sqrt{\beta_*^2 - h^2}}, \end{aligned} \quad (7.5)$$

where α_* is defined in Remark 5.6 and $\beta_* := \frac{t_*}{|\theta_*|}$. We have the following lemma for the limit of the integral operator $\mathbb{T}^{\pm\varepsilon}$ as $\varepsilon \rightarrow 0$.

Proposition 7.1. *Let Assumption 2.7 holds along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. Then the following limit holds uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$:*

$$\mathbb{T}^{\pm\varepsilon}(\lambda_* + \varepsilon h) \rightarrow \tilde{\mathbb{T}}^0(\lambda_*) + \beta(h)\mathbb{P} \mp \xi(h)\mathbb{Q} =: \mathbb{U}^\pm(h), \quad (7.6)$$

where the convergence is understood with the operator norm from $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$.

The proof of the proposition is presented in Appendix C. It is based on the representation of the Green functions in the infinite strip in terms of the band modes [38]:

$$\mathcal{S}^{\pm\varepsilon}(\lambda)\phi = \sum_{n \geq 1} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, v_{n, \pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle_\Gamma} v_{n, \pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n, \pm\varepsilon}(\mathbf{p}(\ell)) - \lambda} d\ell, \quad (7.7)$$

$$\mathcal{K}^{\pm\varepsilon}(\lambda)\psi = \sum_{n \geq 1} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\langle \partial_n v_{n, \pm\varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle_\Gamma v_{n, \pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n, \pm\varepsilon}(\mathbf{p}(\ell)) - \lambda} d\ell, \quad (7.8)$$

$$\mathcal{K}^{*,\pm\varepsilon}(\lambda)\phi = \sum_{n \geq 1} \frac{1}{2\pi} \int_{[-\pi,\pi]} \frac{\overline{\langle \phi, v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle_{\Gamma}} \partial_n v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda} d\ell, \quad (7.9)$$

$$\mathcal{N}^{\pm\varepsilon}(\lambda)\psi = \partial_n \left(\sum_{n \geq 1} \frac{1}{2\pi} \int_{[-\pi,\pi]} \frac{\langle \partial_n v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle_{\Gamma} v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda} d\ell, \right) \quad (7.10)$$

and

$$\tilde{\mathcal{S}}^0(\lambda)\phi = \left(\sum_{n \geq 3} + \sum_{n=1,2} \text{p.v.} \right) \frac{1}{2\pi} \int_{[-\pi,\pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle_{\Gamma}} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda} d\ell, \quad (7.11)$$

$$\tilde{\mathcal{K}}^0(\lambda)\psi = \left(\sum_{n \geq 3} + \sum_{n=1,2} \text{p.v.} \right) \frac{1}{2\pi} \int_{[-\pi,\pi]} \frac{\langle \partial_n v_n(\cdot; \mathbf{p}(\ell)), \psi \rangle_{\Gamma} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda} d\ell, \quad (7.12)$$

$$\tilde{\mathcal{K}}^{*,0}(\lambda)\phi = \left(\sum_{n \geq 3} + \sum_{n=1,2} \text{p.v.} \right) \frac{1}{2\pi} \int_{[-\pi,\pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle_{\Gamma}} \partial_n v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda} d\ell, \quad (7.13)$$

$$\tilde{\mathcal{N}}^0(\lambda)\psi = \partial_n \left(\left(\sum_{n \geq 3} + \sum_{n=1,2} \text{p.v.} \right) \frac{1}{2\pi} \int_{[-\pi,\pi]} \frac{\langle \partial_n v_n(\cdot; \mathbf{p}(\ell)), \psi \rangle_{\Gamma} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda} d\ell \right). \quad (7.14)$$

Corollary 7.2. *Let Assumption 2.7 hold along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. The following limits hold under the operator norm from $\mathcal{H}^{-1/2}(\Gamma) \times \mathcal{H}^{1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d} |\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$:*

$$\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h) = \mathbb{U}_s(h) + \mathbb{R}_1(h, \varepsilon), \quad (7.15)$$

$$\mathbb{T}_t^\varepsilon(\lambda_* + \varepsilon h) = \mathbb{U}_t(h) + \mathbb{R}_2(h, \varepsilon), \quad (7.16)$$

$$\mathbb{T}_n^\varepsilon(\lambda_* + \varepsilon h) = \mathbb{U}_n(h) + \mathbb{R}_3(h, \varepsilon). \quad (7.17)$$

Here the limiting operators are

$$\mathbb{U}_s(h) := 2\tilde{\mathbb{T}}^0(\lambda_*) + 2\beta(h)\mathbb{P}, \quad \mathbb{U}_t(h) := \mathbb{I} + 2\xi(h)\mathbb{Q}, \quad \mathbb{U}_n(h) := \mathbb{I} - 2\xi(h)\mathbb{Q}, \quad (7.18)$$

and the remainder terms have the estimate $\|\mathbb{R}_i(h, \varepsilon)\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma) \rightarrow \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)} = o(1)$ as $\varepsilon \rightarrow 0^+$ uniformly for $|h| < \mathfrak{d} |\frac{t_*}{\gamma_*}|$, $i = 1, 2, 3$.

7.2 Properties of the limiting operators \mathbb{U}_s , \mathbb{U}_t and \mathbb{U}_n

Using the definition of c_i in (7.1), the definition of the q-sesquilinear form (5.18), and the relations (5.21) and (5.22), we obtain

$$\begin{aligned} c_1(\vec{v}_1) &= q(v_1, v_1) = \overline{\langle \partial_n v_1, v_1 \rangle_{\Gamma}} - \langle \partial_n v_1, v_1 \rangle_{\Gamma} = i\alpha_*, \\ c_2(\vec{v}_2) &= q(v_2, v_2) = \overline{\langle \partial_n v_2, v_2 \rangle_{\Gamma}} - \langle \partial_n v_2, v_2 \rangle_{\Gamma} = -i\alpha_*, \\ c_i(\vec{v}_j) &= q(v_j, v_i) = \overline{\langle \partial_n v_j, v_i \rangle_{\Gamma}} - \langle \partial_n v_i, v_j \rangle_{\Gamma} = 0 \text{ for } i \neq j, \end{aligned} \quad (7.19)$$

where \vec{v}_i are defined in (7.2). Define the function spaces

$$X := \text{span}\{\vec{v}_1, \vec{v}_2\}, \quad Y := \{\vec{\phi} \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)\}, c_i(\vec{\phi}) = 0, i = 1, 2\}. \quad (7.20)$$

Then Y is the orthogonal complement of X in the sense of dual spaces. We let

$$P_Y(\vec{\phi}) := \vec{\phi} - \frac{c_1(\vec{\phi})}{i\alpha_*} \vec{v}_1 - \frac{c_2(\vec{\phi})}{-i\alpha_*} \vec{v}_2. \quad (7.21)$$

Since $c_i(P_Y(\vec{\phi})) = 0$, $i = 1, 2$, we obtain the following direct sum decomposition:

$$\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma) = X \oplus Y. \quad (7.22)$$

The following fact will be used repeatedly in the sequel. (7.19) implies that \vec{v}_1 and \vec{v}_2 are linearly independent. For the operators defined in (7.3) and (7.4), there holds

$$\mathbb{P}\vec{v}_1 = i\alpha_*\vec{v}_1, \quad \mathbb{P}\vec{v}_2 = -i\alpha_*\vec{v}_2, \quad \mathbb{Q}\vec{v}_1 = i\alpha_*\vec{v}_2, \quad \mathbb{Q}\vec{v}_2 = -i\alpha_*\vec{v}_1, \quad (7.23)$$

and

$$\mathbb{P}Y = \mathbb{Q}Y = 0. \quad (7.24)$$

Lemma 7.3. *The kernel and range of the operator $\tilde{\mathbb{T}}^0$ are*

$$\text{Ker } \tilde{\mathbb{T}}^0(\lambda_*) = X, \quad \text{Ran } \tilde{\mathbb{T}}^0(\lambda_*) = Y. \quad (7.25)$$

Proof. We first show $X \subset \text{Ker}(\tilde{\mathbb{T}}^0(\lambda_*))$. To this end, we establish the following relations:

$$\tilde{\mathbb{T}}^0(\lambda_*)\vec{v}_1 = \left(\mathbb{T}^0(\lambda_*) + \frac{1}{2}\mathbb{I} \right) \vec{v}_1, \quad \tilde{\mathbb{T}}^0(\lambda_*)\vec{v}_2 = \left(\mathbb{T}^0(\lambda_*) - \frac{1}{2}\mathbb{I} \right) \vec{v}_2. \quad (7.26)$$

We see that

$$\begin{aligned} & -\mathcal{K}^0(\lambda_*)(v_1|_\Gamma)(\mathbf{x}) + \mathcal{S}^0(\lambda_*)(\partial_n v_1|_\Gamma)(\mathbf{x}) \\ &= -\tilde{\mathcal{K}}^0(\lambda_*)(v_1|_\Gamma)(\mathbf{x}) - \frac{i}{2\alpha_*} (v_1(\mathbf{x})\langle \partial_n v_1, v_1 \rangle + v_2(\mathbf{x})\langle \partial_n v_2, v_1 \rangle) \\ & \quad + \tilde{\mathcal{S}}^0(\lambda_*)(\partial_n v_1|_\Gamma)(\mathbf{x}) + \frac{i}{2\alpha_*} (v_1(\mathbf{x})\overline{\langle v_1, \partial_n v_1 \rangle} + v_2(\mathbf{x})\overline{\langle v_2, \partial_n v_1 \rangle}), \quad \mathbf{x} \in \Gamma. \end{aligned} \quad (7.27)$$

Using (7.19), we obtain

$$\begin{aligned} & -\mathcal{K}^0(\lambda_*)(v_1|_\Gamma)(\mathbf{x}) + \mathcal{S}^0(\lambda_*)(\partial_n v_1|_\Gamma)(\mathbf{x}) \\ &= -\tilde{\mathcal{K}}^0(\lambda_*)(v_1|_\Gamma)(\mathbf{x}) + \tilde{\mathcal{S}}^0(\lambda_*)(\partial_n v_1|_\Gamma)(\mathbf{x}) - \frac{1}{2}v_1(\mathbf{x}), \quad \mathbf{x} \in \Gamma. \end{aligned} \quad (7.28)$$

Hence, the first relation in (7.26) holds, and the other relation can be shown similarly.

Next we show that

$$\left(\mathbb{T}^0(\lambda_*) + \frac{1}{2} \right) \vec{v}_1 = 0, \quad \left(\mathbb{T}^0(\lambda_*) - \frac{1}{2} \right) \vec{v}_2 = 0. \quad (7.29)$$

For each constant $A \in \mathbb{R}$, define $\Gamma_A := \Gamma + A\mathbf{e}_1$. Integrating by parts, we obtain when $A > 0$ and \mathbf{x} is between Γ and Γ_A ,

$$v_i(\mathbf{x}) = \mathcal{D}^0(\lambda_*)(v_i|_\Gamma)(\mathbf{x}) - \mathcal{S}^0(\lambda_*)(\partial_n v_i|_\Gamma)(\mathbf{x}) + \left(-\mathcal{D}_A^0(\lambda_*)(v_i|_{\Gamma_A})(\mathbf{x}) + \mathcal{S}_A^0(\lambda_*)(\partial_n v_i|_{\Gamma_A})(\mathbf{x}) \right), \quad (7.30)$$

and when $A < 0$ and \mathbf{x} is between Γ and Γ_A ,

$$v_i(\mathbf{x}) = -\mathcal{D}^0(\lambda_*)(v_i|_\Gamma)(\mathbf{x}) + \mathcal{S}^0(\lambda_*)(\partial_n v_i|_\Gamma)(\mathbf{x}) + \left(\mathcal{D}_A^0(\lambda_*)(v_i|_{\Gamma_A})(\mathbf{x}) - \mathcal{S}_A^0(\lambda_*)(\partial_n v_i|_{\Gamma_A})(\mathbf{x}) \right). \quad (7.31)$$

Here $\mathcal{S}_A^0(\lambda_*)$ and $\mathcal{D}_A^0(\lambda_*)$ represents the single and double layer potentials with kernel $G^0(\mathbf{x}, \mathbf{y}; \lambda_*)$ as defined in (5.26) and normal derivative in the direction \mathbf{n} . Set $i = 2$ in (7.30). By the relation (5.28), the decay of $G^{0,+}(\mathbf{x}, \mathbf{y}; \lambda_*)$ and (7.19), the limit of (7.30) when $A \rightarrow +\infty$ gives

$$v_2(\mathbf{x}) = \mathcal{D}^0(v_2|_\Gamma)(\mathbf{x}) - \mathcal{S}^0(\partial_n v_2|_\Gamma)(\mathbf{x}), \quad \mathbf{x} \text{ is to the right of } \Gamma. \quad (7.32)$$

Taking the trace and normal derivative of v_2 from the right of Γ , we obtain the first relation in (7.29). The second equation can be similarly obtained by setting $i = 1$ in (7.31). Combining (7.26) and (7.29), we obtain $X \subset \text{Ker}(\tilde{\mathbb{T}}^0(\lambda_*))$.

The relation $\text{Ker} \tilde{\mathbb{T}}^0(\lambda_*) \subset X$ follows from Lemma 7.4 and the fact that $-\Delta^0$ does not have eigenvalues in the unperturbed strip.

For the range of $\tilde{\mathbb{T}}^0$, we observe

$$\text{Ran } \tilde{\mathbb{T}}^0(\lambda_*) = \left\{ (\psi_1, \phi_1) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma), \overline{\langle \phi_1, \psi_2 \rangle_\Gamma} + \langle \phi_2, \psi_1 \rangle_\Gamma = 0 \text{ for all } (\psi_2, \phi_2) \in \text{Ker} \left(\tilde{\mathbb{T}}^0(\lambda_*) \right)^* \right\}. \quad (7.33)$$

It is straightforward to verify that

$$\left(\tilde{\mathbb{T}}^0(\lambda_*) \right)^* = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tilde{\mathbb{T}}^0(\lambda_*) \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \quad (7.34)$$

Thus

$$\text{Ran } \tilde{\mathbb{T}}^0(\lambda_*) = \left\{ (\psi_1, \phi_1) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma), \overline{\langle \phi_1, \psi_2 \rangle_\Gamma} - \langle \phi_2, \psi_1 \rangle_\Gamma = 0 \text{ for all } (\psi_2, \phi_2) \in \text{Ker } \tilde{\mathbb{T}}^0(\lambda_*) \right\} = Y. \quad (7.35)$$

□

Lemma 7.4. *Suppose $\vec{\phi} \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ satisfies*

$$\tilde{\mathbb{T}}^0(\lambda_*)\vec{\phi} = 0, \quad \vec{\phi} \in Y \text{ (or } c_i(\vec{\phi}) = 0, i = 1, 2). \quad (7.36)$$

Define

$$u(\mathbf{x}) = \begin{cases} [\mathcal{D}^0(\lambda_*)\psi](\mathbf{x}) - [\mathcal{S}^0(\lambda_*)\phi](\mathbf{x}) & \text{on the right of } \Gamma, \\ -[\mathcal{D}^0(\lambda_*)\psi](\mathbf{x}) + [\mathcal{S}^0(\lambda_*)\phi](\mathbf{x}) & \text{on the left of } \Gamma. \end{cases} \quad (7.37)$$

Then $u \in H^1(\Omega^0)$ is an eigenfunction of $-\Delta$ in Ω^0 with eigenvalue λ_* .

Proof. We only need to show that u and $\partial_n u$ are continuous across Γ , u is nonzero, and it decays as $|\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty$.

We first verify the continuity of u and its normal derivatives across Γ . Observe that

$$\mathbb{T}^0(\lambda_*)\vec{\phi} = \tilde{\mathbb{T}}^0(\lambda_*)\vec{\phi} + \frac{i}{2\alpha_*} c_1(\vec{\phi})\vec{v}_1 + \frac{i}{2\alpha_*} c_2(\vec{\phi})\vec{v}_2 = 0. \quad (7.38)$$

Using the relations

$$\begin{pmatrix} u|_\Gamma^+ \\ \partial_n u|_\Gamma^+ \end{pmatrix} = \left(\frac{1}{2}\mathbb{I} - \frac{1}{2}\mathbb{T}^0(\lambda_*) \right) \vec{\phi} = \frac{1}{2}\vec{\phi}, \quad \begin{pmatrix} u|_\Gamma^- \\ \partial_n u|_\Gamma^- \end{pmatrix} = \left(\frac{1}{2}\mathbb{I} + \frac{1}{2}\mathbb{T}^0(\lambda_*) \right) \vec{\phi} = \frac{1}{2}\vec{\phi}, \quad (7.39)$$

we obtain that the jumps in u and $\partial_n u$ are both 0 across Γ and u is nonzero.

Using relations (5.29) and (5.31), we obtain for $\mathbf{x} \cdot \mathbf{e}_1 \rightarrow +\infty$

$$\mathcal{D}^0(\lambda_*)\psi - \mathcal{S}^0(\lambda_*)\phi = \mathcal{D}^{0,+}(\lambda_*)\psi - \mathcal{S}^{0,+}(\lambda_*)\phi + \frac{i}{\alpha_*}c_1(\vec{\phi})v_1 = \mathcal{D}^{0,+}(\lambda_*)\psi - \mathcal{S}^{0,+}(\lambda_*), \quad (7.40)$$

and for $\mathbf{x} \cdot \mathbf{e}_1 \rightarrow -\infty$

$$-\mathcal{D}^0(\lambda_*)\psi + \mathcal{S}^0(\lambda_*)\phi = -\mathcal{D}^{0,-}(\lambda_*)\psi + \mathcal{S}^{0,-}(\lambda_*)\phi + \frac{i}{\alpha_*}c_2(\vec{\phi})v_2 = \mathcal{D}^{0,-}(\lambda_*)\psi - \mathcal{S}^{0,-}(\lambda_*). \quad (7.41)$$

Thus u decays exponentially as $|\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty$. We conclude $u \in H^1(\Omega^0)$ and the proof is complete. \square

Proposition 7.5. *The following holds for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$:*

(i) *The operator $\mathbb{U}_s(h)$ defined in (7.15) is analytic in h and it is a Fredholm operator with index zero.*

(ii) *The only characteristic value of $\mathbb{U}_s(h)$ is $h = 0$, and the kernel of $\mathbb{U}_s(0)$ is given by*

$$\text{Ker } \mathbb{U}_s(0) = \text{span}\{\vec{v}_1, \vec{v}_2\} = X. \quad (7.42)$$

The multiplicity of the characteristic $h = 0$ is 2.

Proof. (i) The operator $\mathbb{T}^0(\lambda_*)$ is a Fredholm operator with index zero because S^0 and N^0 are Fredholm operators with index zero [60, 66] and the operators K^0 and $K^{*,0}$ are compact. Therefore, in view of the relation between $\mathbb{T}^0(\lambda_*)$ and $\tilde{\mathbb{T}}^0(\lambda_*)$ in (7.38) and the fact that the operator \mathbb{P} is compact, we conclude that $\mathbb{U}_s(0)$ is a Fredholm operator with index zero.

(ii) Note that $\beta(0) = 0$, we see that $h = 0$ is a characteristic value of $\mathbb{U}_s(h)$, with $\text{Ker } \mathbb{U}_s(0) = \text{Ker } \tilde{\mathbb{T}}^0(\lambda_*) = X$ by Lemma 7.3. Now we assume $h \neq 0$ is a characteristics of $\mathbb{U}_s(h)$. Then there exists a nontrivial $\vec{\phi}$ that satisfies

$$\left(2\tilde{\mathbb{T}}^0(\lambda_*) + 2\beta(h)\mathbb{P}\right)\vec{\phi} = 0. \quad (7.43)$$

Since $\text{Ran } \mathbb{P} = X$, $\text{Ran } \tilde{\mathbb{T}}^0(\lambda_*) = Y$ and $X \cap Y = \emptyset$, it follows that $\mathbb{P}\vec{\phi} = 0$, which in turn implies $\vec{\phi} = 0$. Thus $h = 0$ is the only characteristic.

The multiplicity of $h = 0$ is at least two, since $\text{Ker } \mathbb{U}_s(0) = \text{Ker } \tilde{\mathbb{T}}^0(\lambda_*) = X$ is two dimensional. We next show that every $\phi \in X$ is an eigenfunction of $\mathbb{U}_s(0)$ of rank 1 (see Appendix A for the definition of rank used here). Let $\vec{\phi}(h)$ be a family of functions in $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ that are analytic in a neighborhood of $h = 0$, and $\vec{\phi} := \vec{\phi}(0) \in \text{Ker } \mathbb{U}_s(0)$. We obtain

$$\frac{d(\mathbb{U}_s(h)\vec{\phi}(h))}{dh}\Big|_{h=0} = \frac{d\mathbb{U}_s(h)}{dh}\Big|_{h=0}\vec{\phi} + \mathbb{U}_s(0)\vec{\phi}'(0) = \frac{1}{\alpha_*\beta_*}\mathbb{P}\vec{\phi} + \mathbb{U}_s(0)\vec{\phi}'(0), \quad (7.44)$$

where we used (7.18) in the last equality above. Since $\text{Ran } \mathbb{P} \subset X$, $\text{Ran } \mathbb{U}_s(0) = \text{Ran } \tilde{\mathbb{T}}^0 = Y$ and $X \cap Y = \emptyset$, we deduce that (7.44) is nonzero unless $\mathbb{P}\vec{\phi} = 0$, which in turn implies $\vec{\phi} = 0$. That is, every $\vec{\phi} \in \text{Ker } \mathbb{U}_s(0)$ has rank 1, thus the multiplicity is exactly two. \square

Proposition 7.6. *Let $h \in \mathbb{C}$ and $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$. The operators $\mathbb{U}_n(h)$ and $\mathbb{U}_t(h)$ defined in (7.17) and (7.16) are analytic in h and are Fredholm operators with index zero. The only characteristic value of each operator is $h = 0$ with a multiplicity of 2. In addition, the kernel of $\mathbb{U}_n(0)$ and $\mathbb{U}_t(0)$ are given by*

$$\text{Ker } \mathbb{U}_n(0) = \text{span}\{\vec{v}_1 + \vec{w}_2\} \quad \text{and} \quad \text{Ker } \mathbb{U}_t(0) = \text{span}\{\vec{v}_1 - \vec{w}_2\} \quad (7.45)$$

respectively.

Proof. Since the structures of $\mathbb{U}_n(h)$ and $\mathbb{U}_t(h)$ are similar, we only give the proof of the claims for $\mathbb{U}_n(h)$.

It is obvious that the operator $\mathbb{U}_n(h)$ is a Fredholm operator since \mathbb{Q} is a finite-rank operator. Observe that for all h , $\mathbb{U}_n(h)|_Y = \mathbb{I}_Y$, thus $\text{Ker } \mathbb{U}_n(h) \subset X$. Under the basis $\{\vec{v}_1, \vec{v}_2\}$ of X , using (7.23), we obtain $\vec{\phi} = a\vec{v}_1 + b\vec{v}_2 \in \text{Ker } \mathbb{U}_n(h)$ if and only if

$$\begin{pmatrix} 1 & 2i\xi(h)\alpha_* \\ -2i\xi(h) & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0. \quad (7.46)$$

It is easy to verify that the determinant of the matrix $1 - 4\alpha_*^2(\xi(h))^2$ is zero if and only if $h = 0$ by (7.5). When $h = 0$, $(a, b) = (1, i)$ spans the kernel since $\xi(0) = \frac{1}{2\alpha_*}$.

For the multiplicity of $h = 0$, we observe

$$\mathbb{U}_n(h)|_{h=0} = \mathbb{I} - \frac{1}{\alpha_*}\mathbb{Q}, \quad \frac{d\mathbb{U}_n(h)}{dh}|_{h=0} = 0, \quad \frac{d^2\mathbb{U}_n(h)}{dh^2}|_{h=0} = -\frac{1}{\alpha_*\beta_*^2}\mathbb{Q}. \quad (7.47)$$

Let $\vec{\phi}(h)$ be a family of $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ operators that is analytic in a neighborhood of $h = 0$, and $\vec{\phi} := \vec{\phi}(0) \in \text{Ker } \mathbb{U}_n(0)$. Then

$$\frac{d(\mathbb{U}_n(h)\vec{\phi}(h))}{dh}|_{h=0} = \mathbb{U}_n(0)\vec{\phi}'(0) = 0 \quad (7.48)$$

can be satisfied by the choice $\vec{\phi}'(0) = \vec{\phi}(0)$. The second derivative is given by

$$\frac{d^2(\mathbb{U}_n(h)\vec{\phi}(h))}{dh^2}|_{h=0} = -\frac{1}{\alpha_*\beta_*^2}\mathbb{Q}\vec{\phi} + (\mathbb{I} - \frac{1}{\alpha_*}\mathbb{Q})\vec{\phi}''(0). \quad (7.49)$$

To make the second derivative zero, $\vec{\phi}''(0)$ must be in $X \supset \text{Ran}(\mathbb{Q})$. Let $\vec{\phi}''(0) = a\vec{v}_1 + b\vec{v}_2$. Then (7.49) is zero if and only if

$$\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\beta_*^2} \begin{pmatrix} 1 \\ i \end{pmatrix}. \quad (7.50)$$

This equation has no solution (not even trivial) because the right-hand side is not in the range of the matrix on the left-hand side. Thus $h = 0$ is a characteristic of multiplicity two. \square

7.3 The characteristic values for the operators \mathbb{T}_s^ε , \mathbb{T}_n^ε and \mathbb{T}_t^ε

Lemma 7.7. *Let Assumption 2.7 hold along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. For sufficiently small positive ε and $|h_0| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, the following holds:*

(i) *The operator*

$$2\tilde{\mathbb{T}}^0(\lambda_*) + P_Y\mathbb{R}_1(h, \varepsilon) : Y \rightarrow Y \quad (7.51)$$

is invertible, where P_Y is the projection defined in (7.21), and $\mathbb{R}_1(h, \varepsilon)$ is the remainder defined in Corollary 7.2.

(ii) *Denote the inverse of the operator in (7.51) by $A(h, \varepsilon) : Y \rightarrow Y$. For each $\vec{\phi}_0 \in X$, define*

$$J_1(h, \varepsilon)[\vec{\phi}_0] = -A(h_0, \varepsilon)P_Y\mathbb{R}_1(h, \varepsilon)\vec{\phi}_0. \quad (7.52)$$

If $\vec{\phi} \in \text{Ker}(\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h_0))$, then

$$\vec{\phi} = \vec{\phi}_0 + J_1(h_0, \varepsilon)[\vec{\phi}_0], \quad (7.53)$$

for some $\vec{\phi}_0 \in X$. Moreover,

$$\|J_1(h, \varepsilon)[\vec{\phi}_0]\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)} = o(1) \cdot \|\vec{\phi}_0\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)} \quad (7.54)$$

uniformly for $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$.

Proof. The invertibility of (7.51) follows from the observation that $2\tilde{\mathbb{T}}^0(\lambda_*) : Y \rightarrow Y$ is invertible and $\|\mathbb{R}_1(h, \varepsilon)\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma) \rightarrow \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)}$ is of order $o(1)$ uniformly for $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$. In addition, the norm for its inverse $\|A(h, \varepsilon)\|_{Y \rightarrow Y} = O(1)$ uniformly for $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$.

If $\vec{\phi} \in \text{Ker}(\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h_0))$, by (7.22) and Corollary 7.2, we have the decomposition

$$\vec{\phi} = \vec{\phi}_0 + \vec{\phi}_1, \quad \vec{\phi}_0 \in X, \quad \vec{\phi}_1 \in Y, \quad (7.55)$$

and

$$\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h_0) = 2\tilde{\mathbb{T}}^0(\lambda_*) + 2\beta(h_0)\mathbb{P} + \mathbb{R}_1(h_0, \varepsilon). \quad (7.56)$$

As such

$$\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h_0)\vec{\phi} = (2\tilde{\mathbb{T}}^0(\lambda_*) + 2\beta(h_0)\mathbb{P} + \mathbb{R}_1(h_0, \varepsilon))(\vec{\phi}_0 + \vec{\phi}_1) = 0. \quad (7.57)$$

Projecting into Y by P_Y , we obtain

$$(2\tilde{\mathbb{T}}^0(\lambda_*) + P_Y\mathbb{R}_1(h_0, \varepsilon))\vec{\phi}_1 + P_Y\mathbb{R}_1(h_0, \varepsilon)\vec{\phi}_0 = 0. \quad (7.58)$$

Thus $\vec{\phi}_1 = J_1(h_0, \varepsilon)[\vec{\phi}_0]$, and the proof is complete. \square

Lemma 7.8. *Let Assumption 2.7 holds along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. For sufficiently small positive ε , and for $|h_0| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, every nontrivial $\vec{\phi} \in \text{Ker}(\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h_0))$ is of rank 1.*

Proof. The goal is to prove that for all $\vec{\phi}(h) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, analytic in h with $\vec{\phi}(h_0) = \vec{\phi}$, there holds

$$\frac{d(\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h)\vec{\phi}(h))}{dh}\Big|_{h=h_0} \neq 0. \quad (7.59)$$

To this end, we only need to show that there is no $\vec{\psi} \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, such that

$$\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h_0)\vec{\psi} + \frac{d(\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h))}{dh}\Big|_{h=h_0}\vec{\phi} = 0. \quad (7.60)$$

Taking the $\mathcal{H}^{-1/2}(\Gamma) \times \mathcal{H}^{1/2}(\Gamma)$ - $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ innerproduct with $\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \vec{\phi}$, we obtain

$$\left\langle \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \vec{\phi}, (2\beta'(h_0)\mathbb{P} + \partial_h \mathbb{R}_1(h_0, \varepsilon))\vec{\phi} \right\rangle_{\mathcal{H}^{-1/2}(\Gamma) \times \mathcal{H}^{1/2}(\Gamma), \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)} = 0, \quad (7.61)$$

where we have used (7.34). Using the Cauchy integral representation of the h partial derivative

$$\partial_h \mathbb{R}_1(h, \varepsilon) = \frac{1}{2\pi i} \int_{|z|=\frac{1+\varepsilon}{2}} \frac{R_1(z, \varepsilon)}{(z-h)^2} dz. \quad (7.62)$$

Thus

$$\|\partial_h \mathbb{R}_1(h, \varepsilon)\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma) \rightarrow \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)} = o(1) \quad (7.63)$$

uniformly for $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$, since $\|\mathbb{R}_1(h, \varepsilon)\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma) \rightarrow \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)}$ is of $o(1)$ uniformly for $|h| < \frac{1+\mathfrak{d}}{2}|\frac{t_*}{\gamma_*}|$ when $\varepsilon > 0$ is sufficiently small. Writing $\vec{\phi}$ in the form of (7.53) with $\vec{\phi}_0 = a\vec{v}_1 + b\vec{v}_2$ for $a, b \in \mathbb{C}$, we obtain

$$2\beta'(h_0)i\alpha_*^2(|a|^2 + |b|^2) + o(1) = 0. \quad (7.64)$$

Since $|\beta'(h_0)| > |\frac{1}{2\alpha_*\beta_*}|$ for $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, the above equation never holds when $\varepsilon > 0$ is sufficiently small unless $a = b = 0$. By (7.53), $\vec{\phi}_0 = 0$, which contradicts that $\vec{\phi}$ is nontrivial. The proof is complete. \square

To study the operators \mathbb{T}_t and \mathbb{T}_n , we decompose the space X further using the basis

$$\mathbf{u}_1 := \vec{v}_1 + i\vec{v}_2, \quad \mathbf{u}_2 := \vec{v}_1 - i\vec{v}_2. \quad (7.65)$$

Define

$$X_i := \text{span}\{\mathbf{u}_i\}, \quad i = 1, 2. \quad (7.66)$$

Then

$$X = X_1 \oplus X_2, \quad \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma) = X_1 \oplus X_2 \oplus Y. \quad (7.67)$$

It follows that

$$\mathbb{P}\mathbf{u}_1 = i\alpha_*\mathbf{u}_2, \quad \mathbb{P}\mathbf{u}_2 = i\alpha_*\mathbf{u}_1, \quad \mathbb{Q}\mathbf{u}_1 = \alpha_*\mathbf{u}_1, \quad \mathbb{Q}\mathbf{u}_2 = -\alpha_*\mathbf{u}_2, \quad \mathbb{P}Y = \mathbb{Q}Y = 0. \quad (7.68)$$

Similar to Lemma 7.7, we have the following characterization of the root functions of $\mathbb{T}_t^\varepsilon(\lambda_* + \varepsilon h_0)$ and $\mathbb{T}_n^\varepsilon(\lambda_* + \varepsilon h_0)$. We will only give the proof of Lemma 7.9 as that of Lemma 7.10 is the same.

Lemma 7.9. *Let Assumption 2.7 holds along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. The following holds for sufficiently small $\varepsilon > 0$ and $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$,*

(i) *The operator*

$$\mathbb{I} - \xi(h)P_{X_2 \oplus Y}\mathbb{Q} + P_{X_2 \oplus Y}\mathbb{R}_3(h, \varepsilon) : X_2 \oplus Y \rightarrow X_2 \oplus Y \quad (7.69)$$

is invertible, where $\mathbb{R}_3(h, \varepsilon)$ is the remainder defined in Corollary 7.2. Denote the inverse by $C(h, \varepsilon) : X_2 \oplus Y \rightarrow X_2 \oplus Y$.

(ii) *Define*

$$J_2(h, \varepsilon)[\mathbf{u}_1] = -C(h, \varepsilon)P_{X_2 \oplus Y}\mathbb{R}_3(h, \varepsilon)\mathbf{u}_1. \quad (7.70)$$

Then $J_2(h, \varepsilon)[\mathbf{u}_1]$ is analytic in h and

$$\|J_2(h, \varepsilon)[\mathbf{u}_1]\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)} = o(1)\|\mathbf{u}_1\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)}, \quad \text{uniformly for } |h| < \mathfrak{d}|\frac{t_*}{\gamma_*}| \text{ as } \varepsilon \rightarrow 0^+. \quad (7.71)$$

Moreover, if $\vec{\phi} \in \text{Ker}(\mathbb{T}_n^\varepsilon(\lambda_ + \varepsilon h_0))$, then up to a constant factor*

$$\vec{\phi} = \mathbf{u}_1 + J_2(h_0, \varepsilon)[\mathbf{u}_1]. \quad (7.72)$$

Proof of Lemma 7.9. The invertibility of (7.69) follows from $P_{X_2 \oplus Y} \mathbb{Q}|_{X_2} = -\alpha_*$, $\xi(h) > 0$, $P_{X_2 \oplus Y} \mathbb{Q}|_Y = 0$ and the uniform smallness of $\mathbb{R}_3(h, \varepsilon)$. The analyticity of $J_2[\vec{\phi}_0](h, \varepsilon)$ in h and the smallness (7.71) follow straightforwardly.

For the statement (7.72), by (7.67) and Corollary 7.2, we have

$$\vec{\phi} = \mathbf{u}_1 + \vec{\phi}_1(h, \varepsilon), \quad \text{for some } \vec{\phi}_1(h, \varepsilon) \in X_2 \bigoplus Y, \quad (7.73)$$

and

$$\mathbb{T}_n^\varepsilon(\lambda_* + \varepsilon h_0) \vec{\phi}(h_0, \varepsilon) = (\mathbb{I} - \xi(h_0) \mathbb{Q} + \mathbb{R}_3(h_0, \varepsilon))(\mathbf{u}_1 + \vec{\phi}_1(h_0, \varepsilon)) = 0. \quad (7.74)$$

Projecting into $X_2 \bigoplus Y$ using $P_{X_2 \oplus Y}$, we have

$$(\mathbb{I} - \xi(h_0) P_{X_2 \oplus Y} \mathbb{Q} + P_{X_2 \oplus Y} \mathbb{R}_3(h_0, \varepsilon)) \vec{\phi}_1(h_0, \varepsilon) + P_{X_2 \oplus Y} \mathbb{R}_3(h_0, \varepsilon) \mathbf{u}_1 = 0. \quad (7.75)$$

By the invertibility of (7.69), $\vec{\phi}_1 = \|J_2[\vec{\phi}_0](h, \varepsilon)$. The proof is concluded. \square

Lemma 7.10. *Let Assumption 2.7 holds along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. Then the following holds for sufficiently small $\varepsilon > 0$ and $|h| < \mathfrak{d} \left| \frac{t_*}{\gamma_*} \right|$:*

(i) *The operator*

$$\mathbb{I} + \xi(h) P_{X_1 \oplus Y} \mathbb{Q} + P_{X_1 \oplus Y} \mathbb{R}_2(h, \varepsilon) : X_1 \bigoplus Y \rightarrow X_1 \bigoplus Y.$$

is invertible, where $\mathbb{R}_2(h, \varepsilon)$ is the remainder defined in Corollary 7.2. Denote the inverse by $B(h, \varepsilon) : X_1 \bigoplus Y \rightarrow X_1 \bigoplus Y$.

(ii) *Let*

$$J_3(h, \varepsilon)[\mathbf{u}_2] = -B(h, \varepsilon) P_{X_1 \oplus Y} \mathbb{R}_2(h, \varepsilon) \mathbf{u}_2. \quad (7.76)$$

Then $\vec{\phi}_1(h, \varepsilon)$ is analytic in h and

$$\|J_3(h, \varepsilon)[\mathbf{u}_2]\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)} = o(1) \|\mathbf{u}_2\|_{\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)}, \quad \text{uniformly for } |h| < \mathfrak{d} \left| \frac{t_*}{\gamma_*} \right| \text{ as } \varepsilon \rightarrow 0^+. \quad (7.77)$$

Furthermore, if $\vec{\phi} \in \text{Ker}(\mathbb{T}_t^\varepsilon(\lambda_ + \varepsilon h_0))$, then*

$$\vec{\phi} = \mathbf{u}_2 + J_3(h_0, \varepsilon)[\mathbf{u}_2]. \quad (7.78)$$

Proposition 7.11. *Let Assumption 2.7 holds along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. For sufficiently small $\varepsilon > 0$, the system*

$$\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h) \vec{\phi} = 0 \quad \text{and} \quad \mathbb{T}_n^\varepsilon(\lambda_* + \varepsilon h) \vec{\phi} = 0 \quad (7.79)$$

attains at most one pair of solution $(h, \vec{\phi})$, with $|h| < \mathfrak{d} \left| \frac{t_}{\gamma_*} \right|$ and $\vec{\phi} \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$. The same holds for the system*

$$\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h) \vec{\phi} = 0 \quad \text{and} \quad \mathbb{T}_t^\varepsilon(\lambda_* + \varepsilon h) \vec{\phi} = 0. \quad (7.80)$$

Proof. We only display the proof on the system (7.79). Suppose $\vec{\phi}$ solves both equations in (7.79). By Lemma 7.9, the solution to the second equation necessarily takes the form $\vec{\phi} = \mathbf{u}_1 + J_2(h, \varepsilon)[\mathbf{u}_1]$ where $J_2(h, \varepsilon)[\mathbf{u}_1]$ is defined in (7.70). Substituting $\vec{\phi}$ into the first equation in (7.79), we obtain

$$(2\tilde{\mathbb{T}}^0(\lambda_*) + 2\beta(h)\mathbb{P} + \mathbb{R}_1(h, \varepsilon))(\mathbf{u}_1 + J_2(h, \varepsilon)[\mathbf{u}_1]) = 0. \quad (7.81)$$

Projecting into X_2 using P_{X_2} , we obtain

$$2i\alpha_*\beta(h)\mathbf{u}_2 + [P_{X_2}\mathbb{R}_1(h, \varepsilon)\mathbf{u}_1 + P_{X_2}(2\beta(h)\mathbb{P} + \mathbb{R}_1(h, \varepsilon))J_2(h, \varepsilon)[\mathbf{u}_1]] = 0. \quad (7.82)$$

Since X_2 is a one-dimensional space, (7.82) becomes

$$2i\alpha_*\beta(h) + r(h, \varepsilon) = 0. \quad (7.83)$$

Note that for each ε , $r(h, \varepsilon)$ is analytic in h , and $|r(h, \varepsilon)| \rightarrow 0$ as $\varepsilon \rightarrow 0^+$ uniformly in $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$. Thus the Rouché Theorem for single-variable complex functions implies that there is exactly one h_0 that solves (7.83) in the region $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$. There is also at most one root function at h_0 , since $\vec{\phi}$ is determined by (7.72) when $h = h_0$. \square

7.4 Proof of Theorem 2.9

Proof of Theorem 2.9. We claim that $\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h)$ is of multiplicity 2 in $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ when $\varepsilon > 0$ is sufficiently small. In Theorem A.1, we identify $z = h$, $X = Y = \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, $V = \{h, |h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|\}$, $A(z) = \mathbb{U}_s(h)$ and $B(z) = \mathbb{R}_1(h, \varepsilon)$. In Proposition 7.5, we have shown that $A(z)$ is analytic and Fredholm of index zero on a neighborhood of \bar{V} , and the multiplicity of $A(z)$ in V is 2. On ∂V , we know $A(z)$ is invertible and is independent of ε , and $B(z)$ converges uniformly to 0 as $\varepsilon \rightarrow 0^+$ by Corollary 7.2. Since $B(z)$ is analytic on a neighborhood of \bar{V} , by Theorem A.1 and the relation $\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h) = A(z) + B(z)$, we conclude the claim.

By Lemma 7.8, there are two pairs $(h_i, \vec{\phi}_i)$ solving $\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h)\vec{\phi} = 0$, $i = 1, 2$. We first show that there is at least one interface mode. Assume u_i generated by $\vec{\phi}_i$ through the expression (6.8) are both equal to zero. Then $(h_i, \vec{\phi}_i)$, $i = 1, 2$ are both solutions to the system (7.80). This contradicts the uniqueness of simultaneous solutions to (7.80) established in Proposition 7.11. Next, we show that there is at most one interface mode. Suppose there are two linearly independent interface modes u_i at h_i respectively, $i = 1, 2$. Denote $\vec{\phi}_i = (u_i|_\Gamma, \partial_n u_i|_\Gamma)$. Then $(h_i, \vec{\phi}_i)$, $i = 1, 2$ are the solutions to the system (7.79). This contradicts the uniqueness of solutions to the system (7.79) established in Proposition 7.11. \square

8 The interface modes along an armchair interface

In this section, we study interface modes along the armchair interface as stated in the eigenvalue problem (2.20) and prove Theorem 2.12. To this end, we extend in parallel the mathematical framework developed in the previous sections for the zigzag interface.

For ease of notation, we will abuse notations $v_i, \vec{v}_i, c_i, \mathbb{P}, \mathbb{Q}, X, \mathbf{u}_i, X_i$ that are introduced in Sections 4, 5, 6, and 7 to represent the quantities relevant to the zigzag interface. In this section, these notations represent the quantities relevant to the armchair interface.

For the eigenvalue problem (2.20), the Floquet theory on the strip $\Omega_a^J = \cup_{n_1 \in \mathbb{Z}} (\mathcal{C}_a + n_1 \mathbf{e}_1^a)$ corresponds to the slice of quasimomenta $\mathbf{p}(\ell) := K + \ell \beta_1^a$. This slice intersects with both $K + \Lambda$ and $K' + \Lambda$, as $\mathbf{p}(0) = K$, and $\mathbf{p}(-\frac{2\pi}{3}) = K' + \beta_1 - \beta_2$. We have the following proposition whose proof is given in Appendix B.

Proposition 8.1. *Let $\boldsymbol{\rho} := (\rho_1, \rho_2)$, where ρ_i are the functions defined in Proposition 3.10 with the normalization such that (4.6) holds. Let $t_*, \gamma_* \in \mathbb{R}$ and $\theta_* \in \mathbb{C}$ be the constants defined in Proposition 4.1. There holds*

$$\langle \boldsymbol{\rho}, \beta_1^a \cdot \nabla_{\mathbf{p}} T(0, \lambda_*, \mathbf{p}) \boldsymbol{\rho} \rangle_{\partial D} |_{\mathbf{p}=K} = \begin{pmatrix} 0 & \sqrt{3}i\bar{\tau}\theta_* \\ -\sqrt{3}i\tau\theta_* & 0 \end{pmatrix}. \quad (8.1)$$

Let $\boldsymbol{\rho}' := (\rho'_1, \rho'_2)$, where

$$\rho'_1(\mathbf{x}) := \bar{\rho}_2(\mathbf{x}), \quad \rho'_2(\mathbf{x}) := \bar{\rho}_1(\mathbf{x}). \quad (8.2)$$

In particular,

$$R\rho'_1(\mathbf{x}) := \rho'_1(R^{-1}\mathbf{x}) = \tau\rho'_1(\mathbf{x}), \quad R\rho'_2(x) := \rho'_2(R^{-1}\mathbf{x}) = \bar{\tau}, \quad \rho'_2(\mathbf{x}) = \rho'_1(F\mathbf{x}). \quad (8.3)$$

The partial derivatives of $\langle \boldsymbol{\rho}', T(\varepsilon, \lambda, \mathbf{p}) \boldsymbol{\rho}' \rangle_{\partial D}$ at $\varepsilon = 0$, $\lambda = \lambda_*$ and $\mathbf{p} = K'$ take the forms

$$\begin{aligned} \langle \boldsymbol{\rho}', \partial_\lambda T(0, \lambda, K') \boldsymbol{\rho}' \rangle_{\partial D} |_{\lambda=\lambda_*} &= \begin{pmatrix} \gamma_* & 0 \\ 0 & \gamma_* \end{pmatrix}, \\ \langle \boldsymbol{\rho}', \beta_1 \cdot \nabla_{\mathbf{p}} T(0, \lambda_*, \mathbf{p}) \boldsymbol{\rho}' \rangle_{\partial D} |_{\mathbf{p}=K'} &= \begin{pmatrix} 0 & -\bar{\theta}_* \\ -\theta_* & 0 \end{pmatrix}, \\ \langle \boldsymbol{\rho}', \partial_\varepsilon T(\varepsilon, \lambda_*, K') \boldsymbol{\rho}' \rangle_{\partial D} |_{\varepsilon=0} &= \begin{pmatrix} -t_* & 0 \\ 0 & t_* \end{pmatrix}. \end{aligned} \quad (8.4)$$

In particular,

$$\langle \boldsymbol{\rho}', \beta_1^a \cdot \nabla_{\mathbf{p}} T(0, \lambda_*, \mathbf{p}) \boldsymbol{\rho}' \rangle_{\partial D} |_{\mathbf{p}=K'} = \begin{pmatrix} 0 & -\sqrt{3}i\bar{\tau}\theta_* \\ \sqrt{3}i\tau\theta_* & 0 \end{pmatrix}. \quad (8.5)$$

Here $\langle \cdot, \cdot \rangle_{\partial D}$ represents the $(H^{-1/2}(\partial D))^2$ - $(H^{1/2}(\partial D))^2$ pairing.

Define

$$\alpha_*^a := \left| \frac{\sqrt{3}i\bar{\tau}\theta_*}{\gamma_*} \right| = \sqrt{3}\alpha_*. \quad (8.6)$$

8.1 Band structure of the periodic strip Ω_a^ε near the Dirac points

We start with the following strip region

$$\Omega_a^\varepsilon := \Omega_a^J \setminus \cup_{m \geq 0} (D^\varepsilon + m\mathbf{e}_1^a). \quad (8.7)$$

When $\varepsilon = 0$, Ω_a^0 represents the region when the rotation angle $\varepsilon = 0$. For $\varepsilon \in \mathbb{R}$, define

$$\begin{aligned} \mathcal{H}_{\text{loc}}^{\varepsilon, a} &:= \{u \in H_{\text{loc}}^1(\Omega_a^\varepsilon) : \Delta u \in L_{\text{loc}}^2(\Omega_a^\varepsilon), \quad u = 0 \text{ on } \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1^a), \\ &u(\mathbf{x} + \mathbf{e}_2) = e^{ik_*^*} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-^a, \quad \partial_{\nu_2} u(\mathbf{x} + \mathbf{e}_2) = e^{ik_*^*} \partial_{\nu_2} u(\mathbf{x}) \text{ for } \mathbf{x} \in \Gamma_-^a\}. \end{aligned} \quad (8.8)$$

We consider the dispersion relation of the operator Δ on $\mathcal{H}_{\text{loc}}^{\varepsilon, a}$, that is, we find $(\lambda, u) \in \mathbb{R} \times \mathcal{H}_{\text{loc}}^{\varepsilon, a}$, such that

$$\begin{aligned} -\Delta u - \lambda u &= 0 && \text{on } \Omega_a^\varepsilon, \\ u &= 0 && \text{on } \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1^a). \end{aligned} \quad (8.9)$$

At $\ell = 0$ and $\mathbf{p}(0) = K$, comparing (8.1) and the second equation in (4.8), $-\sqrt{3}i\tau\theta_*$ is in the place of θ_* . At $\ell = -\frac{2\pi}{3}$ and $\mathbf{p}(-\frac{2\pi}{3}) = K'$, comparing (8.5) the second equation in (4.8), $\sqrt{3}i\tau\theta_*$ is in the place of θ_* . Thus we obtain the following remark and lemma parallel to Remark 5.2 and Lemma 5.4, respectively.

Remark 8.2. *If the Assumption 2.7 holds along β_1^a , then for an arbitrary fixed constant $\mathfrak{d} \in (0, 1)$, when $\varepsilon > 0$ is sufficiently small, the operator Δ on $\Omega_a^{\pm\varepsilon}$ have a common band gap $(\lambda_* - \sqrt{3}\mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \sqrt{3}\mathfrak{d}|\frac{t_*}{\gamma_*}| \varepsilon)$.*

Lemma 8.3. *Let $\mathbf{p}(\ell) := K + \beta_1^a$. For $|\ell| \ll 1$,*

$$\begin{aligned} \mu_1(\mathbf{p}(\ell)) &= \lambda_* + \sqrt{3}|\frac{\theta_*}{\gamma_*}| \ell(1 + O(\ell)) \quad (\text{increasing in } \ell), \\ \mu_2(\mathbf{p}(\ell)) &= \lambda_* - \sqrt{3}|\frac{\theta_*}{\gamma_*}| \ell(1 + O(\ell)) \quad (\text{decreasing in } \ell). \end{aligned} \quad (8.10)$$

The corresponding Bloch modes can be chosen as

$$\begin{aligned} v_1(\mathbf{x}; \mathbf{p}(\ell)) &= \left(\frac{-i\bar{\tau}\theta_*}{|\theta_*|} w_1 - w_2 + O(\ell) \right) \frac{1}{\sqrt{2 + O(\ell)}}, \\ v_2(\mathbf{x}; \mathbf{p}(\ell)) &= \left(\frac{-i\bar{\tau}\theta_*}{|\theta_*|} w_1 + w_2 + O(\ell) \right) \frac{1}{\sqrt{2 + O(\ell)}}. \end{aligned} \quad (8.11)$$

For $|\ell + \frac{2\pi}{3}| \ll 1$,

$$\begin{aligned} \mu_1(\mathbf{p}(\ell)) &= \lambda_* + \sqrt{3}|\frac{\theta_*}{\gamma_*}| (\ell + \frac{2\pi}{3})(1 + O(\ell + \frac{2\pi}{3})) \quad (\text{increasing in } \ell), \\ \mu_2(\mathbf{p}(\ell)) &= \lambda_* - \sqrt{3}|\frac{\theta_*}{\gamma_*}| (\ell + \frac{2\pi}{3})(1 + O(\ell + \frac{2\pi}{3})) \quad (\text{decreasing in } \ell). \end{aligned} \quad (8.12)$$

The corresponding Bloch modes can be chosen as

$$\begin{aligned} \mathbf{b}_1 v_1(\mathbf{x}; \mathbf{p}(\ell)) &= \left(\frac{i\bar{\tau}\theta_*}{|\theta_*|} w_1 - w_2 + O(\ell) \right) \frac{1}{\sqrt{2 + O(\ell + \frac{2\pi}{3})}}, \\ \mathbf{b}_2 v_2(\mathbf{x}; \mathbf{p}(\ell)) &= \left(\frac{i\bar{\tau}\theta_*}{|\theta_*|} w_1 + w_2 + O(\ell) \right) \frac{1}{\sqrt{2 + O(\ell + \frac{2\pi}{3})}}. \end{aligned} \quad (8.13)$$

Here \mathbf{b}_i , $i = 1, 2$, are two phase factors.

In the above, the phase factors show up in (8.13) because $v_n(\mathbf{p}(\ell))$ needs to be smooth for $\ell \in (-\pi, \pi)$ as explained in Section 5.1. Define $v_i := v_i(\mathbf{x}; \mathbf{p}(0)) = v_i(\mathbf{x}; K)$, and $v'_i := \mathbf{b}_i v_i(\mathbf{x}; \mathbf{p}(-\frac{2\pi}{3})) = \mathbf{b}_i v_i(\mathbf{x}; K')$. We obtain the relations

$$\begin{cases} w_1 = \frac{1}{\sqrt{2}} \frac{-i\bar{\tau}\theta_*}{|\theta_*|} (v_1 + v_2) \\ w_2 = \frac{1}{\sqrt{2}} (-v_1 + v_2) \end{cases}, \quad \begin{cases} w'_1 = \frac{1}{\sqrt{2}} \frac{i\bar{\tau}\theta_*}{|\theta_*|} (v'_1 + v'_2) \\ w'_2 = \frac{1}{\sqrt{2}} (-v'_1 + v'_2) \end{cases}. \quad (8.14)$$

8.2 Green's function in the infinite strip and the integral equation formulation

Compared to the Green function (5.26) for the infinite strip Ω^0 considered in Section 5, the Green function in the strip Ω_a^0 contains four propagating modes: $v_i(\mathbf{x}; K)$ and $v_i(\mathbf{x}; K')$ ($i = 1, 2$), due to the fact that $\mathbf{p}(\ell) := K + \beta_1^a \ell$ intersects with both $K + \Lambda$ and $K' + \Lambda$. As a result, it attains the following spectral representation:

$$\begin{aligned} G^{0,a}(\mathbf{x}, \mathbf{y}; \lambda_*) &= \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell + \sum_{n=1,2} \frac{1}{2\pi} \text{p.v.} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell \\ &+ \sum_{n=1,2} \frac{i}{2\alpha_*^a} \overline{v_i(\mathbf{y}; K)} v_i(\mathbf{x}; K) + \sum_{n=1,2} \frac{i}{2\alpha_*^a} \overline{v_i(\mathbf{y}; K')} v_i(\mathbf{x}; K'), \quad \mathbf{x}, \mathbf{y} \in \Omega^0, \end{aligned} \quad (8.15)$$

where its integral part takes the form

$$\tilde{G}^{0,a}(\mathbf{x}, \mathbf{y}; \lambda_*) = \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell + \sum_{n=1,2} \frac{1}{2\pi} \text{p.v.} \int_{[-\pi, \pi]} \frac{\overline{v_n(\mathbf{y}; \mathbf{p}(\ell))} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell. \quad (8.16)$$

The Green function in $\Omega_a^{\pm\varepsilon}$ attains the following spectral representation:

$$G^{\pm\varepsilon,a}(\mathbf{x}, \mathbf{y}; \lambda) = \sum_{n \geq 1} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{v_{n,\pm\varepsilon}(\mathbf{y}; \mathbf{p}(\ell))} v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda} d\ell, \quad \mathbf{x}, \mathbf{y} \in \Omega^0. \quad (8.17)$$

We now investigate the interface modes along the armchair interface. For $s \in \mathbb{R}$, we define the following quasi-periodic Sobolev space on Γ^a :

$$\mathcal{H}^{s,a}(\Gamma^a) := \left\{ u(\mathbf{x}_0 + t\mathbf{e}_2^a) = \sum_{n \in \mathbb{Z}} a_n e^{iK \cdot \mathbf{e}_2^a t} e^{i2\pi n t} : \|u\|_{\mathcal{H}^{s,a}(\Gamma^a)}^2 := \sum_{n \in \mathbb{Z}} |a_n|^2 (1 + n^2)^s \right\}. \quad (8.18)$$

Here $x_0 = -\frac{1}{2}\mathbf{e}_1^a - \frac{1}{2}\mathbf{e}_2^a$.

We define the layer potentials $\mathcal{S}^{\pm\varepsilon,a}(\lambda)$, $\mathcal{D}^{\pm\varepsilon,a}(\lambda)$, $\mathcal{K}^{\pm\varepsilon,a}(\lambda)$, $\mathcal{K}^{*,\varepsilon,a}(\lambda)$ and $\mathcal{N}^{\pm\varepsilon,a}(\lambda)$ parallel to (6.1), where the Green functions are replaced by $G^{\pm\varepsilon,a}(\mathbf{x}, \mathbf{y}, \lambda)$, the integral region is replaced by Γ^a , the integral operators on $\mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a)$ are defined by

$$\mathbb{T}^{\varepsilon,a}(\lambda) := \begin{pmatrix} -\mathcal{K}^{\varepsilon,a}(\lambda) & \mathcal{S}^{\varepsilon,a}(\lambda) \\ -\mathcal{N}^{\varepsilon,a}(\lambda) & \mathcal{K}^{*,\varepsilon,a}(\lambda) \end{pmatrix}, \quad (8.19)$$

and

$$\mathbb{T}_s^{\varepsilon,a}(\lambda) := \mathbb{T}^{\varepsilon,a} + \mathbb{T}^{-\varepsilon,a}, \quad \mathbb{T}_t^{\varepsilon,a}(\lambda) := -\mathbb{T}^{\varepsilon,a} + \mathbb{T}^{-\varepsilon,a} + \mathbb{I}, \quad \mathbb{T}_n^{\varepsilon,a}(\lambda) := \mathbb{T}^{\varepsilon,a} - \mathbb{T}^{-\varepsilon,a} + \mathbb{I}. \quad (8.20)$$

We characterize the interface modes by using boundary integral operators as follows.

Lemma 8.4. *Let $\lambda \in (\lambda_* - \sqrt{3\mathfrak{d}}|\frac{t_*}{\gamma_*}| \varepsilon, \lambda_* + \sqrt{3\mathfrak{d}}|\frac{t_*}{\gamma_*}| \varepsilon)$.*

(i) *There exists an interface mode u satisfying (2.20) if and only if there exists $(\psi, \phi) \in \mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a)$ such that*

$$\mathbb{T}_s^{\varepsilon,a}(\lambda) \begin{pmatrix} \psi \\ \phi \end{pmatrix} = 0, \quad \mathbb{T}_t^{\varepsilon,a}(\lambda) \begin{pmatrix} \psi \\ \phi \end{pmatrix} \neq 0. \quad (8.21)$$

(ii) *If u is an interface mode satisfying (2.20), then $0 \neq (u|_{\Gamma^a}, \partial_n u|_{\Gamma^a}) \in \mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a)$ satisfies*

$$\mathbb{T}_s^{\varepsilon,a}(\lambda) \begin{pmatrix} u|_{\Gamma^a} \\ \partial_n u|_{\Gamma^a} \end{pmatrix} = 0, \quad \mathbb{T}_n^{\varepsilon,a}(\lambda) \begin{pmatrix} u|_{\Gamma^a} \\ \partial_n u|_{\Gamma^a} \end{pmatrix} = 0. \quad (8.22)$$

8.3 Limiting operators

Define

$$c_i(\vec{\phi}) = \overline{\langle \phi, v_i \rangle_{\Gamma^a}} - \langle \partial_n v_i, \psi \rangle_{\Gamma^a}, \quad c'_i(\vec{\phi}) = \overline{\langle \phi, v'_i \rangle_{\Gamma^a}} - \langle \partial_n v'_i, \psi \rangle_{\Gamma^a}, \quad i = 1, 2. \quad (8.23)$$

Here $\langle \cdot, \cdot \rangle_{\Gamma^a}$ represents the $\mathcal{H}^{-1/2,a}(\Gamma^a)$ - $\mathcal{H}^{1/2,a}(\Gamma^a)$ pairing on the armchair interface Γ^a . Define $\vec{v}_i := (v_i|_{\Gamma^a}, \partial_n v_i|_{\Gamma^a})$ and $\vec{v}'_i := (v'_i|_{\Gamma^a}, \partial_n v'_i|_{\Gamma^a})$. Similar to the argument for (7.19), we have

$$\begin{aligned} c_1(\vec{v}_1) &= i\alpha_*^a, & c_2(\vec{v}_2) &= -i\alpha_*^a, & c_i(\vec{v}_j) &= 0 & \text{for } i \neq j, \\ c'_1(\vec{v}'_1) &= i\alpha_*^a, & c'_2(\vec{v}'_2) &= -i\alpha_*^a, & c'_i(\vec{v}'_j) &= 0 & \text{for } i \neq j, \\ c_i(\vec{v}'_j) &= c'_i(\vec{v}_j) = 0 & & & & \text{for } i, j = 1, 2. \end{aligned} \quad (8.24)$$

Define

$$\mathbb{P}\vec{\phi} := c_1(\vec{\phi})\vec{v}_1 + c_2(\vec{\phi})\vec{v}_2, \quad \mathbb{P}'\vec{\phi} := c'_1(\vec{\phi})\vec{v}'_1 + c'_2(\vec{\phi})\vec{v}'_2, \quad (8.25)$$

and

$$\mathbb{Q}\vec{\phi} := c_2(\vec{\phi})\vec{v}_1 + c_1(\vec{\phi})\vec{v}_2, \quad \mathbb{Q}'\vec{\phi} := c'_2(\vec{\phi})\vec{v}'_1 + c'_1(\vec{\phi})\vec{v}'_2. \quad (8.26)$$

Let

$$\beta^a(h) := \frac{1}{2\alpha_*^a} \frac{h}{\sqrt{\beta_*^2 - h^2}}, \quad \xi^a(h) := \frac{\beta_*}{2\alpha_*^a} \frac{1}{\sqrt{\beta_*^2 - h^2}}, \quad (8.27)$$

where α_*^a is defined in (8.6).

Proposition 8.5. *Let Assumption 2.7 hold along β_1^a and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. The following limit holds uniformly for $h \in \mathbb{C}$ satisfying $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$ under the operator norm on $\mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a)$:*

$$\mathbb{T}^{\pm\varepsilon,a}(\lambda_* + \varepsilon h) \rightarrow \mathbb{U}^{\pm}(h), \quad (8.28)$$

where

$$\mathbb{U}^{\pm,a}(h) := \tilde{\mathbb{T}}^{0,a}(\lambda_*) + \beta^a(h)(\mathbb{P} + \mathbb{P}') \mp \xi^a(h)(\mathbb{Q} - \mathbb{Q}'), \quad (8.29)$$

and

$$\tilde{\mathbb{T}}^{0,a}(\lambda) := \begin{pmatrix} -\tilde{\mathcal{K}}^{0,a}(\lambda) & \tilde{\mathcal{S}}^{0,a}(\lambda) \\ -\tilde{\mathcal{N}}^{0,a}(\lambda) & \tilde{\mathcal{K}}^{*,0,a}(\lambda) \end{pmatrix}. \quad (8.30)$$

Here the layer potentials $\tilde{\mathcal{S}}^{0,a}(\lambda)$, $\tilde{\mathcal{D}}^{0,a}(\lambda)$, $\tilde{\mathcal{K}}^{0,a}(\lambda)$, $\tilde{\mathcal{K}}^{*,0,a}(\lambda)$ and $\tilde{\mathcal{N}}^{0,a}(\lambda)$ are defined parallel to (6.1), where the Green functions are replaced by $\tilde{G}^{0,a}(\mathbf{x}, \mathbf{y}, \lambda)$ as defined in (8.16), and the integral region is replaced by Γ^a .

Corollary 8.6. *Let Assumption 2.7 hold along β_1^a and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. We have*

$$\mathbb{T}_s^{\varepsilon,a}(\lambda_* + \varepsilon h) = \mathbb{U}_s^a(h) + \mathbb{R}_1^a(h, \varepsilon), \quad (8.31)$$

$$\mathbb{T}_t^{\varepsilon,a}(\lambda_* + \varepsilon h) = \mathbb{U}_t^a(h) + \mathbb{R}_2^a(h, \varepsilon), \quad (8.32)$$

$$\mathbb{T}_n^{\varepsilon,a}(\lambda_* + \varepsilon h) = \mathbb{U}_n^a(h) + \mathbb{R}_3^a(h, \varepsilon), \quad (8.33)$$

where

$$\mathbb{U}_s^a(h) := 2\tilde{\mathbb{T}}^{0,a}(\lambda_*) + 2\beta^a(h)(\mathbb{P} + \mathbb{P}'), \quad \mathbb{U}_t^a(h) := \mathbb{I} + 2\xi^a(h)(\mathbb{Q} - \mathbb{Q}'), \quad \mathbb{U}_n^a(h) := \mathbb{I} - 2\xi^a(h)(\mathbb{Q} - \mathbb{Q}'), \quad (8.34)$$

and $\|R_i^a(h, \varepsilon)\|_{\mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a) \rightarrow \mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a)} = o(1)$ as $\varepsilon \rightarrow 0^+$ uniformly for $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, $i = 1, 2, 3$.

Define the function spaces

$$X := \text{span}\{\vec{v}_1, \vec{v}_2\}, \quad X' := \text{span}\{\vec{v}'_1, \vec{v}'_2\}, \quad Z := \{\vec{\phi} \in \mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a), c_i(\vec{\phi}) = 0, i = 1, 2\}. \quad (8.35)$$

$$P_Z(\vec{\phi}) := \vec{\phi} - \frac{c_1(\vec{\phi})}{i\alpha_*^a} \vec{v}_1 - \frac{c_2(\vec{\phi})}{-i\alpha_*^a} \vec{v}_2 - \frac{c'_1(\vec{\phi})}{i\alpha_*^a} \vec{v}'_1 - \frac{c'_2(\vec{\phi})}{-i\alpha_*^a} \vec{v}'_2. \quad (8.36)$$

Since $c_i(P_Z(\vec{\phi})) = c'_i(P_Z(\vec{\phi})) = 0$, $i = 1, 2$, we obtain the direct sum decomposition:

$$\mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a) = X \bigoplus X' \bigoplus Z. \quad (8.37)$$

The following fact will be used repeatedly in the proofs. The relations in (8.24) imply that \vec{v}_1 , \vec{v}_2 , \vec{v}'_1 and \vec{v}'_2 are linearly independent. For the operators defined in (7.3) and (7.4),

$$\begin{aligned} \mathbb{P}\vec{v}_1 &= i\alpha_*^a \vec{v}_1, & \mathbb{P}\vec{v}_2 &= -i\alpha_*^a \vec{v}_2, & \mathbb{Q}\vec{v}_1 &= i\vec{v}_2, & \mathbb{Q}\vec{v}_2 &= -i\alpha_*^a \vec{v}_1, \\ \mathbb{P}'\vec{v}'_1 &= i\alpha_*^a \vec{v}'_1, & \mathbb{P}'\vec{v}'_2 &= -i\alpha_*^a \vec{v}'_2, & \mathbb{Q}'\vec{v}'_1 &= i\vec{v}'_2, & \mathbb{Q}'\vec{v}'_2 &= -i\alpha_*^a \vec{v}'_1, \end{aligned} \quad (8.38)$$

and

$$\mathbb{P}X' = \mathbb{Q}X' = 0, \quad \mathbb{P}'X = \mathbb{Q}'X = 0, \quad \mathbb{P}Z = \mathbb{Q}Z = \mathbb{P}'Z = \mathbb{Q}'Z = 0. \quad (8.39)$$

Proposition 8.7. *The following holds for $h \in \mathbb{C}$ satisfying $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$. The operators $\mathbb{U}_s^a(h)$, $\mathbb{U}_t^a(h)$, and $\mathbb{U}_n^a(h)$ are analytic in h and are Fredholm operators with index zero. The only characteristic value of each operator is $h = 0$ and the multiplicity of the characteristic value is 4. In addition, the kernels are $\mathbb{U}_s^a(0)$, $\mathbb{U}_t^a(0)$ and $\mathbb{U}_n^a(0)$ are given by*

$$\begin{aligned} \text{Ker } \mathbb{U}_s^a(0) &= \text{span}\{\vec{v}_1, \vec{v}_2, \vec{v}'_1, \vec{v}'_2\} = X \bigoplus X', \\ \text{Ker } \mathbb{U}_t^a(0) &= \text{span}\{\vec{v}_1 - i\vec{v}_2, \vec{v}'_1 + i\vec{v}'_2\}, \\ \text{Ker } \mathbb{U}_n^a(0) &= \text{span}\{\vec{v}_1 + i\vec{v}_2, \vec{v}'_1 - i\vec{v}'_2\}. \end{aligned}$$

8.4 The characteristic values of the integral operators

Define

$$\mathbf{u}_1 := \vec{v}_1 + i\vec{v}_2, \quad \mathbf{u}_2 := \vec{v}_1 - i\vec{v}_2, \quad \mathbf{u}'_1 := \vec{v}'_1 + i\vec{v}'_2, \quad \mathbf{u}'_2 := \vec{v}'_1 - i\vec{v}'_2, \quad (8.40)$$

and

$$X_i := \text{span}\{\mathbf{u}_i\}, \quad X'_i := \text{span}\{\mathbf{u}'_i\}, \quad i = 1, 2. \quad (8.41)$$

Then

$$X = X_1 \bigoplus X_2, \quad X' = X'_1 \bigoplus X'_2, \quad \mathcal{H}^{1/2,a}(\Gamma^a) \times \mathcal{H}^{-1/2,a}(\Gamma^a) = X_1 \bigoplus X_2 \bigoplus X'_1 \bigoplus X'_2 \bigoplus Z. \quad (8.42)$$

We have

$$\begin{aligned} \mathbb{P}\mathbf{u}_1 &= i\alpha_*^a \mathbf{u}_2, & \mathbb{P}\mathbf{u}_2 &= i\alpha_*^a \mathbf{u}_1, & \mathbb{Q}\mathbf{u}_1 &= \alpha_*^a \mathbf{u}_1, & \mathbb{Q}\mathbf{u}_2 &= -\alpha_*^a \mathbf{u}_2, & \mathbb{P}X' &= \mathbb{Q}X' = 0, \\ \mathbb{P}'\mathbf{u}'_1 &= i\alpha_*^a \mathbf{u}'_2, & \mathbb{P}'\mathbf{u}'_2 &= i\alpha_*^a \mathbf{u}'_1, & \mathbb{Q}'\mathbf{u}'_1 &= \alpha_*^a \mathbf{u}'_1, & \mathbb{Q}'\mathbf{u}'_2 &= -\alpha_*^a \mathbf{u}'_2, & \mathbb{P}'X &= \mathbb{Q}'X = 0, \\ \mathbb{P}Z &= \mathbb{Q}Z = \mathbb{P}'Z &= \mathbb{Q}'Z &= 0 \end{aligned} \quad (8.43)$$

Lemmas 8.8-8.10 are parallel to Lemmas 7.8- 7.10. We state them below without proof.

Lemma 8.8. *Let Assumption 2.7 hold along β_1^a and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. Suppose $|h_0| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ and $0 \neq \vec{\phi} \in \text{Ker } \mathbb{T}_s^{\varepsilon, a}(\lambda_* + \varepsilon h_0)$. When $|\varepsilon| \ll 1$, the rank of $\vec{\phi}$ is 1.*

Lemma 8.9. *Let Assumption 2.7 hold along β_1^a and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. For sufficiently small positive ε and $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, the operator below is invertible*

$$\mathbb{I} + \xi(h)P_{X_1 \oplus X'_2 \oplus Y}(\mathbb{Q} - \mathbb{Q}') + P_{X_1 \oplus X'_2 \oplus Y} \mathbb{R}_2^a(h, \varepsilon) : X_1 \oplus X'_2 \oplus Y \rightarrow X_1 \oplus X'_2 \oplus Y. \quad (8.44)$$

Here $P_{X_1 \oplus X'_2 \oplus Y}$ is the projection onto $X_1 \oplus X'_2 \oplus Y$ associated to the direct sum (8.42), and $\mathbb{R}_2^a(h, \varepsilon)$ is the remainder defined in Corollary 8.6. Denote the inverse by $B^a(h, \varepsilon) : X_1 \oplus X'_2 \oplus Y \rightarrow X_1 \oplus X'_2 \oplus Y$, and define

$$J_4(h, \varepsilon)[\vec{\phi}_0] = -B^a(h, \varepsilon)P_{X_1 \oplus X'_2 \oplus Y} \mathbb{R}_2^a(h, \varepsilon)\vec{\phi}_0, \quad (8.45)$$

for each given $\vec{\phi}_0 \in X_2 \oplus X'_1$. We have $J_4(h, \varepsilon)[\vec{\phi}_0]$ is analytic in h and

$$\|J_4(h, \varepsilon)[\vec{\phi}_0]\|_{\mathcal{H}^{1/2, a}(\Gamma^a) \times \mathcal{H}^{-1/2, a}(\Gamma^a)} = o(1)\|\vec{\phi}_0\|_{\mathcal{H}^{1/2, a}(\Gamma^a) \times \mathcal{H}^{-1/2, a}(\Gamma^a)}, \quad \text{uniformly in } h. \quad (8.46)$$

Moreover, if $\vec{\phi} \in \text{Ker } (\mathbb{T}_t^\varepsilon(\lambda_* + \varepsilon h_0))$, then

$$\vec{\phi} = \vec{\phi}_0 + J_4(h, \varepsilon)[\vec{\phi}_0] \quad (8.47)$$

for some $\vec{\phi}_0 \in X_2 \oplus X'_1$.

Lemma 8.10. *Let Assumption 2.7 hold along β_1^a and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. For sufficiently small positive ε and $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, the operator below is invertible*

$$\mathbb{I} - \xi(h)P_{X_2 \oplus X'_1 \oplus Y}(\mathbb{Q} - \mathbb{Q}') + P_{X_2 \oplus X'_1 \oplus Y} \mathbb{R}_3^a(h, \varepsilon) : X_2 \oplus X'_1 \oplus Y \rightarrow X_2 \oplus X'_1 \oplus Y. \quad (8.48)$$

Here $P_{X_2 \oplus X'_1 \oplus Y}$ is the projection onto $X_2 \oplus X'_1 \oplus Y$ associated to the direct sum (8.42), and $\mathbb{R}_3^a(h, \varepsilon)$ is the remainder defined in Corollary 8.6. Denote the inverse by $C^a(h, \varepsilon) : X_2 \oplus X'_1 \oplus Y \rightarrow X_2 \oplus X'_1 \oplus Y$, and define

$$J_5(h, \varepsilon)[\vec{\phi}_0] = -C^a(h, \varepsilon)P_{X_2 \oplus X'_1 \oplus Y} \mathbb{R}_3^a(h, \varepsilon)\vec{\phi}_0, \quad (8.49)$$

for each given $\vec{\phi}_0 \in X_1 \oplus X'_2$. We have $J_5(h, \varepsilon)[\vec{\phi}_0]$ is analytic in h and

$$\|J_5(h, \varepsilon)[\vec{\phi}_0]\|_{\mathcal{H}^{1/2, a}(\Gamma^a) \times \mathcal{H}^{-1/2, a}(\Gamma^a)} = o(1)\|\vec{\phi}_0\|_{\mathcal{H}^{1/2, a}(\Gamma^a) \times \mathcal{H}^{-1/2, a}(\Gamma^a)}, \quad \text{uniformly in } h. \quad (8.50)$$

Moreover, if $\vec{\phi} \in \text{Ker } (\mathbb{T}_t^\varepsilon(\lambda_* + \varepsilon h_0))$, then

$$\vec{\phi} = \vec{\phi}_0 + J_5(h, \varepsilon)[\vec{\phi}_0] \quad (8.51)$$

for some $\vec{\phi}_0 \in X_1 \oplus X'_2$.

Proposition 8.11. *Let Assumption 2.7 hold along β_1^a and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. For sufficiently small $\varepsilon > 0$, the system*

$$\mathbb{T}_s^{\varepsilon, a}(\lambda_* + \varepsilon h)\vec{\phi} = 0 \quad \text{and} \quad \mathbb{T}_n^{\varepsilon, a}(\lambda_* + \varepsilon h)\vec{\phi} = 0 \quad (8.52)$$

attains at most two pairs of solutions $(h, \vec{\phi})$, with $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ and $\vec{\phi} \in \mathcal{H}^{1/2, a}(\Gamma^a) \times \mathcal{H}^{-1/2, a}(\Gamma^a)$. Moreover, if $h_1 = h_2$, then $\vec{\phi}_1$ and $\vec{\phi}_2$ are linearly independent. The same holds for the system

$$\mathbb{T}_s^{\varepsilon, a}(\lambda_* + \varepsilon h)\vec{\phi} = 0 \quad \text{and} \quad \mathbb{T}_t^{\varepsilon, a}(\lambda_* + \varepsilon h)\vec{\phi} = 0. \quad (8.53)$$

Proof. Suppose $\vec{\phi}$ solves both equations in (8.52). By Lemma 8.10, the solution to the second equation necessarily takes the form $\vec{\phi} = \vec{\phi}_0 + \vec{\phi}_1(h, \varepsilon)$, where $\vec{\phi}_1(h, \varepsilon) = \mathcal{J}_5(h, \varepsilon)[\vec{\phi}_0]$ as defined in (8.49), with $\vec{\phi}_0 = a\mathbf{u}_1 + b\mathbf{u}'_2$ for some $a, b \in \mathbb{C}$. Substituting $\vec{\phi}$ into the first equation, we obtain

$$(2\tilde{\mathbb{T}}^{0,a}(\lambda_*) + 2\beta^a(h)(\mathbb{P} + \mathbb{P}') + \mathbb{R}_1^a(h, \varepsilon))(a\mathbf{u}_1 + b\mathbf{u}'_2 + \vec{\phi}_1(h, \varepsilon)) = 0.$$

Projecting the above onto the space $X_2 \oplus X'_1$ using $P_{X_2 \oplus X'_1}$, we obtain

$$P_{X_2 \oplus X'_1} 2\beta^a(h)(\mathbb{P} + \mathbb{P}')(a\mathbf{u}_1 + b\mathbf{u}'_2) + P_{X_2 \oplus X'_1} \left((2\beta^a(h)(\mathbb{P} + \mathbb{P}') + \mathbb{R}_1^a(h, \varepsilon))\vec{\phi}_1(h, \varepsilon) + \mathbb{R}_1^a(h, \varepsilon)(a\mathbf{u}_1 + b\mathbf{u}'_2) \right) = 0.$$

The projections onto X_2 and X'_1 give

$$(D(h) + E(h, \varepsilon)) \begin{pmatrix} a \\ b \end{pmatrix} = 0, \quad (8.54)$$

where $D(h)$ is defined by

$$\begin{pmatrix} 2i\beta^a(h)\alpha_*^a & 0 \\ 0 & 2i\beta^a(h)\alpha_*^a \end{pmatrix} \quad (8.55)$$

and $E(h, \varepsilon)$ is of higher order in ε .

It is obvious that $D(h)$ is analytic in h in a neighborhood of $\{h \in \mathcal{C}, |h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|\}$. Furthermore, $h = 0$ is the unique characteristic of $D(h)$ in $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, and the multiplicity of $h = 0$ is two. Note that $E(h, \varepsilon)$ is analytic and its matrix norm is of order $o(1)$ uniformly in h as $\varepsilon \rightarrow 0^+$. Thus the generalized Rouché Theorem implies that there are two pairs of $(h_i, (a_i, b_i))$ ($i = 1, 2$) solving (8.54). When $h_1 = h_2$, (a_1, b_1) and (a_2, b_2) are linearly independent. By the independence of \mathbf{u}_2 and \mathbf{u}'_1 , we complete the proof. \square

8.5 Proof of Theorem 2.12

Proof of Theorem 2.12. Using the same argument as that in the proof of Theorem 2.9, by Propositions 8.7 and Theorem A.1, we conclude that $\mathbb{T}_s^{\varepsilon,a}(\lambda_* + \varepsilon h)$ is of multiplicity four in $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$ when $\varepsilon > 0$ is sufficiently small. By Lemma 8.8, there are four pairs $(h_i, \vec{\phi}_i)$ solving $\mathbb{T}_s^{\varepsilon,a}(\lambda_* + \varepsilon h)\vec{\phi} = 0$, $i = 1, \dots, 4$. Moreover, if any of the h_i 's coincide, the corresponding $\vec{\phi}_i$'s form a linearly independent set.

We first show that there are at least two interface modes. Let u_i be generated by $\vec{\phi}_i$ (6.8), where the Green function is replaced by $G^{\pm\varepsilon,a}(\mathbf{x}, \mathbf{y}; \lambda)$ as defined in (8.17), and the integral domain is replaced by Γ^a . Assume u_i , $i = 1, \dots, 4$ represents fewer than two interface modes. Then we have the following two cases:

- (i) All u_i , $i = 1, \dots, 4$ are zero. Then $(h_i, \vec{\phi}_i)$ are four solutions to (8.53), which contradicts with Proposition 8.11.
- (ii) After rearranging, for some $m \in \{2, 3, 4\}$, u_1, u_2, \dots, u_m are nonzero and span a one-dimensional space, and the rest $(4 - m)$ of u_i 's are zero. Then it follows that $h_1 = \dots = h_m$. Also, using $(u_i|_{\Gamma^a}, \partial_n u_i|_{\Gamma^a})$, $i = 1, \dots, m$, we can construct densities $\vec{\phi}'_i$, $i = 1, \dots, m - 1$, which are linearly independent and generates zero modes. Thus we have $(4 - m) + (m - 1) = 3$ simultaneous solutions to (8.53), which contradicts with Proposition 8.11.

Next, we show that there are at most two interface modes. Suppose there are more than two linearly independent interface modes u_i at h_i respectively for $i = 1, 2, 3$. Denote $\vec{\phi}_i = (u_i|_{\Gamma^a}, \partial_n u_i|_{\Gamma^a})$. Then $(h_i, \vec{\phi}_i)$ with $i = 1, 2, 3$ are solutions to the system (8.52), and if $h_i = h_j$, for some $i \neq j$, then $\vec{\phi}_i$ and $\vec{\phi}_j$ are linearly independent. This contradicts with Proposition 8.11. \square

9 Dispersion relations of interface modes

In this section, we investigate the dispersion relation along the zigzag interface as stated in Theorem 2.13. The dispersion relations along the armchair interface and arbitrary rational interfaces as stated in Theorems 2.14, 2.16 and 2.17 are proved in Appendix D.

For ε in a neighborhood of 0, define the Green function on the periodic zigzag strips with quasimomentum $k_{\parallel}^* + \mu$ by

$$\begin{cases} (-\Delta_{\mathbf{x}} - \lambda)G^\varepsilon[\mu](\mathbf{x}, \mathbf{y}; \lambda) = \delta(\mathbf{x} - \mathbf{y}) & \mathbf{x} \in \Omega^\varepsilon, \\ G^\varepsilon[\mu](\mathbf{x}, \mathbf{y}; \lambda) = 0 & \mathbf{x} \in \cup_{m \in \mathbb{Z}} (\partial D^\varepsilon + m\mathbf{e}_1), \\ G^\varepsilon[\mu](\mathbf{x} + \mathbf{e}_2, \mathbf{y}; \lambda) = e^{ik_{\parallel}^* + \mu} G^\varepsilon[\mu](\mathbf{x}, \mathbf{y}; \lambda) & \text{for } \mathbf{x} \in \Gamma_-, \\ \partial_{\nu_2} G^\varepsilon[\mu](\mathbf{x} + \mathbf{e}_2, \mathbf{y}; \lambda) = e^{ik_{\parallel}^* + \mu} \partial_{\nu_2} G^\varepsilon[\mu](\mathbf{x}, \mathbf{y}; \lambda) & \text{for } \mathbf{x} \in \Gamma_-, \\ G^\varepsilon[\mu](\mathbf{x}, \mathbf{y}; \lambda) \text{ satisfies the radiation conditions when } |\mathbf{x} \cdot \mathbf{e}_1| \rightarrow \infty. \end{cases} \quad (9.1)$$

Similar to (5.17) and (8.18), we define the following quasi-periodic Sobolev space on Γ for $s \in \mathbb{R}$

$$\mathcal{H}^s(\Gamma, \mu) := \left\{ u(\mathbf{x}_0 + t\mathbf{e}_2) = \sum_{n \in \mathbb{Z}} a_n e^{i(K + \mu\beta_2) \cdot \mathbf{e}_2 t} e^{i2\pi n t} : \|u\|_{\mathcal{H}^s(\Gamma, \eta)}^2 := \sum_{n \in \mathbb{Z}} |a_n|^2 (1 + n^2)^s \right\}. \quad (9.2)$$

The functions in $\mathcal{H}^s(\Gamma, \mu)$ attain the quasimomentum $k_{\parallel}^* + \mu$ along the zigzag edge \mathbf{e}_2 . In particular, $\mathcal{H}^s(\Gamma, 0) = \mathcal{H}^s(\Gamma)$ in (5.17).

Define the layer potentials $\mathcal{S}^{\pm\varepsilon}(\lambda, \mu)$, $\mathcal{D}^{\pm\varepsilon}(\lambda, \mu)$, $\mathcal{K}^{\pm\varepsilon}(\lambda, \mu)$, $\mathcal{K}^{*,\varepsilon}(\lambda, \mu)$ and $\mathcal{N}^{\pm\varepsilon}(\lambda, \mu)$ in parallel to (6.1), where the Green functions are replaced by $G^{\pm\varepsilon}[\mu](\mathbf{x}, \mathbf{y}, \lambda)$ above. We also define the integral operators on $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ as in (6.12) and (6.13) by

$$\mathbb{T}^\varepsilon(\lambda, \mu) := \begin{pmatrix} -\mathcal{K}^\varepsilon(\lambda, \mu) & \mathcal{S}^\varepsilon(\lambda, \mu) \\ -\mathcal{N}^\varepsilon(\lambda, \mu) & \mathcal{K}^{*,\varepsilon}(\lambda, \mu) \end{pmatrix}, \quad (9.3)$$

and

$$\mathbb{T}_s^\varepsilon(\lambda, \mu) := \mathbb{T}^\varepsilon + \mathbb{T}^{-\varepsilon}, \quad \mathbb{T}_t^\varepsilon(\lambda, \mu) := -\mathbb{T}^\varepsilon + \mathbb{T}^{-\varepsilon} + \mathbb{I}, \quad \mathbb{T}_n^\varepsilon(\lambda, \mu) := \mathbb{T}^\varepsilon - \mathbb{T}^{-\varepsilon} + \mathbb{I}. \quad (9.4)$$

Let $\mathbb{M}(\mu)$ be the operator of multiplication by the factor $e^{-i\mu\beta_2 \cdot \mathbf{x}}$. Since $\phi \in \mathcal{H}^s(\Gamma, \mu)$ if and only if $\mathbb{M}(\mu)\phi \in \mathcal{H}^s(\Gamma)$, we have the following characterization of edge states with quasimomentum $k_{\parallel}^* + \mu$.

Lemma 9.1. *Let $\mu = \varepsilon\zeta$. There exists an interface mode of quasimomentum $k_{\parallel}^* + \mu$ along \mathbf{e}_2 if and only if there exists $(\psi, \phi) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$, such that*

$$\mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \begin{pmatrix} \psi \\ \phi \end{pmatrix} = 0, \quad \mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}_t^\varepsilon(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \begin{pmatrix} \psi \\ \phi \end{pmatrix} \neq 0. \quad (9.5)$$

Moreover, if u is an interface mode with quasimomentum $k_{\parallel}^* + \mu$ along \mathbf{e}_2 , then $0 \neq (u|_{\Gamma}, \partial_n u|_{\Gamma}) \in \mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ satisfies

$$\mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \begin{pmatrix} u|_{\Gamma} \\ \partial_n u|_{\Gamma} \end{pmatrix} = 0, \quad \mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}_n^\varepsilon(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \begin{pmatrix} u|_{\Gamma} \\ \partial_n u|_{\Gamma} \end{pmatrix} = 0. \quad (9.6)$$

Define

$$\begin{aligned} \beta(h, \zeta) &:= \frac{1}{2} \left| \frac{\gamma_*}{\theta_*} \right| \frac{h}{\sqrt{(\frac{t_*}{\gamma_*})^2 + \frac{3}{4} |\frac{\theta_*}{\gamma_*}|^2 \zeta^2 - h^2}} = \frac{1}{2\alpha_*} \frac{h}{\sqrt{\beta_*^2 + \frac{3}{4} \alpha_*^2 \zeta^2 - h^2}}, \\ \xi(h, \zeta) &:= \frac{t_*}{2|\theta_*|} \frac{1}{\sqrt{(\frac{t_*}{\gamma_*})^2 + \frac{3}{4} |\frac{\theta_*}{\gamma_*}|^2 \zeta^2 - h^2}} = \frac{\beta_*}{2\alpha_*} \frac{1}{\sqrt{\beta_*^2 + \frac{3}{4} \alpha_*^2 \zeta^2 - h^2}}, \\ \sigma(h, \zeta) &:= i \frac{\sqrt{3}}{2} \zeta \frac{1}{\sqrt{(\frac{t_*}{\gamma_*})^2 + \frac{3}{4} |\frac{\theta_*}{\gamma_*}|^2 \zeta^2 - h^2}} = i \frac{\sqrt{3}}{2} \zeta \frac{1}{\sqrt{\beta_*^2 + \frac{3}{4} \alpha_*^2 \zeta^2 - h^2}}. \end{aligned} \quad (9.7)$$

Similarly to Proposition 7.1, we obtain the following operator limit.

Proposition 9.2. *Let Assumption 2.7 hold along β_1 and $t_* > 0$. Let $\mathfrak{d} \in (0, 1)$ be a constant. For each constant ζ , the following limit holds uniformly for $|h| < \mathfrak{d} |\frac{t_*}{\gamma_*}|$ as $\varepsilon \rightarrow 0^+$ in the operator norm from $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma) \times \mathcal{H}^{-1/2}(\Gamma)$:*

$$\mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}^{\pm\varepsilon}(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \rightarrow \tilde{\mathbb{T}}^0(\lambda_*) + \beta(h, \zeta)\mathbb{P} \mp \xi(h, \zeta)\mathbb{Q} + \sigma(h, \zeta)\mathbb{O}, \quad (9.8)$$

where

$$\mathbb{O}\vec{\phi} := -c_2(\vec{\phi})\vec{v}_1 + c_1(\vec{\phi})\vec{v}_2. \quad (9.9)$$

In addition, there hold the uniform convergences

$$\mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \rightarrow 2\tilde{\mathbb{T}}^0(\lambda_*) + 2\beta(h, \zeta)\mathbb{P} + 2\sigma(h, \zeta)\mathbb{O} =: \mathbb{U}_s(h, \zeta), \quad (9.10)$$

$$\mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}_t^\varepsilon(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \rightarrow I + 2\xi(h, \zeta)\mathbb{Q} =: \mathbb{U}_t(h, \zeta), \quad (9.11)$$

$$\mathbb{M}^{-1}(\varepsilon\zeta)\mathbb{T}_n^\varepsilon(\lambda_* + \varepsilon h, \varepsilon\zeta)\mathbb{M}(\varepsilon\zeta) \rightarrow I - 2\xi(h, \zeta)\mathbb{Q} =: \mathbb{U}_n(h, \zeta), \quad (9.12)$$

The proof is in Appendix D.

Now we are ready to prove Theorem 2.13.

Proof of Theorem 2.13. Assume $t_* > 0$. We fix an $\zeta \neq 0$ and let $\vec{\phi} = a\vec{v}_1 + b\vec{v}_2$. First, $\mathbb{U}_s(h, \zeta)\vec{\phi} = 0$ yields

$$i\alpha_* \begin{pmatrix} \beta(h, \zeta) & \sigma(h, \zeta) \\ \sigma(h, \zeta) & -\beta(h, \zeta) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0. \quad (9.13)$$

Solving (9.13), we obtain two characteristic values for h . More specifically, $\sigma(h, \zeta) = i\beta(h, \zeta)$ gives that $h = \frac{\sqrt{3}}{2}\alpha_*\zeta$, $(a, b) = (1, i)$; and $\sigma(h, \zeta) = -i\beta(h, \zeta)$ gives that $h = -\frac{\sqrt{3}}{2}\alpha_*\zeta$, $(a, b) = (1, -i)$.

Next, $\mathbb{U}_t(h, \zeta)\vec{\phi} = 0$ yields

$$\begin{pmatrix} 1 & -2i\alpha_*\xi(h, \zeta) \\ 2i\alpha_*\xi(h, \zeta) & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0. \quad (9.14)$$

Solving (9.15), we obtain two characteristic values for h . Indeed, the condition $1 - 4\alpha_*^2(\xi(h, \zeta))^2 = 0$ is achieved if and only if $|2\alpha_*\xi(h, \zeta)| = 1$, which is equivalent to $\frac{3}{4}\alpha_*^2\zeta^2 - h^2 = 0$. For both $h = \pm\frac{\sqrt{3}}{2}\alpha_*\zeta$, $(a, b) = (1, -i)$.

Similarly, $\mathbb{U}_n(h, \zeta)\vec{\phi} = 0$ yields that

$$\begin{pmatrix} 1 & 2i\alpha_*\xi(h, \zeta) \\ -2i\alpha_*\xi(h, \zeta) & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = 0, \quad (9.15)$$

which also gives two characteristic values for h . For both $h = \pm\frac{\sqrt{3}}{2}\alpha_*\zeta$, $(a, b) = (1, i)$.

Thus for a fixed $\zeta \neq 0$, $\mathbb{T}_s^\varepsilon(\lambda_* + \varepsilon h, \zeta)$ has one characteristic value $h \approx \frac{\sqrt{3}}{2}\alpha_*\zeta$, with root function $\vec{\phi} \approx \vec{v}_1 + i\vec{v}_2$. This $\vec{\phi}$ generates a nonzero interface mode since $\mathbb{U}_t(h, \zeta)(\vec{v}_1 + i\vec{v}_2) \neq 0$. The theorem for $t_* > 0$ follows by noting the following relation $\lambda = \lambda_* + \varepsilon h$, $k_{\parallel} = (K + \varepsilon\zeta\beta_2 + \ell\beta_1) \cdot \mathbf{e}_2 = k_{\parallel}^* + \varepsilon\zeta$ and $\alpha_* = m_*|\beta_1|$.

When $t_* < 0$, doing the parallel calculations, we obtain the theorem when $\text{sgn}(t_*) = -1$. \square

Appendix A Gohberg and Sigal theory

We briefly introduce the Gohberg and Sigal theory. We refer to Chapter 1.5 of [2] for a thorough exposition of the topic.

Let X and Y be two Banach spaces. Let $\mathfrak{U}(z_0)$ be the set of all operator-valued functions with values in $\mathcal{B}(X, Y)$, which are holomorphic in some neighborhood of z_0 , except possibly at z_0 . Then the point z_0 is called a **characteristic value** of $A(z) \in \mathfrak{U}(z_0)$ if there exists a vector-valued function $\phi(z)$ with values in X such that

1. $\phi(z)$ is holomorphic at z_0 and $\phi(z_0) \neq 0$,
2. $A(z)\phi(z)$ is holomorphic at z_0 and vanishes at this point.

Here $\phi(z)$ is called a **root function** of $A(z)$ associated with the characteristic value z_0 , and $\phi(z_0)$ is called an **eigenvector**. By this definition, there exists an integer $m(\phi) \geq 1$ and a vector-valued function $\psi(z) \in Y$, holomorphic at z_0 , such that

$$A(z)\phi(z) = (z - z_0)^{m(\phi)}\psi(z), \quad \psi(z_0) \neq 0.$$

The number $m(\phi)$ is called the **multiplicity** of the root function $\phi(z)$. For $\phi_0 \in \text{Ker}A(z_0)$, the **rank** of ϕ_0 , which is denoted by $\text{rank}(\phi_0)$, is defined as the maximum of the multiplicities of all root functions $\phi(z)$ with $\phi(z_0) = \phi_0$.

Suppose that $n = \dim \text{Ker}A(z_0) < +\infty$ and the ranks of all vectors in $\text{Ker}A(z_0)$ are finite. A system of eigenvectors ϕ_0^j ($j = 1, 2, \dots, n$) is called a **canonical system of eigenvectors** of $A(z)$ associated to z_0 if for $j = 1, 2, \dots, n$, $\text{rank}(\phi_0^j)$ is the maximum of the ranks of all eigenvectors in the direct complement in $\text{Ker}A(z_0)$ of the linear span of the vectors $\phi_0^1, \dots, \phi_0^{j-1}$. We call

$$N(A(z_0)) := \sum_{j=1}^n \text{rank}(\phi_0^j)$$

the **null multiplicity** of the characteristic value z_0 of $A(z)$. Suppose that $A^{-1}(z)$ exists and is holomorphic in some neighborhood of z_0 , except possibly at z_0 . Then the number

$$M(A(z_0)) := N(A(z_0)) - N(A^{-1}(z_0))$$

is called the **multiplicity** of z_0 . Note if $A(z)$ is bounded in a neighborhood of z_0 , then $N(A^{-1}(z_0)) = 0$.

Now, let V be a simply connected bounded domain with a rectifiable boundary ∂V . Let $A(z)$ be an operator-valued function that is analytic in a neighborhood of \bar{V} , is Fredholm of index zero in V and is invertible in \bar{V} except at possibly a finite number of points. For such a function $A(z)$, the full multiplicity $\mathcal{M}(A(z); \partial V)$ counts the number of characteristic values of $A(z)$ in V (computed with their multiplicities). Namely,

$$\mathcal{M}(A(z); \partial V) := \sum_{i=1}^{\sigma} M(A(z_i)) = \sum_{i=1}^{\sigma} N(A(z_i)),$$

where z_i ($i = 1, 2, \dots, \sigma$) are all characteristic values of $A(z)$ lying in V . The generalized Rouché theorem for analytic operator-valued functions is stated as follows. This is a special case of the generalized Rouché theorem for finitely meromorphic operator-valued functions [2, Theorem 1.5].

Theorem A.1. *The operator-valued function $A(z)$ is analytic and Fredholm of index zero in a neighborhood of \bar{V} , $A^{-1}(z)$ exists except at a finite number of points in \bar{V} . The operator-valued function $B(z)$ is analytic in a neighborhood of \bar{V} . Suppose*

$$\|A^{-1}(z)B(z)\|_{\mathcal{B}(X,Y)} < 1, \quad z \in \partial V.$$

Then the multiplicity of $A(z)$ in V equals the multiplicity of $A(z) + B(z)$ in V . That is,

$$\mathcal{M}(A(z); \partial V) = \mathcal{M}(A(z) + B(z); \partial V).$$

In addition the multiplicities of $A(z)$ and $A(z) + B(z)$ do not involve their inverses. That is,

$$\begin{aligned} \mathcal{M}(A(z); \partial V) &= \sum_{i=1}^{\sigma} N(A(z_i)), \\ \mathcal{M}((A+B)(z); \partial V) &= \sum_{i=1}^{\sigma'} N((A+B)(z'_i)), \end{aligned}$$

where z_i , $i = 1, \dots, \sigma$ are all characteristic values of $A(z)$ in V , and z'_i , $i = 1, \dots, \sigma'$ are all characteristic values of $(A+B)(z)$ in V .

Appendix B Proof of Propositions 4.1 and 8.1

We first display a set of facts that can be easily checked for the readers' convenience. Define

$$R_s := \begin{pmatrix} \cos s & \sin s \\ -\sin s & \cos s \end{pmatrix}, \quad s \in \mathbb{R}, \quad R := R_{\frac{2\pi}{3}} \quad \text{and} \quad J := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (\text{B.1})$$

Acting on vectors in \mathbb{R}^2 , it holds

$$\begin{aligned} R^3 &= I, \quad I + R + R^2 = 0, \quad R_a R_b = R_b R_a, \quad \frac{\partial}{\partial \varepsilon} R_\varepsilon|_{\varepsilon=0} = J, \\ F^2 &= I, \quad FR_\theta = (R_\theta)^{-1}F, \quad J^{-1} = -J, \quad JR = RJ, \quad FJ = -JF. \end{aligned} \quad (\text{B.2})$$

For all vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^2$,

$$R\mathbf{x} \cdot R\mathbf{y} = \mathbf{x} \cdot \mathbf{y}, \quad F\mathbf{x} \cdot F\mathbf{y} = \mathbf{x} \cdot \mathbf{y}. \quad (\text{B.3})$$

The set $\tilde{\Lambda}^* := \{K + \mathbf{q}, \mathbf{q} \in \Lambda^*\}$ is invariant under R and F as shown in (3.10). The invariance of ∂D under R guarantees a partition

$$\partial D = \sqcup_{n=1,2,3} C_n, \quad \mathbf{x} \in C_n \text{ iff } \mathbf{x} = R^{n-1}\mathbf{x}' \text{ for some } \mathbf{x}' \in C_1. \quad (\text{B.4})$$

We also have the relations

$$\overline{G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})} = G^f(\mathbf{y}, \mathbf{x}; \lambda, \mathbf{p}) \quad \forall \lambda \in \mathbb{R}, \forall \mathbf{p} \in \mathbb{R}^2, \quad (\text{B.5})$$

and

$$\begin{aligned} \overline{\rho_i(R^{-1}\mathbf{x})\rho_i(R^{-1}\mathbf{y})} &= \overline{\rho_i(\mathbf{x})\rho_i(\mathbf{y})}, \quad i = 1, 2, \quad \overline{\rho_1(R^{-1}\mathbf{x})\rho_2(R^{-1}\mathbf{y})} = \overline{\tau^2\rho_1(\mathbf{x})\rho_2(\mathbf{y})}, \\ \overline{\rho_1(F\mathbf{x})\rho_1(F\mathbf{y})} &= \overline{\rho_2(\mathbf{x})\rho_2(\mathbf{y})}, \quad \overline{\rho_1(F\mathbf{x})\rho_2(F\mathbf{y})} = \overline{\rho_2(\mathbf{x})\rho_1(\mathbf{y})}. \end{aligned} \quad (\text{B.6})$$

Since $D = RD = FD$, it is straightforward to verify

$$\begin{aligned} \int_{\partial D} \int_{\partial D} K(\mathbf{x}, \mathbf{y}) \overline{f(\mathbf{y})} g(\mathbf{x}) ds_{\mathbf{x}} ds_{\mathbf{y}} &= \int_{\partial D} \int_{\partial D} K(R^{-1}\mathbf{x}, R^{-1}\mathbf{y}) \overline{f(R^{-1}\mathbf{x})} g(R^{-1}\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} \\ &= \int_{\partial D} \int_{\partial D} K(F\mathbf{x}, F\mathbf{y}) \overline{f(F\mathbf{x})} g(F\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}}. \end{aligned} \quad (\text{B.7})$$

Recall

$$\langle f, T(\varepsilon, \lambda, \mathbf{p})g \rangle_{\partial D} := \int_{\partial D} \int_{\partial D} \overline{f(\mathbf{x})} G^f(R^\varepsilon \mathbf{x}, R^\varepsilon \mathbf{y}; \lambda, \mathbf{p}) g(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}}, \quad (\text{B.8})$$

where $\langle \cdot, \cdot \rangle_{\partial D}$ represents the $H^{-1/2}(\partial D)$ - $H^{1/2}(\partial D)$ pairing.

Lemma B.1. For all $\lambda \in \mathbb{R}$, all quasimomenta \mathbf{p} with $\ell \in \mathbb{R}$, $\varepsilon \in \mathbb{R}$, and $f, g \in H^{-1/2}(\partial D)$,

$$\overline{\langle f, T(\varepsilon, \lambda, \mathbf{p})g \rangle_{\partial D}} = \langle g, T(\varepsilon, \lambda, \mathbf{p})f \rangle_{\partial D}, \quad \text{and} \quad \langle f, T(\varepsilon, \lambda, \mathbf{p})f \rangle_{\partial D} \in \mathbb{R}. \quad (\text{B.9})$$

Proof. By (B.5),

$$\overline{\int_{\partial D} \int_{\partial D} \overline{f(\mathbf{x})} G^f(R^\varepsilon \mathbf{x}, R^\varepsilon \mathbf{y}; \lambda, \mathbf{p}) g(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}}} = \int_{\partial D} \int_{\partial D} f(\mathbf{x}) G^f(R^\varepsilon \mathbf{y}, R^\varepsilon \mathbf{x}; \lambda, \mathbf{p}) \overline{g(\mathbf{y})} ds_{\mathbf{x}} ds_{\mathbf{y}}. \quad (\text{B.10})$$

□

Now we are ready to prove Proposition 4.1.

Proposition 4.1. Since the derivatives in Proposition 4.1 are all with respect to real variables, by Lemma B.1, the four matrices in Proposition 4.1 all take the form

$$\begin{pmatrix} a & c \\ c^* & b \end{pmatrix}, \quad a, b \in \mathbb{R}, \quad c \in \mathbb{C}. \quad (\text{B.11})$$

For the first equation, consider the λ derivative when $\varepsilon = 0$ and $\mathbf{p} = K$. We have

$$\partial_\lambda G^f(\mathbf{x}, \mathbf{y}; \lambda, K) = \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})}. \quad (\text{B.12})$$

We observe that

$$\begin{aligned}\partial_\lambda G^f(R^{-1}\mathbf{x}, R^{-1}\mathbf{y}; \lambda, K) &= \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} = \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot R^{-1}(\mathbf{x} - \mathbf{y})} \\ &= \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{(\lambda - |\mathbf{m}|^2)^2} e^{iR\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} = \partial_\lambda G^f(\mathbf{x}, \mathbf{y}; \lambda, K)\end{aligned}\tag{B.13}$$

and

$$\begin{aligned}\partial_\lambda G^f(F\mathbf{x}, F\mathbf{y}; \lambda, K) &= \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot F(\mathbf{x} - \mathbf{y})} \\ &= \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{1}{(\lambda - |\mathbf{m}|^2)^2} e^{iF\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} = \partial_\lambda G^f(\mathbf{x}, \mathbf{y}; \lambda, K).\end{aligned}\tag{B.14}$$

Here we have used (3.10) and $|\mathbf{m}| = |R\mathbf{m}| = |F\mathbf{m}|$. The diagonal terms are equal because

$$\begin{aligned}\int_{\partial D} \int_{\partial D} \partial_\lambda G^f(\mathbf{x}, \mathbf{y}; \lambda, K) \overline{\rho_1(\mathbf{x})} \rho_1(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} &= \int_{\partial D} \int_{\partial D} \partial_\lambda G^f(F\mathbf{x}, F\mathbf{y}; \lambda, K) \overline{\rho_2(\mathbf{x})} \rho_2(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} \\ &= \int_{\partial D} \int_{\partial D} \partial_\lambda G^f(\mathbf{x}, \mathbf{y}; \lambda, K) \overline{\rho_2(\mathbf{x})} \rho_2(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}}.\end{aligned}\tag{B.15}$$

Here the first equality follows from (B.6) and (B.7), and the second equality follows from (B.14). The off-diagonal terms are zero follows from the relation below and the fact $\bar{\tau}^2 \neq 1$:

$$\begin{aligned}\int_{\partial D} \int_{\partial D} \partial_\lambda G^f(\mathbf{x}, \mathbf{y}; \lambda, K) \overline{\rho_1(\mathbf{x})} \rho_2(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} &= \bar{\tau}^2 \int_{\partial D} \int_{\partial D} \partial_\lambda G^f(R^{-1}\mathbf{x}, R^{-1}\mathbf{y}; \lambda, K) \overline{\rho_1(\mathbf{x})} \rho_2(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} \\ &= \bar{\tau}^2 \int_{\partial D} \int_{\partial D} \partial_\lambda G^f(\mathbf{x}, \mathbf{y}; \lambda, K) \overline{\rho_1(\mathbf{x})} \rho_2(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}}.\end{aligned}\tag{B.16}$$

Here we have used (B.6), (B.7) and (B.13).

For the second equation, consider the $\nabla_{\mathbf{p}}$ derivative when $\varepsilon = 0$ around K

$$\nabla_{\mathbf{p}} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})|_{\mathbf{p}=K} = -\frac{1}{|\mathcal{C}_z|} \sum_{[\mathbf{m}] \in [\tilde{\Lambda}^*]} \frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} \mathbf{m} - \frac{1}{|\mathcal{C}_z|} \sum_{[\mathbf{m}] \in [\tilde{\Lambda}^*]} \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} (\mathbf{x} - \mathbf{y})\tag{B.17}$$

We only need to show that the diagonal terms are zero. Decompose the integral domain into

$$\begin{aligned}\partial D \times \partial D &= ((C_1 \times C_1) \sqcup (C_2 \times C_2) \sqcup (C_3 \times C_3)) \\ &\quad \sqcup ((C_1 \times C_2) \sqcup (C_2 \times C_3) \sqcup (C_3 \times C_2)) \\ &\quad \sqcup ((C_1 \times C_3) \sqcup (C_2 \times C_1) \sqcup (C_3 \times C_2)).\end{aligned}\tag{B.18}$$

Define the vectors

$$I_{i,j} := \int_{C_i} \int_{C_j} \overline{\rho_1(\mathbf{x})} \nabla_{\mathbf{p}} G^f(R^\varepsilon \mathbf{x}, R^\varepsilon \mathbf{y}; \lambda, \mathbf{p}) \rho_1(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}}, \quad i, j = 1, 2, 3.\tag{B.19}$$

We have

$$\begin{aligned}
I_{2,2} &= \\
&- \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \int_{C_2 \times C_2} \left(\frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} \mathbf{m} + \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} (\mathbf{x} - \mathbf{y}) \right) \overline{\rho_1(\mathbf{x})} \rho_1(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} \\
&= - \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \int_{C_1 \times C_1} \left(\frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot R(\mathbf{x}' - \mathbf{y}')} \mathbf{m} + \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot R(\mathbf{x}' - \mathbf{y}')} R(\mathbf{x}' - \mathbf{y}') \right) \overline{\rho_1(R\mathbf{x}')} \rho_1(R\mathbf{y}') ds_{\mathbf{x}'} ds_{\mathbf{y}'} \\
&= - \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \int_{C_1 \times C_1} \left(\frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{iR^2 \mathbf{m} \cdot (\mathbf{x}' - \mathbf{y}')} \mathbf{m} + \frac{i}{\lambda - |\mathbf{m}|^2} e^{iR^2 \mathbf{m} \cdot (\mathbf{x}' - \mathbf{y}')} R(\mathbf{x}' - \mathbf{y}') \right) \overline{\rho_1(\mathbf{x}')} \rho_1(\mathbf{y}') ds_{\mathbf{x}'} ds_{\mathbf{y}'} \\
&= - \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m}' \in \tilde{\Lambda}^*} \int_{C_1 \times C_1} \left(\frac{2}{(\lambda - |\mathbf{m}'|^2)^2} e^{i\mathbf{m}' \cdot (\mathbf{x} - \mathbf{y})} R\mathbf{m}' + \frac{i}{\lambda - |\mathbf{m}'|^2} e^{i\mathbf{m}' \cdot (\mathbf{x} - \mathbf{y})} R(\mathbf{x} - \mathbf{y}) \right) \overline{\rho_1(\mathbf{x}')} \rho_1(\mathbf{y}') ds_{\mathbf{x}} ds_{\mathbf{y}} \\
&= RI_{1,1}.
\end{aligned} \tag{B.20}$$

Similarly we have $I_{3,3} = R^2 I_{1,1}$ and thus $I_{1,1} + I_{2,2} + I_{3,3} = 0$ by $I + R + R^2 = 0$ on vectors as stated in (B.2). Similarly, $I_{1,2} + I_{2,3} + I_{3,1} = I_{1,3} + I_{2,1} + I_{3,2} = 0$. Thus $\langle \rho_1, \nabla_{\mathbf{p}} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})|_{\mathbf{p}=K} \rho_1 \rangle_{\partial D=0}$. The same method gives $\langle \rho_2, \nabla_{\mathbf{p}} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})|_{\mathbf{p}=K} \rho_2 \rangle_{\partial D=0}$.

For the third equation in (4.8), we only need to show

$$\beta_2 \cdot \langle \rho_1, \nabla_{\mathbf{p}} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})|_{\mathbf{p}=K} \rho_2 \rangle_{\partial D=0} = \tau \beta_1 \cdot \langle \rho_1, \nabla_{\mathbf{p}} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})|_{\mathbf{p}=K} \rho_2 \rangle_{\partial D=0} \tag{B.21}$$

This is true since

$$\begin{aligned}
&\sum_{\mathbf{m} \in \tilde{\Lambda}^*} \int_{\partial D \times \partial D} \left(\frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} \mathbf{m} \cdot \beta_2 + \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} (\mathbf{x} - \mathbf{y}) \cdot \beta_2 \right) \overline{\rho_1(\mathbf{x})} \rho_2(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} \\
&= \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \int_{\partial D \times \partial D} \left(\frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} \mathbf{m} \cdot R^{-1} \beta_1 + \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} (\mathbf{x} - \mathbf{y}) \cdot R^{-1} \beta_1 \right) \overline{\rho_1(\mathbf{x})} \rho_2(\mathbf{y}) ds_{\mathbf{x}} ds_{\mathbf{y}} \\
&= \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \int_{\partial D \times \partial D} \left(\frac{2}{(\lambda - |\mathbf{m}|^2)^2} e^{iR\mathbf{m} \cdot R(\mathbf{x} - \mathbf{y})} R\mathbf{m} \cdot \beta_1 + \frac{i}{\lambda - |\mathbf{m}|^2} e^{iR\mathbf{m} \cdot R(\mathbf{x} - \mathbf{y})} R(\mathbf{x} - \mathbf{y}) \cdot R\beta_1 \right) \overline{\rho_1(R^{-1}R\mathbf{x})} \rho_2(R^{-1}R\mathbf{y}) \\
&= \sum_{\mathbf{m}' \in \tilde{\Lambda}^*} \int_{\partial D \times \partial D} \left(\frac{2}{(\lambda - |\mathbf{m}'|^2)^2} e^{i\mathbf{m}' \cdot (\mathbf{x}' - \mathbf{y}')} \mathbf{m}' \cdot \beta_1 + \frac{i}{\lambda - |\mathbf{m}'|^2} e^{i\mathbf{m}' \cdot (\mathbf{x}' - \mathbf{y}')} (\mathbf{x}' - \mathbf{y}') \cdot R\beta_1 \right) \overline{\tau \rho_1(\mathbf{x}')} \bar{\tau} \rho_2(\mathbf{y}') ds_{\mathbf{x}'} ds_{\mathbf{y}'}.
\end{aligned} \tag{B.22}$$

Here we have used (B.17), $\beta_2 = R^{-1} \beta_1$ and $(\bar{\tau})^2 = \tau$.

For the fourth equation, consider the ε derivative when $\mathbf{p} = K$ around $\varepsilon = 0$. Define

$$K(\mathbf{x}, \mathbf{y}) := \partial_{\varepsilon} G^f(R^{\varepsilon} \mathbf{y}, R^{\varepsilon} \mathbf{x}; \lambda, K)|_{\varepsilon=0} = - \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} \mathbf{m} \cdot J(\mathbf{x} - \mathbf{y}). \tag{B.23}$$

We verify

$$\begin{aligned}
K(R^{-1} \mathbf{x}, R^{-1} \mathbf{y}) &= - \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot R^{-1}(\mathbf{x} - \mathbf{y})} \mathbf{m} \cdot JR^{-1}(\mathbf{x} - \mathbf{y}) \\
&= - \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{i}{\lambda - |\mathbf{m}|^2} e^{iR\mathbf{m} \cdot (\mathbf{x} - \mathbf{y})} R\mathbf{m} \cdot J(\mathbf{x} - \mathbf{y}) = K(\mathbf{x}, \mathbf{y})
\end{aligned} \tag{B.24}$$

and

$$\begin{aligned}
K(F\mathbf{x}, F\mathbf{y}) &= -\frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{i}{\lambda - |\mathbf{m}|^2} e^{i\mathbf{m} \cdot F(\mathbf{x}-\mathbf{y})} \mathbf{m} \cdot JF(\mathbf{x}-\mathbf{y}) \\
&= \frac{1}{|\mathcal{C}_z|} \sum_{\mathbf{m} \in \tilde{\Lambda}^*} \frac{i}{\lambda - |\mathbf{m}|^2} e^{iF\mathbf{m} \cdot (\mathbf{x}-\mathbf{y})} F\mathbf{m} \cdot J(\mathbf{x}-\mathbf{y}) = -K(\mathbf{x}, \mathbf{y}).
\end{aligned} \tag{B.25}$$

Here we have used (B.2), (3.10) and $|\mathbf{m}| = |R\mathbf{m}| = |F\mathbf{m}|$. Thus a similar argument as that for the first equation gives opposite diagonal terms are zero off-diagonal terms. \square

Proof of Proposition 8.1. A linear combination of the second and third equations in (4.8) gives (8.1), since $\tilde{\beta}_1 = \beta_1 - \beta_2$.

Observe

$$K' + \Lambda^* = -K + \Lambda^*. \tag{B.26}$$

Using (B.12), (B.17) and (B.23), we know that

$$\begin{aligned}
\partial_\lambda G^f(\mathbf{y}, \mathbf{x}; \lambda, K') &= \overline{\partial_\lambda G^f(\mathbf{y}, \mathbf{x}; \lambda, K)}, \\
\nabla_{\mathbf{p}} G^f(\mathbf{y}, \mathbf{x}; \lambda, \mathbf{p})|_{\mathbf{p}=K'} &= \overline{-\nabla_{\mathbf{p}} G^f(\mathbf{y}, \mathbf{x}; \lambda, \mathbf{p})|_{\mathbf{p}=K}} \\
\partial_\varepsilon G^f(R^\varepsilon \mathbf{y}, R^\varepsilon \mathbf{x}; \lambda, K')|_{\varepsilon=0} &= \overline{\partial_\varepsilon G^f(R^\varepsilon \mathbf{y}, R^\varepsilon \mathbf{x}; \lambda, K)|_{\varepsilon=0}}.
\end{aligned} \tag{B.27}$$

Using $\rho'_1(\mathbf{x}) = \overline{\rho_2(\mathbf{x})}$ and $\rho'_2(\mathbf{x}) = \overline{\rho_1(\mathbf{x})}$, we obtain

$$\langle \rho'_1, \nabla_{\mathbf{p}} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})|_{\mathbf{p}=K'} \rho'_2 \rangle_{\partial D=0} = -\langle \rho_2, \nabla_{\mathbf{p}} G^f(\mathbf{x}, \mathbf{y}; \lambda, \mathbf{p})|_{\mathbf{p}=K} \rho_1 \rangle_{\partial D=0} = -\overline{\theta_*}. \tag{B.28}$$

This finishes the proof of (8.4). \square

Appendix C Proof of Proposition 7.1

In this subsection, all $\langle \cdot, \cdot \rangle$ pairings represent the $\mathcal{H}^{1/2}(\Gamma)$ - $\mathcal{H}^{-1/2}(\Gamma)$ pairing. We prove Proposition 7.1 in this appendix. Recall the definitions of $\mathbb{T}^\varepsilon(\lambda)$ in (6.12) and $\mathbb{U}_\pm(h)$ in (7.1) to (8.29). We are claiming that

$$\begin{aligned}
\left\| \mathcal{S}^{\pm\varepsilon}(\lambda_* + \varepsilon h)\phi - \left(\tilde{\mathcal{S}}^0(\lambda_*)\phi + \beta(h)\overline{\langle \phi, v_1 \rangle} v_1 + \beta(h)\overline{\langle \phi, v_2 \rangle} v_2 \mp \xi(h)\overline{\langle \phi, v_1 \rangle} v_2 \right. \right. \\
\left. \left. \mp \xi(h)\overline{\langle \phi, v_2 \rangle} v_1 \right) \right\|_{\mathcal{H}^{1/2}(\Gamma)} / \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \rightarrow 0.
\end{aligned} \tag{C.1}$$

$$\begin{aligned}
\left\| \mathcal{K}^{\pm\varepsilon}(\lambda_* + \varepsilon h)\psi - \left(\tilde{\mathcal{K}}^0(\lambda_*)\psi + \beta(h)\langle \partial_n v_1, \psi \rangle v_1 + \beta(h)\langle \partial_n v_2, \psi \rangle v_2 \right. \right. \\
\left. \left. \mp \xi(h)\langle \partial_n v_1, \psi \rangle v_2 \mp \xi(h)\langle \partial_n v_2, \psi \rangle v_1 \right) \right\|_{\mathcal{H}^{1/2}(\Gamma)} / \|\psi\|_{\mathcal{H}^{1/2}(\Gamma)} \rightarrow 0,
\end{aligned} \tag{C.2}$$

$$\begin{aligned}
\left\| \mathcal{K}^{*,\pm\varepsilon}(\lambda_* + \varepsilon h)\phi - \left(\tilde{\mathcal{K}}^{*,0}(\lambda_*)\phi + \beta(h)\overline{\langle \phi, v_1 \rangle} \partial_n v_1 + \beta(h)\overline{\langle \phi, v_2 \rangle} \partial_n v_2 \right. \right. \\
\left. \left. \mp \xi(h)\overline{\langle \phi, v_1 \rangle} \partial_n v_2 \mp \xi(h)\overline{\langle \phi, v_2 \rangle} \partial_n v_1 \right) \right\|_{\mathcal{H}^{-1/2}(\Gamma)} / \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \rightarrow 0,
\end{aligned} \tag{C.3}$$

$$\begin{aligned}
\left\| \mathcal{N}^{\pm\varepsilon}(\lambda_* + \varepsilon h)\psi - \left(\tilde{\mathcal{N}}^0(\lambda_*)\psi + \beta(h)\langle \partial_n v_1, \psi \rangle \partial_n v_1 + \beta(h)\langle \partial_n v_2, \psi \rangle \partial_n v_2 \right. \right. \\
\left. \left. \mp \xi(h)\langle \partial_n v_1, \psi \rangle \partial_n v_2 \mp \xi(h)\langle \partial_n v_2, \psi \rangle \partial_n v_1 \right) \right\|_{\mathcal{H}^{-1/2}(\Gamma)} / \|\psi\|_{\mathcal{H}^{-1/2}(\Gamma)} \rightarrow 0,
\end{aligned} \tag{C.4}$$

In subsections C.1-C.3, we focus on $\mathcal{S}^{\pm\varepsilon}(\lambda_* + \varepsilon h)$ in (C.1). Using the representations of $\mathcal{S}^{\pm\varepsilon}(\lambda_* + \varepsilon h)$ in (7.7) and $\tilde{\mathcal{S}}^0(\lambda)$ in (7.11), we will break the integral in $\mathcal{S}^{\pm\varepsilon}(\lambda_* + \varepsilon h)$ into three parts: (a) near the Dirac point given by (C.5), (b) the first two bands away from the Dirac point given by (C.25), and (c) higher bands given by (C.33). The convergence of the other three operators are verified similarly, and are given by Lemma C.4, Lemma C.6, Corollary C.11 and Subsection C.4.

C.1 Near the Dirac point

Lemma C.1. *The following convergence holds in the operator norm from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$ uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, as $\varepsilon \rightarrow 0^+$:*

$$\begin{aligned} & \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\overline{\langle \phi, v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - (\lambda_* + \varepsilon h)} d\ell \\ & \rightarrow \beta(h) \overline{\langle \phi, v_1 \rangle} v_1 + \beta(h) \overline{\langle \phi, v_2 \rangle} v_2 \mp \xi(h) \overline{\langle \phi, v_1 \rangle} v_2 \mp \xi(h) \overline{\langle \phi, v_2 \rangle} v_1. \end{aligned} \quad (\text{C.5})$$

We prove this lemma by proving the next two lemmas.

Lemma C.2. *The following convergence holds in the operator norm from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$ uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, as $\varepsilon \rightarrow 0^+$:*

$$\sum_{n=1,2} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\overline{\langle \phi, v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - (\lambda_* + \varepsilon h)} d\ell \rightarrow a_{\pm}(h) \overline{\langle \phi, w_1 \rangle} w_1 + b_{\pm}(h) \overline{\langle \phi, w_2 \rangle} w_2. \quad (\text{C.6})$$

where

$$a_+(h) = b_-(h) = f_1(h) + f_4(h), \quad b_+(h) = a_-(h) = f_2(h) + f_3(h). \quad (\text{C.7})$$

and

$$\begin{aligned} f_1(h) &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{-\frac{1}{|\gamma_*|} \sqrt{t_*^2 + |\theta_*|^2 \ell^2} - h} \cdot \frac{1}{1 + |L(1, \ell)|^2} d\ell, \\ f_2(h) &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{-\frac{1}{|\gamma_*|} \sqrt{t_*^2 + |\theta_*|^2 \ell^2} - h} \cdot \frac{|L(1, \ell)|^2}{1 + |L(1, \ell)|^2} d\ell, \\ f_3(h) &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{\frac{1}{|\gamma_*|} \sqrt{t_*^2 + |\theta_*|^2 \ell^2} - h} \cdot \frac{1}{1 + |L(1, \ell)|^2} d\ell. \\ f_4(h) &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1}{\frac{1}{|\gamma_*|} \sqrt{t_*^2 + |\theta_*|^2 \ell^2} - h} \cdot \frac{|L(1, \ell)|^2}{1 + |L(1, \ell)|^2} d\ell, \end{aligned} \quad (\text{C.8})$$

and $L(\varepsilon, \ell) = L(\varepsilon, \ell, 0)$ and $L(\varepsilon, \ell, \mu)$ is defined in (4.12). Note that the individual integrals in (C.8) are all divergent, but $f_1(h) + f_4(h)$ and $f_2(h) + f_3(h)$ are convergent.

Proof. Define

$$I_i^{\pm\varepsilon}(h) := \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\overline{\langle \phi, v_{i,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} v_{i,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{i,\pm\varepsilon}(\mathbf{p}(\ell)) - (\lambda_* + \varepsilon h)} d\ell. \quad (\text{C.9})$$

Using (5.11), (5.12), Remark 5.5 and

$$0 \leq L(\varepsilon, \ell) \leq 1,$$

$$\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} (1 + O(\varepsilon, \ell)) \pm \varepsilon h = \left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} \pm \varepsilon h \right) (1 + O(\varepsilon, \ell)), \quad |h| < \mathfrak{d} \left| \frac{t_*}{\gamma_*} \right|,$$

$$\frac{1}{|1 + |L(\varepsilon, \ell)|^2 + O(\varepsilon, \ell)|} = \frac{1}{|1 + |L(\varepsilon, \ell)|^2|} (1 + O(\varepsilon, \ell)),$$
(C.10)

we obtain

$$I_1^\varepsilon(h) = -\frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\overline{\langle \phi, w_1 \rangle} w_1 + \overline{L(\varepsilon, \ell)} \overline{\langle \phi, w_2 \rangle} w_1 + L(\varepsilon, \ell) \overline{\langle \phi, w_1 \rangle} w_2 + |L(\varepsilon, \ell)|^2 \overline{\langle \phi, w_2 \rangle} w_2 + O(\varepsilon, \ell) \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} (1 + O(\varepsilon, \ell))}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} + \varepsilon h \right) (|1 + |L(\varepsilon, \ell)|^2|)} dl.$$
(C.11)

The fact that $\frac{L(\varepsilon, \ell)}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} \pm \varepsilon h \right)}$ is odd in ℓ implies that

$$-\frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\overline{\langle \phi, w_1 \rangle} w_1 + \overline{L(\varepsilon, \ell)} \overline{\langle \phi, w_2 \rangle} w_1 + L(\varepsilon, \ell) \overline{\langle \phi, w_1 \rangle} w_2 + |L(\varepsilon, \ell)|^2 \overline{\langle \phi, w_2 \rangle} w_2}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} + \varepsilon h \right) (|1 + |L(\varepsilon, \ell)|^2|)} dl$$
(C.12)

$$= -\frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\overline{\langle \phi, w_1 \rangle} w_1 + |L(\varepsilon, \ell)|^2 \overline{\langle \phi, w_2 \rangle} w_2}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} + \varepsilon h \right) (|1 + |L(\varepsilon, \ell)|^2|)} dl$$

Using

$$L(\varepsilon, \ell) = L(1, \ell/\varepsilon), \quad \frac{1}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} + \varepsilon h \right)} dl = \frac{1}{\left(\frac{1}{|\gamma_*|} \sqrt{t_*^2 + |\theta_*|^2 (\ell/\varepsilon)^2} + h \right)} dl/\varepsilon,$$
(C.13)

we see that $f_1(h)$ and $f_2(h)$ emerge as the coefficients of $\overline{\langle \phi, w_1 \rangle} w_1$ and $\overline{\langle \phi, w_2 \rangle} w_2$ as $\varepsilon \rightarrow 0$. A similar argument for $I_2^\varepsilon(h)$ gives that

$$I_1^\varepsilon(h) + I_2^\varepsilon(h) = I^\varepsilon(h) + \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{O(\varepsilon, \ell) \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)}}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} + \varepsilon h \right) (|1 + |L(\varepsilon, \ell)|^2|)} dl,$$
(C.14)

where

$$I^\varepsilon(h) \rightarrow f_1(h) \overline{\langle \phi, w_1 \rangle} w_1 + f_2(h) \overline{\langle \phi, w_2 \rangle} w_2 + f_4(h) \overline{\langle \phi, w_1 \rangle} w_1 + f_3(h) \overline{\langle \phi, w_2 \rangle} w_2, \quad \text{as } \varepsilon \rightarrow 0.$$
(C.15)

Thus to establish the $+\varepsilon$ identity in (C.6), we only need to show

$$\int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{O(\varepsilon, \ell)}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} + \varepsilon h \right) (|1 + |L(\varepsilon, \ell)|^2|)} dl \rightarrow 0, \quad \text{as } \varepsilon \rightarrow 0.$$
(C.16)

This is true because $O(\varepsilon, \ell) = O(\varepsilon^{1/3})$ within the integral domain, the integral domain is of size $\varepsilon^{1/3}$, and

$$\int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{1}{\left(\frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\theta_*|^2 \ell^2} \right)} dl = \left| \frac{\gamma_*}{\theta_*} \right| \int_{[-\left| \frac{\theta_*}{t_*} \right| \varepsilon^{-2/3}, \left| \frac{\theta_*}{t_*} \right| \varepsilon^{-2/3}]} \frac{1}{\sqrt{1+x^2}} dx = O(\ln \varepsilon).$$
(C.17)

Here we have used $\int \frac{1}{\sqrt{1+x^2}} dx = \ln(x + \sqrt{x^2+1})$.

The $-\varepsilon$ identity in (C.6) can be shown similarly. □

Lemma C.3. *The coefficients defined in (C.7) are equal to*

$$a_+(h) = b_-(h) = \beta(h) - \xi(h), \quad b_+(h) = a_-(h) = \beta(h) + \xi(h), \quad (\text{C.18})$$

where $\beta(h)$ and $\xi(h)$ are defined in (7.5). There holds the identity

$$a_{\pm}(h) \overline{\langle \phi, w_1 \rangle} w_1 + b_{\pm}(h) \overline{\langle \phi, w_2 \rangle} w_2 = \beta(h) \overline{\langle \phi, v_1 \rangle} v_1 + \beta(h) \overline{\langle \phi, v_2 \rangle} v_2 \mp \xi(h) \overline{\langle \phi, v_1 \rangle} v_2 \mp \xi(h) \overline{\langle \phi, v_2 \rangle} v_1 \quad (\text{C.19})$$

Proof. We first derive the simplified forms of the coefficients $a_{\pm}(h)$ and $b_{\pm}(h)$. Direct calculation shows

$$\begin{aligned} 2\pi(f_1(h) + f_4(h)) &= \int_{\mathbb{R}} \frac{1}{-\frac{1}{|\gamma_*|} \sqrt{t_*^2 + |\theta_*|^2 \ell^2} - h} \cdot \frac{1}{1 + |L(1, \ell)|^2} d\ell + \int_{\mathbb{R}} \frac{1}{\frac{1}{\gamma_*} \sqrt{t_*^2 + |\theta_*|^2 \ell^2} - h} \cdot \frac{|L(1, \ell)|^2}{1 + |L(1, \ell)|^2} d\ell, \\ &= - \int_{\mathbb{R}} \frac{1 - |L(1, \ell)|^2}{1 + |L(1, \ell)|^2} \cdot \frac{\frac{1}{\gamma_*} \sqrt{t_*^2 + |\theta_*|^2 \ell^2}}{(\frac{1}{\gamma_*})^2 (t_*^2 + |\theta_*|^2 \ell^2) - h^2} d\ell + \int_{\mathbb{R}} \frac{h}{(\frac{1}{\gamma_*})^2 (t_*^2 + |\theta_*|^2 \ell^2) - h^2} d\ell \end{aligned} \quad (\text{C.20})$$

Using

$$\begin{aligned} 1 - |L(1, \ell)|^2 &= \frac{2t_*}{t + \sqrt{t_*^2 + |\theta_*|^2 \ell^2}}, \\ 1 + |L(1, \ell)|^2 &= \frac{2\sqrt{t_*^2 + |\theta_*|^2 \ell^2}}{t + \sqrt{t_*^2 + |\theta_*|^2 \ell^2}}, \\ \frac{1 - |L(1, \ell)|^2}{1 + |L(1, \ell)|^2} &= \frac{t_*}{\sqrt{t_*^2 + |\theta_*|^2 \ell^2}}, \\ \int_{\mathbb{R}} \frac{1}{(\frac{1}{\gamma_*})^2 (t_*^2 + |\theta_*|^2 \ell^2) - h^2} d\ell &= \frac{|\gamma_*|}{|\theta_*|} \frac{1}{\sqrt{(\frac{t_*}{\gamma_*})^2 - h^2}} \pi, \end{aligned} \quad (\text{C.21})$$

we obtain the first equation in (C.18). The second equation in (C.18) can be similarly obtained.

The relation (C.19) can be obtained using the relation between w_i and v_i (5.16). \square

Using the same method, we obtain the convergence of the first two bands close to the Dirac point in the other operators.

Lemma C.4. *The following convergences hold in the operator norm from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$, from $\mathcal{H}^{1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$ and from $\mathcal{H}^{1/2}(\Gamma)$ to $\mathcal{H}^{-1/2}(\Gamma)$ respectively uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d} |\frac{t_*}{\gamma_*}|$, as $\varepsilon \rightarrow 0^+$:*

$$\begin{aligned} \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\overline{\langle v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle} \partial_n v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \\ \rightarrow \beta(h) \langle \partial_n v_1, \psi \rangle v_1 + \beta(h) \langle \partial_n v_2, \psi \rangle v_2 \mp \xi(h) \langle \partial_n v_1, \psi \rangle v_2 \mp \xi(h) \langle \partial_n v_2, \psi \rangle v_1 \end{aligned} \quad (\text{C.22})$$

$$\begin{aligned} \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\langle \partial_n v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \\ \beta(h) \overline{\langle \phi, v_1 \rangle} \partial_n v_1 + \beta(h) \overline{\langle \phi, v_2 \rangle} \partial_n v_2 \mp \xi(h) \overline{\langle \phi, v_1 \rangle} \partial_n v_2 \mp \xi(h) \overline{\langle \phi, v_2 \rangle} \partial_n v_1 \end{aligned} \quad (\text{C.23})$$

$$\begin{aligned} \partial_n \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{\langle \partial_n v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell), \psi) \rangle v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \\ \beta(h) \langle \partial_n v_1, \psi \rangle \partial_n v_1 + \beta(h) \langle \partial_n v_2, \psi \rangle \partial_n v_2 \mp \xi(h) \langle \partial_n v_1, \psi \rangle \partial_n v_2 \mp \xi(h) \langle \partial_n v_2, \psi \rangle \partial_n v_1 \end{aligned} \quad (\text{C.24})$$

C.2 The first two bands away from the Dirac point

Lemma C.5. *The following convergence holds in the operator norm from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$ uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, as $\varepsilon \rightarrow 0$:*

$$\sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\overline{\langle \phi, v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \sum_{n=1,2} \frac{1}{2\pi} p.v. \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell. \quad (\text{C.25})$$

Proof. We show that among the following five quantities, the difference between each adjacent pair converges to zero in operator norm as $\varepsilon \rightarrow 0$. The five quantities are

$$\begin{aligned} I_1\phi &:= \sum_{n=1,2} \lim_{\delta \rightarrow 0^+} \frac{1}{2\pi} \int_{[-\pi, -\delta] \cup [\delta, \pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell, \\ I_2\phi &:= \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell, \\ I_3\phi &:= \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\overline{\langle \phi, u_n(\cdot; \mathbf{p}(\ell)) \rangle} u_n(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_n(\mathbf{p}(\ell)) - \lambda_*} d\ell, \\ I_4\phi &:= \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\overline{\langle \phi, u_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell, \\ I_5\phi &:= \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\overline{\langle \phi, v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell. \end{aligned} \quad (\text{C.26})$$

For $I_1 - I_2 \rightarrow 0$, we define $f(\mathbf{x}, \ell) := \overline{\langle \phi, v_1(\cdot; \mathbf{p}(\ell)) \rangle} v_1(\mathbf{x}; \mathbf{p}(\ell))$. From the analyticity of $v_1(\cdot; \mathbf{p}(\ell))$ in ℓ in a neighborhood of \mathbb{R} as $H^1(\mathcal{C}_z \setminus D)$ functions as stated above (5.6), we know $\|\frac{d}{d\ell} v_1(\cdot; \mathbf{p}(\ell))\|_{H^1(\mathcal{C}_z \setminus D)}$ is bounded on $\ell \in [0, 1]$, thus

$$\begin{aligned} \|f(\cdot, \ell)\|_{\mathcal{H}^{1/2}(\Gamma)} &\leq \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \max_{|\ell| \leq 1} (\|v_1(\cdot, \ell)\|_{H^1(\mathcal{C}_z \setminus D)} \|v_1(\cdot, \ell)\|_{H^1(\mathcal{C}_z \setminus D)}), \\ \|\frac{d}{d\ell} f(\cdot, \ell)\|_{\mathcal{H}^{1/2}(\Gamma)} &= \|\overline{\langle \phi, \frac{d}{d\ell} v_1(\cdot; \mathbf{p}(\ell)) \rangle} v_1(\mathbf{x}; \mathbf{p}(\ell)) + \overline{\langle \phi, v_1(\cdot; \mathbf{p}(\ell)) \rangle} \frac{d}{d\ell} v_1(\mathbf{x}; \mathbf{p}(\ell))\|_{\mathcal{H}^{1/2}(\Gamma)} \\ &\leq 2\|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \max_{|\ell| \leq \varepsilon^{1/3}} (\|\frac{d}{d\ell} v_1(\cdot, \ell)\|_{\mathcal{H}^{1/2}(\Gamma)} \|v_1(\cdot, \ell)\|_{\mathcal{H}^{1/2}(\Gamma)}) \\ &\leq 2\|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \max_{|\ell| \leq 1} (\|\frac{d}{d\ell} v_1(\cdot, \ell)\|_{H^1(\mathcal{C}_z \setminus D)} \|v_1(\cdot, \ell)\|_{H^1(\mathcal{C}_z \setminus D)}). \end{aligned} \quad (\text{C.27})$$

Thus

$$\begin{aligned}
& \left\| \lim_{\delta \rightarrow 0^+} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, -\delta] \cup [\delta, \varepsilon^{1/3}]} \frac{\overline{\langle \phi, v_1(\cdot; \mathbf{p}(\ell)) \rangle} v_1(\mathbf{x}; \mathbf{p}(\ell))}{\mu_1(\mathbf{p}(\ell)) - \lambda_*} d\ell \right\|_{\mathcal{H}^{1/2}(\Gamma)} / \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \\
&= \left\| \lim_{\delta \rightarrow 0^+} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, -\delta] \cup [\delta, \varepsilon^{1/3}]} \frac{f(\mathbf{x}, \ell)}{|\alpha_*| \ell} (1 + O(\ell)) d\ell \right\|_{\mathcal{H}^{1/2}(\Gamma)} / \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \\
&= \left\| \lim_{\delta \rightarrow 0^+} \frac{1}{2\pi} \int_{[\delta, \varepsilon^{1/3}]} \frac{f(\mathbf{x}, \ell) - f(\mathbf{x}, -\ell)}{|\alpha_*| \ell} + O(\ell) \frac{f(\mathbf{x}, \ell)}{|\alpha_*| \ell} + O(\ell) \frac{f(\mathbf{x}, -\ell)}{|\alpha_*| \ell} d\ell \right\|_{\mathcal{H}^{1/2}(\Gamma)} / \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \\
&= O(\varepsilon^{1/3}) \left(\max_{|\ell| \leq \varepsilon^{1/3}} \left\| \frac{d}{d\ell} f(\cdot, \ell) \right\|_{\mathcal{H}^{1/2}(\Gamma)} + \max_{|\ell| \leq \varepsilon^{1/3}} \|f(\cdot, \ell)\|_{\mathcal{H}^{1/2}(\Gamma)} \right) / \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)} \rightarrow 0.
\end{aligned} \tag{C.28}$$

From Fig. 5.1, we observe I_2 and I_3 are the same, and I_4 and I_5 are the same. Finally, on the integral domain,

$$\begin{aligned}
|\lambda_n(\mathbf{p}(\ell)) - \lambda_*| &\gtrsim \varepsilon^{1/3}, \quad |\lambda_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h| \gtrsim \varepsilon^{1/3}, \\
\|u_{n, \pm \varepsilon}(\cdot; \mathbf{p}(\ell)) - \alpha u_n(\cdot; \mathbf{p}(\ell))\|_{H^1(\mathcal{C}_z)} &= O(\varepsilon), \\
\lambda_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \varepsilon h - \lambda_n(\mathbf{p}(\ell)) &= O(\varepsilon).
\end{aligned} \tag{C.29}$$

Here α is a phase factor that depends on $\pm \varepsilon$, n and ℓ as remarked on Remark 5.5. Thus by elementary insertion and grouping, $I_3 - I_4 = O(\varepsilon^{1/3}) \rightarrow 0$. \square

Using the same method, we obtain the convergence of the first two bands away from the Dirac point in the other operators.

Lemma C.6. *The following convergences hold in the operator norm from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$, from $\mathcal{H}^{1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$ and from $\mathcal{H}^{1/2}(\Gamma)$ to $\mathcal{H}^{-1/2}(\Gamma)$ respectively uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d} \frac{t_*}{\gamma_*}$, as $\varepsilon \rightarrow 0$:*

$$\begin{aligned}
& \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\overline{\langle v_{n, \pm \varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle} \partial_n v_{n, \pm \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \\
& \rightarrow \sum_{n=1,2} \frac{1}{2\pi} p.v. \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle} \partial_n v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell.
\end{aligned} \tag{C.30}$$

$$\begin{aligned}
& \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\langle \partial_n v_{n, \pm \varepsilon}(\cdot; \mathbf{p}(\ell), \psi) \rangle v_{n, \pm \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \\
& \sum_{n=1,2} \frac{1}{2\pi} p.v. \int_{[-\pi, \pi]} \frac{\langle \partial_n v_n(\cdot; \mathbf{p}(\ell)), \psi \rangle v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell,
\end{aligned} \tag{C.31}$$

$$\begin{aligned}
& \partial_n \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\pi, -\varepsilon^{1/3}] \cup [\varepsilon^{1/3}, \pi]} \frac{\langle \partial_n v_{n, \pm \varepsilon}(\cdot; \mathbf{p}(\ell), \psi) \rangle v_{n, \pm \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \\
& \partial_n \sum_{n=1,2} \frac{1}{2\pi} p.v. \int_{[-\pi, \pi]} \frac{\langle \partial_n v_n(\cdot; \mathbf{p}(\ell)), \psi \rangle v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell.
\end{aligned} \tag{C.32}$$

C.3 Higher bands

In this section, we will prove Lemma C.7 and Lemma C.11.

Lemma C.7. *The following convergence holds in the operator norm from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$ uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, as $\varepsilon \rightarrow 0$:*

$$\sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, v_{n, \pm \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} v_{n, \pm \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell. \quad (\text{C.33})$$

(C.33) is equivalently be represented by

$$\sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, u_{n, \pm \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n, \pm \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, u_n(\cdot; \mathbf{p}(\ell)) \rangle} u_n(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_n(\mathbf{p}(\ell)) - \lambda_*} d\ell, \quad (\text{C.34})$$

where $\lambda_{n, \pm \varepsilon}$ and λ_n are ranked increasingly as introduced in Section 5.1.

Remark C.8. *The limits in Lemma C.7 do not depend on the sign of ε . Thus we will work with ε with sufficiently small absolute values. We also use $\lambda_n = \lambda_{n,0}$ and $u_n = u_{n,0}$ when convenient.*

Notice that $u_{n, \varepsilon}$ are supported on different domains $\mathcal{C}_z \setminus D^\varepsilon$ as ε varies. Instead of extending them by 0 into D^ε as done in (4.4), we convert them to the same support $\mathcal{C}_z \setminus D$ through diffeomorphisms, where results in [47, p.423] and [52] can be applied. Let \mathbf{x} and \mathbf{y}^ε be the Euclidean coordinates of $\mathcal{C}_z \setminus D$ and $\mathcal{C}_z \setminus D^\varepsilon$. Fix an open set \mathcal{O} compactly supported in \mathcal{C}_z and containing D^ε for all ε . There is a smooth bijective map from $\mathcal{C}_z \setminus D$ to $\mathcal{C}_z \setminus D^\varepsilon$ that is analytic in ε , denoted by $y^\varepsilon = y^\varepsilon(x)$. Moreover, we may require that $\mathbf{y}^\varepsilon(\mathbf{x})$ satisfy the following conditions: (i) $\mathbf{y}^\varepsilon(\mathbf{x}) = \mathbf{x}$ for $\mathbf{x} \in \mathcal{O}$, (ii) $|\mathbf{y}^\varepsilon(\mathbf{x}) - \mathbf{x}| \rightarrow 0$ uniformly in $\mathcal{C}_z \setminus D$ as $\varepsilon \rightarrow 0$, and (iii) the Jacobian $|\frac{\partial \mathbf{y}^\varepsilon(\mathbf{x})}{\partial \mathbf{x}}| \rightarrow 0$ uniformly in $\mathcal{C}_z \setminus D$ as $\varepsilon \rightarrow 0$. Every function $u(\mathbf{y}^\varepsilon)$ on $\mathcal{C}_z \setminus D^\varepsilon$ can be treated as a function $u(\mathbf{y}^\varepsilon(\mathbf{x}))$ on $\mathcal{C}_z \setminus D$.

Since $\mathbf{y}^\varepsilon(\mathbf{x}) = \mathbf{x}$ in a neighborhood of Γ , Lemma C.7 follows from the following lemma and taking trace to Γ .

Lemma C.9. *As $\varepsilon \rightarrow 0$, the following convergence holds uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$*

$$\|\mathbb{S}^{\varepsilon, \text{evan}}(\lambda_* + \varepsilon h) - \mathbb{S}^{0, \text{evan}}(\lambda_*)\|_{\mathcal{H}^{-1/2}(\Gamma) \rightarrow H^1(\mathcal{C}_z \setminus D)} \rightarrow 0, \quad (\text{C.35})$$

where

$$\begin{aligned} \mathbb{S}^{\varepsilon, \text{evan}}(\lambda_* + \varepsilon h)\phi(\mathbf{x}) &:= \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, u_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n, \varepsilon}(\mathbf{y}^\varepsilon(\mathbf{x}); \mathbf{p}(\ell))}{\lambda_{n, \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell, \\ \mathbb{S}^{0, \text{evan}}(\lambda_*)\phi(\mathbf{x}) &:= \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, u_n(\cdot; \mathbf{p}(\ell)) \rangle} u_n(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_n(\mathbf{p}(\ell)) - \lambda_*} d\ell. \end{aligned} \quad (\text{C.36})$$

We will prove Lemma C.9 using the dominant convergence theorem and the following results.

Lemma C.10. *Let $\mathbb{S}^{\varepsilon, \text{evan}}(\lambda_* + \varepsilon h, \mathbf{p}(\ell))$ and $\mathbb{S}^{0, \text{evan}}(\lambda_*, \mathbf{p}(\ell))$ be operators from $\mathcal{H}^{-1/2}(\Gamma)$ to $H^1(\mathcal{C}_z \setminus D)$ that are defined by*

$$\begin{aligned} \mathbb{S}^{\varepsilon, \text{evan}}(\lambda_* + \varepsilon h, \mathbf{p})\phi(\mathbf{x}) &:= \sum_{n \geq 3} \frac{\overline{\langle \phi, v_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} v_{n, \varepsilon}(\mathbf{y}^\varepsilon(\mathbf{x}); \mathbf{p}(\ell))}{\mu_{n, \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h}, \\ \mathbb{S}^{0, \text{evan}}(\lambda_*, \mathbf{p})\phi(\mathbf{x}) &:= \sum_{n \geq 3} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle} v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*}. \end{aligned} \quad (\text{C.37})$$

There is a constant ε_1 , such that the following three statements hold uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$.

1. For each $|\varepsilon| < \varepsilon_1$, $\mathbb{S}^{\varepsilon, \text{evan}}(\lambda_* + \varepsilon h, \mathbf{p}(\ell))$ are continuous in ℓ in the operator norm.
2. $\mathbb{S}^{\varepsilon, \text{evan}}(\lambda_* + \varepsilon h, \mathbf{p}(\ell))$ are uniformly bounded in the operator norm over ℓ and over $|\varepsilon| < \varepsilon_1$.
3. For each $\ell \neq 0$, $\mathbb{S}^{\varepsilon, \text{evan}}(\lambda_* + \varepsilon h, \mathbf{p}(\ell))$ converge to $\mathbb{S}^{0, \text{evan}}(\lambda_*, \mathbf{p}(\ell))$ in the operator norm as $\varepsilon \rightarrow 0$.

To prepare for the proof of Lemma C.10, we introduce the following functions for each fixed ℓ :

$$w^\varepsilon(\mathbf{x}) := \sum_{n \geq 3} \frac{\langle \phi, u_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle u_{n, \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_{n, \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} \quad (\text{C.38})$$

and

$$\hat{w}^\varepsilon(\mathbf{x}) := \sum_{n \geq 3} \frac{\langle \phi, u_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle u_{n, \varepsilon}(\mathbf{y}^\varepsilon(\mathbf{x}); \mathbf{p}(\ell))}{\lambda_{n, \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h}. \quad (\text{C.39})$$

We introduce the following function spaces, whose more detailed properties can be found in [60, 66]. Let $H^s(\ell)$ be the Sobolev space on \mathbb{R}^2 of order s that is quasiperiodic with quasimomenta $\mathbf{p}(\ell) \cdot \mathbf{e}_i$ in \mathbf{e}_i , $i = 1, 2$. Let $L^{2, \varepsilon}(\ell) = H^{0, \varepsilon}(\ell)$ be $H^0(\ell)$ functions that are supported on $\mathbb{R}^2 \setminus \cup_{n_1, n_2 \in \mathbb{Z}} (D^\varepsilon + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2)$, $H^{1, \varepsilon}(\ell)$ be $H^1(\ell)$ functions that are supported on $\overline{\mathbb{R}^2 \setminus \cup_{n_1, n_2 \in \mathbb{Z}} (D^\varepsilon + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2)}$, and $H^{-1, \varepsilon}(\ell)$ distributions on $\mathbb{R}^2 \setminus \cup_{n_1, n_2 \in \mathbb{Z}} (\overline{D^\varepsilon} + n_1 \mathbf{e}_1 + n_2 \mathbf{e}_2)$ who can be extended to distributions in $H^{-1}(\ell)$. The dual space of $H^{1, \varepsilon}(\ell)$ is $H^{-1, \varepsilon}(\ell)$.

The pairings on these spaces are defined through their quasiperiodic Fourier expansions. Denote the $L^{2, \varepsilon}(\ell)$ - $L^{2, \varepsilon}(\ell)$ pairing by $\langle \cdot, \cdot \rangle_\varepsilon$, and the $H^{-1, \varepsilon}(\ell)$ - $H^{1, \varepsilon}(\ell)$ pairing by $(\cdot, \cdot)_\varepsilon$. The inner product on $H^{1, \varepsilon}(\ell)$ is given by $\langle \nabla u, \nabla v \rangle_\varepsilon + \langle u, v \rangle_\varepsilon$.

Define the operators $(-\Delta_\varepsilon(\ell))^{-1} : H^{-1, \varepsilon}(\ell) \rightarrow H^{1, \varepsilon}(\ell)$ by

$$(-\Delta_\varepsilon(\ell))^{-1} f = u \text{ if and only if } \langle \nabla u, \nabla v \rangle_\varepsilon = (f, v)_\varepsilon \quad \forall v \in H^{1, \varepsilon}(\ell). \quad (\text{C.40})$$

Notice that when restricted on $H^{1, \varepsilon}(\ell)$, the operator $(-\Delta_\varepsilon(\ell))^{-1} : H^{1, \varepsilon}(\ell) \rightarrow H^{1, \varepsilon}(\ell)$ is bounded, selfadjoint, compact and positive. Thus there exists an orthogonal eigensystem of $(-\Delta_\varepsilon(\ell))^{-1}$ that is complete in $H^{1, \varepsilon}(\ell)$. This eigensystem coincides with $\lambda_{n, \varepsilon} := \lambda_{n, \varepsilon}(\mathbf{p}(\ell))$ and $u_{n, \varepsilon} := u_{n, \varepsilon}(\mathbf{x}, \mathbf{p}(\ell))$ that are defined in Section 5.1. We have

$$\begin{aligned} (-\Delta_\varepsilon(\ell))^{-1} u_{n, \varepsilon}(\ell) &= \frac{1}{\lambda_{n, \varepsilon}(\ell)} u_n(\ell), \quad 0 < \lambda_{1, n}(\ell) \leq \lambda_{2, \varepsilon}(\ell) \leq \dots \rightarrow \infty, \\ \langle \nabla u_{n, \varepsilon}(\ell), \nabla u_{m, \varepsilon}(\ell) \rangle_\varepsilon + \langle u_{n, \varepsilon}(\ell), u_{m, \varepsilon}(\ell) \rangle_\varepsilon &= (1 + \lambda_{n, \varepsilon}(\ell)) \delta_{m, n}. \end{aligned} \quad (\text{C.41})$$

We have the expansion

$$\forall f \in H^{1, \varepsilon}(\ell), \quad f = \sum_{n \geq 1} \langle u_{n, \varepsilon}(\ell), f \rangle_\varepsilon u_{n, \varepsilon}(\ell), \text{ which converges in } H^{1, \varepsilon}(\ell). \quad (\text{C.42})$$

By the density of $H^{1, \varepsilon}(\ell)$ in $L^2(C^\varepsilon)$ and $H^{-1, \varepsilon}(\ell)$, we also have

$$\forall f \in L^2(C^\varepsilon), \quad f = \sum_{n \geq 1} \langle u_{n, \varepsilon}(\ell), f \rangle_\varepsilon u_{n, \varepsilon}(\ell), \text{ which converges in } L^2(\mathcal{C}_z \setminus D^\varepsilon), \quad (\text{C.43})$$

and

$$\forall f \in H^{-1,\varepsilon}(\ell), \quad f = \sum_{n \geq 1} \overline{(f, u_{n,\varepsilon}(\ell))_\varepsilon} u_{n,\varepsilon}(\ell), \quad \text{which converges in } H^{-1,\varepsilon}(\ell). \quad (\text{C.44})$$

For $A \subset \mathbb{Z}^+$, define the projection operator $P_{n \in A, \varepsilon, \ell} : H^{1,\varepsilon}(\ell) \rightarrow H^{1,\varepsilon}(\ell)$ by

$$P_{n \in A, \varepsilon, \ell} f = \sum_{n \in A} \langle u_{n,\varepsilon}(\ell), f \rangle_\varepsilon u_{n,\varepsilon}(\ell). \quad (\text{C.45})$$

It is straightforward to verify that the function w^ε in (C.38) solves the following problem

$$\begin{aligned} (I - (\lambda_* + \varepsilon h)(-\Delta_\varepsilon(\ell))^{-1})w(\mathbf{x}) &= (-\Delta_\varepsilon(\ell))^{-1} \left(\phi\delta(\Gamma) - \sum_{n \geq 1, 2} \overline{\langle \phi, u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) \right) \\ &= P_{n \geq 3, \varepsilon, \ell} (-\Delta_\varepsilon(\ell))^{-1} (\phi\delta(\Gamma)). \end{aligned} \quad (\text{C.46})$$

This can be equivalently represented as

$$(-\Delta - (\lambda_* + \varepsilon h))w(\mathbf{x}) = \phi\delta(\Gamma) - \sum_{n \geq 1, 2} \overline{\langle \phi, u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)). \quad (\text{C.47})$$

Here we have used $\phi\delta(\Gamma) \in H^{-1,\varepsilon}(\ell)$ and

$$\overline{(\phi\delta(\Gamma), u_{n,\varepsilon})_\varepsilon} = \overline{\langle \phi, u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle}. \quad (\text{C.48})$$

The diffeomorphism $\mathbf{y}^\varepsilon(\mathbf{x})$ converts (C.38) to (C.39). We have the following change of variables formulas

$$\begin{aligned} \int_{\mathcal{C}_z \setminus D^\varepsilon} \overline{u}(\mathbf{y}^\varepsilon) v(\mathbf{y}^\varepsilon) d\mathbf{y}^\varepsilon &= \int_{\mathcal{C}_z \setminus D} \overline{u(\mathbf{y}^\varepsilon(\mathbf{x}))} v(\mathbf{y}^\varepsilon(\mathbf{x})) \left| \left(\frac{\partial \mathbf{y}^\varepsilon}{\partial \mathbf{x}} \right) \right| d\mathbf{x}, \\ \int_{\mathcal{C}_z \setminus D^\varepsilon} \nabla_{\mathbf{y}^\varepsilon} \overline{u(\mathbf{y}^\varepsilon)} \cdot \nabla_{\mathbf{y}^\varepsilon} v(\mathbf{y}^\varepsilon) d\mathbf{y}^\varepsilon &= \int_{\mathcal{C}_z \setminus D} \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}^\varepsilon} \right) \nabla_{\mathbf{x}} \overline{u(\mathbf{y}^\varepsilon(\mathbf{x}))} \cdot \left(\frac{\partial \mathbf{x}}{\partial \mathbf{y}^\varepsilon} \right) \nabla_{\mathbf{x}} v(\mathbf{y}^\varepsilon(\mathbf{x})) \left| \left(\frac{\partial \mathbf{y}^\varepsilon}{\partial \mathbf{x}} \right) \right| d\mathbf{x}. \end{aligned} \quad (\text{C.49})$$

Thus

$$\|u(\mathbf{y}^\varepsilon(\cdot))\|_{H^{k,0}(\ell)} = \|u(\cdot)\|_{H^{k,\varepsilon}(\ell)} (1 + O(\varepsilon)), \quad k = -1, 0, 1. \quad (\text{C.50})$$

Define $(-\tilde{\Delta}_\varepsilon)^{-1} : H^{-1,0}(\ell) \rightarrow H^{1,0}(\ell)$ by

$$\begin{aligned} (-\tilde{\Delta}_\varepsilon(\ell))^{-1} f = u \text{ if and only if} \\ \int_{\mathcal{C}_z \setminus D} \left(\frac{\partial x}{\partial y^\varepsilon} \right) \nabla_x \overline{u(x)} \cdot \left(\frac{\partial x}{\partial y^\varepsilon} \right) \nabla_x v(x) \left| \left(\frac{\partial y^\varepsilon}{\partial x} \right) \right| dx = \int_{\mathcal{C}_z \setminus D} \overline{f(x)} v(x) \left| \left(\frac{\partial y^\varepsilon}{\partial x} \right) \right| dx. \end{aligned} \quad (\text{C.51})$$

Then we have

$$(-\tilde{\Delta}_\varepsilon(\ell))^{-1} f(\mathbf{y}^\varepsilon(\cdot)) = u(\mathbf{y}^\varepsilon(\cdot)) \text{ if and only if } (-\Delta_\varepsilon(\ell))^{-1} f(\cdot) = u(\cdot). \quad (\text{C.52})$$

Combining with (C.47), we obtain that (C.39) solves

$$(-\tilde{\Delta}_\varepsilon - (\lambda_* + \varepsilon h))\hat{w}(\mathbf{x}) = \phi\delta(\Gamma) - \sum_{n \geq 1, 2} \overline{\langle \phi, u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n,\varepsilon}(\mathbf{y}^\varepsilon(\mathbf{x}); \mathbf{p}(\ell)). \quad (\text{C.53})$$

We are ready to prove Lemma C.10.

Proof of Lemma C.10. We know that there are constants $\varepsilon_1, \mathbf{c}_1, \mathbf{c}_2 > 0$ and a family of constants $\mathbf{c}_3(\ell) > 0$ depending on ℓ such that

$$\begin{aligned} \lambda_{n,\varepsilon}(\ell) &> \mathbf{c}_1 \quad \text{for all } |\varepsilon| < \varepsilon_1, \quad n \geq 1, \quad \ell \in [-\pi, \pi]; \\ \lambda_{n,\varepsilon}(\ell) &> \lambda_* + \frac{1+\mathfrak{d}}{2} \left| \frac{t_*}{\gamma_*} \right|, \quad \text{for all } |\varepsilon| < \varepsilon_1, \quad n \geq 3, \quad \ell \in [-\pi, \pi]; \\ |\lambda_{n,\varepsilon}(\ell) - \lambda| &> \mathbf{c}_2 \quad \text{for all } |\varepsilon| < \varepsilon_1, |\lambda - \lambda_*| < \mathfrak{d} \left| \frac{t_*}{\gamma_*} \right| \varepsilon, \quad n \geq 3, \quad \ell \in [-\pi, \pi]; \end{aligned}$$

for each $\ell \neq 0$, $\left| 1 - \frac{\lambda}{\lambda_{n,\varepsilon}(\ell)} \right| > \mathbf{c}_3(\ell)$ for all $|\varepsilon| < \varepsilon_1, |\lambda - \lambda_*| < \mathfrak{d} \left| \frac{t_*}{\gamma_*} \right| \varepsilon, \quad n \geq 1.$ (C.54)

Statement 1 follows from the analyticity in $\mathbf{p}(\ell)$ through gauge transformations [64, 38, 47].

For statement 2, before the diffeomorphism, treated as functions on $\mathcal{C}_z \setminus D^\varepsilon$, (C.46) gives

$$v = (I - (\lambda_* + \varepsilon h)(-\Delta_\varepsilon(\ell))^{-1})^{-1} P_{n \geq 3, \varepsilon, \ell} (-\Delta_\varepsilon(\ell))^{-1} (\phi \delta(\Gamma)). \quad (\text{C.55})$$

We have

$$\begin{aligned} \|\phi \delta(\Gamma)\|_{H^{-1, \varepsilon}(\ell)} &\leq C \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)}, \\ \|(-\Delta_\varepsilon(\ell))^{-1}\|_{H^{-1, \varepsilon}(\ell) \rightarrow H^{1, \varepsilon}(\ell)} &= \sup_n \left| \frac{1 + \lambda_{n, \varepsilon}(\ell)}{\lambda_{n, \varepsilon}(\ell)} \right| \leq \frac{1 + \mathbf{c}_1}{\mathbf{c}_1}, \\ \|P_{n \geq 3, \varepsilon, \ell}\|_{H^{-1, \varepsilon}(\ell) \rightarrow H^{1, \varepsilon}(\ell)} &\leq 1, \\ \|(I - (\lambda_* + \varepsilon h)(-\Delta_\varepsilon(\ell))^{-1})^{-1}\|_{P_{n \geq 3, \varepsilon, \ell} H^{1, \varepsilon}(\ell) \rightarrow H^{1, \varepsilon}(\ell)} &= \sup_{n \geq 3} \left| \left(1 - \frac{\lambda_* + \varepsilon h}{\lambda_{n, \varepsilon}(\ell)} \right)^{-1} \right| < \frac{1}{1 - (\lambda_* + \mathfrak{d} \left| \frac{t_*}{\gamma_*} \right|) / (\lambda_* + \frac{1+\mathfrak{d}}{2} \left| \frac{t_*}{\gamma_*} \right|)}. \end{aligned} \quad (\text{C.56})$$

Since the operator norms are related by a factor of $(1 + O(\varepsilon))$ uniformly when treated as maps between functions on $\mathcal{C}_z \setminus D$ through the diffeomorphisms, the proof of Statement 2 is complete.

For Statement 3, for each fixed ℓ , we apply Lemma 4.4 to

$$\begin{aligned} A_\varepsilon &= -\tilde{\Delta}_\varepsilon - \lambda_* - \varepsilon h, \\ A_0 &= -\tilde{\Delta}_0 - \lambda_*, \\ f_\varepsilon &= \phi \delta(\Gamma) - \sum_{n \geq 1, 2} \overline{\langle \phi, u_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n, \varepsilon}(\mathbf{y}^\varepsilon(\mathbf{x}); \mathbf{p}(\ell)), \\ f_0 &= \phi \delta(\Gamma) - \sum_{n \geq 1, 2} \overline{\langle \phi, u_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n, \varepsilon}(\mathbf{x}; \mathbf{p}(\ell)). \end{aligned} \quad (\text{C.57})$$

The forms defined in (C.51) are analytic in ε . Thus by [47], each pair of eigenvalue and eigeneigenfunction $\lambda_{n, \varepsilon}, u_{n, \varepsilon}$ converges to λ_n, u_n in $\mathbb{R} \times H^1(\mathcal{C}_z \setminus D)$ at a rate of $O(\varepsilon)$. Thus it is straight forward to verify that when ε_1 is sufficiently small, $|\varepsilon| < \varepsilon_1, |h| < \mathfrak{d} \left| \frac{t_*}{\gamma_*} \right|$, for each $\ell \neq 0$, there exists a constant $C(\ell)$, such that

$$\begin{aligned} \|A_0^{-1}\|_{H^{-1, 0}(\ell) \rightarrow H^{1, 0}(\ell)}, \|A_\varepsilon^{-1}\|_{H^{-1, 0}(\ell) \rightarrow H^{1, 0}(\ell)} &\leq C(\ell), \\ \|f_0\|_{H^{-1, 0}(\ell)}, \|f_\varepsilon\|_{H^{-1, 0}(\ell)} &\leq C(\ell) \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)}, \\ \|f_\varepsilon - f_0\|_{H^{-1, 0}(\ell)} &\leq \varepsilon C(\ell) \|\phi\|_{\mathcal{H}^{-1/2}(\Gamma)}, \\ \|A_\varepsilon - A_0\|_{H^{1, 0}(\ell) \rightarrow H^{-1, 0}(\ell)} &\rightarrow 0. \end{aligned} \quad (\text{C.58})$$

Thus we obtain Statement 3. □

Since we showed convergence in H^1 , taking the normal derivatives and using the jump relations, we obtain the following corollary.

Corollary C.11. *The following convergence holds in the operator norm from $\mathcal{H}^{-1/2}(\Gamma)$ to $\mathcal{H}^{-1/2}(\Gamma)$ uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, as $\varepsilon \rightarrow 0$:*

$$\sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle v_{n, \pm \varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle} \partial_n v_{n, \pm \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n, \pm \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\overline{\langle \phi, v_n(\cdot; \mathbf{p}(\ell)) \rangle} \partial_n v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell. \quad (\text{C.59})$$

C.4 Double layer potential and the convergence of higher bands

Let $\psi \in \mathcal{H}^{1/2}(\Gamma)$. Denote the part of $\mathcal{C}_z \setminus D^\varepsilon$ to the left of Γ by \mathcal{L}^ε and that to the right of Γ by \mathcal{R}^ε . Using (C.41), we know that when $\varepsilon \neq 0$ or $\ell \neq 0$, $\lambda_* + \varepsilon h \neq \lambda_{n, \varepsilon}(\ell)$ for all n ,

$$v(\mathbf{x}) := \sum_{n \geq 3} \frac{\langle \partial_n u_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle u_{n, \varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_{n, \varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} \quad (\text{C.60})$$

is the unique function that satisfies

$$\begin{aligned} [v] &= \psi, \quad [\partial_n v] = 0, \\ (-\Delta - \lambda_* - \varepsilon h)v &= - \sum_{n=1,2} \langle \partial_n u_{n, \varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle u_{n, \varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) \quad \mathbf{x} \in \mathcal{L}^\varepsilon \cup \mathcal{R}^\varepsilon. \end{aligned} \quad (\text{C.61})$$

Here $[\cdot]$ represents the jump of the quantity across Γ . The uniqueness follows from that the difference between two such functions is a Floquet mode of quasimomentum $\mathbf{p}(\ell)$ and energy $\lambda_* + \varepsilon h$ on $\mathcal{C}_z \setminus D^\varepsilon$.

We next decompose v as the sum of two functions \tilde{u} and w which are introduced below. Let $E : \mathcal{H}^{1/2}(\Gamma) \rightarrow H^{1, \varepsilon}(\ell)$ be an extension operator which is a right inverse of the trace operator, for which functions in its image are supported in a neighborhood \mathcal{O}_1 of Γ that does not intersect \mathcal{O} . Thus this extension operator stays the same for all ℓ . Define

$$u := \chi_{\mathcal{R}^\varepsilon} E\psi, \quad (\text{C.62})$$

where $\chi_{\mathcal{R}^\varepsilon}$ is the characteristic function of \mathcal{R}^ε . Then u satisfies

$$\begin{aligned} [u] &= \psi, \quad [\partial_n u] = -\partial_n E\psi, \\ (-\Delta - \lambda_* - \varepsilon h)u &= \chi_{\mathcal{R}^\varepsilon} (-\Delta - \lambda_* - \varepsilon h)E\psi \quad \mathbf{x} \in \mathcal{L}^\varepsilon \cup \mathcal{R}^\varepsilon. \end{aligned} \quad (\text{C.63})$$

We have that there exists a constant C , such that for all ε , $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, and ℓ ,

$$\|u\|_{H^1(\mathcal{R}^\varepsilon)}, \|u\|_{H^1(\mathcal{L}^\varepsilon)} \leq C\|\psi\|_{\mathcal{H}^{1/2}(\Gamma)}, \quad \|(-\Delta - \lambda_* - \varepsilon h)u\|_{H^{-1}(\mathcal{L}^\varepsilon \cup \mathcal{R}^\varepsilon)} \leq C\|\psi\|_{\mathcal{H}^{1/2}(\Gamma)}. \quad (\text{C.64})$$

Next we shift u along $u_{n, \varepsilon}(\ell)$, $n = 1, 2$, to make sure the source for the rest of v does not have components in these two directions. Define

$$\tilde{u} := \chi_{\mathcal{R}^\varepsilon} E\psi - \sum_{n=1,2} \langle u_{n, \varepsilon}(\ell), \chi_{\mathcal{R}^\varepsilon} E\psi \rangle_\varepsilon u_{n, \varepsilon}(\ell) \quad (\text{C.65})$$

Then \tilde{u} satisfies

$$\begin{aligned} [\tilde{u}] &= \psi, \quad [\partial_n \tilde{u}] = -\partial_n E\psi, \\ (-\Delta - \lambda_* - \varepsilon h)\tilde{u} &= \chi_{\mathcal{R}^\varepsilon}(-\Delta - \lambda_* - \varepsilon h)E\psi - \sum_{n=1,2} (\lambda_{n,\varepsilon} - \lambda_* - \varepsilon h)\langle u_{n,\varepsilon}(\ell), \chi_{\mathcal{R}^\varepsilon} E\psi \rangle_\varepsilon u_{n,\varepsilon}(\ell), \quad \mathbf{x} \in \mathcal{L}^\varepsilon \cup \mathcal{R}^\varepsilon. \end{aligned} \quad (\text{C.66})$$

Let $w \in H^{1,\varepsilon}(\ell)$ be the solution to

$$\begin{aligned} [w] &= 0, \quad [\partial_n w] = \partial_n E\psi, \\ (-\Delta - \lambda_* - \varepsilon h)w &= - \sum_{n=1,2} \overline{\langle \partial_n E\psi, u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) - \chi_{\mathcal{R}^\varepsilon}(-\Delta - \lambda_* - \varepsilon h)E\psi \\ &\quad + \sum_{n=1,2} (\lambda_{n,\varepsilon} - \lambda_* - \varepsilon h)\langle u_{n,\varepsilon}(\ell), \chi_{\mathcal{R}^\varepsilon} E\psi \rangle_\varepsilon u_{n,\varepsilon}(\ell), \quad \mathbf{x} \in \mathcal{L}^\varepsilon \cup \mathcal{R}^\varepsilon. \end{aligned} \quad (\text{C.67})$$

Then $w \in H^{1,\varepsilon}(\ell)$ is the solution to the PDE below on the entire $\mathcal{C}_z \setminus D^\varepsilon$

$$\begin{aligned} (-\Delta - \lambda_* - \varepsilon h)w &= (\partial_n E\psi)\delta(\Gamma) - \sum_{n=1,2} \overline{\langle \partial_n E\psi, u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} u_{n,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell)) - \chi_{\mathcal{R}^\varepsilon}(-\Delta - \lambda_* - \varepsilon h)E\psi \\ &\quad + \sum_{n=1,2} (\lambda_{n,\varepsilon} - \lambda_* - \varepsilon h)\langle u_{n,\varepsilon}(\ell), \chi_{\mathcal{R}^\varepsilon} E\psi \rangle_\varepsilon u_{n,\varepsilon}(\ell), \quad \mathbf{x} \in \mathcal{C}_z \setminus D^\varepsilon. \end{aligned} \quad (\text{C.68})$$

It can be checked that the right hand side of (C.68) is orthogonal to $u_{n,\varepsilon}(\ell)$, $n = 1, 2$, thus w can be treated using the procedure shown in Section C.3.

Integration by parts gives

$$\overline{\langle \partial_n E\psi, u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)) \rangle} - \langle \partial_n u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle = \langle u_{n,\varepsilon}, (-\Delta - \lambda_* - \varepsilon h)\chi_{\mathcal{R}^\varepsilon} E\psi \rangle - (\lambda_{n,\varepsilon} - \lambda_* - \varepsilon h)\langle u_{n,\varepsilon}, \chi_{\mathcal{R}^\varepsilon} E\psi \rangle \quad (\text{C.69})$$

Thus we see

$$v = \tilde{u} + w.$$

Treating $v - \chi_{\mathcal{R}^\varepsilon} E\psi$ using the procedures in Section C.3, we conclude the convergence of

$$\frac{1}{2\pi} \sum_{n \geq 3} \int_{-\pi, \pi} \frac{\langle \partial_n u_{n,\varepsilon}(\cdot; \mathbf{p}(\ell)), \psi \rangle u_{n,\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_{n,\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \frac{1}{2\pi} \sum_{n \geq 3} \int_{-\pi, \pi} \frac{\langle \partial_n u_n(\cdot; \mathbf{p}(\ell)), \psi \rangle u_n(\mathbf{x}; \mathbf{p}(\ell))}{\lambda_n(\mathbf{p}(\ell)) - \lambda_*} d\ell \quad (\text{C.70})$$

in H^1 on the right of Γ in the proper sense through diffeomorphism. Taking the traces and the normal derivatives, we obtain the following convergences.

Lemma C.12. *The following convergences hold in the operator norm from $\mathcal{H}^{1/2}(\Gamma)$ to $\mathcal{H}^{1/2}(\Gamma)$ and from $\mathcal{H}^{1/2}(\Gamma)$ to $\mathcal{H}^{-1/2}(\Gamma)$ respectively uniformly for $h \in \mathbb{C}$ that satisfy $|h| < \mathfrak{d}|\frac{t_*}{\gamma_*}|$, as $\varepsilon \rightarrow 0$:*

$$\sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\langle \partial_n v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell), \psi) \rangle v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\langle \partial_n v_n(\cdot; \mathbf{p}(\ell), \psi) \rangle v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell, \quad (\text{C.71})$$

$$\partial_n \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\langle \partial_n v_{n,\pm\varepsilon}(\cdot; \mathbf{p}(\ell), \psi) \rangle v_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell))}{\mu_{n,\pm\varepsilon}(\mathbf{p}(\ell)) - \lambda_* - \varepsilon h} d\ell \rightarrow \partial_n \sum_{n \geq 3} \frac{1}{2\pi} \int_{[-\pi, \pi]} \frac{\langle \partial_n v_n(\cdot; \mathbf{p}(\ell), \psi) \rangle v_n(\mathbf{x}; \mathbf{p}(\ell))}{\mu_n(\mathbf{p}(\ell)) - \lambda_*} d\ell. \quad (\text{C.72})$$

Appendix D Proof of Propositions 9.2, and Theorems 2.16, 2.17 and 2.14.

Proof of Proposition 9.2. The proof is similar to that of Proposition 7.1. The leading order term in the limit comes from the integrals close to the Dirac points. We only display this calculation below.

Using (4.9), (4.13) and (4.14),

$$\begin{aligned}
& e^{i\varepsilon\zeta\beta_2\cdot\mathbf{x}} \sum_{n=1,2} \frac{1}{2\pi} \int_{[-\varepsilon^{1/3}, \varepsilon^{1/3}]} \frac{u_{n,\pm\varepsilon}(\mathbf{x}; \mathbf{p}(\ell, \varepsilon\zeta)) \overline{u_{n,\pm\varepsilon}(\mathbf{y}; \mathbf{p}(\ell, \varepsilon\zeta))}}{\lambda_{n,\pm\varepsilon}(\mathbf{p}(\ell, \varepsilon\zeta)) - (\lambda_* + \varepsilon h)} d\ell e^{-i\varepsilon\zeta\beta_2\cdot\mathbf{y}} \\
& \rightarrow F_1^\pm(h, \zeta) w_1(\mathbf{x}) \overline{w_1(\mathbf{y})} + F_2^\pm(h, \zeta) w_2(\mathbf{x}) \overline{w_2(\mathbf{y})} + F_3^\pm(h, \zeta) w_2(\mathbf{x}) \overline{w_1(\mathbf{y})} \\
& \quad + F_4^\pm(h, \zeta) w_1(\mathbf{x}) \overline{w_2(\mathbf{y})} + o(1) \|\phi\|_{\mathcal{H}^{1/2}(\Gamma)}.
\end{aligned} \tag{D.1}$$

Here

$$\begin{aligned}
F_1^+(h, \zeta) &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{1 - |L(\varepsilon, \ell, \varepsilon\zeta)|^2}{1 + |L(\varepsilon, \ell, \varepsilon\zeta)|^2} \cdot \frac{J(\varepsilon, \ell, \varepsilon\zeta)}{-(J(\varepsilon, \ell, \varepsilon\zeta))^2 + \varepsilon^2 h^2} + \frac{-\varepsilon h}{-(J(\varepsilon, \ell, \varepsilon\zeta))^2 + \varepsilon^2 h^2} d\ell, \\
F_2^+(h, \zeta) &= \frac{1}{2\pi} \int_{\mathbb{R}} -\frac{1 - |L(\varepsilon, \ell, \varepsilon\zeta)|^2}{1 + |L(\varepsilon, \ell, \varepsilon\zeta)|^2} \cdot \frac{J(\varepsilon, \ell, \varepsilon\zeta)}{-(J(\varepsilon, \ell, \varepsilon\zeta))^2 + \varepsilon^2 h^2} + \frac{-\varepsilon h}{-(J(\varepsilon, \ell, \varepsilon\zeta))^2 + \varepsilon^2 h^2} d\ell, \\
F_3^+(h, \zeta) &= \frac{1}{2\pi} \int_{\mathbb{R}} \frac{L(\varepsilon, \ell, \varepsilon\zeta)}{1 + |L(\varepsilon, \ell, \varepsilon\zeta)|^2} \cdot \frac{2J(\varepsilon, \ell, \varepsilon\zeta)}{-(J(\varepsilon, \ell, \varepsilon\zeta))^2 + \varepsilon^2 h^2} d\ell, \\
F_4^+(h, \zeta) &= \overline{F_3^+(h, \zeta)},
\end{aligned} \tag{D.2}$$

$$F_1^-(h, \zeta) = F_2^+(h, \zeta), \quad F_2^-(h, \zeta) = F_1^+(h, \zeta), \quad F_3^-(h, \zeta) = F_3^+(h, \zeta), \quad F_4^-(h, \zeta) = F_4^+(h, \zeta), \tag{D.3}$$

$L(\varepsilon, \ell, \varepsilon\zeta)$ is defined in (4.12) and

$$J(\varepsilon, \ell, \mu) = \frac{1}{|\gamma_*|} \sqrt{\varepsilon^2 t_*^2 + |\ell + \mu\bar{\tau}|^2 |\theta_*|^2}. \tag{D.4}$$

Note it turns out that the functions F_i^\pm are independent of $\varepsilon > 0$. This is because

$$\begin{aligned}
\frac{L(\varepsilon, \ell, \varepsilon\zeta)}{1 + |L(\varepsilon, \ell, \varepsilon\zeta)|^2} &= \frac{\theta_*(\ell + \varepsilon\zeta\bar{\tau})}{2\gamma_*(\varepsilon, \ell, \varepsilon\zeta)}, \\
\frac{1 - |L(\varepsilon, \ell, \varepsilon\zeta)|^2}{1 + |L(\varepsilon, \ell, \varepsilon\zeta)|^2} &= \frac{\varepsilon t_*}{\gamma_* J(\varepsilon, \ell, \varepsilon\zeta)}.
\end{aligned} \tag{D.5}$$

Observing

$$|\ell + \varepsilon\zeta\tau|^2 = \left(\ell - \frac{1}{2}\varepsilon\zeta\right)^2 + \frac{3}{4}(\varepsilon\zeta)^2, \tag{D.6}$$

We set $\tilde{\ell} = \ell - \frac{1}{2}\varepsilon\zeta$. Using

$$\frac{1}{\pi} \int_{\mathbb{R}} \frac{1}{\frac{1}{(\gamma_*)^2} (t_*^2 + \frac{3}{4}|\theta_*|^2\zeta^2 + |\theta_*|^2\tilde{\ell}^2) - h^2} d\tilde{\ell} = \left| \frac{\gamma_*}{\theta_*} \right| \frac{1}{\sqrt{(\frac{t_*}{\gamma_*})^2 + \frac{3}{4}|\frac{\theta_*}{\gamma_*}|^2\zeta^2 - h^2}}, \tag{D.7}$$

we obtain

$$F_1^+(h, \zeta) = -\xi(h, \zeta) + \beta(h, \zeta), \quad F_2^+(h, \zeta) = \xi(h, \zeta) + \beta(h, \zeta), \quad F_3^+(h, \zeta) = \frac{\theta_*}{|\theta_*|} \sigma(h, \zeta), \quad F_4^+(h, \zeta) = \frac{\bar{\theta}_*}{|\theta_*|} \overline{\sigma(h, \zeta)}. \quad (\text{D.8})$$

Here $\xi(h, \zeta)$, $\beta(h, \zeta)$ and $\sigma(h, \zeta)$ are defined in (9.7). A coincidence is that $\sigma(h, \zeta) \in \mathbb{C}$, which implies $\overline{\sigma(h, \zeta)} = -\sigma(h, \zeta)$.

Finally using

$$\begin{aligned} w_1 \bar{w}_1 &= \frac{1}{2} (v_1 \bar{v}_1 + v_2 \bar{v}_2 + v_2 \bar{v}_1 + v_1 \bar{v}_2), \\ w_2 \bar{w}_2 &= \frac{1}{2} (v_1 \bar{v}_1 + v_2 \bar{v}_2 - v_2 \bar{v}_1 - v_1 \bar{v}_2), \\ w_2 \bar{w}_1 &= \frac{1}{2} \frac{\bar{\theta}_*}{|\theta_*|} (-v_1 \bar{v}_1 + v_2 \bar{v}_2 + v_2 \bar{v}_1 - v_1 \bar{v}_2), \\ w_1 \bar{w}_2 &= \frac{1}{2} \frac{\theta_*}{|\theta_*|} (-v_1 \bar{v}_1 + v_2 \bar{v}_2 - v_2 \bar{v}_1 + v_1 \bar{v}_2), \end{aligned} \quad (\text{D.9})$$

we finish the proof. □

Proof of Theorem 2.16. Along the rational edge, we need to consider the quasimomenta

$$\ell \beta_1^r + \mu \beta_2^r = \ell (b \beta_1 - a \beta_2) + \mu (-d \beta_1 + c \beta_2) \quad (\text{D.10})$$

The leading order term in the counter part of matrix (4.25) is

$$\begin{pmatrix} t_* \varepsilon + \gamma_* \lambda^{(1)} & (\ell + \mu \tau) \bar{\theta}_* \\ (\ell + \mu \bar{\tau}) \theta_* & -t_* \varepsilon + \gamma_* \lambda^{(1)} \end{pmatrix}. \quad (\text{D.11})$$

Thus in the counter parts of L defined in (4.12) and J defined in (D.4), we have the replacement

$$\ell + \mu \bar{\tau} \rightarrow \ell (b - a \bar{\tau}) + \mu (-d + c \bar{\tau}) =: A \ell + B \mu, \quad (\text{D.12})$$

where $A := b - a \bar{\tau}$ and $B := -d + c \bar{\tau}$. Since

$$|A \ell + B \mu|^2 = |A|^2 \left(\ell + \frac{\text{Re}(A \bar{B})}{|A|^2} \mu \right)^2 + \left(|B|^2 - |A|^2 \left(\frac{\text{Re}(A \bar{B})}{|A|^2} \right)^2 \right) \mu^2, \quad (\text{D.13})$$

we rewrite

$$A \ell + B \mu = A \left(\ell + \frac{\text{Re}(A \bar{B})}{|A|^2} \mu \right) + \mathfrak{f}^r \mu, \quad (\text{D.14})$$

where \mathfrak{f}^r is defined in (2.24). So we set $\tilde{\ell} := \ell + \frac{\text{Re}(A \bar{B})}{|A|^2} \varepsilon \zeta$ when $\mu = \varepsilon \zeta$. It can be shown that $|\mathfrak{f}^r|^2 = |B|^2 - |A|^2 \left(\frac{\text{Re}(A \bar{B})}{|A|^2} \right)^2$. Define

$$C^r(h, \zeta) := \frac{1}{\pi} \int_{\mathbb{R}} \frac{1}{\frac{1}{(\gamma_*)^2} \left(t_*^2 + |\theta_*|^2 |A|^2 \tilde{\ell}^2 + |\theta_*|^2 |\mathfrak{f}^r|^2 \zeta^2 \right) - h^2} d\tilde{\ell} = \frac{1}{2} \left| \frac{\gamma_*}{\theta_*} \right| \frac{1}{\sqrt{\left(\frac{t_*}{\gamma_*} \right)^2 + \frac{3}{4} \left| \frac{\theta_* A}{\gamma_*} \right|^2 \zeta^2 - h^2}}. \quad (\text{D.15})$$

We use the superscript r to denote operators corresponding to $(\mathbb{M}(\varepsilon\zeta))^{-1}\mathbb{T}^{\pm\varepsilon}(\lambda_* + \varepsilon h, \varepsilon\zeta)(\mathbb{M})(\varepsilon\zeta)$ defined in (9.8). The limits are

$$(\mathbb{M}^r(\varepsilon\zeta))^{-1}\mathbb{T}^{\pm\varepsilon,r}(\lambda_* + \varepsilon h, \varepsilon\zeta)(\mathbb{M}^r)(\varepsilon\zeta) \rightarrow \tilde{\mathbb{T}}^{0,r}(\lambda_*) + \beta^r(h, \zeta)\mathbb{P} \mp \xi^r(h, \zeta)\mathbb{Q} + \sigma_1^r(h, \zeta)\mathbb{O}_1 + \sigma_2^r(h, \zeta)\mathbb{O}_2, \quad (\text{D.16})$$

where

$$\begin{aligned} \mathbb{O}_1\vec{\phi} &:= c_1(\vec{\phi})\vec{v}_1 - c_2(\vec{\phi})\vec{v}_2, & \mathbb{O}_2\vec{\phi} &:= -c_2(\vec{\phi})\vec{v}_1 + c_1(\vec{\phi})\vec{v}_2, \\ \beta^r(h, \zeta) &= hC^r(h, \zeta), & \beta^r(h, \zeta) &= \frac{t_*}{|\gamma_*|}C^r(h, \zeta), \\ \sigma_1^r(h, \zeta) &= \text{Re}(\mathfrak{f}^r)\zeta\left|\frac{\theta_*}{\gamma_*}\right|C^r(h, \zeta), & \sigma_2^r(h, \zeta) &= \text{Im}(\mathfrak{f}^r)\zeta\left|\frac{\theta_*}{\gamma_*}\right|C^r(h, \zeta). \end{aligned} \quad (\text{D.17})$$

A calculation similar to the proof of Proposition 2.13 produces the result. \square

Proof of Theorem 2.17. Comparing to (4.8) and (8.4), we observe that at K and K' , the signs of θ_* and t_* are opposite. Thus the edge states bifurcating from K and K' have opposite dispersion slopes. \square

Proof of Theorem 2.14. The dispersion relations on the zigzag interface and the armchair interface in Theorems 2.13 and 2.14 are special cases of Propositions 2.16 and 2.17.

For the zigzag interface $a = 0, b = 1, c = 1, d = 0$ and $A = 1, B = \bar{\tau}, \mathfrak{f}^r = \frac{1}{2} + \bar{\tau}$ and $|\mathfrak{f}^r| = \frac{\sqrt{3}}{2}$.

For the armchair interface, $a = 1, b = 1, c = 1, d = 0$ and $A = 1 - \bar{\tau}, B = \bar{\tau}, \mathfrak{f}^r = \frac{1+\bar{\tau}}{2}$ and $|\mathfrak{f}^r| = \frac{1}{2}$. \square

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