Spectra of Periodic Schrödinger Operators on the Octagonal Lattice

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(ABSTRACT)

We consider the spectrum of the Schrödinger operator on an octagonal lattice using the Floquet-Bloch transform of the Laplacian. We will first consider the spectrum of the Laplacian in detail and prove various properties thereof, including spectral-band limits and locations of singularities. In addition, we will prove that Schrödinger operators with 1-1 periodic potentials can open at most two gaps in the spectrum precisely at energies ± 1, and that a third gap can open at 0 for 2-2 periodic potentials. We describe in detail the structure of these operators for higher periods, and motivate our expectations of their spectra.

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(GENERAL AUDIENCE ABSTRACT)

In quantum physics, we would like the capability to model environments, such as magnetic fields, that interact with electrons or other quantum entities. The fields of graph theory and functional analysis within mathematics provide tools which relate well-understood mathematical concepts to these physical interactions. In this work, we use these tools to describe these environments using previously employed techniques in new ways.

Dedication

To my Lord and Savior Jesus Christ, all glory and honor to You.

To my parents, for always believing in me and encouraging me.

To my husband-to-be, for your patience, grace, and kindness in all circumstances.

To my siblings, for reminding me that I'm smart, but not *that* smart.

Acknowledgments

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Contents

List of Figures

List of Tables

Chapter 1

Introduction

1.1 Relevant Theory and Background

In both quantum and classical physics, one would often like to quantify the energy of a system, given information regarding the states of its components. In classical mechanics, the Hamiltonian operator gives this relation; for example, a system of N bodies in $\mathbb{R}^3$, $\{x_i\}_{i=1}^N$ with masses m_i, under the influence of a potential $Q(x)$, has energy

$$H(x) = \sum_{i=1}^{N} \frac{1}{2m_i} \sum_{j=1}^{3} p(x_{i,j})^2 + Q(x),$$

where $p(x_{ij})$ gives the j^{th} component of the momentum of the i^{th} body [9]. However, in quantum mechanics, the Heisenberg uncertainty principle inhibits our ability to have information on both the position and momentum of the electrons simultaneously, and so, presuming we instead consider a set of electrons under an appropriate potential Q, we find that the system's energy is given by the operator that exchanges the momenta of the $\{x_{ij}\}$ for the respective differential operator:

$$\begin{aligned} H &= -\sum_{i=1}^{N} \sum_{j=1}^{3} \frac{\partial^2}{\partial x_{ij}^2} + Q \\ &= -\Delta + Q. \end{aligned}$$

In non-relativistic settings, H is known as the Schrödinger operator [9]. Even though this operator is defined in terms of the negative *Laplacian*, $-\Delta$, from the perspective of spectral theory the negative sign is easy to account for, so we drop it to simplify some formulae. We will make this clear and more precise in later sections (see Proposition 2.5).

In this manuscript, we examine the spectrum of the discrete Schrödinger operator acting upon a periodic graph, which we will refer to as the octagonal lattice. The study of such operators has applications in a variety of fields; Kuchment mentions in his survey [7] recent areas of relevance including photonic crystals and carbon nanostructures, amongst others.

A notable result in this area of spectral theory is the recently resolved Bethe-Sommerfeld conjecture, which states that for dimensions $n \geq 2$, a periodic function Q will induce a Schrödinger operator whose spectrum contains at most finitely many *gaps*, or intervals of finite length that do not lie in the spectrum of the operator. See [6] for proof of this conjecture, as well as [1, 2, 3], which have expanded upon this result in the discrete setting.

Embree and Fillman [1] were able to show that the spectrum of the Schrödinger operator on the $\mathbb{Z}^2$ lattice with a (p, q)-periodic potential contains at most one gap, which can only open if both p and q are even. Similar results were proven by Han and Jitomirskaya in [3] for the general $\mathbb{Z}^d$ lattice, $d \geq 2$, and by Fillman and Han for the triangular lattice. We will make progress towards a similarly general result on the octagonal lattice, though our result allows for at most three gaps in the spectrum, with two gaps possible for general periods and a third gap possible when the period is even.

The goal of this manuscript is to examine the spectrum of the Schrödinger operator on periodic graphs, as in [1, 2, 3], but in a more complex setting. In these papers, the graphs under consideration either contain exactly one vertex in the fundamental domain, or can be reduced to such a case via direct products. Here, we consider a graph Γ whose structure, while still periodic, does not enjoy quite as strong a criterion. We will make this property of Γ precise in the next section.

An essential component to our discussion throughout will be Floquet theory, which formulates solutions to periodic systems in terms of solutions on compact domains with suitable boundary conditions. For a nice introduction to this in a general setting, see [7]; for an overview of the theory applied to Schrödinger operators on periodic graphs, see [2]. We will include references to larger results from the general theory that already apply to the octagonal lattice, and derive results specifically pertaining to the octagonal lattice as they are useful to us.

1.2 The Octagonal Lattice in $\mathbb{R}^2$

We examine the spectra of Schrödinger operators on the graph $\Gamma = (\mathcal{V}, \mathcal{E})$ associated with an octagonal lattice, realized as embedded in $\mathbb{R}^2$ (Figure 1.1). We first define explicitly the vertices and edges of Γ, as they exist in $\mathbb{R}^2$.

Letting $\lambda = \frac{1}{2+\sqrt{2}}$, we set

$$\mathcal{V} = \{(n, m \pm \lambda) : n, m \in \mathbb{Z}\} \cup \{(n \pm \lambda, m) : n, m \in \mathbb{Z}\},$$
$$\mathcal{E} = \{(u, v) : u, v \in \mathcal{V}, \|u - v\| = \sqrt{2}\lambda\}.$$

Labelling $N = (0, \lambda)$, $E = (\lambda, 0)$, $S = (0, -\lambda)$, and $W = (-\lambda, 0)$, we note that Γ is periodic: there exist linearly independent translations, which by our definition of Γ are conveniently

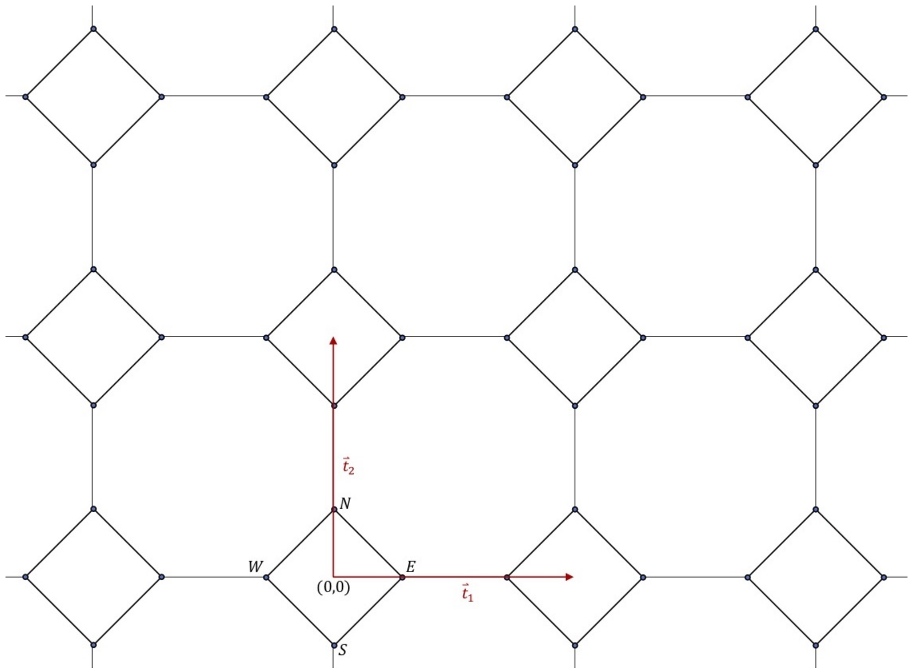

Figure 1.1: Octagonal lattice embedded in $\mathbb{R}^2$

$\boldsymbol{t}_1 = [1,0]^\top$ and $\boldsymbol{t}_2 = [0,1]^\top$, such that for every $v \in \mathcal{V}$ with coordinates in $\mathbb{R}^2$ and $n_1, n_2 \in \mathbb{Z}$, any linear combination $v + n_1\boldsymbol{t}_1 + n_2\boldsymbol{t}_2$ is also in $\mathcal{V}$, with a similar statement holding for edges. We will use the notation $v = X + \boldsymbol{n} = X_{\boldsymbol{n}}$ to denote any vertex, where $X \in \{N, E, S, W\}$.

We may further formalize the periodicity of Γ by considering translations of Γ as a group action $\circlearrowleft$ on Γ by $\mathbb{Z}^2$. Given $u, v \in \mathcal{V}$ (viewed as ordered pairs in $\mathbb{R}^2$ with the standard basis) and $\boldsymbol{n} \in \mathbb{Z}^2$ (viewed as an ordered pair with respect to the basis $T = \{\boldsymbol{t}_1, \boldsymbol{t}_2\}$),

$$\boldsymbol{n} \circlearrowleft v = v + \boldsymbol{n},$$
$$\boldsymbol{n} \circlearrowleft (u, v) = (\boldsymbol{n} \circlearrowleft u, \boldsymbol{n} \circlearrowleft v).$$

It is worth noting explicitly that our choice of T is only unique up to integer multiples of $\boldsymbol{t}_1$ and $\boldsymbol{t}_2$.

Viewing the periodicity of Γ as a group action helps us define concretely the *fundamental domain* with respect to our translation basis T, which we will denote as Γ_f^T. In this case, since T is also the standard basis in $\mathbb{R}^2$, we drop the T superscript for cleaner notation; however, we will specify the translation basis when it differs from the standard basis.

Denote the group orbit of a particular vertex v as $\mathcal{O}(v) = \{\boldsymbol{n} \circlearrowleft v : \boldsymbol{n} \in \mathbb{Z}^2\}$, and denote the group orbit of a particular edge analogously. The graph Γ has four distinct vertex orbits,

$$\mathcal{O}(N),\ \mathcal{O}(S),\ \mathcal{O}(E),\ \text{and}\ \mathcal{O}(W),$$

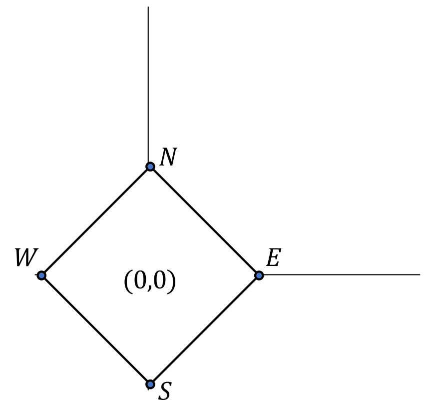

Figure 1.2: Γ_f with respect to T

and six distinct edge orbits,

$$\mathcal{O}(N,E),\ \mathcal{O}(E,S),\ \mathcal{O}(E,W),\ \mathcal{O}(W,N),\ \mathcal{O}(N,S_{(0,1)}),\ \text{and } \mathcal{O}(E,W_{(1,0)}).$$

We will define the *fundamental domain vertices and edges* to include exactly one representative from each respective orbit. For the sake of simplicity, we choose

$$\begin{aligned}\mathcal{V}_f &= \{N,E,S,W\},\\ \mathcal{E}_f &= \{(N,E),(E,S),(S,W),(W,N),(N,S_{(0,1)}),(E,W_{(1,0)})\},\\ \Gamma_f &= (\mathcal{V}_f,\mathcal{E}_f).\end{aligned}$$

See Figure 1.2 for an illustration of Γ_f.

Our current translation basis gives us the "smallest" possible fundamental domain, in that

$$\bigcap_{\substack{S=\{\boldsymbol{s}_1,\boldsymbol{s}_2\}:\\ \boldsymbol{s}_1,\boldsymbol{s}_2\in\mathbb{Z}^2}} \Gamma_f^S = \Gamma_f^T.$$

In later sections we will expand our study to include fundamental domains with translation basis vectors that are larger integer multiples of $\boldsymbol{t}_1,\boldsymbol{t}_2$. (These fundamental domains correspond to potentials of higher period, which we will discuss in later chapters.)

We would like to study the Schrödinger operator $H_Q : \ell^2(\mathcal{V}) \to \ell^2(\mathcal{V})$ on Γ,

$$[H_Q]\psi = \Delta\psi + Q\psi,$$

where $\psi \in \ell^2(\mathcal{V})$, Δ is the discrete Laplacian on Γ, and $Q(v)$ is a real-valued, periodic potential function on $\mathcal{V}$.

Definition 1.1. A function $f : \ell^2(\mathcal{V}) \to \ell^2(\mathcal{V})$ is said to be **periodic** with respect to Γ_f if $f(v) = f(X)$ for all $v \in \mathcal{O}(X),\ X \in \mathcal{V}_f$.

Notation: We will write $u \sim v$ to denote that $(u, v) \in \mathcal{E}$, and σ to denote the spectrum of an operator.

Normally, the graph Laplacian Δ takes the form $[\Delta\psi](v) = \sum\limits_{u \sim v} \big(\psi(u) - \psi(v)\big)$. However, since $\deg v = 3$ for all $v \in \mathcal{V}$, we may write

$$[\Delta\psi](v) = \left(\sum_{u \sim v} \psi(u)\right) - 3\psi(v). \tag{1.1}$$

Defining the operator $[\kappa\psi](v) = \sum_{u \sim v} \psi(u)$, we note that $\sigma(\Delta) = \sigma(\kappa) - 3$; that is, the spectra of these two operators are identical up to a shift. For the remainder of this paper we therefore take $[\Delta\psi](v) := [\kappa\psi](v)$ to simplify notation and computation. Explicitly, then,

$$[\Delta\psi](X_{n,m}) = \begin{cases} \psi(E_{n,m}) + \psi(W_{n,m}) + \psi(S_{n,m+1}), & X = N; \\ \psi(N_{n,m}) + \psi(S_{n,m}) + \psi(W_{n+1,m}), & X = E; \\ \psi(W_{n,m}) + \psi(E_{n,m}) + \psi(N_{n,m-1}), & X = S; \\ \psi(N_{n,m}) + \psi(S_{n,m}) + \psi(E_{n-1,m}), & X = W. \end{cases}$$

To study the full Laplacian, we will use its Floquet decomposition, which we now describe.

Given $\phi \in \ell^1(\mathcal{V})$, $X \in \mathcal{V}_f$, and $\boldsymbol{\theta} = (\theta_1, \theta_2) \in \mathbb{T}^2 := \left(\mathbb{R}/2\pi\mathbb{Z}\right)^2$, let $\widehat{\phi}(\boldsymbol{\theta}) \in \mathbb{C}^{\mathcal{V}_f} \cong \mathbb{C}^4$ be defined coordinatewise as

$$\widehat{\phi}_X(\boldsymbol{\theta}) := \sum_{\boldsymbol{n} \in \mathbb{Z}^2} \phi(X_{\boldsymbol{n}}) e^{-i\langle \boldsymbol{n}, \boldsymbol{\theta}\rangle},$$

so that

$$\widehat{\phi}(\boldsymbol{\theta}) = [\widehat{\phi}_N(\boldsymbol{\theta}),\ \widehat{\phi}_E(\boldsymbol{\theta}),\ \widehat{\phi}_S(\boldsymbol{\theta}),\ \widehat{\phi}_W(\boldsymbol{\theta})]^\top.$$

(We establish (N, E, S, W) as the default ordering of the basis elements of $\mathbb{C}^{\mathcal{V}_f} = \mathbb{C}^4$.) Then, for any $\phi \in \ell^1(\mathcal{V})$, define the Floquet transformation $\mathcal{F} : \ell^1(\mathcal{V}) \to L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}_f})$ by

$$\mathcal{F}\phi = \widehat{\phi}. \tag{1.2}$$

For clarity, we define

$$L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}_f}) := \left\{ g : \mathbb{T}^2 \to \mathbb{C}^{\mathcal{V}_f} : \|g\|^2 := \frac{1}{4\pi^2} \int_{\mathbb{T}^2} \|g(\boldsymbol{\theta})\|^2_{\mathbb{C}^{\mathcal{V}_f}} \, d\boldsymbol{\theta} < \infty \right\}.$$

To show that $\mathcal{F}$ is unitary, it is sufficient to show that $\mathcal{F}$ applied to an orthonormal basis $\{\delta_{X_{\boldsymbol{n}}}\}_{\substack{X \in \mathcal{V}_f \\ \boldsymbol{n} \in \mathbb{Z}^2}}$ on $\ell^1(\mathcal{V})$ is an orthonormal basis for $L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}_f})$. Given a particular $X_{\boldsymbol{n}} \in \mathcal{V}$, and denoting the standard basis on $\mathbb{C}^{V_f}$ as $\delta_N = [1,0,0,0]^\top$, $\delta_E = [0,1,0,0]^\top$, etc., we have the equivalence

$$\begin{aligned}[\mathcal{F}\delta_{X_{\boldsymbol{n}}}](\boldsymbol{\theta}) &= \delta_X \cdot \sum_{\boldsymbol{m}\in\mathbb{Z}^2} \delta_{X_{\boldsymbol{n}}}(X_{\boldsymbol{m}})\; e^{-i\langle \boldsymbol{m},\boldsymbol{\theta}\rangle} \\ &= \delta_X \cdot e^{-i\langle \boldsymbol{n},\boldsymbol{\theta}\rangle},\end{aligned}$$

which is a natural orthonormal basis for $L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}_f})$. Hence $\mathcal{F}$ is unitary, and by the density of $\ell^1(\mathcal{V})$ in $\ell^2(\mathcal{V})$, $\mathcal{F}$ *extends* to a unitary operator from $\ell^2(\mathcal{V})$ to $L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}})$. (Recall that we initially only defined $\mathcal{F}$ on $\ell^1(\mathcal{V})$.) Therefore we can define $\mathcal{F}^{-1} : L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}_f}) \to \ell^2(\mathcal{V})$ by

$$[\mathcal{F}^{-1}\widehat{\phi}](X_{\boldsymbol{n}}) = \int_{\mathbb{T}^2} e^{i\langle \boldsymbol{n},\boldsymbol{\theta}\rangle} \widehat{\phi}_X(\boldsymbol{\theta})\; d\boldsymbol{\theta}.$$

We make use of the Floquet transformation through the following theorem, which will allow us to study the spectrum of the infinite dimensional operator Δ in a finite dimensional setting.

Theorem 1.2.

$$\sigma(\Delta) = \bigcup_{\boldsymbol{\theta}\in\mathbb{T}^2} \sigma\left([\mathcal{F}\Delta\mathcal{F}^{-1}](\boldsymbol{\theta})\right).$$

Proof. See Theorem 3.3 of [6]. □

Let us now find an explicit representation of the operator $\widehat{\Delta} := \mathcal{F}\Delta\mathcal{F}^{-1}$. By our definitions, for a given $\phi \in \ell^1(\mathcal{V})$, we have

$$\begin{aligned}[\mathcal{F}\Delta\mathcal{F}^{-1}\widehat{\phi}]_N(\boldsymbol{\theta}) &= [\mathcal{F}\Delta\phi]_N(\boldsymbol{\theta}) \\ &= \sum_{\boldsymbol{n}\in\mathbb{Z}^2} [\Delta\phi](N_{\boldsymbol{n}}) e^{-i\langle \boldsymbol{n},\boldsymbol{\theta}\rangle} \\ &= \sum_{\boldsymbol{n}\in\mathbb{Z}^2} \big(\phi(E_{\boldsymbol{n}}) + \phi(W_{\boldsymbol{n}}) + \phi(S_{\boldsymbol{n}+[0,1]})\big) e^{-i\langle \boldsymbol{n},\boldsymbol{\theta}\rangle} \\ &= \Bigg(\sum_{\boldsymbol{n}\in\mathbb{Z}^2} \phi(E_{\boldsymbol{n}}) e^{-i\langle \boldsymbol{n},\boldsymbol{\theta}\rangle} + \sum_{\boldsymbol{n}\in\mathbb{Z}^2} \phi(W_{\boldsymbol{n}}) e^{-i\langle \boldsymbol{n},\boldsymbol{\theta}\rangle} \\ &\qquad + \sum_{\boldsymbol{n}\in\mathbb{Z}^2} \phi(S_{\boldsymbol{n}+[0,1]}) e^{-i\langle \boldsymbol{n}+[0,1],\boldsymbol{\theta}\rangle} e^{i\langle (0,1),\boldsymbol{\theta}\rangle} \Bigg) \\ &= \widehat{\phi}_E(\boldsymbol{\theta}) + \widehat{\phi}_W(\boldsymbol{\theta}) + \widehat{\phi}_S(\boldsymbol{\theta}) e^{i\theta_2}.\end{aligned}$$

Similar calculations gives that

$$[\mathcal{F}\Delta\mathcal{F}^{-1}\widehat{\phi}]_E(\boldsymbol{\theta}) = \widehat{\phi}_N(\boldsymbol{\theta}) + \widehat{\phi}_S(\boldsymbol{\theta}) + \widehat{\phi}_W(\boldsymbol{\theta}) e^{i\theta_1},$$

$$[\mathcal{F}\Delta\mathcal{F}^{-1}\widehat{\phi}]_S(\boldsymbol{\theta}) = \widehat{\phi}_E(\boldsymbol{\theta}) + \widehat{\phi}_W(\boldsymbol{\theta}) + \widehat{\phi}_N(\boldsymbol{\theta})e^{-i\theta_2},$$
$$[\mathcal{F}\Delta\mathcal{F}^{-1}\widehat{\phi}]_W(\boldsymbol{\theta}) = \widehat{\phi}_N(\boldsymbol{\theta}) + \widehat{\phi}_S(\boldsymbol{\theta}) + \widehat{\phi}_E(\boldsymbol{\theta})e^{-i\theta_1}.$$

By continuity, these relations extend from $\phi \in \ell^1(\mathcal{V})$ to arbitrary elements of $\ell^2(\mathcal{V})$, and thus we have the equivalence

$$[\mathcal{F}\Delta\mathcal{F}^{-1}\widehat{\phi}](\boldsymbol{\theta}) = \begin{bmatrix} 0 & 1 & e^{i\theta_2} & 1 \\ 1 & 0 & 1 & e^{i\theta_1} \\ e^{-i\theta_2} & 1 & 0 & 1 \\ 1 & e^{-i\theta_1} & 1 & 0 \end{bmatrix} \widehat{\phi}(\boldsymbol{\theta}). \tag{1.3}$$

From now on, we will refer to the matrix in (1.3) as the Floquet matrix, and will distinguish it from the Laplacian by denoting it as $\widehat{\Delta}(\boldsymbol{\theta})$.

For a real-valued potential function $Q : \mathcal{V} \to \mathbb{R}$ that is periodic with respect to Γ_f, Q is of the form

$$Q(v) = \begin{cases} a, & \text{if } v \in \mathcal{O}(N); \\ b, & \text{if } v \in \mathcal{O}(E); \\ c, & \text{if } v \in \mathcal{O}(S); \\ d, & \text{if } v \in \mathcal{O}(W). \end{cases}$$

It is routine to check that

$$[\mathcal{F}Q\mathcal{F}^{-1}](\boldsymbol{\theta}) = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{bmatrix}. \tag{1.4}$$

Therefore, the Schrödinger operator is now

$$[\widehat{H}_Q](\boldsymbol{\theta}) = [\widehat{\Delta} + \widehat{Q}](\boldsymbol{\theta}), \tag{1.5}$$

where $\widehat{Q}(\boldsymbol{\theta}) = [\mathcal{F}Q\mathcal{F}^{-1}](\boldsymbol{\theta})$.

1.3 Summary of Main Results of This Thesis

In the following chapters we will show that the spectrum of the Laplacian on the octagonal lattice is the interval $[-3, 3]$, and that perturbation of the Laplacian by a sufficiently small periodic potential Q (i.e., the Schrödinger operator) on the smallest possible fundamental domain can open at most two gaps in the resulting spectrum, and that these gaps must have opened at energies ± 1. Furthermore, we will show that there are choices of periodic potentials on larger fundamental domains that allow a third gap in the spectrum to open at 0. In Chapter 6, we explore what generalizations of these results should look like for arbitrary fundamental domains.

Following this analysis of the spectrum of Schrödinger operators on the octagonal lattice, we will take a closer look at the spectrum of the Laplacian. Our main result here is a proof that, on the smallest fundamental domain, the dispersion relation of the Laplacian has singularities.

Chapter 2

The Spectrum of $\widehat{\Delta}$

Our goal is to study the behavior of the spectrum of $\widehat{H}_Q$ for small potentials Q, to which end we employ the following strategy. Given a relevant potential Q, we analyze $\sigma(\widehat{H}_{tQ}) = \sigma(\widehat{\Delta} + t\widehat{Q})$ for real-valued t in ϵ-neighborhoods of 0. As such, it is therefore pertinent to study the spectrum of $H_{(0)Q}$, the free Laplacian, before continuing to the spectrum of $\widehat{H}_{tQ}$ for $t > 0$. In this section, we sharply characterize the spectral bands of Δ by inspecting the characteristic polynomial of $\widehat{\Delta}(\boldsymbol{\theta})$ and taking advantage of the unitary equivalence between $\widehat{\Delta}$ and $-\widehat{\Delta}$.

Theorem 2.1. *The spectrum of the Laplacian $\sigma(\Delta)$ is the interval* $[-3, 3]$.

The proof of the theorem will be an obvious consequence of Propositions 2.4, 2.6, and 2.7, which give sharp bounds for each spectral band $B_j = \{\lambda_j \in \sigma(\widehat{\Delta}(\boldsymbol{\theta})) : \boldsymbol{\theta} \in \mathbb{T}^2\}$. We will enumerate eigenvalues of $\widehat{\Delta}(\boldsymbol{\theta})$ in order of descending value, so that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$.

Theorem 2.2. *The characteristic polynomial of $\widehat{\Delta}(\boldsymbol{\theta})$ is given by*

$$P_{\boldsymbol{\theta}}(z) = z^4 - 6z^2 - 4z(\cos\theta_1 + \cos\theta_2) - 4\cos\theta_1\cos\theta_2 + 1.$$

Proof. By definition, $P_{\boldsymbol{\theta}}(z) = \det(z - \widehat{\Delta}(\boldsymbol{\theta}))$. By cofactor expansion of $z - \widehat{\Delta}(\boldsymbol{\theta})$, we get that

$$\begin{aligned}
\det(z - \widehat{\Delta}(\boldsymbol{\theta})) &= -z \det \begin{bmatrix} -z & 1 & e^{i\theta_1} \\ 1 & -z & 1 \\ e^{-i\theta_1} & 1 & -z \end{bmatrix} - \det \begin{bmatrix} 1 & 1 & e^{i\theta_1} \\ e^{-i\theta_2} & -z & 1 \\ 1 & 1 & -z \end{bmatrix} \\
&\quad + e^{i\theta_2} \det \begin{bmatrix} 1 & -z & e^{i\theta_1} \\ e^{-i\theta_2} & 1 & 1 \\ 1 & e^{-i\theta_1} & -z \end{bmatrix} - \det \begin{bmatrix} 1 & -z & 1 \\ e^{-i\theta_2} & 1 & -z \\ 1 & e^{-i\theta_1} & 1 \end{bmatrix} \\
&= -z[-z(z^2 - 1) - (-z - e^{-i\theta_1}) + e^{i\theta_1}(1 + ze^{-i\theta_1})] \\
&\quad - [(z^2 - 1) - (-e^{-i\theta_2}z - 1) + e^{i\theta_1}(e^{-i\theta_2} + z)]
\end{aligned}$$

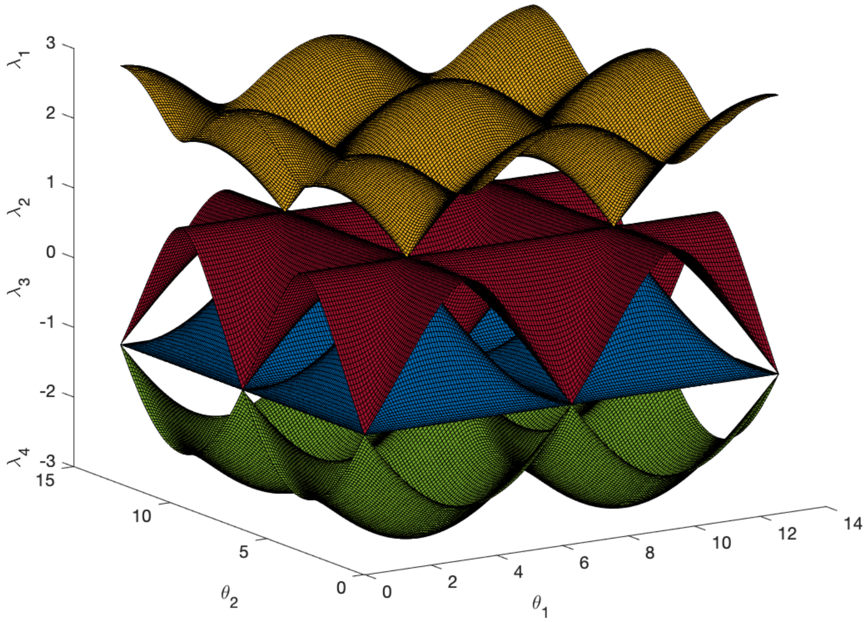

Figure 2.1: The eigenvalues of $\sigma(\widehat{\Delta}(\boldsymbol{\theta}))$ for $\boldsymbol{\theta} \in \mathbb{T}^2$

$$
\begin{aligned}
&+ e^{i\theta_2}[(-z - e^{-i\theta_1}) + z(-e^{-i\theta_2}z - 1) + e^{i\theta_1}(e^{-i(\theta_1+\theta_2)} - 1)] \\
&- [(1 + ze^{-i\theta_1}) + z(e^{-i\theta_2} + z) + (e^{-i(\theta_1+\theta_2)} - 1)] \\
= {}& z^4 - 3z^2 - z(e^{i\theta_1} + e^{i\theta_2}) - z^2 - z(e^{-i\theta_2} + e^{i\theta_1}) - e^{i(\theta_1-\theta_2)} \\
&- z^2 - z(e^{-i\theta_2}) - e^{-i(\theta_1-\theta_2)} - e^{i(\theta_1+\theta_2)} + 1 \\
&- z^2 - z(e^{-i\theta_1} + e^{-i\theta_2}) - e^{-i(\theta_1+\theta_2)} \\
= {}& z^4 - 6z^2 - 2z(e^{i\theta_1} + e^{-i\theta_1} + e^{i\theta_2}e^{-i\theta_2}) \\
&+ e^{i(\theta_1+\theta_2)} + e^{i(\theta_1-\theta_2)} + e^{-i(\theta_1-\theta_2)} + e^{-i(\theta_1+\theta_2)} \\
= {}& z^4 - 6z^2 - 4z(\cos\theta_1 + \cos\theta_2) - 4\cos\theta_1\cos\theta_2 + 1. \qquad (2.1)
\end{aligned}
$$

□

In particular, letting $\mathbf{0} = (0,0)$ and $\boldsymbol{\pi} = (\pi,\pi)$, we look at $\widehat{\Delta}(\mathbf{0})$ and $\widehat{\Delta}(\boldsymbol{\pi})$, which will become useful in the following propositions.

Proposition 2.3. *Enumerating eigenvalues according to their multiplicity,* $\sigma(\widehat{\Delta}(\mathbf{0})) = \{3, -1, -1, -1\}$ *and* $\sigma(\widehat{\Delta}(\boldsymbol{\pi})) = \{-3, 1, 1, 1\}$.

Proof. Evaluating the characteristic polynomial given in the previous theorem, we see

$$P_{(0,0)}(z) = z^4 - 6z^2 - 4z(\cos(0) + \cos(0)) - 4\cos(0)\cos(0) + 1$$

$$\begin{aligned} &= z^4 - 6z^2 - 8z - 3 \\ &= (z-3)(z+1)^3, \end{aligned}$$

and

$$\begin{aligned} P_{(\pi,\pi)}(z) &= z^4 - 6z^2 - 4z(\cos(\pi) + \cos(\pi)) - 4\cos(\pi)\cos(\pi) + 1 \\ &= z^4 - 6z^2 + 8z - 3 \\ &= (z+3)(z-1)^3. \end{aligned}$$

Thus we have that $\sigma(\widehat{\Delta}(\mathbf{0})) = \{3, -1, -1, -1\}$ and $\sigma(\widehat{\Delta}(\boldsymbol{\pi})) = \{-3, 1, 1, 1\}$. □

Proposition 2.4. *The band B_1 formed by the largest eigenvalue of $\widehat{\Delta}(\boldsymbol{\theta})$ satisfies $B_1 = [1, 3]$.*

Proof. For any particular $\boldsymbol{\theta} \in \mathbb{T}^2$, it is clear by Gershgorin's Theorem that $\sigma(\widehat{\Delta}(\boldsymbol{\theta})) \subseteq [-3, 3]$. Since $\sigma(\widehat{\Delta}) = \bigcup_{\boldsymbol{\theta}\in[0,2\pi]^2} \sigma(\widehat{\Delta}(\boldsymbol{\theta}))$, we also have that $\sigma(\widehat{\Delta}) \subseteq [-3, 3]$. In particular, the largest eigenvalue of $\widehat{\Delta}(\boldsymbol{\theta})$ satisfies $\lambda_1 \leq 3$.

Since $\widehat{\Delta}(\boldsymbol{\theta})$ is Hermitian, we may apply the Rayleigh Principle, which tells us that $\lambda_1 = \max_{||v||=1}(\widehat{\Delta}(\boldsymbol{\theta})v, v)$. Denote any such unit vector as $v = (w,\ x,\ y,\ z)^\top$. Then

$$\begin{aligned} \lambda_1 &= \max_{v\in\mathbb{C}^4:||v||=1} (\widehat{\Delta}(\boldsymbol{\theta})v, v) \\ &\geq \max_{v\in\mathbb{R}^4:||v||=1} (\widehat{\Delta}(\boldsymbol{\theta})v, v) \\ &= \max_{v\in\mathbb{R}^4:||v||=1} \left(\begin{bmatrix} 0 & 1 & e^{i\theta_2} & 1 \\ 1 & 0 & 1 & e^{i\theta_1} \\ e^{-i\theta_2} & 1 & 0 & 1 \\ 1 & e^{-i\theta_1} & 1 & 0 \end{bmatrix} \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix}, \begin{bmatrix} w \\ x \\ y \\ z \end{bmatrix} \right) \\ &= \max_{v\in\mathbb{R}^4:||v||=1} 2[(w+y)(x+z) + xz\cos\theta_1 + wy\cos\theta_2]. \end{aligned}$$

For ease of notation let $G(v, \boldsymbol{\theta}) = 2[(w+y)(x+z) + xz\cos\theta_1 + wy\cos\theta_2]$. Since $u = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \end{bmatrix}^\top$ has 2-norm equal to 1,

$$\begin{aligned} \max_{v\in\mathbb{R}^4:||v||=1} G(v, \boldsymbol{\theta}) &\geq G(u, \boldsymbol{\theta}) \\ &= 2\left[\left(\frac{1}{2} + \frac{1}{2}\right)\left(\frac{1}{2} + \frac{1}{2}\right) + \left(\frac{1}{2}\right)\left(\frac{1}{2}\right)\cos\theta_1 + \left(\frac{1}{2}\right)\left(\frac{1}{2}\right)\cos\theta_2 \right] \\ &= 2 + \frac{\cos\theta_1 + \cos\theta_2}{2} \\ &\geq 1 \end{aligned}$$

Therefore, $\lambda_1 \in [1, 3]$.

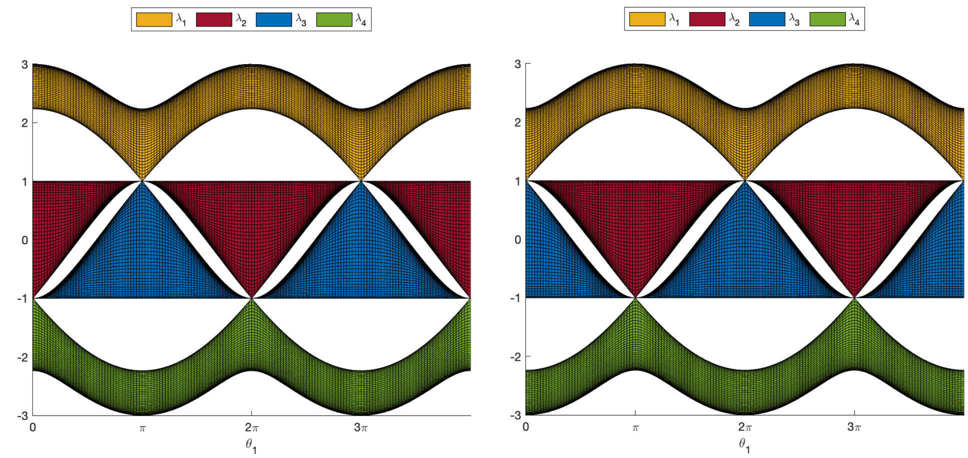

Figure 2.2: $\sigma(\widehat{\Delta})$ and $\sigma(-\widehat{\Delta})$

By Proposition 2.3, $\widehat{\Delta}(\mathbf{0})$ has $\lambda_1 = 3$, and $\widehat{\Delta}(\boldsymbol{\pi})$ has $\lambda_1 = 1$. Therefore since the entries of $\widehat{\Delta}(\boldsymbol{\theta})$ change continuously with respect to (θ_1, θ_2), (see Chapter 2 of [4] for proof), and again $\sigma(\widehat{\Delta}(\boldsymbol{\theta})) \subseteq [-3, 3] \subseteq \mathbb{R}$, for any $z \in [1, 3]$ there exists $\boldsymbol{\theta^*}$ such that $\widehat{\Delta}(\boldsymbol{\theta^*})$ has $\lambda_1 = z$. $\square$

Proposition 2.5. *There is a unitary transformation* $U : L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}_f}) \to L^2(\mathbb{T}^2, \mathbb{C}^{\mathcal{V}_f})$ *such that for all* $\boldsymbol{\theta} \in \mathbb{T}^2$*, there exists* $\boldsymbol{\theta'} \in \mathbb{T}^2$ *such that* $[U\widehat{\Delta}U^*](\boldsymbol{\theta}) = -\Delta(\boldsymbol{\theta'})$.

Note: Since similar operators have the same spectra, this proposition justifies our omission of the negative sign in our definition of the Schrödinger operator.

We are interested in the unitary transformation from $\widehat{\Delta}$ to $-\widehat{\Delta}$ because this transformation allows us to take advantage of the inherent symmetry of $\sigma(\widehat{\Delta})$. This strong symmetry is clear in the plots of the spectra of both $\widehat{\Delta}$ and $-\widehat{\Delta}$ in θ_1-θ_2-λ space projected onto the θ_1-λ plane. We have thus included them in Figure 2.2 to illuminate the inner workings of our argument.

Proof of Proposition 2.5. Let $U = \operatorname{diag}(1, -1, 1, -1)$, and let $\boldsymbol{\theta'} = \boldsymbol{\theta} + \boldsymbol{\pi}$, where $\boldsymbol{\pi} = (\pi, \pi)$.

Then

$$[U\widehat{\Delta}U^*](\boldsymbol{\theta}) = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \begin{bmatrix} 0 & 1 & e^{i\theta_2} & 1 \\ 1 & 0 & 1 & e^{i\theta_1} \\ e^{-i\theta_2} & 1 & 0 & 1 \\ 1 & e^{-i\theta_1} & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & -1 & e^{i\theta_2} & -1 \\ -1 & 0 & -1 & e^{i\theta_1} \\ e^{-i\theta_2} & -1 & 0 & -1 \\ -1 & e^{-i\theta_1} & -1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & -1 & e^{i(\theta_2'-\pi)} & -1 \\ -1 & 0 & -1 & e^{i(\theta_1'-\pi)} \\ e^{-i(\theta_2'-\pi)} & -1 & 0 & -1 \\ -1 & e^{-i(\theta_1'-\pi)} & -1 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & -1 & -e^{i\theta_2'} & -1 \\ -1 & 0 & -1 & -e^{i\theta_1'} \\ -e^{-i\theta_2'} & -1 & 0 & -1 \\ -1 & -e^{-i\theta_1'} & -1 & 0 \end{bmatrix}$$

$$= -\widehat{\Delta}(\boldsymbol{\theta'}).$$

□

Proposition 2.6. *The band traced out by the smallest eigenvalue of $\widehat{\Delta}(\boldsymbol{\theta})$ is $B_4 = [-3, -1]$.*

Proof. By the unitary equivalence of $\widehat{\Delta}$ and $-\widehat{\Delta}$, in addition to the fact that $\sigma(\widehat{\Delta}(\boldsymbol{\theta})) = -\sigma(-\widehat{\Delta}(\boldsymbol{\theta}))$, we have that

$$\lambda_1(\widehat{\Delta}(\boldsymbol{\theta})) = \lambda_1(-\widehat{\Delta}(\boldsymbol{\theta}+\boldsymbol{\pi})) = -\lambda_4(\widehat{\Delta}(\boldsymbol{\theta}+\boldsymbol{\pi})))$$

for all $\boldsymbol{\theta} \in \mathbb{T}^2$. Thus, $B_4 = -B_1 = [-3, -1]$. □

Proposition 2.7. *The bands B_1 and B_2 traced out by the middle eigenvalues of $\widehat{\Delta}(\boldsymbol{\theta})$ are $B_2 = B_3 = [-1, 1]$.*

Proof. We first note that, again by the unitary equivalence of $\widehat{\Delta}$ and $-\widehat{\Delta}$, we get

$$\lambda_2(\widehat{\Delta}(\boldsymbol{\theta})) = \lambda_2(-\widehat{\Delta}(\boldsymbol{\theta}+\boldsymbol{\pi})) = -\lambda_3(\widehat{\Delta}(\boldsymbol{\theta}+\boldsymbol{\pi})))$$

for all $\boldsymbol{\theta} \in \mathbb{T}^2$. Thus $B_2 = -B_3$.

Also observe that $\mathrm{Tr}(\widehat{\Delta}(\boldsymbol{\theta})) = 0$, which implies that for any $\boldsymbol{\theta} \in \mathbb{T}^2$, $\lambda_1+\lambda_2+\lambda_3+\lambda_4 = 0$. Since $\lambda_1 \in [1, 3]$ and $\lambda_4 \in [-3, -1]$, we get that

$$\lambda_2 + \lambda_3 \in [-2, 2]. \tag{2.2}$$

We now show that both λ_2 and λ_3 are less than or equal to 1. By the spectral theorem, $\det(\widehat{\Delta}(\boldsymbol{\theta}) - 1) = \prod_{j=1}^4 (1 - \lambda_j) = \prod_{j=1}^4 (\lambda_j - 1)$. We calculate that

$$\begin{aligned} \det(1 - \widehat{\Delta}(\boldsymbol{\theta})) = P_{\boldsymbol{\theta}}(1) &= 1^4 - 6(1)^2 - 4(1)(\cos\theta_1 + \cos\theta_2) - 4\cos\theta_1\cos\theta_2 + 1 \\ &= -4 - 4(\cos\theta_1 + \cos\theta_2) - 4\cos\theta_1\cos\theta_2 \end{aligned}$$

$$\begin{aligned} &= -4(1 + \cos\theta_1 + \cos\theta_2 + \cos\theta_1\cos\theta_2) \\ &= -4(\cos\theta_1 + 1)(\cos\theta_2 + 1) \\ &\leq 0. \end{aligned} \tag{2.3}$$

Thus we now have that

$$\prod_{j=1}^{4}(\lambda_j - 1) \leq 0. \tag{2.4}$$

We consider the following 2 cases:

Case 1: $\lambda_1 = 1$.

If $\lambda_1 = 1$, then naturally λ_2 and λ_3 are less than or equal to 1, since λ_1 is the largest eigenvalue. (Note that we consider this case because if $\lambda_1 = 1$, the left-hand side of (2.4) vanishes and we cannot determine anything about the values of λ_2 and λ_3.)

Case 2: $\lambda_1 \neq 1$.

If $\lambda_1 \neq 1$, then $\lambda_1 \in (1, 3]$ and $\lambda_4 \in [-3, -1]$, which implies $\lambda_1 - 1 \in (0, 2]$ and $\lambda_4 - 1 \in [-4, -2]$. As a result, $(\lambda_1 - 1)(\lambda_4 - 1) < 0$, and thus by (2.4), we conclude that $(\lambda_2 - 1)(\lambda_3 - 1) \geq 0$. This implies $(\lambda_2 - 1)$ and $(\lambda_3 - 1)$ are either both non-negative or both non-positive.

If both $\lambda_2 - 1$ and $\lambda_3 - 1$ are non-negative, then it must be that both λ_2, $\lambda_3 \geq 1$. Since we know $\lambda_2 + \lambda_3 \in [-2, 2]$, it must be that $\lambda_2 = \lambda_3 = 1$. If both $\lambda_2 - 1$ and $\lambda_3 - 1$ are non-positive, then it must be that $\lambda_2 \leq 1$ and $\lambda_3 \leq 1$. In both cases, we get our desired result, that $\lambda_2, \lambda_3 \leq 1$.

Since $B_2 = -B_3$, and λ_2 and λ_3 are both bounded above by 1, we conclude $B_2, B_3 \subseteq [-1, 1]$.

By Proposition 2.3, $\widehat{\Delta}(\mathbf{0})$ has $\lambda_2 = \lambda_3 = -1$, and $\widehat{\Delta}(\boldsymbol{\pi})$ has $\lambda_2 = \lambda_3 = 1$. Since $\lambda_j(\widehat{\Delta}(\boldsymbol{\theta}))$ is continuously dependent on $\boldsymbol{\theta}$, and $\sigma(\widehat{\Delta}(\boldsymbol{\theta})) \subseteq \mathbb{R}$, we conclude $B_2, B_3 \supseteq [-1, 1]$, and thus $B_2 = B_3 = [-1, 1]$. $\square$

Proof of Theorem 2.1. By Propositions 2.4, 2.6, and 2.7, and Theorem 1.2,

$$\sigma(\Delta) = \bigcup_{\boldsymbol{\theta} \in \mathbb{T}^2} \sigma(\widehat{\Delta}(\boldsymbol{\theta})) = \bigcup_{j=1}^{4} B_j = [-3, -1] \cup [-1, 1] \cup [1, 3] = [-3, 3].$$

$\square$

Chapter 3

The Spectrum of the Schrödinger Operator

Now that we know the spectrum of Δ, as well as the precise intervals for each of its spectral bands, we seek to see if the addition of small potentials to Δ can open gaps in the spectrum. For the following two theorems, refer back to Equations (1.4) and (1.5) for definitions of $\widehat{H}_Q$ and $\widehat{Q}$.

Theorem 3.1. *If $Q : \mathcal{V} \to \mathbb{R}$ is periodic with respect to Γ_f and $\|Q\|_\infty \leq 1$, then the spectrum of H_Q has at most two gaps, which may only open at eigenvalues ± 1.*

Theorem 3.2. *There exists a potential $Q : \mathcal{V} \longrightarrow \mathbb{R}$ that is periodic with respect to Γ_f with $\|Q\|_\infty = 1$ such that $\sigma(H_{tQ})$ has two gaps for $0 < t < 1$.*

To prove Theorem 3.2, we will evaluate the characteristic polynomial of $\widehat{H}_{tQ}(\boldsymbol{\theta})$ along a specified line whose image for small t is contained in the interior of $\sigma(\Delta)$. By showing that the characteristic polynomial has no roots on this line, we will be able to conclude that every value the line takes on is not an eigenvalue of $\widehat{H}_{tQ}(\boldsymbol{\theta})$ for any $\boldsymbol{\theta} \in \mathbb{T}^2$, and hence does not lie in $\sigma(H_{tQ})$. As long as the line does not lie strictly above the largest or below the smallest spectral band of H_{tQ} for $t < 1$, this will be sufficient to prove that the addition of Q to Δ opens a gap in the spectrum.

First we prove Theorem 3.1, which specifies for which values in the spectrum of Δ gaps can open.

Proof of Theorem 3.1. Suppose Q satisfies the hypothesis of the theorem, with $\|Q\|_\infty \leq 1$. Theorem 2.4 gives that the first band of Δ is $B_1(\Delta) = [1, 3]$. By a standard result in perturbation theory (see Theorem V.3.4.10 of [4]) we then have

$$[1 + t, 3 - t] \subseteq B_1(\Delta + tQ) \subseteq [1 - t, 3 + t].$$

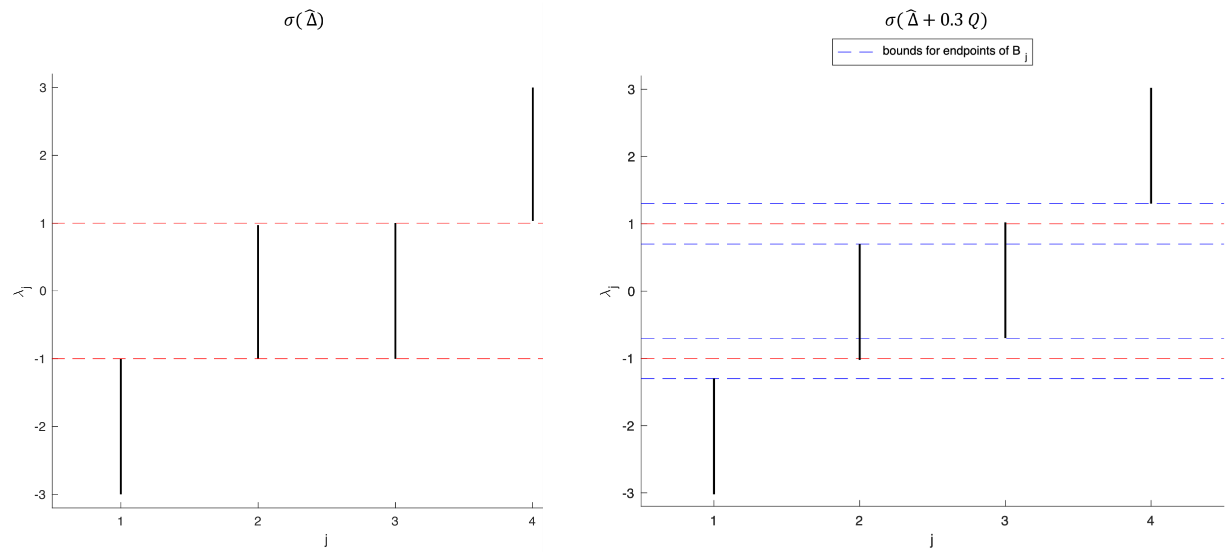

Figure 3.1: *Spectral band gaps of H_Q for Γ_f.* Here, we use the potential $\widehat{Q} = [1, 1, -1, -1]$. The left figure shows the spectrum of H with 0 potential (i.e. the free Laplacian) enumerated by eigenvalue. The right figures shows the spectrum of $H_{0.3Q}$ enumerated by eigenvalue.

Similarly,

$$\begin{aligned}
[-1+t, 1-t] &\subseteq B_2(\Delta + tQ) \subseteq [-1-t, 1+t],\\
[-1+t, 1-t] &\subseteq B_3(\Delta + tQ) \subseteq [-1-t, 1+t],\\
[-3+t, -1-t] &\subseteq B_4(\Delta + tQ) \subseteq [-3-t, -1+t].
\end{aligned}$$

At a particular $s \in (0, 1]$, each B_i is an interval, and so we conclude that any gap in $\sigma(\Delta + sQ)$ opening at $t = 0$ must have opened at some $z_0 \in (-1-s, -1+s) \cup (1-s, 1+s)$. Letting $s \to 0$, we conclude $z_0 = \pm 1$. $\square$

Lemma 3.3. *The characteristic polynomial of $\widehat{H}_{tQ}(\boldsymbol{\theta})$ for $\widehat{Q} = \mathrm{diag}(1, 1, -1, -1)$ is*

$$P_{\boldsymbol{\theta}}(z) = t^4 + t^2(2 - 2z^2) + z^4 - 6z^2 - 4z\left(\cos\theta_2 - \cos\theta_1\right) - 4\cos\theta_1\cos\theta_2 + 1.$$

Proof. The formula can be easily verified by Mathematica or (laboriously) by hand. $\square$

Proof of Theorem 3.2. Let $\widehat{Q}$ =diag$(1, 1, -1, -1)$ and let $s(t) = t/2$. We will show that for any $t > 0$ and any $\boldsymbol{\theta} \in \mathbb{T}^2$, $1 + s(t) \notin \sigma(\widehat{H}_{tQ}(\boldsymbol{\theta}))$ (see Figure 3.2).

The characteristic polynomial of $\widehat{H}_{tQ}(\boldsymbol{\theta})$ on the line $z = 1 + s(t)$ is

$$P_{\boldsymbol{\theta}}(1 + s(t)) = \frac{9}{16}t^4 - \frac{3}{2}t^3 - 4(1 + \cos\theta_1)(1 + \cos\theta_2) - 2t(2 + \cos\theta_1 + \cos\theta_2). \tag{3.1}$$

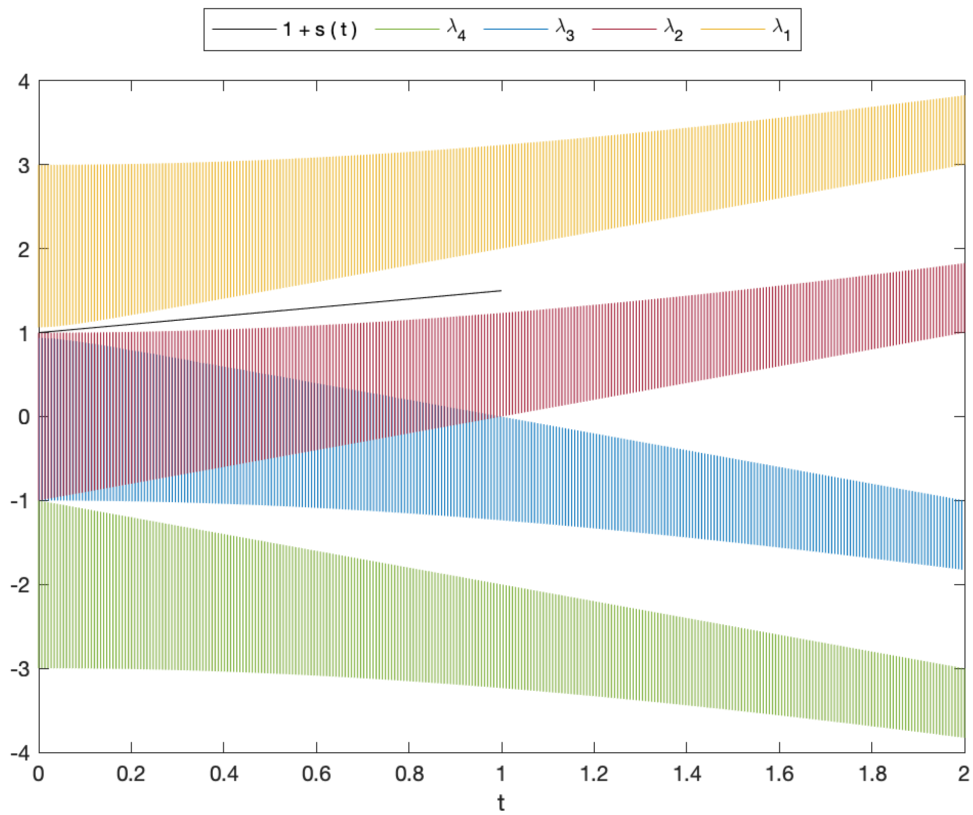

Figure 3.2: $\sigma(H_{tQ})$, for $t \in [0,2]$, $\widehat{Q} = \mathrm{diag}(1,1,-1,-1)$

Under our restriction $0 < t < 1$, it is easy to see that

$$-4(1+\cos\theta_1)(1+\cos\theta_2) \in [-16, 0]$$
$$-2t(2+\cos\theta_1+\cos\theta_2) \in [-8t, 0], \text{ and}$$
$$\frac{9}{16}t^4 - \frac{3}{2}t^3 = t^3\left(\frac{9}{16}t - \frac{3}{2}\right) \in [(-3/2)t^3, (-15/16)t^3],$$

which together imply that $P_{\boldsymbol{\theta}}(1+s(t))$ is strictly negative for all $\boldsymbol{\theta}$. Since we have shown that $P_{\boldsymbol{\theta}}$ has no root on the line $1+s(t)$ for $t > 0$, we have found a gap in the spectrum that opens at $z = 1$.

□

Chapter 4

Higher Periods of Γ_f

4.1 Structure of Γ_f and $\widehat{\Delta}(\boldsymbol{\theta})$ for $p \geq 3$

Letting $pT := \{p\boldsymbol{t}_1, p\boldsymbol{t}_2\}$ for any integer $p \geq 3$, we will now consider in more detail Γ_f^{pT}, which we will call the general $p \times p$ fundamental domain of Γ. It is of course possible to consider non-square fundamental domains by using a translation basis $\{p\boldsymbol{t}_1, q\boldsymbol{t}_2\}$, $p \neq q$, but these domains can be considered "square" by adjusting the translation basis accordingly. We simplify our notation to $\Gamma_f^{pT} = \Gamma_f^p$. Recall that we define Γ_f^p in terms of the distinct orbits with respect to the group action of $p\mathbb{Z}^2$ on Γ: $\Gamma_f^p = (\mathcal{V}_f^p, \mathcal{E}_f^p)$, where $\mathcal{V}_f^p$ consists of exactly one representative from each distinct vertex orbit $\mathcal{O}^p(v)$, and $\mathcal{E}_f^p$ consists of exactly one representative from each distinct edge orbit $\mathcal{O}^p(e)$. Note that Γ_f^1 agrees with our definition from earlier sections.

For $0 \leq n, m \leq p-1$, we first denote $\gamma_{(n,m)} := \Gamma_f^1 + n\boldsymbol{t}_1 + m\boldsymbol{t}_2 \subseteq \Gamma_f^p$ and $\gamma := \gamma_{(0,0)} \subseteq \Gamma_f^p$ (see Figure 4.1). Each Γ_f^p contains p^2 copies of γ, and thus $\mathcal{V}_f^p$ has $4p^2$ vertices. We want to examine the structure of the matrix $\widehat{\Delta}(\boldsymbol{\theta})$ on Γ_f^p for $p \geq 3$, so we take a moment to relabel the vertices in Γ_f^p consecutively.

Denote any $X_{(n,m)} \in \mathcal{V}_f^p$ as $v_{\iota(X_{(n,m)})}$, where

$$\iota(X_{(n,m)}) = \begin{cases} 4pm + 4n + 1, & \text{if } X \in \mathcal{O}^1(N); \\ \iota(N_{(n,m)}) + 1, & \text{if } X \in \mathcal{O}^1(E); \\ \iota(N_{(n,m)}) + 2, & \text{if } X \in \mathcal{O}^1(S); \\ \iota(N_{(n,m)}) + 3, & \text{if } X \in \mathcal{O}^1(W). \end{cases}$$

Intuitively, this indexing labels vertices in $\mathcal{O}^1(N)$ in Γ_f^p increasingly from left to right, bottom to top, and vertices in each $\gamma_{(n,m)}$ clockwise beginning with $N_{(n,m)}$ (see Figure 4.1). The j^{th} column/row of $\widehat{\Delta}(\boldsymbol{\theta})$ will correspond to v_j as indexed by ι.

Before we continue, it will become helpful to define a function that gives the relative

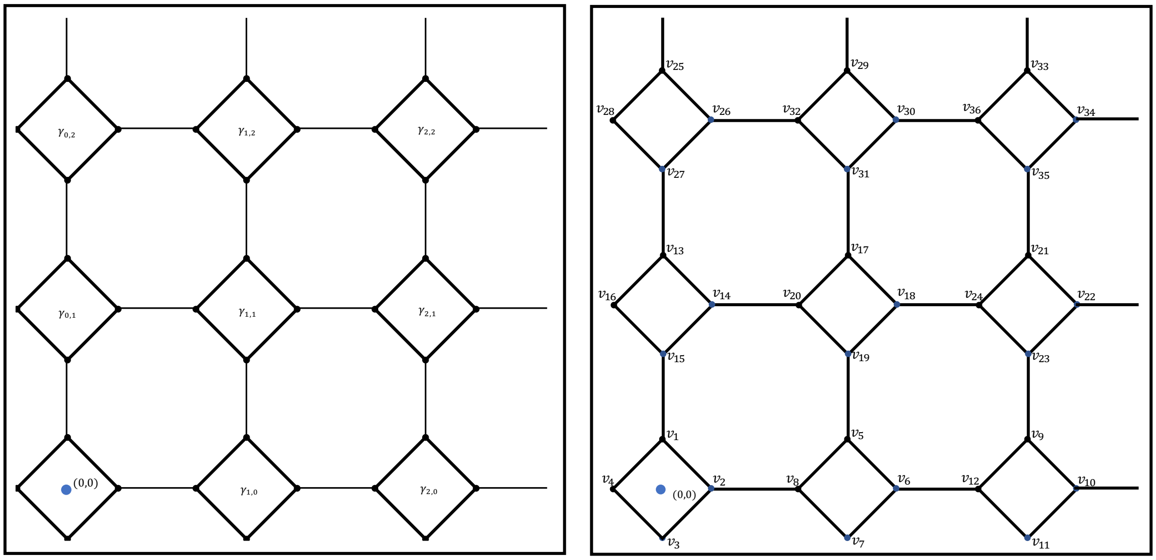

Figure 4.1: Γ_f^3

position of one vertex to another in Γ. Given $u = X_{(n_1,n_2)}, v = Y_{(m_1,m_2)}$ where $X, Y \in \mathcal{V}_f^p$ and $(n_1, n_2), (m_1, m_2) \in p\,\mathbb{Z}^2$, let $\tau : \mathcal{V}^2 \to \mathbb{Z}^2$ be defined by

$$\tau(u, v) = \frac{1}{p}\ (m_1 - n_1, m_2 - n_2).$$

The function τ essentially gives a"position vector" relating $\Gamma_f^p + n_1\boldsymbol{t}_1 + n_2\boldsymbol{t}_2$ and $\Gamma_f^p + m_1\boldsymbol{t}_1 + m_2\boldsymbol{t}_2$. In particular, we note that for any two vertices $u, v \in \Gamma_f^p$, we have $\tau(u, v) = 0$.

Definition 4.1. An edge (u, v) is called a *bridge* if $\tau(u, v) \neq 0$.

We now present a formal definition for $\widehat{\Delta}(\boldsymbol{\theta})$, as given by Korotyaev and Saburova in [5].

Definition 4.2. The $(\ell, j)^{th}$ entry of the Floquet matrix $\widehat{\Delta}(\boldsymbol{\theta})$ on Γ_f^p for $0 \le \ell, j \le p-1$ is

$$[\widehat{\Delta}(\boldsymbol{\theta})]_{\ell,j} = \begin{cases} \exp\big(i\langle\tau(v_\ell, v_j), \boldsymbol{\theta}\rangle\big), & \text{if } (v_\ell, v_j) \in \mathcal{E}_f^p; \\ 0, & \text{if } (v_\ell, v_j) \notin \mathcal{E}_f^p. \end{cases}$$

Note that our definition for $\widehat{\Delta}(\boldsymbol{\theta})$ on Γ_f^1 (see equation (1.3)) agrees with this definition.

Since the entries of $\widehat{\Delta}(\boldsymbol{\theta})$ only depend on the relative indices given by τ, we can immediately make the following remarks regarding the structure of $\widehat{\Delta}(\boldsymbol{\theta})$.

Remark 4.3. The $(\ell, j)^{th}$ entry of $\widehat{\Delta}(\boldsymbol{\theta})$ is non-zero *if and only if* v_ℓ and v_j share an edge. This is clear by the definition of $\widehat{\Delta}(\boldsymbol{\theta})$.

Remark 4.4. If v_ℓ and v_j are in Γ_f^p, then, because $\tau(v_\ell, v_j) = 0$, we have that $\widehat{\Delta}(\boldsymbol{\theta})_{\ell,j} \in \{0,1\}$; if v_ℓ and v_j share an edge, $[\widehat{\Delta}(\boldsymbol{\theta})]_{\ell,j} = 1$, and if not, $[\widehat{\Delta}(\boldsymbol{\theta})]_{\ell,j} = 0$. This implies that the only $\boldsymbol{\theta}$-dependent entries of $\widehat{\Delta}(\boldsymbol{\theta})$ correspond to bridges.

Remark 4.5. Since $\tau(v_\ell, v_j) = -\tau(v_j, v_\ell)$, we notice that $[\widehat{\Delta}(\boldsymbol{\theta})]_{\ell,j} = \overline{[\widehat{\Delta}(\boldsymbol{\theta})]}_{j,\ell}$; that is, $\widehat{\Delta}(\boldsymbol{\theta})$ is a Hermitian matrix.

These remarks, together with the periodicity and inherent symmetry of Γ, create the nested block structure found in $\widehat{\Delta}(\boldsymbol{\theta})$. We now investigate this structure algebraically and pictorially.

To aid in this discussion, we make notation for a "submatrix" of a general $m \times n$ matrix M: if $\mathcal{S} \subseteq \{1, 2, \ldots, m\}$ and $\mathcal{T} \subseteq \{1, 2, \ldots, n\}$, then we define $M_{\mathcal{S},\mathcal{T}}$ to be the $|\mathcal{S}| \times |\mathcal{T}|$ submatrix of M formed from the rows of M with indices in $\mathcal{S}$ and the columns of M with indices in $\mathcal{T}$.

First, we take a closer look at 4×4 blocks of the form $\Delta_{\mathcal{S}_k,\mathcal{S}_k}$, where

$$\mathcal{S}_k := 4k + \{1, 2, 3, 4\}, \text{ where } k \in \{0, 1 \ldots, p^2 - 1\}.$$

These blocks have columns and rows associated with the four vertices in a particular $\gamma_{(n,m)}$ within Γ_f^p, and have the following form (which we call "form (0)"):

$$\textit{(0)} : \widehat{\Delta}_{\mathcal{S}_k,\mathcal{S}_k}(\boldsymbol{\theta}) = \begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix} =: A. \tag{4.1}$$

Note that A is independent of $\boldsymbol{\theta}$ (see Remark 4.4). More importantly, this matrix is also independent of k, because the interaction of $\gamma_{(n,m)}$ with itself is independent of n and m: $\widehat{\Delta}_{\mathcal{S}_k,\mathcal{S}_k}$ does not depend on where $\gamma_{(n,m)}$ "sits" in Γ_f^p.

Now consider blocks taking either form

$$\textit{(i)}\ \widehat{\Delta}_{\mathcal{S}_k,\mathcal{S}_{k+1}} \text{ for } k \in \{\{0, 1, \ldots, p^2 - 1\} : k \neq p - 1 \mod p\};$$
$$\textit{(ii)}\ \widehat{\Delta}_{\mathcal{S}_k,\mathcal{S}_{k-p+1}} \text{ for } k \in \{\{0, 1, \ldots, p^2 - 1\} : k = p - 1 \mod p\}.$$

A block of either form represents the interaction between a copy $\gamma_{(n,m)}$ and the copy γ to its right. The block to the right of $\gamma_{n,m}$ is $\gamma_{n+1,m}$, where we add indices mod p. This modular arithmetic accounts for the case when $\gamma_{(n,m)}$ lies on the far right column of γ in Γ_f^p (i.e., when the corresponding block is of form *(ii)*), and the immediate right-hand neighbor of $\gamma_{n,m}$ actually wraps around and sits in the far left column of γ of Γ_f^p in the same row. In both forms *(i)* and *(ii)*, the only edge connecting γ to its right-hand "neighbor" γ is the edge from $E \in \gamma_{(n,m)}$ to $W \in \gamma_{(n+1,m)}$. This gives us the following matrix structures, denoted by

R for *right*:

$$\text{Form } (i):\ R_0 := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},\ \text{Form } (ii):\ R_{\theta_1} := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\theta_1} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Note that the form (i) of R is not $\boldsymbol{\theta}$-dependent, but the form (ii) of R is $\boldsymbol{\theta}$-dependent (see Remark 4.4).

Naturally then, we also have blocks of the forms

$$(iii)\ \widehat{\Delta}_{S_k,S_{k-1}} \text{ for } k \in \{\{0,1,\dots,p^2-1\} : k \neq 0 \mod p\};$$
$$(iv)\ \widehat{\Delta}_{S_k,S_{k+p-1}} \text{ for } k \in \{\{0,1,\dots,p^2-1\} : k = 0 \mod p\}),$$

which are equal to the conjugate transpose of R, denoted as $L := R^*$ for *left*. Analogously, these blocks represent the interaction between $\gamma_{(n,m)}$ and the copy of γ that sits to its left:

$$\text{Form } (iii):\ L_0 := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},\ \text{Form } (iv):\ L_{\theta_1} := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & e^{-i\theta_1} & 0 & 0 \end{bmatrix}.$$

We can similarly define the blocks relating $\gamma_{(n,m)}$ to the copy of γ above $\gamma_{(n,m)}$,

$$(v)\ \widehat{\Delta}_{S_k,S_{k+p}}(\boldsymbol{\theta}) \text{ for } k \in \{0,1,\dots,p^2-p-1)\};$$
$$(vi)\ \widehat{\Delta}_{S_k,S_{k-p^2+p}}(\boldsymbol{\theta}) \text{ for } k \in \{p^2-p,\dots,p^2-1\},$$

which we denote by U for *up*:

$$\text{Form } (v):\ U_0 := \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},\ \text{Form } (vi):\ U_{\theta_2} := \begin{bmatrix} 0 & 0 & e^{i\theta_2} & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Analogous to U, we have blocks of the forms

$$(vii)\ \widehat{\Delta}_{S_k,S_{k-p}}(\boldsymbol{\theta}) \text{ for } k \in \{p,\dots,p^2-1)\} \text{ and}$$
$$(viii)\ \widehat{\Delta}_{S_k,S_{k+p^2-p}}(\boldsymbol{\theta}) \text{ for } k \in \{0,\dots,p-1\},$$

which relate $\gamma_{(n,m)}$ to the block theoretically below $\gamma_{(n,m)}$. Denoting $D = U^*$ for *down*, we have

$$\text{Form } (vii):\ D_0 := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},\ \text{Form } (viii):\ D_{\theta_2} := \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{-i\theta_2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

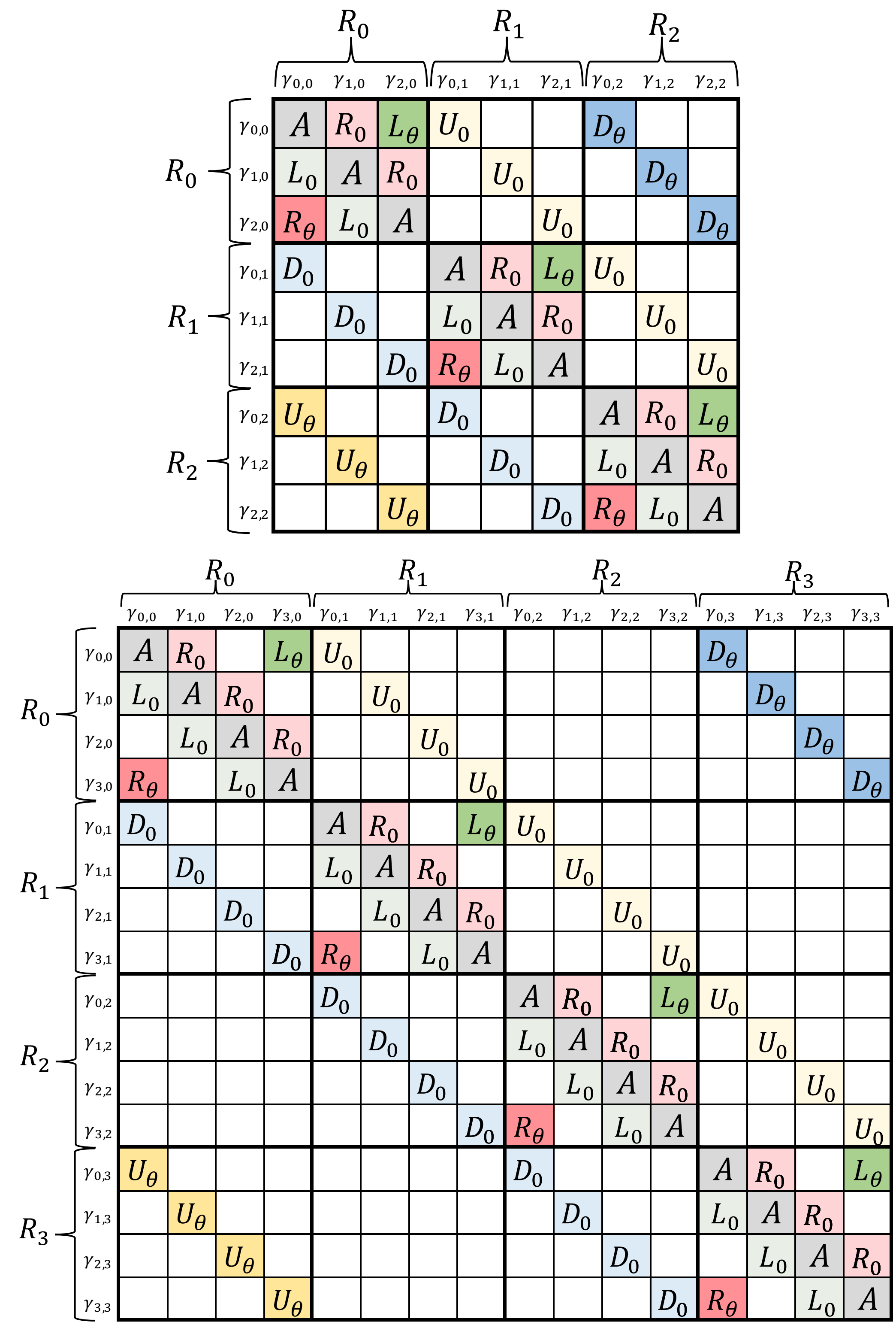

Figure 4.2: Block structure of $\widehat{\Delta}(\boldsymbol{\theta})$ for Γ_f^3 (top) and Γ_f^4 (bottom)

```
function M = myFloquetMat(p,t1,t2)
M=zeros(4*p^2);
A = [0 1 0 1; 1 0 1 0; 0 1 0 1; 1 0 1 0];
U = @(t1, t2) [0 0 exp(1i*t2) 0; 0 0 0 0; 0 0 0 0; 0 0 0 0];
R = @(t1, t2) [0 0 0 0; 0 0 0 exp(1i*t1); 0 0 0 0; 0 0 0 0];
L = @(t1, t2) R(t1,t2)';
D = @(t1, t2) U(t1,t2)';

DiagBlock=zeros(4*p);
%Puts Left in top right position and Right in bottom-left position
DiagBlock(1:4,(4*p-3):4*p)=L(t1,t2);
DiagBlock((4*p-3):4*p,1:4)=R(t1,t2);

%Constructs Main Diag pxp block:
for i=1:p
    %Puts A's on main diagonal of 4x4
    DiagBlock(4*i-3:4*i,4*i-3:4*i)=A;
    if i<p
        %Puts Left's under main diagonal of 4x4
        DiagBlock(4*(i+1)-3:4*(i+1),4*i-3:4*i)=L(0,0);
    end
    if i>1
        %Puts the Right's above main diagonal
        DiagBlock(4*(i-1)-3:4*(i-1),4*i-3:4*i)=R(0,0);
    end
end
%Constructs 4px4p Block with U's on the diagonal evaluated at t1,t2
UBlock=zeros(4*p);
for i=1:p
    UBlock(4*i-3:4*i,4*i-3:4*i)=U(t1,t2);
end

%Constructs 4px4p Block with U's on the diagonal evaluated at 0,0
UBlock0=zeros(4*p);
for i=1:p
    UBlock0(4*i-3:4*i,4*i-3:4*i)=U(0,0);
end

%Constructs 4px4p Block with D's on the diagonal evaluated at t1,t2
DBlock=zeros(4*p);
for i=1:p
    DBlock(4*i-3:4*i,4*i-3:4*i)=D(t1,t2);
end

%Constructs 4px4p Block with D's on the diagonal evaluated at 0,0
DBlock0=zeros(4*p);
for i=1:p
    DBlock0(4*i-3:4*i,4*i-3:4*i)=D(0,0);
end

%Situates UBlock0's on the supdiagonal of M, Dblocks on the subdiagonal of
%M, and DiagBlock's on the diagonal of M
for i=1:p
    M((4*p*i-(4*p-1)):4*p*i,(4*p*i-(4*p-1)):4*p*i)=DiagBlock;
    if i<p
        M((4*p*(i+1)-(4*p-1)):4*p*(i+1),(4*p*i-(4*p-1)):4*p*i)=DBlock0;
    end
    if i>1
        M((4*p*(i-1)-(4*p-1)):4*p*(i-1),(4*p*i-(4*p-1)):4*p*i)=UBlock0;
    end
end

%Puts a Dblock in the upper right hand corner of M and a Ublock in the
%lower left hand corner of M.
M(1:4*p,(4*p^2-(4*p-1):4*p^2))=DBlock;
M((4*p^2-(4*p-1):4*p^2),1:4*p)=UBlock;
end
```

Figure 4.3: MATLAB code to construct $\widehat{\Delta}(\boldsymbol{\theta})$ for given p

Finally, for any blocks $\widehat{\Delta}_{\mathcal{S}_k,\mathcal{S}_\ell}$ that are not of forms *(0)-(viii)*, $\widehat{\Delta}_{\mathcal{S}_k,\mathcal{S}_\ell} = \mathbf{0}_{4\times 4}$. This makes sense, since, if the copy of γ associated with $\mathcal{S}_\ell$ is not left, right, up, or down from the copy of γ associated with $\mathcal{S}_k$, there are no connecting edges between the two copies of γ, and thus the corresponding block should be identically 0 (Remark 4.3).

We will now examine the larger symmetry of Γ_f^p by defining formally the notion of a "row" in Γ_f^p. Let

$$\mathcal{R}_k := \{4pk+1, 4pk+2, \ldots, 4pk+4p\}.$$

The set $\mathcal{R}_k$ corresponds to the indices of vertices in the k^{th} row from the bottom in Γ_f^p. Blocks of the form $\widehat{\Delta}_{\mathcal{R}_k,\mathcal{R}_\ell}$ cannot be defined indepently of p, as $\widehat{\Delta}_{\mathcal{S}_k,\mathcal{S}_\ell}$ could; at the very least, their dimension is p-dependent ($\widehat{\Delta}_{\mathcal{R}_k,\mathcal{R}_\ell} \in \mathbb{C}^{4p\times 4p}$). However, these blocks still contain describable structure (see Figure 4.2).

Viewing $\widehat{\Delta}(\boldsymbol{\theta})$ as a $p\times p$ block matrix in which the j^{th} column or row of $\widehat{\Delta}(\boldsymbol{\theta})$ corresponds to the j^{th} row of γ in Γ_f^p, it is intuitive to construct the block entries of $\widehat{\Delta}(\boldsymbol{\theta})$; for example, if we consider $\widehat{\Delta}_{\mathcal{R}_0,\mathcal{R}_1}$, we expect "up" blocks on the diagonal entries, because $\gamma_{(0,1)}$ is above $\gamma_{(0,0)}$, $\gamma_{(1,1)}$ is above $\gamma_{(1,0)}, \ldots$, and $\gamma_{(p,1)}$ is above $\gamma_{(p,0)}$. Therefore, rather than giving algebraic formulae for the construction of a single $\widehat{\Delta}_{\mathcal{R}_k,\mathcal{R}_k}$ here, we include the Matlab code that constructs $\widehat{\Delta}(\boldsymbol{\theta})$ for a given period p, which gives the algebraic structure inherently. See Figure 4.2 for examples, and Figure 4.3 for precise construction of $\widehat{\Delta}(\boldsymbol{\theta})$ with $\widehat{\Delta}_{\mathcal{R}_k,\mathcal{R}_\ell}$ blocks.

4.2 Structure of Γ_f and $\widehat{\Delta}(\boldsymbol{\theta})$ for $p = 2$

The case of $p = 2$ is very similar to that of $p \geq 3$, but there is a slightly different structure.

For $p \geq 3$, a block corresponding to the interaction between $\gamma_{(n,m)}$ and $\gamma_{(r,s)}$ can have at most one of the forms $(0) - (viii)$ given in the previous section. However, when $p = 2$, the addition modulo two allows certain pairs of indices to satisfy more than one form. For example, $\gamma_{(0,0)}$ is both to the right and left of $\gamma_{(1,0)}$. Therefore letting $F = \{0, i, ii, ..., vii, viii\}$, we may define blocks (with the same definition for $\mathcal{S}_k$):

$$\Delta_{\mathcal{S}_k,\mathcal{S}_\ell} = \sum_{\substack{j\in F\ s.t.\\ k,\ell \text{ satisfy form } (j)}} \text{Matrix corresponding to form } (j). \tag{4.2}$$

We acknowledge that this definition is perhaps not the clearest, so we explicitly include the 2-period Floquet matrix in Figure 4.4.

$$
\begin{array}{cc|cccc|cccc|cccc|cccc|}
 & & \multicolumn{4}{c|}{\gamma_{(0,0)}} & \multicolumn{4}{c|}{\gamma_{(1,0)}} & \multicolumn{4}{c|}{\gamma_{(0,1)}} & \multicolumn{4}{c|}{\gamma_{(1,1)}} \\
 & & N & E & S & W & N_{(1,0)} & E_{(1,0)} & S_{(1,0)} & W_{(1,0)} & N_{(0,1)} & E_{(0,1)} & S_{(0,1)} & W_{(0,1)} & N_{(1,1)} & E_{(1,1)} & S_{(1,1)} & W_{(1,1)} \\
\hline
\gamma_{(0,0)} & N & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
 & E & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & S & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & e^{-i\theta_2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & W & 1 & 0 & 1 & 0 & 0 & e^{-i\theta_1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
\gamma_{(1,0)} & N_{(1,0)} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
 & E_{(1,0)} & 0 & 0 & 0 & e^{i\theta_1} & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 & S_{(1,0)} & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & e^{-i\theta_2} & 0 & 0 & 0 \\
 & W_{(1,0)} & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
\gamma_{(0,1)} & N_{(0,1)} & 0 & 0 & e^{i\theta_2} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
 & E_{(0,1)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
 & S_{(0,1)} & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\
 & W_{(0,1)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & e^{-i\theta_1} & 0 & 0 \\
\hline
\gamma_{(1,1)} & N_{(1,1)} & 0 & 0 & 0 & 0 & 0 & 0 & e^{i\theta_2} & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
 & E_{(1,1)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & e^{i\theta_1} & 1 & 0 & 1 & 0 \\
 & S_{(1,1)} & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\
 & W_{(1,1)} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\
\hline
\end{array}
$$

Figure 4.4: $\widehat{\Delta}(\boldsymbol{\theta})$ for $p = 2$

The formula (4.2) also holds for the 1-period Floquet Matrix (Equation (1.3)). In this case, it is easy to see that $\widehat{\Delta}(\boldsymbol{\theta})$ is simply the sum of all matrix forms $(0), (i), (ii), \ldots, (vii), (viii)$.

4.3 Spectrum of the Schrödinger Operator on Γ_f^2

Now that we have an explicit definition of $\widehat{\Delta}(\boldsymbol{\theta})$ for Γ_f^2, as well as a broader understanding of the construction of $\widehat{\Delta}(\boldsymbol{\theta})$ for general periods, we begin to investigate the spectrum resulting from a perturbation of Δ by a periodic Q, as we did in Chapter 2 for Γ_f^1. We will prove an analog of Theorem 3.2 for $p = 2$, but do not prove an analog of Theorem 3.1, as we have not yet built the tools to prove this. We address this in detail in Chapter 6.

Definition 4.6. A function $f : \mathcal{V} \to \mathbb{C}$ is (p, q)-periodic if it is periodic (Definition 1.1) with respect to $\Gamma_f^{\{p\boldsymbol{t}_1, q\boldsymbol{t}_2\}}$.

Theorem 4.7. *There is a constant $\epsilon > 0$ and a $(2, 2)$-periodic potential $Q : \mathcal{V} \longrightarrow \mathbb{R}$ with $\|Q\|_\infty = 1$ such that $\sigma(H_{tQ})$ has three gaps when $0 < t < \epsilon$; these gaps open at eigenvalues*

$z = 0, \pm 1$.

Lemma 4.8. *Let* $\widehat{Q} = \operatorname{diag}(0,0,-1,1,0,-1,1,0,1,0,0,-1,-1,1,0,0)$. *There is a constant* ϵ *such that if* $t \in (0,\epsilon)$, *then* $z = 1 + t/2 \notin \sigma(\widehat{H}_{tQ})$.

To prove Lemma 4.8, we first analyze the characteristic polynomial of $\widehat{H}_{tQ}(\boldsymbol{\theta})$ for our chosen potential, $\widehat{Q}$ (see Figure 4.5) along the line $z(t) = 1 + t/2$. We rely on Mathematica to derive the expression, a real-valued polynomial in t of degree 16:

$$P_{\boldsymbol{\theta}}(t) = \sum_{j=0}^{16} c_j(\boldsymbol{\theta}) t^j. \tag{4.3}$$

Here $c_0, \ldots, c_9$ are $\boldsymbol{\theta}$-dependent expressions (some of which are formulated in Table 4.1) and $c_{10}, \ldots, c_{16}$ are constants that are not relevant to our argument. We note several properties regarding these coefficients.

Table 4.1: Coefficients of the characteristic polynomial of $\widehat{H}_{tQ}(\boldsymbol{\theta})$ evaluated on the line $z(t) = 1 + t/2$, along with their images of the interior of $\mathbb{T}^2$ and $\mathbf{0}$.

	Expression for c_j	$c_j((0,2\pi)^2)$	$c_j(\mathbf{0})$
c_0	$256\sin^4(\theta_1/2)\sin^4(\theta_2/2)$	(0,256]	0
c_1	$-256(-2+\cos\theta_1+\cos\theta_2)\sin^2(\theta_1/2)\sin^2(\theta_2/2)$	(0,1024]	0
c_2	$32(12+\cos(2\theta_1)-10\cos\theta_2+2\cos\theta_1(-5+3\cos\theta_2)+\cos(2\theta_2))$	(0,1280]	0
c_3	$-32(-7+3\cos\theta_2+\cos\theta_1(3+\cos\theta_2))$	(0,384]	0
c_4	$4(-11+3\cos\theta_2+\cos\theta_1(3+5\cos\theta_2))$	$[-64,0)$	0
c_5	$20(5+\cos\theta_1(-3+\cos\theta_2)-3\cos\theta_2)$	[0, 240]	0
c_6	$89+\cos\theta_1(-13+\cos\theta_2)-13\cos\theta_2$	(64,116]	64

Lemma 4.9. *We have the following inequalities, which hold independently of* $\boldsymbol{\theta}$*:*

1. $c_0, c_1, c_2, c_3, c_5 \geq 0$.
2. $c_4 \leq 0$.
3. $c_6 \geq 64$.

The only of these inequalities that are not clear from their respective formulae are $c_2 \geq 0$ and $c_5 \geq 0$, so we include a short proof.

Proof for $c_2 \geq 0$. We wish to find the extrema of c_2, so we set its partial derivatives equal to 0, ignoring the scalar multiple:

$$\frac{\partial c_2}{\partial \theta_1} = 10\sin\theta_1 - 2\sin(2\theta_1) - 6\sin\theta_1\cos\theta_2 = 0, \tag{4.4}$$

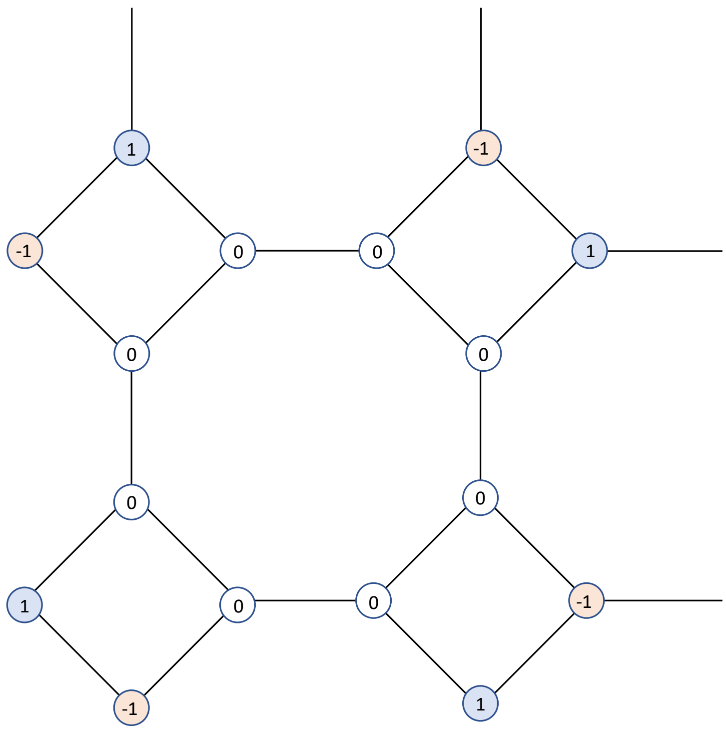

Figure 4.5: Potential $\widehat{Q}$ illustrated on Γ_f^2.

$$\frac{\partial c_2}{\partial \theta_2} = 10\sin\theta_2 - 2\sin(2\theta_2) - 6\cos\theta_1\sin\theta_2 = 0. \tag{4.5}$$

It is clear that (4.4) is satisfied when $\theta_1 = 0, \pi$ and (4.5) is satisfied when $\theta_2 = 0, \pi$. We evaluate c_2 along these lines:

$$\begin{aligned} c_2(\theta_1, 0) &= 256\sin^4\left(\frac{\theta_1}{2}\right) \geq 0, \\ c_2(\theta_1, \pi) &= 32(23 - 16\cos\theta_1 + \cos(2\theta_1)) \geq 192, \\ c_2(0, \theta_2) &= 256\sin^4\left(\frac{\theta_2}{2}\right) \geq 0, \\ c_2(\pi, \theta_2) &= 32(23 - 16\cos\theta_2 + \cos(2\theta_2)) \geq 192. \end{aligned}$$

In particular, c_2 is nonnegative here. To extend our search for the minimum to the remainder of $\mathbb{T}^2$, we note that since we are not considering $\boldsymbol{\theta}$ with $\theta_1, \theta_2 \in \{0, \pi\}$, we may divide Equation (4.4) by $\sin\theta_1$ and Equation (4.5) by $\sin\theta_2$, so that our previous system becomes

$$10 - 4\cos\theta_1 - 6\cos\theta_2 = 0,$$

$$10 - 4\cos\theta_2 - 6\cos\theta_1 = 0.$$

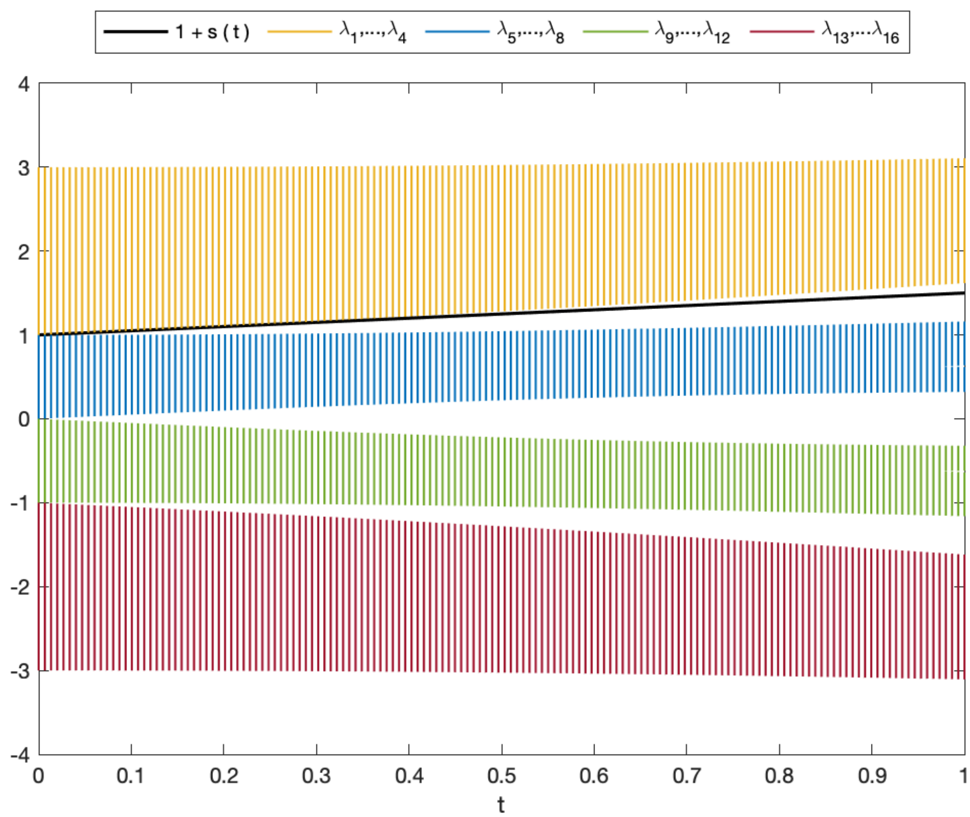

Figure 4.6: $\sigma(\widehat{H}_{tQ})$, for $t \in [0,1]$, $\widehat{Q} = \mathrm{diag}(0,0,0,1,0,-1,0,0,0,0,0,-1,0,1,0,0)$, computed in MATLAB.

Rearranging this system to

$$\frac{10 - 4\cos\theta_1}{6} = \cos\theta_2,$$

$$\frac{10 - 4\cos\theta_2}{6} = \cos\theta_1,$$

it becomes clear that this solution is only solvable when $\cos\theta_1 = \cos\theta_2 = 1$, which implies $\theta_1, \theta_2 \in \{0, \pi\}$, contrary to our assumption. Therefore c_2 attains its minimum value at $\boldsymbol{\omega} = (\omega_1, \omega_2)$, where at least one of $\omega_1, \omega_2 \in \{0, \pi\}$. We conclude that c_2 is nonnegative for all $\boldsymbol{\theta} \in \mathbb{T}^2$. $\square$

Proof for $c_5 \geq 0$. We do not include the details of this proof, as the argument is analogous to the previous argument, and in fact is much simpler. $\square$

Proof of Lemma 4.8. Our goal is to prove that there is an $\epsilon > 0$ such that if $0 < t < \epsilon$ and

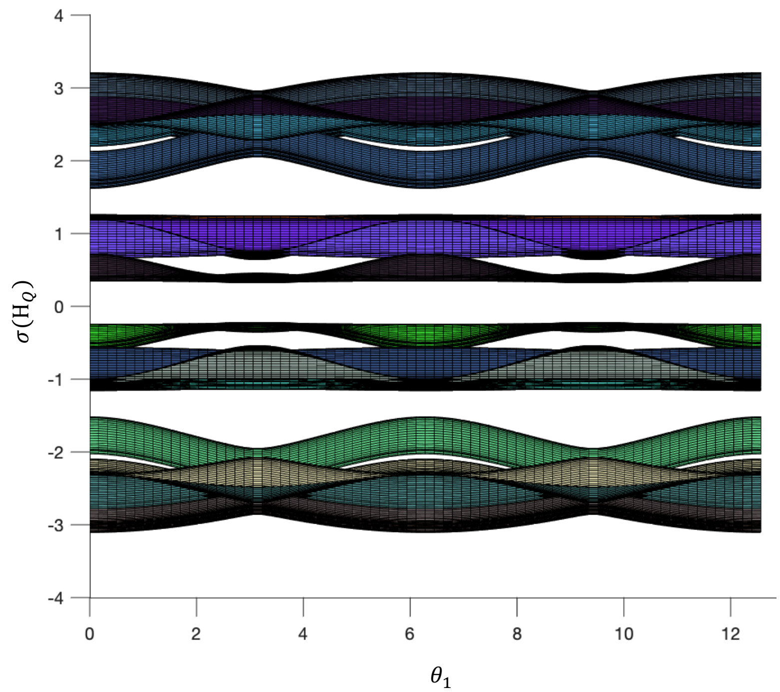

Figure 4.7: Spectral bands of H_Q $(t = 1)$ on Γ_f^2 viewed as a projection onto the θ_1-z plane. Notice three gaps in the spectrum.

$z = 1 + t/2$, the characteristic polynomial $P_{\boldsymbol{\theta}}$ has no roots. We reassociate $P_{\boldsymbol{\theta}}$ as follows:

$$\begin{aligned} P_{\boldsymbol{\theta}}(t) &= \sum_{\substack{j=1 \\ j\neq 3,4}}^{16} c_j(\boldsymbol{\theta})t^j + t^3(c_3(\boldsymbol{\theta}) + tc_4(\boldsymbol{\theta})) \\ &=: \rho_{\boldsymbol{\theta}}(t) + t^3(c_3(\boldsymbol{\theta}) + tc_4(\boldsymbol{\theta})). \end{aligned}$$

Since we are concerned with $t \ll 1$, there is a threshold $\eta > 0$ such that if $0 < t < \eta$, $\sum_{j=7}^{16} c_j(\boldsymbol{\theta})t^j$ is negligible in the sum $\rho_{\boldsymbol{\theta}}(t)$. Since $c_0, c_1, \ldots, c_3, c_5 \geq 0$ and $c_6 > 0$, it follows that $\rho_{\boldsymbol{\theta}}(t) > 0$ for $0 < t < \eta$. It remains to show that our adjusted coefficient on t_3, which we denote as $l_{\boldsymbol{\theta}}(t) = c_3(\boldsymbol{\theta}) + tc_4(\boldsymbol{\theta})$, is nonnegative for some $0 < \epsilon < \eta$. Our bounds for $c_3(\boldsymbol{\theta})$ and $c_4(\boldsymbol{\theta})$ mandate that every $l_{\boldsymbol{\theta}}$ is a line with negative slope that intersects the nonnegative z-axis.

If the slope $c_4(\boldsymbol{\theta}) = 0$, then the corresponding $l_{\boldsymbol{\theta}}$ is a nonnegative constant, and thus clearly satisfies $l_{\boldsymbol{\theta}} \geq 0$ for all $0 < t < \eta$. Otherwise, $l_{\boldsymbol{\theta}}$ has a single t-intercept, given by

$$\begin{aligned} t_0(\boldsymbol{\theta}) = \frac{-c_3(\boldsymbol{\theta})}{c_4(\boldsymbol{\theta})} &= \frac{8(-7 + 3\cos\theta_2 + \cos\theta_1(3 + \cos\theta_2))}{-11 + 3\cos\theta_2 + \cos\theta_1(3 + 5\cos\theta_2)} \\ &= 4 + \frac{-12(1 - \cos\theta_1)(1 - \cos\theta_2)}{3(\cos\theta_1 - 1) + 3(\cos\theta_2 - 1) + 5(\cos\theta_1\cos\theta_2 - 1)} \end{aligned}$$

$$:= 4 + \frac{\mathcal{N}(\boldsymbol{\theta})}{\mathcal{D}(\boldsymbol{\theta})}. \tag{4.6}$$

This simplification of $t_0(\boldsymbol{\theta})$ was obtained with the combined efforts of Mathematica and our own brute force.

It is clear from the simplified expression that t_0 is continuous on $\mathbb{T}^2 \setminus \{\mathbf{0}\}$ (i.e., $\mathcal{D}(\boldsymbol{\theta}) = 0$ if and only if $\boldsymbol{\theta} = \mathbf{0}$). We argue that $\boldsymbol{\theta} = \mathbf{0}$ is a removable singularity of t_0. Letting $\theta_1 = r\cos\phi$, $\theta_2 = r\sin\phi$, we have that

$$\begin{aligned}
\frac{\partial^2}{\partial r^2}(\mathcal{N}(r\cos\phi, r\sin\phi)) &= -\cos^2\phi\cos(r\cos\phi)(\cos(r\sin\phi)-1) \\
&\quad - (\cos(r\cos\phi)-1)\cos(r\sin\phi)\sin^2\phi \\
&\quad + \sin(2\phi)\sin(r\cos\phi)\sin(r\sin\phi), \\
\frac{\partial^2}{\partial r^2}(\mathcal{D}(r\cos\phi, r\sin\phi)) &= -\cos^2\phi\cos(r\cos\phi)(3+5\cos(r\sin\phi)) \\
&\quad - (3+5\cos(r\cos\phi))\cos(r\sin\phi)\sin^2\phi \\
&\quad + 5\sin(2\phi)\sin(r\cos\phi)\sin(r\sin\phi).
\end{aligned}$$

(We skipped straight to the second derivatives because the first derivatives $\frac{\partial \mathcal{N}}{\partial r}$ and $\frac{\partial \mathcal{D}}{\partial r}$ evaluated at $r = 0$ both equal 0, and thus provide us no additional information.) Therefore

$$\lim_{r\to 0}\frac{\mathcal{N}(r\cos\phi, r\sin\phi)}{\mathcal{D}(r\cos\phi, r\sin\phi)} = \left.\frac{\frac{\partial^2}{\partial r^2}(\mathcal{N}(r\cos\phi, r\sin\phi))}{\frac{\partial^2}{\partial r^2}(\mathcal{D}(r\cos\phi, r\sin\phi))}\right|_{r=0} = \frac{0}{-8} = 0.$$

Thus we can define $\widehat{t_0}$ to be the continuous extension of t_0 to all of $\mathbb{T}^2$ by setting $\widehat{t_0}(\mathbf{0}) = 4$.

It is easily checked that $\widehat{t_0}(\boldsymbol{\theta}) = 4$ for all $\boldsymbol{\theta} \in \partial\,\mathbb{T}^2$. We check for critical points on the interior of $\mathbb{T}^2$ by calculating the partial derivatives of $\widehat{t_0}$:

$$\begin{aligned}
\frac{\partial t_0}{\partial \theta_1} &= \frac{384\sin\theta_1\sin^4(\theta_2/2)}{(3(\cos\theta_1-1)+3(\cos\theta_2-1)+5(\cos\theta_1\cos\theta_2))^2} \\
\frac{\partial t_0}{\partial \theta_2} &= \frac{384\sin\theta_2\sin^4(\theta_1/2)}{(3(\cos\theta_1-1)+3(\cos\theta_2-1)+5(\cos\theta_1\cos\theta_2-1))^2}.
\end{aligned}$$

It is clear from these expressions that for $\boldsymbol{\theta}$ in the interior of $\mathbb{T}^2$, (i.e., when $\theta_1 \neq 0, 2\pi$ and $\theta_2 \neq 0, 2\pi$), both partials are zero if and only if both $\sin\theta_1 = 0$ and $\sin\theta_2 = 0$, and therefore the only critical point occurs at $\boldsymbol{\pi}$. We calculate that $\widehat{t_0}(\boldsymbol{\pi}) = 8$, and thus conclude that the minimum value of t_0, achieved on $\partial\,\mathbb{T}^2$, is 4. Hence, if $t < 4$, $l_{\boldsymbol{\theta}}(t) \geq 0$.

Therefore, for all $\boldsymbol{\theta} \in \mathbb{T}^2$ and $0 < t < 4$, the modified coefficient $l_{\boldsymbol{\theta}}(t)$ of t^3 in $P_{\boldsymbol{\theta}}$ is nonnegative. Letting $\epsilon = \min\{\eta, 4\}$ we have that $P_{\boldsymbol{\theta}}(t) > 0$ for $0 < t < \epsilon$. $\square$

Lemma 4.10. *Let* $\widehat{Q} = \mathrm{diag}(0,0,-1,1,0,-1,1,0,1,0,0,-1,-1,1,0,0)$. *There is a constant* ϵ *such that if* $t \in (0,\epsilon)$, *then* $z = -1 - t/2 \notin \sigma(\widehat{H}_{tQ})$.

Proof. This is analogous to the proof of Lemma 4.8. □

Lemma 4.11. *Let* $\widehat{Q} = \mathrm{diag}(0,0,-1,1,0,-1,1,0,1,0,0,-1,-1,1,0,0)$. *There is a constant* ϵ *such that if* $t \in (0,\epsilon)$, *then* $z = 0 \notin \sigma(\widehat{H}_{tQ})$.

Proof. The characteristic polynomial of $\widehat{H}_{tQ}$ evaluated at $z = 0$ is, as expected, (relatively) simple:

$$\begin{aligned} P_{\boldsymbol{\theta}}(0) = 16t^6 &+ 2t^4\Big(28 + \cos(2\theta_1) + 12\cos\theta_2 + 4\cos\theta_1(3+\cos\theta_2) + \cos(2\theta_2)\Big) \\ &+ t^2\Big(64 + 60\cos\theta_2 + 8\cos(2\theta_1)(1+\cos\theta_2) + \cos\theta_1(60 + 64\cos\theta_2) \\ &\qquad + 16\cos^2(\theta_1/2)\cos(2\theta_2)\Big) \\ &+ (3 + 4\cos\theta_2 + 4\cos\theta_1(1+\cos\theta_2))^2. \end{aligned}$$

The constant term of this polynomial is squared and thus nonnegative, and similar arguments to those given in the proof of Lemma 4.9 verify that the coefficients of t^2 and t^4 are also nonnegative. Similar to our previous argument, since the leading coefficient is strictly positive for all $\boldsymbol{\theta} \in \mathbb{T}^2$ and $0 < t < 1$, $P_{\boldsymbol{\theta}}$ is also strictly positive for $0 < t < 1$, and thus we have found a gap in the spectrum opening at $z = 0$. □

Proof of Theorem 4.7. This result now follows immediately from the previous lemmas. □

Chapter 5

Characterization of $\sigma[\Delta(\theta_1, \pi)]$ on Γ_f^1

As we explored the spectrum of Δ on Γ_f^1, we began to search for explicit formulae $z_i(\boldsymbol{\theta})$ that would give the i^{th} eigenvalue of $\widehat{\Delta}(\boldsymbol{\theta})$ as a function of $\boldsymbol{\theta}$. We began our search for such formulae by writing code in MATLAB to approximate the eigensurface $z_1(\boldsymbol{\theta})$ by a two-dimensional Fourier series, with the hope that only a few coefficients would be non-zero, and the few non-zero coefficients would be "nice" numbers. However, the Fourier coefficients we found did not behave in this way; for a 2π-periodic function that was apparently smooth, the coefficients decayed rather slowly, as shown in Figure 5.1.

As a result, we began to suspect that the surface z_1 was not smooth everywhere, as we had originally assumed, but in fact had a conical singularity at $\boldsymbol{\pi}$. In this chapter, we make some progress towards this result.

Theorem 5.1. *$z_1(\boldsymbol{\theta})$ is not differentiable at $\boldsymbol{\theta} = \boldsymbol{\pi}$.*

To assist the reader, we lay out a roadmap of sorts for the proof.

1. Derive an explicit formula $z_1(\theta_1)$ for the largest eigenvalue of $\widehat{\Delta}(\theta_1, \pi)$ as a function of θ_1. (We will also give formulae for the smaller eigenvalues of $\widehat{\Delta}(\theta_1)$ as well, though that is for completeness (grammatically speaking) and is not necessary for the proof of the theorem.)

2. Verify that the formula for $z_1(\theta_1)$ does in fact give the largest eigenvalue of $\widehat{\Delta}(\theta_1, \pi)$.

3. Differentiate z_1 with respect to θ_1.

4. Show that the right- and left-hand limits of the derivative of $z_1(\theta_1)$ do not agree.

We now proceed to the proof.

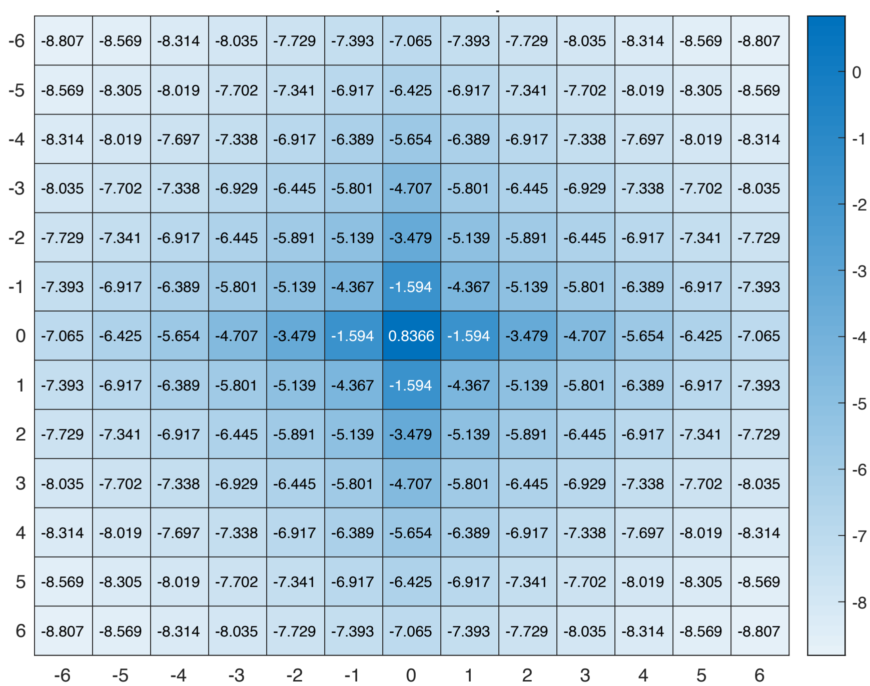

Figure 5.1: Fourier coefficients for approximation of $z_1(\boldsymbol{\theta})$.
A cell (ℓ, k) in this heat-map contains $\log_{10}(\mathcal{C}_{\ell,k})$, where $\mathcal{C}_{\ell,k}$ is the numerically computed coefficient of $e^{-i\langle(\ell,k),\boldsymbol{\theta}\rangle}$ in the Fourier expansion of $z_1(\boldsymbol{\theta})$.

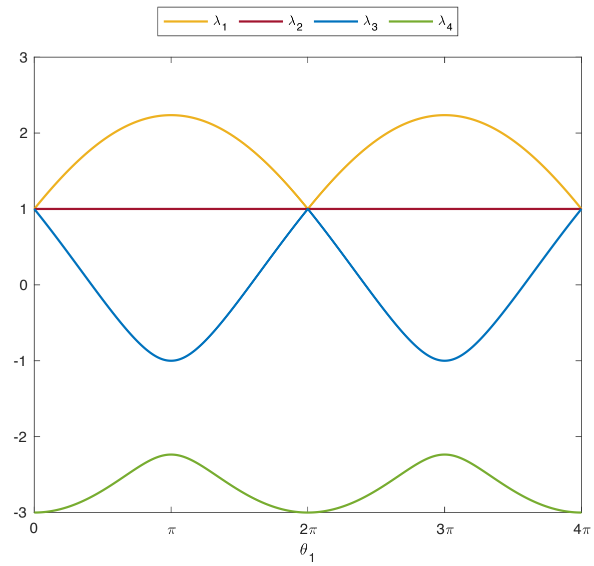

Figure 5.2: $\sigma(\widehat{\Delta}(\theta_1, \pi))$.

5.1 Steps 1 and 2: Formulae for Eigenvalues of $\widehat{\Delta}(\theta_1, \pi)$

Fixing $\theta_2 = \pi$, from our previous calculation of the characteristic polynomial of $\Delta(\boldsymbol{\theta})$, we have that

$$\begin{aligned} P_{(\theta_1,\pi)}(z) &= z^4 - 6z^2 - 4z(\cos\theta_1 + \cos\pi) - 4\cos\theta_1\cos\pi + 1 \\ &= (z-1)(z^3 + z^2 - 5z - 4\cos\theta_1 - 1). \end{aligned} \tag{5.1}$$

We will give explicit formulas for the eigenvalues of $\widehat{\Delta}(\theta_1, \pi)$ as a function of θ_1.

Theorem 5.2. *The eigenvalues of $\widehat{\Delta}(\theta_1, \pi)$ are given by the functions*

$$\begin{aligned} z_1(\theta_1) &= \frac{1}{3}\left(8\cos(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)) - 1\right), \\ z_2(\theta_1) &\equiv 1, \\ z_3(\theta_1) &= \frac{1}{3}\left(8\cos\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right) - \frac{\pi}{3}\right) + 1\right), \\ z_4(\theta_1) &= \frac{1}{3}\left(8\cos\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right) + \frac{\pi}{3}\right) + 1\right). \end{aligned}$$

Proof. From the characteristic polynomial (5.1), it is clear that we have a constant eigenvalue $z_2 \equiv 1$, independent of θ_1, so we turn our focus to the other three roots of $P_{(\theta_1,\pi)}$. (We will prove later that this labelling reflects the ordering of the eigenvalues.) Removing $(z-1)$ from $P_{(\theta_1,\pi)}$, it must be that z_1, z_3, and z_4 solve the equation

$$p_{\boldsymbol{\theta}}(z) := z^3 + z^2 - 5z - 4\cos\theta_1 - 1 = 0.$$

It is tedious but possible to check that the proposed expressions are in fact roots of $p_{\theta_1}(z)$; we will show the details for z_1. However, we will also provide a bit of context for their derivation. Mathematica provides the following expression for the first root of $p_{\theta_1}(z)$:

$$\begin{aligned} z_1(\theta_1) = -\frac{1}{3} &+ \frac{8\cdot 2^{2/3}}{3\left[-5+27\cos\theta_1+3\sqrt{3}\sqrt{-37-10\cos\theta_1+27\cos^2\theta_1}\right]^{1/3}} \\ &+ \frac{2^{1/3}}{3}\left[-5+27\cos\theta_1+3\sqrt{3}\sqrt{-37-10\cos\theta_1+27\cos^2\theta_1}\right]^{1/3}. \end{aligned}$$

To simplify this expression, we first take a closer look at the expression which we will denote as

$$a(\theta_1) = -5+27\cos\theta_1+3\sqrt{3}\sqrt{-37-10\cos\theta_1+27\cos^2\theta_1},$$

so that

$$z_1(\theta_1) = -\frac{1}{3} + \frac{8\cdot 2^{2/3}}{3a(\theta_1)^{1/3}} + \frac{2^{1/3}a(\theta_1)^{1/3}}{3}. \tag{5.2}$$

We notice that $\max_{\theta_1\in[0,2\pi]}\left\{-37-10\cos\theta_1+27\cos^2\theta_1\right\} = 0$ (achieved when $\cos\theta_1=-1$), and so by factoring out -1 from the argument of the square root in $a(\theta_1)$ we can write $a(\theta_1)$ in the form $x+iy$, where $x,y\in\mathbb{R}$, as

$$a(\theta_1) = -5+27\cos\theta_1+i\left(3\sqrt{3}\sqrt{37+10\cos\theta_1-27\cos^2\theta_1}\right).$$

From here, we can easily characterize the magnitude of a via

$$\begin{aligned} |a(\theta_1)|^2 &= (27\cos\theta_1-5)^2+\left(3\sqrt{3}\sqrt{37+10\cos\theta_1-27\cos^2\theta_1}\right)^2 \\ &= 25-270\cos\theta_1+27^2\cos^2\theta_1+27(37+10\cos\theta_1-27\cos^2\theta_1) \\ &= 25+27\cdot 37 \\ &= 1024, \end{aligned}$$

and so $|a(\theta_1)| = 32$. Next, we find the argument of $a(\theta_1)$ in the complex plane, which we denote as $\alpha(\theta_1)$:

$$\alpha(\theta_1) = \arccos\left(\frac{\operatorname{Re} a(\theta_1)}{|a(\theta_1)|}\right) = \arccos\left(\frac{27\cos\theta_1-5}{32}\right).$$

Therefore a has the complex polar representation $a(\theta_1) = 32e^{i\alpha(\theta_1)}$, and thus by Equation (5.2), $z_1(\theta_1)$ becomes

$$z_1(\theta_1) = -\frac{1}{3} + \frac{8\cdot 2^{2/3}}{3\big(32\exp(i\alpha(\theta_1))\big)^{1/3}} + \frac{2^{1/3}\big(32\exp\big(i\alpha(\theta_1)\big)\big)^{1/3}}{3}$$

$$\begin{aligned}
&= -\frac{1}{3} + \frac{4}{3}\exp\left(\frac{-i\alpha(\theta_1)}{3}\right) + \frac{4}{3}\exp\left(\frac{i\alpha(\theta_1)}{3}\right) \\
&= \frac{1}{3}\left(-1 + 4\cdot 2\ \mathrm{Re}\exp\left(\frac{-i\alpha(\theta_1)}{3}\right)\right) \\
&= \frac{1}{3}\left(8\cos\left(\frac{-\alpha(\theta_1)}{3}\right) - 1\right) \\
&= \frac{1}{3}\left[8\cos\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)\right) - 1\right],
\end{aligned}$$

our proposed expression for z_1. We now algebraically check that this expression for $z_1(\theta)$ is in fact a root of p_{θ_1}. Make the substitution $A(\theta_1) = \frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)$, and we then have that

$$z_1(\theta_1) = \frac{1}{3}\left(8\cos A - 1\right).$$

Note the following equivalence, which results from the use of standard trigonometric identities:

$$\begin{aligned}
4\cos^3 A - 3\cos A &= 2\cos A(\cos 2A + 1) - 3\cos A \\
&= 2\cos A \cdot \cos 2A + 2\cos A - 3\cos A \\
&= \cos A + \cos 3A - \cos A \\
&= \cos 3A.
\end{aligned}$$

Hence

$$\begin{aligned}
p_{\theta_1}(z_1(\theta_1)) &= \frac{1}{27}\left(8\cos A - 1\right)^3 + \frac{1}{9}\left(8\cos A - 1\right)^2 - \frac{5}{3}\left(8\cos A - 1\right) - 4\cos\theta_1 - 1 \\
&= \frac{1}{27}\left(47 + 128\left(4\cos^3 A - 3\cos A\right)\right) - 4\cos\theta_1 - 1 \\
&= \frac{1}{27}\left(47 + 128\left(\cos 3A\right)\right) - 4\cos\theta_1 - 1 \\
&= \frac{1}{27}\left(47 + 128\cos\left(3\cdot\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)\right)\right) - 4\cos\theta_1 - 1 \\
&= \frac{1}{27}\left(47 + 128\left(\frac{27\cos\theta_1 - 5}{32}\right)\right) - 4\cos\theta_1 - 1 \\
&= \frac{1}{27}\left(27 + 4\cdot 27\cos\theta_1\right) - 4\cos\theta_1 - 1 \\
&= 0,
\end{aligned}$$

as desired.

Turning now to z_3 and z_4, the proof is largely analogous. Immediately making the identical substitutions of α and a into the expression given by Mathematica for z_3, we simplify to obtain the desired expression for z_3:

$$\begin{aligned}
z_3(\theta_1) &= -\frac{1}{3} - \frac{4 \cdot 2^{2/3}(1+i\sqrt{3})}{3a(\theta_1)^{1/3}} - \frac{(1-i\sqrt{3})a(\theta_1)^{1/3}}{3 \cdot 2^{2/3}} \\
&= -\frac{1}{3}\left[1 + \frac{2^{8/3} \cdot 2\exp(i\pi/3)}{2^{5/3}\exp\left(i\alpha(\theta_1)\right)} + \frac{2\exp(-i\pi/3)\ 2^{5/3}\ \exp(i\alpha(\theta_1)/3)}{2^{2/3}}\right] \\
&= -\frac{1}{3}\left[1 + 4\exp\left(i\ \frac{\pi-\alpha(\theta_1)}{3}\right) + 4\exp\left(-i\ \frac{\pi-\alpha(\theta_1)}{3}\right)\right] \\
&= -\frac{1}{3}\left[1 + 2\mathrm{Re}\left(4\exp\left(i\ \frac{\pi-\alpha(\theta_1)}{3}\right)\right)\right] \\
&= -\frac{1}{3}\left[1 + 8\cos\left(\frac{-\alpha(\theta_1)+\pi}{3}\right)\right] \qquad (5.3)\\
&= \frac{1}{3}\left[1 + 8\cos\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right) - \frac{\pi}{3}\right)\right].
\end{aligned}$$

Similarly, given Mathematica's expression for z_4, it is exactly analogous to our calculations for z_3 to see that

$$\begin{aligned}
z_4(\theta_1) &= -\frac{1}{3} - \frac{4 \cdot 2^{2/3}(1-i\sqrt{3})}{3a(\theta_1)^{1/3}} - \frac{(1+i\sqrt{3})a(\theta_1)^{1/3}}{3 \cdot 2^{2/3}} \\
&= \frac{1}{3}\left[1 + 8\cos\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right) + \frac{\pi}{3}\right)\right].
\end{aligned}$$

We skip checking that z_3 and z_4 are in fact roots of p_{θ_1}, as the calculation is similar to that for z_1. □

Theorem 5.3. *For any $\theta_1 \in [0, 2\pi]$, we have that $z_1 \geq z_2 \geq z_3 \geq z_4$.*

Proof. Let $\theta_1 \in [0, 2\pi]$. Then working from the inside out, we have

$$\begin{aligned}
\frac{27\cos\theta_1 - 5}{32} \in \left[-1, \frac{22}{32}\right] &\implies \arccos\left(\frac{27\cos\theta_1 - 5}{32}\right) \in [\arccos(22/32), \pi] \\
&\implies \frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right) \in [\arccos(22/32)/3, \pi/3] \\
&\implies \cos\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)\right) \in \left[1/2, \cos\left(\frac{1}{3}\arccos\frac{22}{32}\right)\right] \\
&\implies 8\cos\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)\right) - 1 \in \left[3, 8\cos\left(\frac{1}{3}\arccos\frac{22}{32}\right) - 1\right] \\
&\implies z_1(\theta_1) \in \left[1, \frac{8}{3}\cos\left(\frac{1}{3}\arccos\frac{22}{32}\right) - \frac{1}{3}\right].
\end{aligned}$$

Since z_1 has a lower bound of 1, z_1 must always give the maximum eigenvalue; if λ is any other eigenvalue of $\widehat{\Delta}(\theta_1, \pi)$, Propositions 2.6 and 2.7 imply that

$$\lambda \leq 1 \leq z_1(\theta).$$

A similar argument shows that $z_4(\theta_1) \leq -1$, which gives that z_4 is always the minimum eigenvalue. Since $z_2 \equiv 1$ is an upper bound of the inner eigenvalues, we have the ordering $z_1 \geq z_2 \equiv 1 \geq z_3 \geq z_4$. □

5.2 Steps 3 and 4: Evaluation and Discontinuity of $\frac{\partial z_1}{\partial \theta_1}$

Proof of Theorem 5.1. By Theorem 5.2 we have an explicit formula for $z_1(\theta_1, \pi)$, which we may differentiate as

$$\begin{aligned} \frac{d}{d\theta_1}\left(z_1(\theta_1,\pi)\right) &= \frac{d}{d\theta_1}\left(\frac{1}{3}\left(8\cos\left(-\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)\right) - 1\right)\right) \\ &= -\frac{8}{3}\sin\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)\right)\cdot\frac{-\sin\theta_1}{\sqrt{1-\left(\frac{27\cos\theta_1-5}{32}\right)^2}}\cdot\frac{27}{32}\cdot\frac{1}{3}. \end{aligned}$$

To simplify our task, we note that

$$\begin{aligned} \lim_{\theta_1\to\pi}\left[\frac{8}{3}\cdot\frac{27}{32}\cdot\frac{1}{3}\sin\left(\frac{1}{3}\arccos\left(\frac{27\cos\theta_1 - 5}{32}\right)\right)\right] &= \frac{3}{4}\sin\left(\frac{1}{3}\arccos\left(\frac{27\cos\pi - 5}{32}\right)\right) \\ &= \frac{3}{4}\sin\left(\frac{1}{3}\arccos(-1)\right) \\ &= \frac{3}{4}\sin\frac{\pi}{3} \\ &= \frac{3\sqrt{3}}{8}, \end{aligned} \tag{5.4}$$

(i.e., we have evaluated the clearly continuous portion of the derivative), and thus it is just left for us to show that the remaining term,

$$f(\theta_1) := \frac{\sin\theta_1}{\sqrt{1-\left(\frac{27\cos\theta_1-5}{32}\right)^2}}$$

is discontinuous at $\theta_1 = \pi$.

Define the norm of f, $N : [3\pi/4, 5\pi/4] \to \mathbb{R}$, by

$$N(\theta_1) = \begin{cases} |f(\theta_1)|, & \theta_1 \neq \pi; \\ \lim_{\theta_1\to\pi}|f(\theta_1)|, & \theta_1 = \pi; \end{cases}$$

$$= \begin{cases} \frac{|\sin\theta_1|}{\sqrt{1-\left(\frac{27\cos\theta_1-5}{32}\right)^2}}, & \theta_1 \neq \pi; \\ \lim_{\theta_1\to\pi} |f(\theta_1)|, & \theta_1 = \pi. \end{cases} \tag{5.5}$$

(Note here that the argument of the square root in (5.5) cannot be negative, and so we need not worry about taking its complex modulus. Also note that N is well defined at π since for $\theta_1 + \delta$, with $\delta > 0$ sufficiently small, the denominator of $N(\theta_1)$ is non-zero, and $N(\pi + \delta) = N(\pi - \delta)$, implying equivalence of the right- and left-hand limits at π.)

We first consider the left-hand limit. As $\theta_1 \to \pi^-$, $\sin\theta_1 > 0$, and thus $\lim_{\theta_1\to\pi^-} f(\theta_1) = \lim_{\theta_1\to\pi} N(\theta_1)$. Using l'Hôpital's rule and (5.5), we have that

$$\begin{aligned} N(\pi) &= \lim_{\theta_1\to\pi^-} \frac{\sin\theta_1}{\sqrt{1-\left(\frac{27\cos\theta_1-5}{32}\right)^2}} \\ &= \lim_{\theta_1\to\pi^-} \frac{\cos\theta_1}{\frac{1}{\sqrt{1-\left(\frac{27\cos\theta_1-5}{32}\right)^2}} \cdot \frac{27\cos\theta_1-5}{32} \cdot \frac{27\sin\theta_1}{32}} \\ &= \lim_{\theta_1\to\pi^-} \frac{\cos\theta_1}{\frac{N(\theta_1)}{|\sin\theta_1|} \cdot \frac{27\cos\theta_1-5}{32} \cdot \frac{27\sin\theta_1}{32}} \\ &= \lim_{\theta_1\to\pi^-} \frac{\cos\theta_1}{N(\theta_1) \cdot \frac{27\cos\theta_1-5}{32} \cdot \frac{27}{32}}, \end{aligned}$$

where this last step used $\sin\theta_1/|\sin\theta_1| = 1$ as $\theta_1 \to \pi^-$. We also observe here that $N(\pi) < \infty$; if not, this sequence of calculations would equate 0 and ∞. Continuing, we have

$$\begin{aligned} \lim_{\theta_1\to\pi^-} \frac{\cos\theta_1}{N(\theta_1) \cdot \frac{27\cos\theta_1-5}{32} \cdot \frac{27}{32}} &= \frac{\cos\pi}{N(\pi) \cdot \frac{27\cos\pi-5}{32} \cdot \frac{27}{32}} \\ &= \frac{-1}{N(\pi)(-1)(\frac{27}{32})} \\ &= \frac{32}{27N(\pi)}. \end{aligned}$$

Therefore, $N(\pi) = \frac{32}{27N(\pi)}$, which implies that $N(\pi) = \sqrt{32/27}$. (Recall $N(\pi) \geq 0$.) Hence, we have that

$$\lim_{\theta_1\to\pi^-} f(\theta) = N(\pi) = \frac{\sqrt{32}}{\sqrt{27}}. \tag{5.6}$$

We now consider the right-hand limit, and note that this limit calculation is identical to that of the left-hand limit, save that when $\theta_1 \to \pi^+$, $\sin\theta_1/|\sin\theta_1| = -1$. Therefore,

$$\lim_{\theta_1 \to \pi^+} f(\theta) = -\frac{\sqrt{32}}{\sqrt{27}}. \tag{5.7}$$

Readdressing our original limit, we see that by (5.4), (5.6), and (5.7),

$$\lim_{\theta_1 \to \pi^-} \frac{dz_1}{d\theta_1} = \frac{3\sqrt{3}}{8} \cdot \frac{\sqrt{32}}{\sqrt{27}} = \frac{\sqrt{2}}{2},$$

while

$$\lim_{\theta_1 \to \pi^+} \frac{dz_1}{d\theta_1} = \frac{3\sqrt{3}}{8} \cdot \frac{-\sqrt{32}}{\sqrt{27}} = -\frac{\sqrt{2}}{2}.$$

Therefore $z_1(\boldsymbol{\theta})$ is non-differentiable at $\boldsymbol{\pi}$. □

5.3 Corollaries and Implications

We now include a few corollaries that follow immediately from Theorem 5.1 and generalize where singularities of the spectrum occur; it might be helpful to refer back to Figures 2.2 and 2.1, as well as refer forward to Figure 5.3.

Corollary 5.4. *$z_1(\boldsymbol{\theta})$ is not differentiable at $\boldsymbol{\theta} = 2\pi\boldsymbol{n} + \boldsymbol{\pi}$ for $\boldsymbol{n} \in \mathbb{Z}^2$.*

Proof. This follows from the $2\boldsymbol{\pi}$ periodicity of $\widehat{\Delta}(\boldsymbol{\theta})$. □

Corollary 5.5. *$z_4(\boldsymbol{\theta})$ is not differentiable at $\boldsymbol{\theta} = 2\pi\boldsymbol{n}$ for $\boldsymbol{n} \in \mathbb{Z}^2$.*

Proof. This follows from Corollary 5.4 and the unitary equivalence relation between $\widehat{\Delta}$ and $-\widehat{\Delta}$ given in Proposition 2.5. □

Note: This singularity in z_4 does not appear when $\theta_2 = \pi$; that is, the formula for $z_4(\boldsymbol{\theta})$ given in Theorem 5.2 does not have a singularity at $\theta_1 = 0$. Thus, this singularity does not appear in the left-hand plot of Figure 5.3. If we view the spectrum on the $\theta_2 = 0$ cross section, as in the right-hand plot of Figure 5.3, we can see the singularity.

Remark 5.6. The similarity in structure of the formula of z_3 to that of z_1 warrants the presumption that z_3 is not differentiable at $\boldsymbol{\pi} + \pi\boldsymbol{n}$. We did not pursue this result directly, but suspect that a proof analogous to the proof of Theorem 5.1 can be successfully applied here. By the unitary equivalence between $\widehat{\Delta}$ and $-\widehat{\Delta}$, this result would imply an analog of Theorem 5.5 for z_2.

Remark 5.7. Even though we have shown that $z_1(\boldsymbol{\theta})$ is not differentiable at $\boldsymbol{\pi}$, we would need to show that z_1 is not differentiable in every direction (i.e., not just in the direction of θ_1) to show that the singularity is conical, that is, that $\boldsymbol{\theta} = \boldsymbol{\pi}$ is a *Dirac point*. It appears

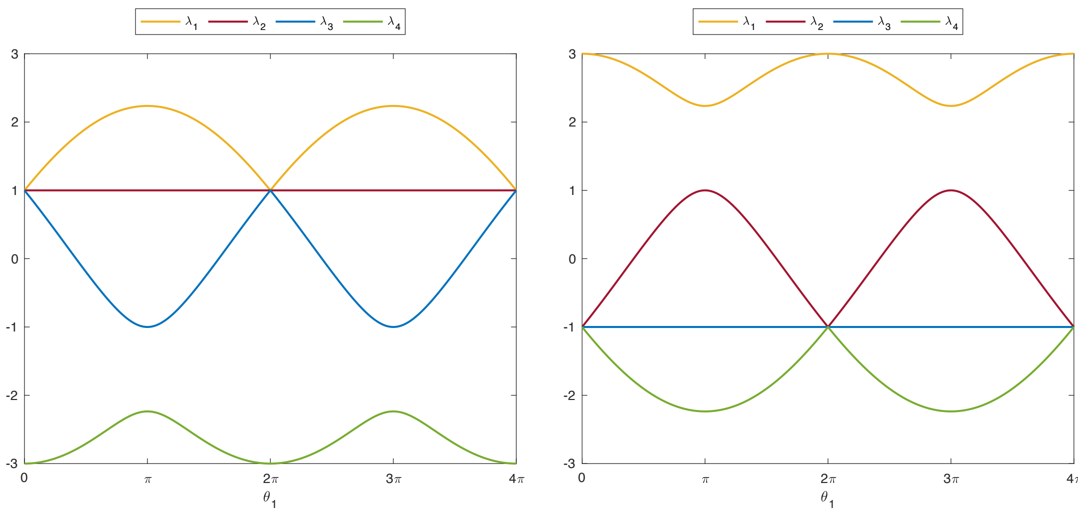

Figure 5.3: *Left*: $\sigma(\widehat{\Delta}(\theta_1, \pi))$; *Right*: $\sigma(\widehat{\Delta}(\theta_1, 0))$.

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that $\boldsymbol{\pi}$ is a Dirac point by inspection of Figure 2.1, but of course more work needs to be done to investigate this result further. This result would be of interest to the physics community, as Dirac points have exciting properties from the point of view of electronic transport. In particular, electrons with energies near the Dirac point can behave as if they are massless [8].

Chapter 6

Future Directions

We have been able to make several large steps towards a result regarding the spectra of Schrödinger operators for a (p, p)-periodic potential on an octagonal lattice. Most notably, we have shown where gaps of the spectrum can open for sufficiently small $(1, 1)$-periodic potentials, and have exhibited that a third gap can open for a sufficiently small $(2, 2)$-periodic potential. Furthermore, we have been able to find singularities in the dispersion relation of the Laplacian on Γ_f^1. We now pose what we believe to be the logical next steps for this study.

6.1 Bethe-Sommerfeld Conjecture for the Octagonal Lattice

We do not include any formal proofs in this section, but postulate our expectations for the spectrum of H_Q on a general fundamental domain Γ_f^p by extrapolation from our own work and the literature.

Conjecture 6.1. *Let Q be (p, p)-periodic with sufficiently small norm.*

a) If p is odd, then the spectrum of $\widehat{H}_Q$ has at most two gaps, which may only open at eigenvalues ± 1.

b) If p is even, then the spectrum of $\widehat{H}_Q$ has at most three gaps, which may only open at eigenvalues ± 1 and 0.

This conjecture is very much in the spirit of Theorem 1.1 of [1] (Embree-Fillman) and Theorem 1.1 of [3] (Han-Jitomirskaya), which are both discrete analogs of the Bethe-Sommerfeld conjecture on $\ell^2(\mathbb{Z}^d)$, $d \geq 2$. To explore how the behavior described in these theorems would or would not manifest on the octagonal lattice, we created a code that plots the j^{th} spectral band of $\widehat{\Delta}$ as a function of j. Figure 6.1 shows the results for $3 \leq p \leq 10$.

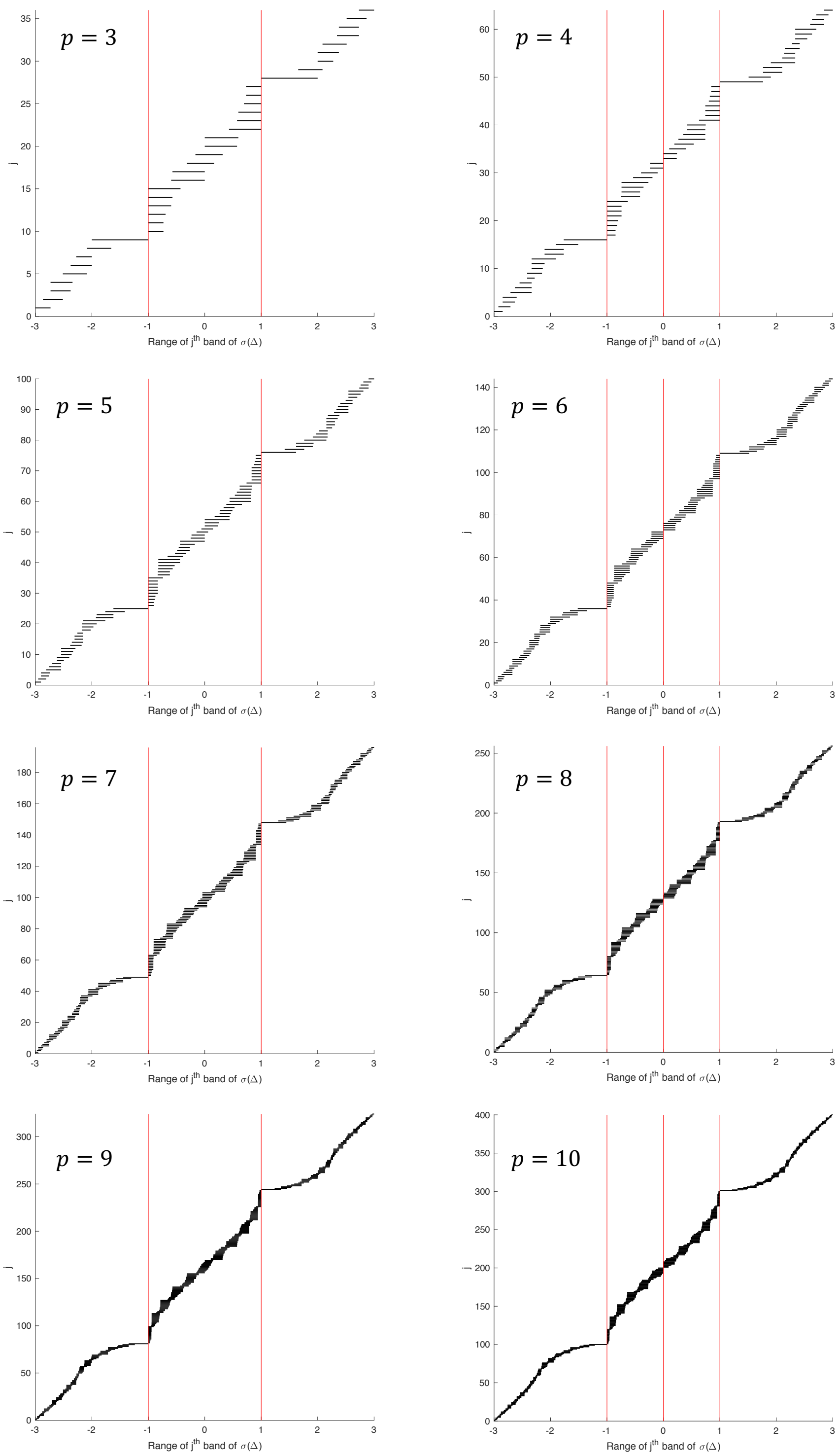

Figure 6.1: Spectral bands of $\widehat{\Delta}(\boldsymbol{\theta})$ for $3 \leq p \leq 10$

We notice numerically that for all p, odd or even, $B_{p^2} \cap B_{p^2+1} = \{-1\}$ and $B_{3p^2} \cap B_{3p^2+1} = \{1\}$. (See the locations of the outer red vertical lines in Figure 6.1.) This is what initially led us to believe that a potential $\widehat{Q}$ could be engineered in such a way that the addition of $\widehat{Q}$ to $\widehat{\Delta}$ would perturb these two bands apart in the resulting spectrum. We demonstrated this in previous chapters for both $p = 1$ and $p = 2$.

The same behavior can be observed for B_{2p^2} and B_{2p^2+1} when p is even; the intersection of these particular bands is the single point 0, and thus we anticipate that gaps can be opened here (as we showed for $p = 2$).

However, when p is odd, the middle two bands ($j = 2p^2$ and $j = 2p^2 + 1$), have intersection which is an interval with positive length. Since for any sufficiently small perturbation of $\widehat{\Delta}$ (in this case the addition of a potential $\widehat{Q}$ of norm ϵ), the spectral bands will likewise perturb minimally, we could choose ϵ so small that B_{2p^2} and B_{2p^2+1} still overlap, and thus a gap cannot be opened. This "overlapping" phenomena would appear to occur for all other pairs of consecutive bands, and which is why the conjecture requires that gaps cannot open at other values of the spectrum, regardless of the parity of p.

6.2 The Dispersion Relation of $\widehat{\Delta}$

We were able to show that the dispersion relation of $\widehat{\Delta}$ on Γ_f^1 has singularities, but, as we mentioned at the close of Chapter 5, the next step would be to show that these singularities are Dirac points, that is, that the singularities are conical. We include a few ideas for such a proof:

- Formulate the largest eigenvalue z_1 of $\widehat{\Delta}(\theta_1, \theta_2 \tan s)$, where $0 \leq s < \pi/2$, and try to apply a similar technique to that given in the proof of Theorem 5.1.
- Experiment with changes of variables $u(\boldsymbol{\theta})$ in order to simplify the formulation and differentiation of z_1. Proceed using a similar technique to that given in the proof of Theorem 5.1, or, in a neighborhood of $\boldsymbol{\theta} = \boldsymbol{\pi}$, produce a continuous mapping from z_1 to a cone.

Additionally, we did not attempt any analysis of dispersion relations of the Laplacian for higher period fundamental domains. It would be nice to be able to generalize locations of singularities of the dispersion relation of $\widehat{\Delta}$ on Γ_f^p, either dependently or independently of p.

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