Schrödinger Operators with Lattice Invariant Potentials

Curtiss Lyman

A dissertation
submitted in partial fulfillment of the
requirements for the degree of

Doctor of Philosophy

University of Washington

2025

Reading Committee:

Alexis Drouot, Chair

Stefan Steinerberger

Bobby Wilson

Robin Graham

Program Authorized to Offer Degree:

Mathematics

University of Washington

Abstract

Schrödinger Operators with Lattice Invariant Potentials

Curtiss Lyman

Chair of the Supervisory Committee:
Professor Alexis Drouot
Mathematics

We develop a systematic framework to study the dispersion surfaces of Schrödinger operators $H = -\Delta + V$, where the potential $V \in C^\infty(\mathbb{R}^n, \mathbb{R})$ is both periodic with respect to a lattice $\Lambda \subset \mathbb{R}^n$ and respects its symmetries. Our analysis relies on an abstract result, previously proven by Franz Rellich [Rel40] and which we prove using an alternative approach inspired by methods developed by Tosio Kato [Kat95]: if a self-adjoint operator depends analytically on a parameter, then so do its eigenvalues and eigenprojectors in a neighborhood of the real line. Using this and techniques from Floquet-Bloch theory and representation theory, we prove a series of results that can be used to analyze the operator H where the lattice Λ is arbitrary. As an application of this framework, we describe the generic structure of some singularities in the band spectrum of Schrödinger operators invariant under various two- and three-dimensional lattices. Specifically, we study the square, hexagonal, rectangular, simple cubic, body-centered cubic, face-centered cubic, and stacked hexagonal lattices, in the process reproducing results due to [Kel+18] and [FW12], and also proving a conjecture of [GZZ22].

TABLE OF CONTENTS

Page

LIST OF FIGURES

Figure Number | Page

LIST OF TABLES

Table Number | Page

NOTATION

- $H = -\Delta + V$
- For $z \in \mathbb{C}$, $H_z = -\Delta + zV$
- $\mathbb{B}_\varepsilon(z_0) = \{z \in \mathbb{C} \ : \ |z - z_0| < \varepsilon\}$
- $\mathbb{P}_\varepsilon(z_0) = \mathbb{B}_\varepsilon(z_0) \setminus \{z' \ : \ \Re(z') = z_0, \Im(z') \geq 0\}$
- For $v_1, \ldots, v_n \in \mathbb{R}^n$, $\Lambda = \oplus_{j=1}^n \mathbb{Z} v_j$
- $\Lambda^* = \oplus_{j=1}^n \mathbb{Z} k_j$, where $k_1, \ldots, k_n$ satisfy $k_j \cdot v_\ell = 2\pi\delta_{j\ell}$
- $\Omega = \left\{ \sum_{j=1}^n \theta_j v_j \ \middle| \ \theta_j \in [0,1], \ j = 1, \ldots, n \right\}$
- $\mathcal{B} = \left\{ k \in \mathbb{R}^n \ \middle| \ : ||k|| \leq ||k - k'|| \ \forall k' \in \Lambda^* \right\}$
- $V(\mathcal{B})$ is the set of vertices of $\mathcal{B}$
- For $k \in \mathbb{R}^n$, $L^2_k = \{f \in L^2_{\text{loc}}(\mathbb{R}^n) \ : \ f(x + v) = e^{ik \cdot v} f(x) \ \forall v \in \Lambda\}$
- For $k \in \mathbb{R}^n$ and $s \in \mathbb{N}$, $H^s_k = \{f \in L^2_k \ : \ \partial^\alpha f \in L^2_k \ \forall |\alpha| \leq s\}$
- $\mathcal{S}(\mathbb{R}^n) = \{f \in C^\infty(\mathbb{R}^n) \ : \ \forall \alpha, \beta \in \mathbb{N}^n, \sup_{x \in \mathbb{R}^n} |x^\alpha \partial_\beta f(x)| < \infty\}$
- $\langle f, g \rangle_{L^2_k} = \frac{1}{|\Omega|} \int_\Omega \overline{f(x)} g(x) dx$
- For $m \in \mathbb{Z}^n$ and $k_1, \ldots, k_n \in \mathbb{R}^n$, $mk := \sum_{j=1}^n m_j k_j$
- For $k \in \mathbb{R}^n$, $[k] = \{k' \in k + \Lambda^* \ : \ ||k'|| = ||k||\}$

ACKNOWLEDGMENTS

First, I would like to express my gratitude to my advisor Alexis Drouot. His expertise, advice, and support were invaluable during my time here, and I will forever appreciate him taking me on as his first advisee. I also would never have reached this point without the support of numerous other professors, colleagues, and friends in the University of Washington's math department. I especially would like to thank Julia Pevtsova, Robin Graham, Stefan Steinerberger, Bobby Wilson, Monty McGovern, Andy Loveless, Max Lieblich, Jack Lee, James Zhang, Cody Tipton, and Sarah Garner (who I suspect is not told thank you nearly enough!). Having started my career with a Bachelor's in Psychology, I am also indebted to the math department at Western Washington University for taking a chance and accepting me into their Master's program. In particular, the mentorship of Professors Stephen McDowall, Richard Gardner, Edoh Amiran, Amites Sarkar, and David Hartenstine, along with the support of my cohort including Riley Abel, Chris Murphy, Krista Steuben, Lindsay Skinner, Dania Morales, Evan Gates, Josh Hansen, Garrett Nelson, Seth Greendale, Dan Baron, and Eun Hee Kim, were pivotal in helping me find my passion for mathematics and teaching. Looking to the future, I am also grateful for the guidance of Michael Weinstein from Columbia University as I went through the job application process, and am beyond excited to be joining him in the Applied Physics and Applied Mathematics Department at Columbia. In addition, I am thankful for the support of the National Science Foundation DMS-2054589, which partially funded this dissertation.

As much as I truly love mathematics, I could not have finished this dissertation if my entire life revolved around it. Thus, I will be eternally grateful to my wonderful community outside of academia, who helped me get out of the house and enjoy everything else life has to offer. I want to give a special shout-out to the Famtrak group and my board-gaming friends, including Lauren Laxton, Tom Mitchell, Michael and Taylor Legore, Jenny Salatovka, Andrew Smart, Avery Hall, Matty Stepenski, Ali Aqel, Caroline Sprague, Berk Erkul, Jane Novotny, Isaac Westland, Natasha Bourgeois, Johnny Lee, Jon Moon, Erman Akbay, Jackie Lang, Chris Lacorte, Ronak Shah, Brooke Cheng, Alex Schokking, and Amy Edwards. I would also like to thank my parents, Heidi and Frank Lyman, who have supported and encouraged me through more years of school than any of us ever thought I would do, and always stepped in to help with rides, home-cooked meals, and watching my lovable but crazy dog Zelda. Last but not least, I want to thank my partner (soon to be spouse!) Gillian Raposo, who has stuck with me from start to finish – I could not have done this without you!

DEDICATION

To my parents,
Heidi and Frank Lyman,
and my partner,
Gillian Raposo.

Chapter 1

INTRODUCTION

Analyzing the behavior of waves in periodic structures is a central theme in condensed matter physics, electromagnetism, and photonics. This includes, for instance, the flow of electrons through a metal, i.e., electricity. In the context of quantum mechanics, these waves solve the *time-dependent Schrödinger equation*

$$i\partial_t \psi = (-\Delta + V)\psi, \qquad \text{where:} \tag{1.1}$$

- the potential V is periodic with respect to a lattice Λ;
- the function ψ is the wavefunction of the electron, so that $|\psi(t,x)|^2$ is the density of probability of finding the electron at position x, at time t.

Solutions of (1.1) can be written as superpositions of time-harmonic waves: functions of the form $e^{-i\mu t}\phi(x)$, where ϕ and μ solve the *time-independent Schrödinger equation*

$$\mu\phi = (-\Delta + V)\phi. \tag{1.2}$$

Since the potential V is periodic, the operator $-\Delta + V$ has absolutely continuous spectrum on L^2 [RS04, Theorem XIII.100]. The corresponding *generalized eigenstates* are themselves superpositions over $k \in \mathbb{R}^n$ of *Floquet-Bloch modes*: solutions $\phi(x;k)$ to

$$\begin{aligned} (-\Delta + V)\phi(x;k) &= \mu(k)\phi(x;k), \quad x \in \mathbb{R}^n, \\ \phi(x+v;k) &= e^{ik\cdot v}\phi(x;k), \quad v \in \Lambda. \end{aligned} \tag{1.3}$$

For each $k \in \mathbb{R}^n$, the problem (1.3) has a discrete set of solutions $\mu(k)$, which corresponds to the spectrum of $-\Delta + V$ on the space of quasiperiodic functions

$$L^2_k = \left\{ f \in L^2_{\text{loc}}(\mathbb{R}^n, \mathbb{C}) : \ f(x+v) = e^{ik\cdot v} f(x), \ v \in \Lambda \right\}.$$

The primary focus of this work will be on the eigenvalue problem (1.3), and specifically the maps $k \mapsto \mu(k)$ – which are called *dispersion surfaces* – as their local properties control the effective dynamics of wavepackets [AP05]. The set $\cup_k \mu(k)$ will then be a union of intervals of $\mathbb{R}$, which is called the *band spectrum* of $-\Delta + V$. Singularities in the band spectrum (i.e., intersections of the dispersion surfaces) typically result in unusual behavior of waves (see Section 2.4 for examples).

The mathematical analysis of band spectrum singularities started with the seminal work of Fefferman-Weinstein [FW12], who proved genericity of Dirac points (see Definition 1.1) in honeycomb lattices. This has sparked various mathematical investigations of spectral degeneracies in other low-dimensional lattices, which all share a common strategy. First, they prove results for small values of the perturbation parameters using symmetry arguments. Second, they refer to [FW12] for details about extending their results to generic values of z using an analyticity argument, although the setup of each is technically different.

For instance, in two dimensions, [LWZ19; CW21] generalized the result of [FW12] to photonic operators, [Kel+18] showed that Schrödinger operators invariant under the Lieb lattice have quadratic degeneracies, and [CW24] studied the stability of these degeneracies and showed they split to tilted Dirac cones under parity-breaking perturbations. In three dimensions, [GZZ22] showed that Schrödinger operators with small potentials, periodic with respect to the body-centered cubic lattice and invariant under the octahedral group, present a three-fold Weyl point – see Definition 1.1 and Figure 1.1. In [GZZ22, §5.2], they *conjectured* that this extends to *large* potentials.

The general framework developed herein aims to exempt the above works from providing further details, by proving general results that can be applied regardless of the lattice in question – see Theorem 1.2 and Section 4.4. To demonstrate applications of this framework, we provide results on the band spectrum singularities of Schrödinger operators invariant under the square, hexagonal, rectangular, simple cubic, body-centered cubic, face-centered cubic, and stacked hexagonal lattices: Theorem 1.3. In so doing, we prove the conjecture of [GZZ22] and also reproduce results due to [Kel+18] and [FW12].

1.1 Main Results

The primary goal of this work is the development of a unified framework for the generic analysis of band spectrum singularities in lattice-invariant Schrödinger operators $H = -\Delta + V$. To find such singularities, our strategy will be to instead look at

$$H_z = -\Delta + zV \tag{1.4}$$

on L^2_k for varying $k \in \mathbb{R}^n$ and $z \in \mathbb{C}$. With this in mind, our first main result describes the behavior of eigenvalues and eigenprojectors of general families of analytic operators. More generally, this result applies to families of operators $T(z)$ for $z \in \mathbb{C}$ that satisfy the following two assumptions:

Assumption A1: *$\mathcal{H}$ is a Hilbert space, $\mathcal{D}$ is a dense subspace of $\mathcal{H}$, and $T(z), z \in \mathbb{C}$ is a family of closed operators on $\mathcal{H}$ with domain $\mathcal{D}$ such that:*

(i) $T(z)$ is analytic in z: $\forall f \in \mathcal{D}$, $g \in \mathcal{H}$, $z \mapsto \langle T(z)f, g\rangle$ is an analytic function on $\mathbb{C}$;

(ii) For each $z \in \mathbb{R}$, $T(z)$ is self-adjoint and has discrete spectrum;

(iii) There exists $C > 0$ such that $||T'(z)|| \leq C$ for all $z \in \mathbb{C}$.

Assumption A2: *$\mu : (a, b) \to \mathbb{R}$ is a continuous function on an open interval $(a, b) \subset \mathbb{R}$, such that for all $z \in (a, b)$, $\mu(z)$ is an eigenvalue of $T(z)$ of constant multiplicity m.*

Our first main result is then:

Theorem 1.1. *Let $T(z)$ satisfy A1 and let $\mu : (a, b) \to \mathbb{R}$ satisfy A2. There exist a discrete set $D \subset \mathbb{R}$ and an open connected neighborhood $U \subset \mathbb{C}$ of $\mathbb{R} \setminus D$ containing (a, b), such that μ extends to an analytic function on U and:*

- *$\mu(z)$ is an eigenvalue of $T(z)$ of multiplicity m for all $z \in U$;*
- *The eigenprojector $\pi(z)$ associated to $\mu(z)$ is analytic in $z \in U$.*

For transparency, after we proved the above theorem, it was brought to our attention that a similar and admittedly stronger result was proven by Franz Rellich [Rel40] using different methods from those presented herein. Specifically, Rellich showed that if $T(z)$ is a *holomorphic family of operators of type A* (as defined in [Kat95], and which includes all families of operators satisfying A1) that is self-adjoint for $z \in \mathbb{R}$ and has compact resolvent for some $z_0 \in \mathbb{C}$, then the eigenvalues and eigenvectors of $T(z)$ can be chosen to be analytic in a neighborhood of $\mathbb{R}$. From this, it is not difficult to show that the eigenvalues then have constant (algebraic) multiplicity away from a discrete set.

Inspired by this result, we use techniques developed by [Kat95] to give the following stronger version of 1.1, which in particular shows that the eigenvalue μ and corresponding eigenprojector π are in fact analytic at points $z_0 \in D \cap \mathbb{R}$.

Theorem 1.2. *Let $T(z)$ satisfy A1 and let $\mu : (a, b) \to \mathbb{R}$ satisfy A2. There exists an open connected neighborhood $U \subset \mathbb{C}$ of $\mathbb{R}$ containing (a, b) and a discrete set $D \subset \mathbb{R}$, such that μ extends to an analytic function on U and:*

- *$\mu(z)$ is an eigenvalue of $T(z)$ for all $z \in U$ and has multiplicity m for all $z \in U \setminus D$;*
- *The eigenprojector $\pi(z)$ associated to $\mu(z)$ is analytic on U.*

We then apply Theorems 1.1 and 1.2 to the analytic family H_z defined in (1.4). The most interesting case consists of potentials V that are invariant under the symmetries of the corresponding lattice (see Definition 4.2). This is because additional symmetries come with higher multiplicities of eigenvalues, which translate to singularities in the band spectrum and exotic behavior of waves. In Chapter 4 we use these theorems to prove a series of general results regarding lattice-invariant Schrödinger operators. As an application of this framework, we study band spectrum singularities for Schrödinger operators invariant under the square, hexagonal, rectangular, simple cubic, body-centered cubic, face-centered cubic, and stacked hexagonal lattices. To formulate our conclusions, we need the following definitions.

Definition 1.1. *Let $E \in \mathbb{R}, K \in \mathbb{R}^n$. We say that a Schrödinger operator H has:*

- *An m-fold quadratic point at (K, E) if E is a L^2_K-eigenvalue of H of multiplicity $m > 1$ and the Floquet-Bloch problem (1.3) has m solutions $\mu_1(k), \ldots, \mu_m(k)$:*

$$\mu_j(K+\kappa) = E + \mathcal{O}(||\kappa||^2), \quad j = 1, \ldots, m, \quad \kappa \to 0.$$

- *A Dirac point at (K, E) if $n = 2$, E is a double L^2_K-eigenvalue of H, and there exists some $\alpha \neq 0 \in \mathbb{R}$ such that the Floquet-Bloch problem (1.3) has 2 solutions $\mu_+(k), \mu_-(k)$:*

$$\mu_\pm(K+\kappa) = E \pm \alpha||\kappa|| + \mathcal{O}(||\kappa||^2), \quad \kappa \to 0.$$

- *A (two-fold) basin point at (K, E) if $n = 3$, E is a double L^2_K-eigenvalue of H, and there exists some $v \neq 0 \in \mathbb{R}^3$ such that for κ satisfying $v \cdot \kappa \neq 0$, the Floquet-Bloch problem (1.3) has 2 solutions $\mu_+(k), \mu_-(k)$:*

$$\mu_\pm(K+\kappa) = E \pm |v \cdot \kappa| + \mathcal{O}(||\kappa||^2), \quad \kappa \to 0.$$

- *A (two-fold) valley point at (K, E) if $n = 3$, E is a double L^2_K-eigenvalue of H, and there exists some diagonal, rank two matrix D such that for κ satisfying $D\kappa \neq 0$, the Floquet-Bloch problem (1.3) has 2 solutions $\mu_+(k), \mu_-(k)$:*

$$\mu_\pm(K+\kappa) = E \pm ||D\kappa|| + \mathcal{O}(||\kappa||^2), \quad \kappa \to 0.$$

- *A Weyl point at (K, E) if $n = 3$, E is a double L^2_K-eigenvalue of H, and there exists some $\alpha \neq 0 \in \mathbb{R}$ such that the Floquet-Bloch problem (1.3) has 2 solutions $\mu_+(k), \mu_-(k)$:*

$$\mu_\pm(K+\kappa) = E \pm \alpha||\kappa|| + \mathcal{O}(||\kappa||^2), \quad \kappa \to 0.$$

- *A three-fold Weyl point at (K, E) if $n = 3$, E is a triple L^2_K-eigenvalue of H, and there exists some $\alpha \neq 0 \in \mathbb{C}$ such that the Floquet-Bloch problem (1.3) has 3 solutions $\mu_1(k), \mu_2(k), \mu_3(k)$:*

$$\mu_j(K+\kappa) = E + \lambda_{\alpha,j}(\kappa) + \mathcal{O}(||\kappa||^2), \quad j = 1, 2, 3, \quad \kappa \to 0,$$

  where $\lambda_{\alpha,j}(\kappa)$ are the three roots of the polynomial $\lambda^3 - 4|\alpha|^2||\kappa||^2\lambda + 16\,\mathrm{Im}(\alpha^3)\kappa_1\kappa_2\kappa_3$.

See Figure 1.1 for examples of a basin point and three-fold Weyl point. Our second main result then demonstrates the existence of these exotic points in the band spectra of Schrödinger operators with potentials V periodic with respect to and sharing the same symmetries as the following lattices.

Theorem 1.3. *Let Λ be a square, hexagonal, simple cubic, body-centered cubic, face-centered cubic, or stacked hexagonal lattice, and let G be its point group. Then for generic potentials V periodic with respect to Λ and invariant under G, and generic values of $z \in \mathbb{R}$, the band spectrum of $H_z = -\Delta + zV$ has at least:*

(i) one two-fold quadratic point if Λ is the square lattice;

(ii) one Dirac point if Λ is the hexagonal lattice;

(iii) two three-fold quadratic points if Λ is the simple cubic lattice;

(iv) one three-fold Weyl point as well as one two-fold and one three-fold quadratic point if Λ is the body-centered cubic lattice;

(v) one basin point if Λ is the face-centered cubic lattice;

(vi) one valley point if Λ is the stacked hexagonal lattice.

In Theorem 1.3, "generic potentials $V \in C^\infty(\mathbb{R}^n, \mathbb{R})$" means all of $C^\infty(\mathbb{R}^n, \mathbb{R})$ but a finite union of hyperplanes, and "generic values of $z \in \mathbb{R}$" means all of $\mathbb{R}$ away from a discrete set. In particular, Theorem 1.3 (i) and (ii) reproduce results due to [Kel+18] and [FW14], respectively, and (iv) proves the conjecture formulated in [GZZ22, §5.2].

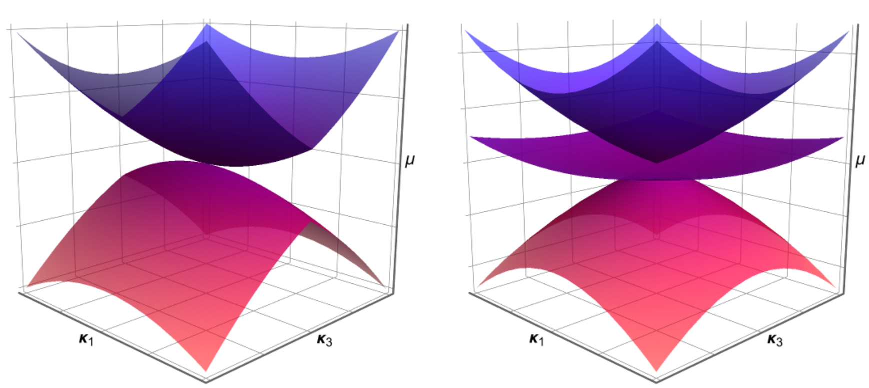


Figure 1.1: Cross sections of a Basin point (left) and a three-fold Weyl point (right).

1.2 Organization

This work is roughly split into three parts. The first part discusses analytic families of operators, and culminates with a proof of Theorem 1.2. The second part then formulates a general framework for analyzing Schrödinger operators with lattice-invariant potentials, and is the primary focus of this work. The last part applies this framework to various lattices, leading us to Theorem 1.3. With this in mind, the main chapters are organized as follows.

In Chapter 2, we review the relevant theory we will need to prove our main results. In particular, in Section 2.1 we discuss lattice theory, the focus of which will be the definition and classification of *Bravais lattices* – Definition 2.2 and Theorem 2.1 – which provides us with a finite list of lattices that need to be considered. We give an explicit proof of this classification in two dimensions, the primary tool for which will be the crystallographic restriction theorem (Theorem 2.2). We also discuss the *Brillouin zone* $\mathcal{B}$, and prove a result which will later imply that the vertices of $\mathcal{B}$ have a high degree of symmetry (Proposition 2.1). In Section 2.2, we discuss Floquet-Bloch theory following [RS04], and show that one can recover the spectral theory of H on L^2 from the spectral theory of H on L^2_k for $k \in \mathcal{B}$, thus motivating our analysis of the eigenvalue problem (1.3). We then discuss representation theory in Section 2.3, and provide a proof from [DF03] of Maschke's theorem (Theorem 2.5) and some of its consequences, which will enable us to further reduce the problem (1.3) to the invariant subspaces of an appropriately chosen group representation. In addition, we briefly discuss *corepresentations*, which we suspect will help us further develop our general framework and is the focus of one of our current projects. Finally, in Section 2.4 we give explicit examples of how dispersion surfaces can control the effective dynamics of wavepackets, thus providing some additional motivation for our analysis.

In Chapter 3, we discuss families of operators satisfying A1. We start with a finite-dimensional analogue of Theorem 1.2, and show that analytic families of matrices can be analytically diagonalized in a neighborhood of the real line – see section 3.1 and Theorem 3.4. To prove this result, we look at the characteristic polynomial of this family and use the fact that polynomials depending analytically on a parameter admit an analytic factorization when the parameter is away from a discrete set – Theorem 3.1, which we prove in Section 3.2. To extend the finite-dimensional case to the general case, we require several additional results from the theory of variation of eigenvalues, which we present in Section 3.3. Lastly, in Section 3.4, we prove our first two main results: Theorems 1.1 and 1.2.

In Chapter 4 we then develop our general framework for lattice-invariant Schrödinger operators, inspired by the work of Fefferman-Weinstein [FW12]. We first give an explicit diagonalization of $H_0 = -\Delta$ in Section 4.1, and then define lattice-invariant potentials in Section 4.2 – see Definition 4.2. A consequence of this definition is that when the potential V is lattice-invariant, the Schrödinger operator H_z will commute with representations of subgroups of the symmetry group G. This enables us to further reduce the Floquet-Bloch problem (1.3) to the invariant subspaces of these representations in Section 4.3. In Section 4.4 we then present a series of key lemmas, Lemmas 4.2 – 4.6, which form the core of our general framework. We conclude this chapter by proving these lemmas in Section 4.5.

Chapters 5 and 6 are then dedicated to proving Theorem 1.3 for the listed two- and three-dimensional lattices, respectively. The proof of this theorem follows the framework established in Chapter 4, and consists of analogous steps for each of the lattices under consideration. First, we describe the multiplicities of L^2_K-eigenvalues of H_z for fixed $K \in \mathcal{B}$ and for small values of z using a perturbative argument justified by Lemma 4.3, together with a representation-theoretic argument that relies on the specific symmetries of V. We will focus on eigenvalues that have multiplicities higher than one, as they correspond to intersections of dispersion surfaces at K, hence to band spectrum singularities near K. Due to Theorem 1.2, these multiplicities will in fact be constant for generic values of z, and the corresponding eigenvalues and eigenprojectors will be analytic in a neighborhood of the real line. We finish by studying the dispersion surfaces $\mu(k)$ in the vicinity of K, i.e. the $L^2_{K+\kappa}$-eigenvalues of H_z for κ small. This again relies on a perturbative procedure, this time with respect to κ. In particular, Lemmas 4.4 and 4.6 enable us to produce effective equations for these dispersion surfaces, as in Definition 1.1. The coefficients of these effective equations will depend on the eigenprojector $\pi(z)$, and consequently will be nonzero away from a discrete set – Lemma 4.5. The corresponding band spectrum singularities will therefore persist for generic values of z.

1.3 Future Projects

The investigation of Dirac cones in honeycomb structures [FW12] sparked a multitude of mathematical works beside band spectrum singularities: behavior of wavepackets [FW14], tight-binding analysis [FLW18], emergence of edge states [FLW16; Dro19a; DW20], propagation of edge states in Dirac systems [Bal+23; BBD24; Dro22; Bal24; HXZ23], computation of topological invariants [Dro19b; AK24] and Dirac cones in other setups [BC18; Amm+20; LLZ23]. The framework developed in Chapter 4, along with Theorems 1.2 and 1.3, provides a foundation upon which one can now produce similar results for other lattices and their corresponding band spectrum singularities. We conclude this chapter by describing four potential projects that build upon this work.

Project 1: Weyl Points. The three-dimensional analogue of Dirac cones are Weyl points. We believe they are the only stable type of spectral degeneracies in three dimensions – see [Dro21] for an analysis on discrete models. But to the best of our knowledge, one has yet to produce a Schrödinger operator with Weyl points. We plan to use the current paper as a stepping stone. Since band spectrum singularities other than Weyl points are believed to be unstable, they should generically split into Weyl points under perturbations. So adding e.g. a parity-breaking term to the Schrödinger operators discussed in Theorem 1.3 should produce Weyl points. This belief is reinforced by a two-dimensional analysis of Chaban-Weinstein [CW24], who demonstrated that the quadratic degeneracies of Schrodinger operators invariant under square lattices become Dirac cones after adding an odd potential. Constructing Schrödinger operators with Weyl points has the potential to spark a number of mathematical investigations, such as wavepacket analysis [FW14], study of surface states (the 3D analogues of edge states), and computation of topological invariants [FMP16].

Project 2: Wavepacket Analysis. In [FW14], Fefferman-Weinstein showed that Dirac cones give rise to Dirac-like propagation of wavepackets, thus explaining the relativistic behavior of electrons observed in graphene. Grégoire Allaire and Andrey Piatnitski performed a similar wavepacket analysis in [AP05], showing that initial conditions *localized at a frequency* $\mu(K)$, where $\mu(k)$ has multiplicity one in a neighborhood of K, and initial conditions *localized at a spectral band gap edge* give rise to ballistic propagation and an effective mass Schrödinger evolution, respectively – see Section 2.4 for more details. The general framework developed herein, and specifically Theorem 1.3, demonstrates the existence of other types of band spectrum singularities besides Dirac cones, which in turn will induce other types of wavepacket behavior. In particular, this could lead to the construction of materials with unique electronic or conductive properties.

Project 3: Tight Binding Models. In [FLW18], the authors show that honeycomb Schrödinger operators converge, in an appropriate sense and in the tight binding limit, to the Wallace model. As an application, they obtain that the set of values of z for which an additional band comes to perturb a Dirac cone is *finite.* This complements Theorem 1.3, which shows that the set is discrete. It would be enlightening to perform a similar tight-binding analysis for the other lattices considered in Theorem 1.3, with the analogue of the Wallace model given by the graph Laplacian. Ideally, some form of general analysis could be formulated to determine if this set is always finite, regardless of the lattice in question.

Project 4: Corepresentation Theory. In [BC18], Gregory Berkolaiko and Andrew Comech observed that, since the potential V is typically assumed to be real, the relevant symmetries include both the symmetry group of the lattice and complex conjugation; consequently, the corresponding representations of the *point group* (the subgroup of the symmetry group which keeps the origin fixed) should include both unitary and antiunitary operators. Such representations have been fully classified by Eugene Wigner [Wig59], who called them *corepresentations* – see Section 2.4 and specifically Definition 2.4 and Theorem 2.7. In [BC18] they specifically apply this theory to honeycomb lattice potentials, but using the general framework established herein, one could apply this theory to other two- and three-dimensional lattices. In addition, since this general framework largely depends on representation theory, we suspect that the implementation of corepresentation theory could lead to an alternative or perhaps stronger formulation of some of the presented results.

Chapter 2

PRELIMINARY RESULTS AND MOTIVATION

The results presented herein build upon and combine techniques from various fields, including lattice theory, Floquet-Bloch theory, and representation theory. We therefore briefly introduce each of these fields in the following sections, listing some of the key definitions and results that we will need later. We finish this chapter with some motivation for our study of dispersion surfaces by giving explicit examples of wave dynamics that can occur.

2.1 Lattice Theory

Let us begin with a review of lattice theory.

Definition 2.1. *Given n linearly independent vectors $v_1, \dots, v_n \in \mathbb{R}^m$, the lattice generated by them is the set*

$$\Lambda(v_1, \dots, v_n) = \left\{ \sum_{j=1}^{n} m_j v_j \;\middle|\; m_j \in \mathbb{Z} \right\} = \bigoplus_{j=1}^{n} \mathbb{Z} v_j,$$

where we denote the lattice simply by Λ when the context is clear. In this context, we then say that $(v_1, \dots, v_n)$ is a basis for Λ, the rank of Λ is n, its dimension is m, its span is the linear space spanned by its vectors (i.e. $\operatorname{span}\Lambda = \operatorname{span}(v_1, \dots, v_n)$), and the lattice is said to be full-rank if $m = n$. The symmetry group of Λ is the group G of isometries on $\mathbb{R}^n$ which send Λ to itself. The fundamental period cell of Λ is the set

$$\Omega = \left\{ \sum_{j=1}^{n} \theta_j v_j \;:\; \theta_j \in [0,1],\ j = 1, \dots, n \right\}.$$

Assuming Λ is full-rank, the dual lattice to Λ (also often referred to as the reciprocal lattice) is defined to be

$$\Lambda^* = \left\{ \sum_{j=1}^{n} m_j k_j \;:\; m_j \in \mathbb{Z} \right\} = \bigoplus_{j=1}^{n} \mathbb{Z} k_j,$$

where $k_1, \dots, k_n$ satisfy the relation $k_j \cdot v_\ell = 2\pi\delta_{j\ell}$. The Brillouin zone is the set

$$\mathcal{B} = \left\{ k \in \mathbb{R}^n \;:\; ||k|| \leq ||k - k'|| \;\forall k' \in \Lambda^* \right\},$$

i.e. $\mathcal{B}$ *is the set of points in* $\mathbb{R}^n$ *closer to the origin than any other point of* Λ^**. Lastly, we say* $k \in \mathbb{R}^n$ *is a Voronoi vector if the (hyper)plane defined by the equation* $x \cdot k = \frac{1}{2}||k||^2$ *has a non-empty intersection with* $\mathcal{B}$*, and we say* k *is Voronoi relevant if this intersection is a (hyper)face of* $\mathcal{B}$*.*

Unless stated otherwise, we will always assume our lattices are full-rank. Later, we will see that the lattice's symmetry group plays a significant role in the spectrum of Schrödinger operators with periodic potentials. This naturally leads us to the notion of a Bravais lattice.

Definition 2.2. *A Bravais lattice is an equivalence class of lattices, where* $\Lambda \sim \Lambda'$ *if the symmetry groups of* Λ *and* Λ' *are isomorphic. Furthermore, the point group of a lattice is the subgroup of its symmetry group which keeps the origin fixed; we then say that* Λ, Λ' *belong to the same lattice system if their point groups are isomorphic.*

Note that an immediate consequence of the definition of a point group is that such a group consists of linear isometries, and thus can always be represented by a subgroup of the orthogonal group $O(n)$. Furthermore, the point group is always finite, as the following lemma demonstrates.

Lemma 2.1. *Let* $\Lambda \subset \mathbb{R}^n$ *be a lattice and let* G *denote its point group; then* $|G| < \infty$*.*

Proof. Let $(v_1, \dots, v_n)$ be a basis for Λ, and let $g \in G$. Then viewing g as a linear transformation on $\mathbb{R}^n$, g must send the basis $(v_1, \dots, v_n)$ to another basis of $\mathbb{R}^n$ consisting of vectors in Λ. However, if we let $C = \max_j ||v_j||$, then since g is an isometry we must have that $||gv_j|| = ||v_j|| \leq C$ for $j = 1, \dots, n$. As a result, $g \cdot \{v_1, \dots, v_n\} \subset \mathbb{B}_C(0) \cap \Lambda$, and since $\mathbb{B}_C(0) \cap \Lambda$ is necessarily finite, this implies there are only finitely many lattice vectors to which g can send each basis element. Since each g is determined by where it sends a basis, this tells us that there are only finitely many such g, so the group G must also be finite. □

Although Bravais lattices are technically defined in any dimension, the study of Bravais lattices typically focuses on lattices in two and three dimensions. In addition, these objects are well-understood and have been completely classified in dimensions up to four [Kit12; BBN78], as described in the following theorem.

Theorem 2.1. *In two dimensions, there are 5 Bravais lattices grouped into four lattice systems, which are listed in Table 2.1. Similarly, in three dimensions, there are 14 Bravais lattices grouped into seven lattice systems, which are listed in Table 2.2. In four dimensions, there are 64 Bravais lattices grouped into 33 lattice systems.*

The proof of this theorem relies on the following two results [Jr72]:

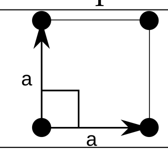
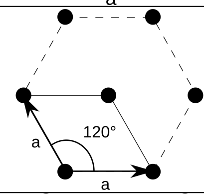
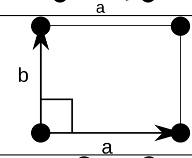
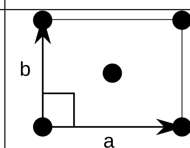
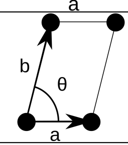
Lattice System	Point Group	List of Bravais Lattices	
		Simple	Centered
Square	D_4		–
Hexagonal	D_6		–
Rectangular	$\mathbb{Z}_2^2$		
Oblique	$\mathbb{Z}_2$		–

Table 2.1: Classification of two-dimensional Bravais lattices. Here D_n refers to the dihedral group of order $2n$, or equivalently the group of symmetries of an n-gon. The images of the unit cells are from [Wik25].

Theorem 2.2. (Crystallographic Restriction Theorem) *Let $\Lambda \subset \mathbb{R}^n$ be a lattice and let G denote its point group. If $r \in G$ is a non-trivial rotation, then r has order 2, 3, 4, or 6.*

Proof. Let $n = |r|$, i.e. the order of r, so that r is a rotation by $2\pi/n$, and let $v \in \Lambda$ such that $cv \notin \Lambda$ for any $|c| < 1$. Then since r is a symmetry of Λ, both $rv, r^{-1}v \in \Lambda$, and therefore $rv + r^{-1}v \in \Lambda$ as well. Moreover, $rv + r^{-1}v$ lies in the line spanned by v, and thus must satisfy $gv + g^{-1}v = mv$ for some $m \in \mathbb{Z}$. Since r is a rotation, and in particular an orthogonal transformation, $||rv|| = ||r^{-1}|| = ||v||$, and therefore

$$m||v|| = ||rv|| \cos \frac{2\pi}{n} + ||r^{-1}v|| \cos \frac{2\pi}{n} = 2||v|| \cos \frac{2\pi}{n}.$$

Since m must be an integer, it follows that $m \in \{-2, -1, 0, 1, 2\}$. Solving for n and using that r is assumed to be a non-trivial rotation (so that $n \neq 1$), we conclude that $n = 2, 3, 4$, or 6. □

Lemma 2.2. *Let G denote the point group of a lattice $\Lambda \subset \mathbb{R}^d$ for $d = 2$ (respectively 3). If there exists a rotation $r \in G$, $|r| > 2$, then G contains a reflection across a line through the origin (respectively a plane containing the axis of rotation).*

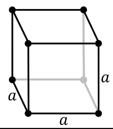
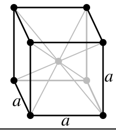
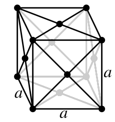
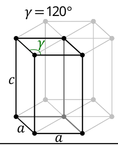
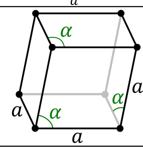
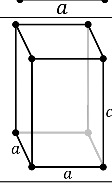
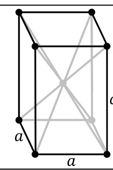
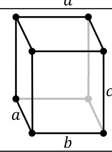
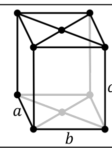
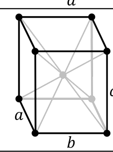
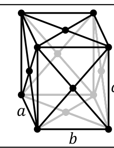
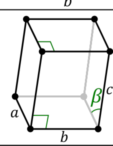
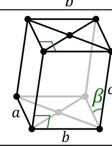
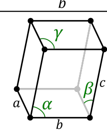
Lattice System	Point Group	List of Bravais Lattices			
		Simple	Base-Centered	Body-Centered	Face-Centered
Cubic	$S_4 \times \mathbb{Z}_2$		–		
Hexagonal	$D_6 \times \mathbb{Z}_2$		–	–	–
Rhombohedral	D_6		–	–	–
Tetragonal	$D_4 \times \mathbb{Z}_2$		–		–
Orthorhombic	$\mathbb{Z}_2^3$				
Monoclinic	$\mathbb{Z}_2^2$			–	–
Triclinic	$\mathbb{Z}_2$		–	–	–

Table 2.2: Classification of three-dimensional Bravais lattices. Here D_n again refers to the dihedral group of order $2n$, and S_n is the symmetric group of order $n!$. To distinguish the two- and three-dimensional hexagonal lattices from each other, we shall henceforth refer to the three-dimensional hexagonal lattice as the *stacked hexagonal lattice.* The images of the unit cells are from [Wik25].

Proof. We can treat the $d = 2, 3$ cases simultaneously by identifying $\mathbb{R}^2$ with the x_1x_2-plane in $\mathbb{R}^3$, in which case the x_3-axis becomes the axis of rotation for a rotation in $\mathbb{R}^2$, and any plane containing this axis restricts to a line through the origin in $\mathbb{R}^2$. Now let r be the given rotation, so that r is a rotation by $2\pi/n$ for $n > 2$, let L denote the corresponding axis of rotation, and let Q be the plane perpendicular to L passing through the origin. Then if $u \in \Lambda \setminus L$, it follows that $ru - u \in \Lambda \cap Q$, and so Q has nonzero lattice vectors.

Let v_1 be a nonzero vector of minimum length in $\Lambda \cap Q$, and let $v_2 = rv_1$; then $\Lambda \cap Q$ is a lattice of rank 2 with basis (v_1, v_2) (if (v_1, v_2) were not a basis, there would exist $u \in \Lambda \cap Q$ such that $u = c_1 v_1 + c_2 v_2$ for $0 < c_1, c_2 < 1$, which in turn implies there exists a vector $u' \in \Lambda \cap Q$ such that $||u'|| < ||v_1||$, a contradiction). We can then extend (v_1, v_2) to a basis (v_1, v_2, v_3) for Λ, where $v_3 \in \Lambda \setminus Q$. Consequently, we can write

$$v_3 = u + v,$$

where u, v are the projections of v_3 onto L and Q, respectively (and as such they are not necessarily lattice vectors).

From here, observe that since $rv_3 - v_3 \in \Lambda \cap Q$ and $ru = u$, there exist integers m_1, m_2 such that

$$rv - v = m_1 v_1 + m_2 v_2 = m_1 v_1 + m_2 r v_1. \tag{2.1}$$

Multiplying both sides by r^{-1} and subtracting from (2.1), we get

$$rv + r^{-1} v - 2v = m_2 r v_1 + m_1 r^{-1} v_1 + (m_1 - m_2) v_1. \tag{2.2}$$

However, the same trigonometry argument as in the proof of Theorem 2.2 yields that

$$rv + r^{-1} v = 2\cos(2\pi/n) v,$$
$$rv_1 + r^{-1} v_1 = 2\cos(2\pi/n) v_1.$$

Plugging these into (2.2) gives us

$$2(\cos(2\pi/n) - 1) v = (m_1 - m_2 - 2m_1 \cos(2\pi/n)) v_1 + (m_1 + m_2) v_2. \tag{2.3}$$

Now let f be the reflection across the plane containing L and perpendicular to v_1; then by construction $fv_1 = -v_1$, and thus to show that $f \in G$, it suffices to show that $fv_j \in \Lambda$ for $j = 2, 3$. Since we are assuming $n > 2$, together with Theorem 2.2 this implies we only need to consider the cases where $n = 3, 4$, and 6:

- if $n = 3$, then $fv_2 = v_2 + v_1$,
- if $n = 4$, then $fv_2 = v_2$,
- if $n = 6$, then $fv_2 = v_2 - v_1$.

Therefore, in all three cases, $fv_2 \in \Lambda$, as desired. To compute fv_3, we write $fv_2 = v_2 + mv_1$ for $m \in \{-1, 0, 1\}$ and plug this into (2.3) to get

$$\begin{aligned}
2(\cos(2\pi/n) - 1)fv &= (m_1 - m_2 - 2m_1\cos(2\pi/n))fv_1 + (m_1 + m_2)fv_2 \\
&= -(m_1 - m_2 - 2m_1\cos(2\pi/n))v_1 + (m_1 + m_2)(v_2 + mv_1) \\
&= \Big[(m_1 - m_2 - 2m_1\cos(2\pi/n))v_1 + (m_1 + m_2)v_2\Big] \\
&\quad - 2(m_1 - m_2 - 2m_1\cos(2\pi/n))v_1 + m(m_1 + m_2)v_1) \\
&= 2(\cos(2\pi/n) - 1)v \\
&\quad + \Big[(m+2)m_1 + (m+2)m_2 + 4m_1(\cos(2\pi/n) - 1)\Big]v_1.
\end{aligned}$$

Dividing both sides by $2(\cos(2\pi/n) - 1)$ gives us

$$fv = v + \left(\frac{(m+2)m_1 + (m+2)m_2}{2(\cos(2\pi/n) - 1)} + 2m_1\right)v_1. \tag{2.4}$$

Let $c(n, m)$ be the coefficient of v_1 in equation (2.4), so that $fv = v + c(n, m)v_1$. We now again consider the three cases $n = 3, 4$, and 6, and compute that

- if $n = 3$, then $m = 1$ and $c(3, 1) = \frac{3m_1 + 3m_2}{-3} + 2m_1 = m_1 - m_2$,
- if $n = 4$, then $m = 0$ and $c(4, 0) = \frac{2m_1 + 2m_2}{-2} + 2m_1 = m_1 - m_2$,
- if $n = 6$, then $m = -1$ and $c(6, -1) = \frac{m_1 + m_2}{-1} + 2m_1 = m_1 - m_2$.

Therefore, in all three cases

$$fv_3 = u + fv = u + v + (m_1 - m_2)v_1 = v_3 + (m_1 - m_2)v_1 \in \Lambda,$$

and so $f \in G$. □

Using Theorem 2.2 and Lemma 2.2, we now prove Theorem 2.1 for two-dimensional lattices.

Proof of Theorem 2.1 for two-dimensional lattices. Let $\Lambda \subset \mathbb{R}^2$ be a lattice, let G be its point group, and let $G_0 = \ker(\det)$, where we are viewing the determinant as a group homorphism from G to $\{\pm 1\}$. Then G_0 is a finite subgroup of $SO(2)$, and as such consists of rotations and is isomorphic to a cyclic group of finite order. Let r be a generator of G_0; then by the crystallographic restriction theorem (Theorem 2.2), r must have order $1, 2, 3, 4$, or 6. However, $|r| \geq 2$, for if $v \in \Lambda$, then by definition so too is $-v$, which implies $f := -I$, i.e. rotation by π, is contained in G_0. In addition, $|r| \neq 3$, for if it did, then $fr = -r$ is in G_0 as a product of elements in G_0 and has order 6, contradicting our assumption that r generates G_0. Therefore, the only possibilities are $|r| = 2, 4$, or 6.

Now let v_1 be a nonzero vector of minimal length a in Λ; then by Lemma 2.2 and its proof, if $r = 4$ or 6, G must contain the reflection f_1 across the line perpendicular to v_1. As a result, G_0 is a proper subgroup of G, and moreover, as a set, $G = G_0 \cup f_1 G_0$. It follows that if G contains a rotation of order 4 or 6, then $G \cong D_4$ or D_6, respectively. If on the other hand $|r| = 2$, then there are two possibilities: either $G_0 = G$, in which case $G \cong \mathbb{Z}_2$, or G_0 is a proper subgroup of G, in which case there exists some $f_2 \in G$ such that $|f_2| = 2$ and $\det f_2 = -1$, which implies $G_0 \cong \mathbb{Z}_2^2$. We address each of these four cases separately.

$G \cong \mathbb{Z}_2$: Extend v_1 to a basis (v_1, v_2) for Λ, and let θ denote the angle between them. By replacing v_2 with $v_2 + nv_1$ for some integer n, we may assume that $\theta \in (0, \pi/2]$. However, θ cannot equal $\pi/2$, for then v_1 and v_2 would be perpendicular, in which case f_1 (the reflection across the line perpendicular to v_1) would be contained in G, a contradiction. Therefore, we must have that $\theta \in (0, \pi/2)$. In addition, if $\theta = \pi/6$, then $||v_2|| \neq ||v_1||$, for otherwise G would contain a rotation of order 6. Similarly, $v_1 \cdot v_2/||v_j||^2 \neq \frac{1}{2}$ for $j = 1, 2$, for otherwise G would again contain a reflection. Letting $b = ||v_2||$, we see that Λ must be isometric to a lattice of the form shown in row 4 of Table 2.1, and so Λ is an oblique lattice.

$G \cong \mathbb{Z}_2^2$: Extend v_1 to a basis (v_1, v_2) for Λ, and let $f_1 \in G$ be a reflection (which exists since G is not isomorphic to a cyclic group). As previously noted, G must contain $f = -I$, and thus must also contain the reflection $f_2 := -f_1$. Note that the lines across which f_1, f_2 reflect, which we denote by L_1, L_2, respectively, are necessarily orthogonal: if $u_j \in L_j$ then $f_j u_j = u_j$ for $j = 1, 2$, and consequently

$$u_1 \cdot u_2 = u_1 \cdot f_2 u_2 = -f_1 u_1 \cdot u_2 = -(u_1 \cdot u_2),$$

which implies $u_1 \cdot u_2 = 0$.

We now consider two possibilities: either $L_1 \cup L_2$ contains (v_1, v_2) or it does not. In the first case, since v_1, v_2 are linearly independent, precisely one of these vectors lies in each of the lines L_1 and L_2. Since (v_1, v_2) is assumed to be a basis, this implies Λ must be isometric to a lattice of the form shown in row 3, column 1 of Table 2.1, and so Λ is a simple rectangular lattice.

On the other hand, if $L_1 \cup L_2$ does not contain (v_1, v_2), then there exists $v \in \Lambda$ such that $v \notin L_1 \cup L_2$. Since

$$f_1(v + f_1 v) = f_1 v + f_1^2 v = v + f_1 v,$$

this implies $v + f_1 v \in L_1$, and so $L_1 \cap \Lambda \neq \emptyset$. Replace v_1 with some minimal vector in $L_1 \cap \Lambda$ (where we still let $a = ||v_1||$), and extend to basis (v_1, v_2) by replacing v_2 if necessary. We can then write

$$v_2 = u_1 + u_2,$$

where $u_j \in L_j$, for $j = 1, 2$. In addition, both u_1, u_2 must be nonzero, for otherwise (v_1, v_2) would be a basis contained in $L_1 \cup L_2$, a contradiction. Since $v_2 + f_1 v_2 \in L_1 \cap \Lambda$, we deduce that

$$mv_1 = v_2 + f_1 v_2 = (u_1 + u_2) + (u_1 - u_2) = 2u_1$$

for some nonzero $m \in \mathbb{Z}$, so that

$$v_2 = \frac{m}{2} v_1 + u_2.$$

However, we can replace v_2 with $v_2 - m' v_1$ and (v_1, v_2) will still be a basis for Λ, so without loss of generality we may assume $0 < m/2 < 1$, which implies $m = 1$. If we then let $b = ||v_2||$, Λ must be isometric to a lattice of the form shown in row 3, column 2 of Table 2.1, and so Λ is a centered rectangular lattice.

$G \cong D_4$: Let $r \in G$ such that $|r| = 4$; then, as noted in the proof of Lemma 2.2, if we let $v_2 = rv_1$ it follows that (v_1, v_2) form a basis for Λ. Consequently, Λ must be isometric to a lattice of the form shown in row 1 of Table 2.1, and so Λ is a square lattice.

$G \cong D_6$: Let $r \in G$ such that $|r| = 6$; then if again let $v_2 = rv_1$, (v_1, v_2) form a basis for Λ. Consequently, Λ must be isometric to a lattice of the form shown in row 2 of Table 2.1, and so Λ is a hexagonal lattice. □

The proof of Theorem 2.1 for three and four-dimensional lattices uses similar techniques, but requires addressing significantly more cases, and thus we refer the interested reader to [Jr72] and [BBN78], respectively. In addition, we note that the classification of three-dimensional lattices by lattice system and centering type as in Table 2.2 is not necessarily unique, but merely helpful. For example, it can be shown that by choosing a different basis for the base-centered monoclinic lattice, it can also be described as a body-centered monoclinic lattice. For the rest of this paper, however, we shall refer to each lattice by the names given in Tables 2.1 and 2.2.

We finish this section with two results regarding the Brillouin zone $\mathcal{B}$, the first of which is due to Christoph Hunkenschröder, Gina Reuland, and Matthias Schymura (see [HRS20] for a proof).

Theorem 2.3. *Every lattice of rank at most 4 has a basis of Voronoi relevant vectors.*

Proposition 2.1. *Let $K \in \mathcal{B}$ and let m be the number of (hyper)faces of $\mathcal{B}$ which contain K. If $m > 0$, then there exist nonzero vectors $K_1, \ldots, K_m \in \Lambda^*$ such that $K - K_j$ also lies on m (hyper)faces of $\mathcal{B}$ and $||K - K_j||^2 = ||K||^2$ for $j = 1, \ldots, m$.*

Proof. Let $K \in \mathcal{B}$ such that K lies on m (hyper)faces of $\mathcal{B}$ for some $m > 0$. Denote these (hyper)faces by $F_1, \ldots, F_m$; then our assumption that $K \in F_j$ for $1 \leq j \leq m$ implies that there exists a vector K_j such that K lies on the (hyper)plane defined by $x \cdot K_j = \frac{1}{2}||K_j||^2$, which when intersected with $\mathcal{B}$ is precisely F_j. Then for $j = 1, \ldots, m$

$$\begin{aligned} ||K - K_j||^2 &= ||K||^2 - 2K \cdot K_j + ||K_j||^2 \\ &= ||K||^2 - ||K_j||^2 + ||K_j||^2 \\ &= ||K||^2. \end{aligned} \tag{2.5}$$

To prove that $K - K_j$ also lies on m (hyper)faces of $\mathcal{B}$, observe that since $K \in \mathcal{B}$, it follows that,

$$||K - K_j||^2 = ||K||^2 \leq ||(K - K_j) - K||^2, \quad \forall K \in \Lambda^*, \tag{2.6}$$

which implies $K - K_j \in \mathcal{B}$. Furthermore, we have that

$$(K - K_j) \cdot (-K_j) = -K \cdot K_j + ||K_j||^2 = -\frac{1}{2}||K_j||^2 - ||K_j||^2 = \frac{1}{2}||K_j||^2, \tag{2.7}$$

and for all $\ell \neq j$,

$$\begin{aligned} (K - K_j) \cdot (K_\ell - K_j) &= K \cdot K_\ell - K \cdot K_j - K_j \cdot K_\ell + ||K_j||^2 \\ &= \frac{1}{2}||K_\ell||^2 - \frac{1}{2}||K_j||^2 - K_j \cdot K_\ell + ||K_j||^2 \\ &= \frac{1}{2}\left(||K_\ell||^2 - 2K_j \cdot K_\ell + ||K_j||^2\right) \\ &= \frac{1}{2}||K_\ell - K_j||^2. \end{aligned} \tag{2.8}$$

Therefore $K - K_j$ lies on the m (hyper)planes defined by $x \cdot (-K_j) = \frac{1}{2}||K_j||^2$ and $x \cdot (K_j - K_\ell) = \frac{1}{2}||K_j - K_\ell||^2$ for $\ell \neq j$.

We now seek to show that each of these (hyper)planes defines a (hyper)face of $\mathcal{B}$. To start, for $j = 0, \ldots, m$ and $\ell = 1, \ldots, m$, let

$$P_{j\ell} = \begin{cases} \{x \in \mathbb{R}^n \ : \ x \cdot K_\ell = \frac{1}{2}||K_\ell||^2\} & j = 0 \\ \{x \in \mathbb{R}^n \ : \ -x \cdot K_j = \frac{1}{2}||K_j||^2\} & j \neq 0, \ell = j \\ \{x \in \mathbb{R}^n \ : \ x \cdot (K_\ell - K_j) = \frac{1}{2}||K_j - K_\ell||^2\} & j \neq 0, \ell \neq j, \end{cases}$$

and suppose $k' \in P_{0\ell} \cap \mathcal{B}$ for some ℓ. Then the same computations as in (2.5)-(2.6), but with K replaced with k', imply that $k' - K_j \in \mathcal{B}$ for $j = 1, \ldots, m$. Similarly, (2.7) with K replaced with k' implies $k' - K_j \in P_{jj}$, and (2.8) with K replaced with k implies $k' - K_j \in P_{j\ell}$ for $j \neq \ell, 0$. As a result, for $j = 1, \ldots, m$,

$$(P_{0\ell} \cap \mathcal{B}) - K_j = P_{j\ell} \cap \mathcal{B}.$$

By construction, $P_{0\ell} \cap \mathcal{B} = F_\ell$, and since $P_{j\ell} \cap \mathcal{B}$ is an isometric set and contained in the boundary of $\mathcal{B}$, it follows that $P_{j\ell} \cap \mathcal{B}$ is in fact a (hyper)face of $\mathcal{B}$ as well. Therefore, $K - K_j$ lies on m (hyper)faces of $\mathcal{B}$. □

2.2 *Floquet-Bloch Theory*

Let Λ be a lattice with fundamental period cell Ω and Brillouin zone $\mathcal{B}$. Using the structure of Λ, we can reduce the time-independent Schrödinger equation (1.1) to the Floquet-Bloch eigenvalue problem (1.3), which we make explicit in this section.

First, note that the space of locally square integrable functions, periodic with respect to Λ, is given by

$$L^2(\mathbb{R}^n/\Lambda) = \{f \in L^2_{\text{loc}} \,:\, f(x+v) = f(x)\ \forall v \in \Lambda\}.$$

More generally, recall that the space of k-quasiperiodic functions with respect to Λ is

$$L^2_{k,\Lambda} = \{f \in L^2_{\text{loc}}(\mathbb{R}^n) \,:\, f(x+v) = e^{ik\cdot v} f(x)\ \forall v \in \Lambda\}.$$

We shall suppress the dependence on the lattice Λ, and simply write L^2_k, when the choice of lattice is clear. In this context, we refer to k as the *quasi-momentum* of functions $f \in L^2_k$. It then follows that $L^2_0 = L^2(\mathbb{R}^n/\Lambda)$, and furthermore L^2_k and L^2_0 are isomorphic via the unitary map $F : L^2_k \to L^2_0$ given by $F(f) = e^{-ik\cdot x} f$. This isomorphism then induces an inner product on L^2_k given by

$$\langle f, g\rangle_{L^2_k} = \frac{1}{|\Omega|} \int_\Omega \overline{f(x)} g(x) dx.$$

We similarly define Sobolev spaces H^s_k, $s \in \mathbb{N}$ by

$$H^s_k = \{f \in L^2_k \,:\, \partial^\alpha f \in L^2_k\ \forall |\alpha| \le s\}.$$

We now consider the Schrödinger operator $H = -\Delta + V$, where V is smooth and periodic with respect to Λ. We can then write the Floquet-Bloch eigenvalue problem (1.3) at quasi-momentum $k \in \mathbb{R}^n$ as

$$\begin{aligned} H\phi(x;k) &= \mu(k)\phi(x;k), \quad x \in \mathbb{R}^n, \\ \phi(x+v;k) &= e^{ik\cdot v}\phi(x;k), \quad v \in \Lambda. \end{aligned}$$

The operator H is a self-adjoint unbounded operator on L^2_k (respectively L^2) with domain H^2_k (respectively H^2). By elliptic regularity, the operator $(H-i)^{-1}$ is a bijection from L^2_k to H^2_k, which when composed with the isomorphism F together with the compact injection of H^2_0 into $L^2(\Omega)$, implies that H has a compact resolvent. As a result, H has a discrete spectrum and the corresponding set of normalized eigenfunctions $\{\phi_b(x;k)\}_{b\ge 1}$ form a complete orthonormal basis in L^2_k [Hel13]. In addition, since the problem (1.3) is invariant under the change $k \mapsto k + k'$ for $k' \in \Lambda^*$, we can restrict our attention to k varying over the Brillouin zone $\mathcal{B}$ (See Definition 2.1).

The eigenvalue problem (1.3) has another formulation, which we shall not directly use, but provides some motivation for the framework developed in Chapter 4 and is commonly used in the literature. For $k \in \mathcal{B}$, let $\phi \in L^2_k$ be a Floquet-Bloch state, and set $p(x;k) = F\phi(x;k) = e^{-ik\cdot x}\phi(x;k)$. Then $p(x;k)$ satisfies the periodic boundary value problem:

$$\begin{aligned} H(k)p(x;k) &= \mu(k)p(x;k), \quad x \in \mathbb{R}^2, \\ p(x+v;k) &= p(x;k), \quad v \in \Lambda, \end{aligned} \tag{2.9}$$

where

$$H(k) := -(\nabla + ik)\cdot(\nabla + ik) + V(x). \tag{2.10}$$

An important consequence of this formulation is that, as an operator on L^2_k, $H = F^{-1}H(k)F$. As a result $\sigma_{L^2_k}(H) = \sigma_{L^2_0}(H(k))$, which together with (2.10) implies that the eigenvalues of H are continuous in k.

The reason the Floquet-Bloch problem (1.3) and its alternative formulation (2.9) are helpful is that they allow us to recover the spectral theory of H on $L^2(\mathbb{R}^n)$. To make this explicit we proceed in two steps, following the work of [RS04]: first, we construct an operator $\widetilde{H}$ such that $\sigma(\widetilde{H}) = \cup_{k\in\mathcal{B}}\, \sigma_{L^2_k}(H)$, and second, we construct a unitary operator U satisfying $H = U^{-1}\widetilde{H}U$, which implies $\sigma_{L^2(\mathbb{R}^n)}(H) = \cup_{k\in\mathcal{B}}\, \sigma_{L^2_k}(H)$ and which we use to show that the eigenfunctions $\{\phi_b(x;k)\}_{b\geq 1}$ are "complete" in $L^2(\mathbb{R}^n)$ in an appropriate sense (see Theorem 2.4).

Towards that end, we define a Hilbert space $\mathcal{H}$ by

$$\mathcal{H} = L^2(\mathcal{B}; L^2_k),$$

where we view $f \in \mathcal{H}$ as functions of $x \in \mathbb{R}^n$ parameterized by $k \in \mathcal{B}$, with an inner product given by

$$\langle f, g\rangle_{\mathcal{H}} = \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} \langle f(\cdot;k), g(\cdot;k)\rangle_{L^2_k}\, dk.$$

We also let $\widetilde{H}$ be the operator on $\mathcal{H}$ given by $(\widetilde{H}f)(x;k) = Hf(x;k)$, i.e. $\widetilde{H}$ acts pointwise as H on L^2_k, with domain

$$\operatorname{dom}(\widetilde{H}) = \left\{ f \in \mathcal{H} \;:\; f(x;k) \in H^2_k \text{ almost everywhere and } ||\widetilde{H}f||^2_{\mathcal{H}} < \infty \right\}.$$

Note that, by construction, the domain of $\widetilde{H}$ is dense in $\mathcal{H}$. The space $\mathcal{H}$ and the operator $\widetilde{H}$ are referred to as the *direct integrals* of L^2_k and H (viewed as an operator on L^2_k), respectively, and are often denoted by $\mathcal{H} = \int_{\mathcal{B}}^{\oplus} L^2_k dk$ and $\widetilde{H} = \int_{\mathcal{B}}^{\oplus} H dk$.

Lemma 2.3. *The operator $\widetilde{H}$ is self-adjoint and its spectrum is given by*

$$\sigma(\widetilde{H}) = \bigcup_{k\in\mathcal{B}} \sigma_{L^2_k}(H)$$

Proof. First, to show that $\widetilde{H}$ is self-adjoint, we start by showing that range$(\widetilde{H} \pm i) = \mathcal{H}$. Let $f \in \mathcal{H}$; then since H is self-adjoint on L^2_k, $(H+i)^{-1}$ is well-defined and bounded, say by C, and thus we can let $g(x;k) = (H+i)^{-1} f(x;k)$. It follows from elliptic regularity that $g(x;k) \in H^2_k$ almost everywhere, and

$$\begin{aligned} ||\widetilde{H}g||^2_{\mathcal{B}} &= \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} ||H(H+i)^{-1} f(\cdot;k)||^2_{L^2_k} dk \\ &= \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} ||(H+i-i)(H+i)^{-1} f(\cdot;k)||^2_{L^2_k} dk \\ &\leq (1+C)^2 \int_{\mathcal{B}} ||f(\cdot;k)||^2_{L^2_k} dk \\ &= (1+C)^2 ||f||^2_{\mathcal{H}} < \infty. \end{aligned}$$

Therefore $g \in \text{dom}(\widetilde{H})$, and since $f \in \mathcal{H}$ was arbitrary, this shows that range$(\widetilde{H}+i) = \mathcal{H}$; an identical argument shows that range$(\widetilde{H}-i) = \mathcal{H}$ as well.

We then claim that this implies $\widetilde{H}$ is self-adjoint. We note that $\widetilde{H}$ is symmetric since H is, meaning that dom$(\widetilde{H})$ is dense in $\mathcal{H}$ and for all $f, g \in \text{dom}(\widetilde{H})$, $\langle f, \widetilde{H}g \rangle_{\mathcal{H}} = \langle \widetilde{H}f, g \rangle_{\mathcal{H}}$. As a result, dom$(\widetilde{H}^*) \supset \text{dom}(\widetilde{H})$ and $\widetilde{H}^* f = \widetilde{H}f$ for all $f \in \text{dom}(\widetilde{H})$, from which it follows that dom$((\widetilde{H}-i)^*) = \text{dom}(\widetilde{H}^*+i) \supset \text{dom}(\widetilde{H}+i)$ and $(\widetilde{H}^*+i)f = (\widetilde{H}+i)f$ for all $f \in \text{dom}(\widetilde{H}+i) = \text{dom}(\widetilde{H})$. Using the fact that range$(\widetilde{H}+i) = \mathcal{H}$, we deduce that range$(\widetilde{H}^*+i) = \mathcal{H}$ as well, and thus $\widetilde{H}^*+i$ is surjective. However, it must also be injective, and therefore bijective, since a straightforward computation shows that $\ker(\widetilde{H}^*+i) = \text{range}(\widetilde{H}-i)^{\perp} = 0$. This in turn implies that dom$(\widetilde{H}^*+i) = \text{dom}(\widetilde{H}+i)$, for if dom$(\widetilde{H}^*+i) \supsetneq \text{dom}(\widetilde{H}+i)$ then for f dom$(\widetilde{H}^*+i) \setminus \text{dom}(\widetilde{H}+i)$ by surjectivity of $\widetilde{H}+i$ there would exist $g \in \text{dom}(\widetilde{H}+i)$ such that

$$(\widetilde{H}^*+i)f = (\widetilde{H}+i)g = (\widetilde{H}^*+i)g,$$

contradicting injectivity. Therefore dom$(\widetilde{H}^*+i) = \text{dom}(\widetilde{H}+i)$, and so dom$(\widetilde{H}^*) = \text{dom}(\widetilde{H})$, from which we conclude that $\widetilde{H}$ is self-adjoint.

Next, to compute the spectrum of $\widetilde{H}$, let $\mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}$ denote the indicator function on the interval $(\lambda-\varepsilon, \lambda+\varepsilon)$ and let $f \in \text{dom}(\widetilde{H})$. Then

$$\left(\mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}(\widetilde{H})f\right)(x;k) = \mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}(H)f(x;k);$$

this follows from the Helffer-Sjöstrand formula – see [Hel13, (8.1.12)] – and the fact that $\mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}$ can be approximated by a sequence of smooth, compactly supported functions.

We therefore get the following string of equivalences:

$$\begin{aligned}\lambda \in \sigma(\widetilde{H}) &\Leftrightarrow \mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}(\widetilde{H}) \neq 0 \text{ for all } \varepsilon > 0\\ &\Leftrightarrow |\{k \in \mathcal{B} \ : \ \mathbb{1}_{(\lambda-\varepsilon,\lambda+\varepsilon)}(H) \neq 0\}| > 0 \text{ for all } \varepsilon > 0\\ &\Leftrightarrow |\{k \in \mathcal{B} \ : \ (\lambda-\varepsilon,\lambda+\varepsilon) \cap \sigma_{L^2_k}(H) \neq \emptyset\}| > 0 \text{ for all } \varepsilon > 0\\ &\Leftrightarrow \lambda \in \sigma_{L^2_k}(H) \text{ for some } k \in \mathcal{B},\end{aligned}$$

where the last equivalence follows from continuity of eigenvalues. As a result,

$$\sigma(\widetilde{H}) = \bigcup_{k\in\mathcal{B}} \sigma_{L^2_k}(H),$$

as claimed. □

We now define a unitary operator $U : L^2(\mathbb{R}^n) \to \mathcal{H}$ by first defining U on the Schwartz space $\mathcal{S}(\mathbb{R}^n)$ (i.e. the space of rapidly decreasing functions on $\mathbb{R}^n$) by

$$Uf(x;k) = \sqrt{|\Omega|}\sum_{v\in\Lambda} e^{-ik\cdot v} f(x+v) \tag{2.11}$$

and then extending to $L^2(\mathbb{R}^n)$ by continuity. To see that U is well-defined, note that since $f \in \mathcal{S}(\mathbb{R}^n)$, the sum in (2.11) is uniformly convergent. To show that $Uf \in \mathcal{H}$, we first show that, for a fixed $k \in \mathcal{B}$, $Uf(x;k) \in L^2_k$: let $v' \in \Lambda$, then using the substitution $u = v' + v$, we compute that

$$\begin{aligned}Uf(x+v';k) &= \sqrt{|\Omega|}\sum_{v\in\Lambda} e^{-ik\cdot v} f(x+v'+v)\\ &= e^{ik\cdot v'}\sqrt{|\Omega|}\sum_{u\in\Lambda} e^{-ik\cdot u} f(x+u) = e^{ik\cdot v'}Uf(x;k).\end{aligned}$$

Next, using Fubini's theorem, we show that Uf is square integrable:

$$\begin{aligned}||Uf||^2_{\mathcal{H}} &= \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} ||Uf(\cdot;k)||^2_{L^2_k} dk = \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} \frac{1}{|\Omega|}\int_{\Omega} |Uf(x;k)|^2 dx dk\\ &= \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}}\int_{\Omega}\left|\sum_{v\in\Lambda} e^{-ik\cdot v} f(x+v)\right|^2 dx dk\\ &= \int_{\Omega}\sum_{v\in\Lambda}\sum_{v'\in\Lambda}\left(\frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} e^{-ik\cdot(v-v')}dk\right)\overline{f(x+v)}f(x+v')dx\\ &= \int_{\Omega}\sum_{v\in\Lambda}\sum_{v'\in\Lambda}\delta_{v-v'}\overline{f(x+v)}f(x+v')dx\\ &= \sum_{v\in\Lambda}\int_{\Omega}|f(x+v)|^2 dx = \int_{\mathbb{R}^n}|f(x)|^2 dx\\ &= ||f||^2_{L^2}.\end{aligned}$$

Thus Uf is square-integrable and therefore in $\mathcal{H}$, and moreover this shows that U is an isometry.

To compute U^*, note that for any $x \in \mathbb{R}^n$, there exists a unique $x_0 \in \Omega$ and $v \in \Lambda$ such that $x = x_0 + v$, and thus we define $U^* f$ for $f \in \mathcal{H}$ by

$$U^* f(x) = \frac{1}{|\mathcal{B}|\sqrt{|\Omega|}} \int_{\mathcal{B}} e^{ik\cdot v} f(x_0; k) dk.$$

To show that U^* is in fact the adjoint of U, we compute the following:

$$\begin{aligned}
\langle g, Uf \rangle_{\mathcal{H}} &= \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} \langle g(\cdot; k), Uf(\cdot; k) \rangle_{L^2_k} dk \\
&= \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} \frac{1}{|\Omega|} \int_{\Omega} \overline{g(x; k)} Uf(x; k) dx dk \\
&= \frac{1}{|\mathcal{B}|\sqrt{|\Omega|}} \int_{\mathcal{B}} \int_{\Omega} \overline{g(x; k)} \sum_{v \in \Lambda} e^{-ik\cdot v} f(x+v) dx dk \\
&= \sum_{v \in \Lambda} \int_{\Omega} \overline{\left(\frac{1}{|\mathcal{B}|\sqrt{|\Omega|}} \int_{\mathcal{B}} e^{ik\cdot v} g(x; k) dk \right)} f(x+v) dx \\
&= \sum_{v \in \Lambda} \int_{\Omega} \overline{U^* g(x+v)} f(x+v) dx \\
&= \int_{\mathbb{R}^n} \overline{U^* g(x)} f(x) dx = \langle U^* g, f \rangle_{L^2}.
\end{aligned}$$

Furthermore, $U^* = U^{-1}$ since

$$\begin{aligned}
U^* Uf(x) &= \frac{1}{|\mathcal{B}|\sqrt{|\Omega|}} \int_{\mathcal{B}} e^{ik\cdot v} Uf(x_0; k) dk = \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} e^{ik\cdot v} \sum_{v' \in \Lambda} e^{-ik\cdot v'} f(x_0 + v') dk \\
&= \sum_{v' \in \Lambda} \left(\frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} e^{-ik\cdot (v'-v)} dk \right) f(x_0 + v') \\
&= \sum_{v' \in \Lambda} \delta_{v'-v} f(x_0 + v') = f(x_0 + v) \\
&= f(x),
\end{aligned}$$

which shows that $U^* U = \mathrm{Id}_{L^2(\mathbb{R}^n)}$, and an identical argument shows that $UU^* = \mathrm{Id}_{\mathcal{H}}$. Therefore, U is a unitary operator, as claimed.

Using the operator U, we are now able to prove that one can recover the spectral theory of H on $L^2(\mathbb{R}^n)$ from the spectral theory of H on L^2_k for $k \in \mathcal{B}$.

Theorem 2.4. *Let Λ be a lattice and let $H = -\Delta + V$ for V smooth and periodic with respect to Λ. Then*

(1)

$$\sigma_{L^2(\mathbb{R}^n)}(H) = \bigcup_{k\in\mathcal{B}} \sigma_{L^2_k}(H) = \bigcup_{k\in\mathcal{B}} \sigma_{L^2_0}(H(k)),$$

(2) for each $k \in \mathcal{B}$, let $\{\phi_b(x;k)\}_{b\geq 1}$ be an orthonormal basis of eigenvectors for H on L^2_k; then the set

$$\bigcup_{b\geq 1}\bigcup_{k\in\mathcal{B}} \{\phi_b(x;k)\},$$

is complete in $L^2(\mathbb{R}^n)$ in the following sense: for any $f \in L^2(\mathbb{R}^n)$,

$$f(x) = \frac{1}{|\mathcal{B}||\Omega|}\sum_{b\geq 1}\int_{\mathcal{B}} \langle f, \phi_b(\cdot;k)\rangle_{L^2}\phi_b(x;k)dk,$$

and

$$||f||_{L^2} = \frac{1}{|\mathcal{B}|}\sum_{b\geq 1}\int_{\mathcal{B}} |\langle f, \phi_b(\cdot;k)\rangle_{L^2}|^2 dk.$$

Proof. To prove (1), we first show that $\widetilde{H}U = UH$ on $\mathcal{S}(\mathbb{R}^n)$. Since H is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^n)$ and $\widetilde{H}$ is self-adjoint on $\mathcal{H}$ by Lemma 2.3, the uniqueness of self-adjoint extensions of essentially self-adjoint operators then implies that $\widetilde{H}U = UH$ on $L^2(\mathbb{R}^n)$. To show this, first note that $Uf \in \mathrm{dom}(\widetilde{H})$ since Uf is given by the uniformly convergent sum (2.11), and each term in this sum is in $C^\infty(\Omega)$ since $f \in \mathcal{S}(\mathbb{R}^n)$. Therefore the expression $\widetilde{H}Uf$ is well-defined, and is equal to

$$(\widetilde{H}U)f(x) = \widetilde{H}\left(\sqrt{|\Omega|}\sum_{v\in\Lambda} e^{-ik\cdot v} f(x+v)\right) = \sqrt{|\Omega|}\sum_{v\in\Lambda} e^{-ik\cdot v} Hf(x+v) = (UH)f(x).$$

Therefore $H = U^{-1}\widetilde{H}U$, and consequently $\sigma_{L^2(\mathbb{R}^n)}(H) = \sigma_{\mathcal{H}}(\widetilde{H})$. In addition, recall that as an operator on L^2_k, $H = F^{-1}H(k)F$, and so $\sigma_{L^2_k}(H) = \sigma_{L^2_0}(H(k))$. Therefore, by Lemma 2.3, we compute that

$$\sigma_{L^2(\mathbb{R}^n)}(H) = \sigma_{\mathcal{H}}(\widetilde{H}) = \bigcup_{k\in\mathcal{B}} \sigma_{L^2_k}(H) = \bigcup_{k\in\mathcal{B}} \sigma_{L^2_0}(H(k)).$$

To prove (2), let $\{\phi_b(x;k)\}_{b\geq 1}$ be an orthonormal basis of eigenvectors for H on L^2_k for each $k \in \mathcal{B}$. As noted following (2.10), the eigenvalues of H on L^2_k are continuous in k, and so the functions $\phi_b(x;k)$ can be chosen to be continuous in k as well, and in particular measurable. In addition, by quasiperiodicity, we can extend each of these functions to all of $\mathbb{R}^n$.

To prove (2), we first consider $f \in \mathcal{S}(\mathbb{R}^n)$. Since $\mathcal{S}(\mathbb{R}^n) \subset L^2(\mathbb{R}^n)$, $Uf \in \mathcal{H}$, and so for each $k \in \mathcal{B}$ we can write

$$\begin{aligned} Uf(x;k) &= \sum_{b\geq 1} \langle Uf(\cdot;k), \phi_b(\cdot;k)\rangle_{L^2_k}\, \phi_b(x_0;k), \\ ||Uf(\cdot;k)||^2_{L^2_k} &= \sum_{b\geq 1} |\langle Uf(\cdot;k), \phi_b(\cdot;k)\rangle_{L^2_k}|^2. \end{aligned}$$

In addition, although the functions $\{\phi_b(x;k)\}_{b\geq 1}$, viewed as function on $\mathbb{R}^n$, are not contained in $L^2(\mathbb{R}^n)$, the expression $\langle f, \phi_b\rangle_{L^2}$ is still well-defined since by quasiperiodicity there exists $C_b > 0$ such that $|\phi_b(x;k)|^2 \leq C_b$, and consequently

$$\int_{\mathbb{R}^n} \left|\overline{f(x)}\phi_b(x;k)\right|^2 dx \leq C_b \int_{\mathbb{R}^n} |f(x)|^2 dx < \infty.$$

Therefore, by continuity, we can extend $\langle f, \phi_b\rangle_{L^2}$ to $f \in L^2(\mathbb{R}^n)$. As a result, for $f \in L^2(\mathbb{R}^n)$,

$$\begin{aligned} f(x) = U^*Uf(x) &= \frac{1}{|\mathcal{B}|\sqrt{|\Omega|}} \int_{\mathcal{B}} e^{ik\cdot v} Uf(x_0;k)dk \\ &= \frac{1}{|\mathcal{B}|\sqrt{|\Omega|}} \int_{\mathcal{B}} e^{ik\cdot v} \sum_{b\geq 1} \langle Uf(\cdot;k), \phi_b(\cdot;k)\rangle_{L^2_k}\, \phi_b(x_0;k)dk \\ &= \frac{1}{|\mathcal{B}||\Omega|} \sum_{b\geq 1} \int_{\mathcal{B}} \left(\sum_{v'\in\Lambda} e^{-ik\cdot v'} \int_{\Omega} \overline{f(y+v')}\phi_b(y;k)dy \right) e^{ik\cdot v}\phi_b(x_0;k)dk \\ &= \frac{1}{|\mathcal{B}||\Omega|} \sum_{b\geq 1} \int_{\mathcal{B}} \left(\sum_{v'\in\Lambda} \int_{\Omega} \overline{f(y+v')}\phi_b(y+v';k)dy \right) \phi_b(x;k)dk \\ &= \frac{1}{|\mathcal{B}||\Omega|} \sum_{b\geq 1} \int_{\mathcal{B}} \left(\int_{\mathbb{R}^n} \overline{f(y)}\phi_b(y;k)dy \right) \phi_b(x;k)dk \\ &= \frac{1}{|\mathcal{B}||\Omega|} \sum_{b\geq 1} \int_{\mathcal{B}} \langle f, \phi_b(\cdot;k)\rangle_{L^2}\, \phi_b(x;k)dk. \end{aligned}$$

By similar computations, we also have that

$$\begin{aligned} ||f||^2_{L^2} = ||Uf||^2_{\mathcal{H}} &= \frac{1}{|\mathcal{B}|} \int_{\mathcal{B}} ||Uf(\cdot;k)||^2_{L^2_k} dk \\ &= \frac{1}{|\mathcal{B}|} \sum_{b\geq 1} \int_{\mathcal{B}} |\langle Uf(\cdot;k), \phi_b(\cdot;k)\rangle_{L^2_k}|^2 dk \\ &= \frac{1}{|\mathcal{B}|} \sum_{b\geq 1} \int_{\mathcal{B}} |\langle f, \phi_b(\cdot;k)\rangle_{L^2}|^2 dk. \end{aligned}$$

□

2.3 Representation Theory

In the previous section we discussed how one can use Floquet-Bloch theory to reduce the eigenvalue problem $\mu\phi = H\phi$ from the space $L^2(\mathbb{R}^n)$ to the space L^2_k when the potential V is periodic with respect to a lattice Λ. If we also assume V has the same symmetries as Λ, the point group G of Λ can be used to further reduce this problem using techniques from representation theory. We will particularly be interested in the representation theory of abelian groups, as their representations can be decomposed into subrepresentations of dimension one (see Corollary 2.2 and Remark 2.6), corresponding to a maximal reduction of the problem.

In practice, the potential V is also typically assumed to be real. Consequently, the relevant symmetries include the group G together with complex conjugation, which implies the corresponding representations should include both unitary and antiunitary operators. Such representations have been fully classified in [Wig59], who called them *corepresentations*, which we briefly introduce in the latter half of this section. So far this theory has only been applied to honeycomb lattice potentials [BC18], but using the general framework established herein, one could apply this theory to other two- and three-dimensional lattices.

Definition 2.3. *Let G be a group and let X be a vector space. A representation of G over a field $\mathbb{F}$ is a group homomorphism $\rho : G \to \mathrm{GL}(X)$, meaning that for $g_1, g_2 \in G$, $\rho(g_1 g_2) = \rho(g_1)\rho(g_2)$. When the homomorphism is clear from the context, we shall typically refer to X as the representation, and denote $\rho(g)v$ by gv. We then say that the dimension of the representation is the dimension of X as a vector space. If X is finite dimensional, the character of the representation is the map $\chi_\rho : G \to \mathbb{F}$ given by*

$$\chi_\rho(g) = \mathrm{Tr}(\rho(g)).$$

Given two representations $\rho_1 : G \to \mathrm{GL}(X_1)$, $\rho_2 : G \to \mathrm{GL}(X_2)$, a G-homomorphism (or simply a homomorphism when the group G is clear) is a linear map $T : X_1 \to X_2$ such that

$$\rho_2(g)T = T\rho_1(g) \quad \text{for all } g \in G.$$

We then say that X_1 and X_2 are isomorphic if there exists a homomorphism $T : X_1 \to X_2$ that is also a vector space isomorphism (in this case, a straightforward computation shows that T^{-1} is a homomorphism as well). A subrepresentation of a representation X is a vector subspace $X' \subset X$ such that $gv \in X'$ for all $g \in G$ and $v \in X'$.

Lastly, we say that a representation X is irreducible if it has no proper, nontrivial subrepresentations.

Henceforth, when referring to a representation, we shall take the field $\mathbb{F}$ to be $\mathbb{C}$. By definition, a representation X also necessarily defines a group action on X, and as such we can define

1. the orbit of a vector $v \in X$: $G \cdot v = \{gv \;:\; g \in G\}$,

2. the stabilizer subgroup of a subset $S \subset X$: $G_S = \{g \in G \;:\; gS \subset S\}$,

3. invariant subsets $S \subset X$, which satisfy $G \cdot S \subset S$.

Using this terminology, a subrepresentation can then equivalently be defined as an invariant vector subspace.

To analyze the representation theory of abelian groups, we need two key results: Maschke's Theorem and Schur's Lemma (Theorem 2.5 and Lemma 2.4, respectively). We include proofs adapted from [DF03]; in particular, the idea of "averaging" in the proof of Maschke's Theorem motivates an approach we will later use to construct an explicit basis consisting of eigenvectors of $-\Delta$ for representations of k-invariant subgroups (see Definition 4.1 and Lemma 4.2).

Theorem 2.5. (Maschke's Theorem) *Let G be a finite group and let X be a G-representation. If $X_1 \subset X$ is a G-subrepresentation, then there exists a G-subrepresentation $X_2 \subset X$ such that $X = X_1 \oplus X_2$*[1].

Proof. We seek to construct a G-homomorphism $\pi : X \to X_1$ such that π is a projection. If we can do so, then we can let $X_2 = \ker \pi$, from which it follows that X_2 is a G-subrepresentation. In addition, if $v \in X_1 \cap X_2$, then $\pi(v) = v$ since π is a projection onto X_1 and $\pi(v) = 0$ since $v \in \ker \pi$, which implies that $v = 0$ and so $X_1 \cap X_2 = 0$. Lastly, for any $v \in X$, we can write $\pi(v) + (v - \pi(v))$, and since $\pi(v - \pi(v)) = \pi(v) - \pi(v) = 0$, this implies that $v \in X_1 + X_2$. Therefore, it suffices to construct the homomorphism π to prove the theorem.

Towards that end, let X_2 be a vector space complement to X_1, so that $X = X_1 \oplus X_2$ (note that X_2 is not necessarily a G-subrepresentation), and let $\pi_0 : X \to X_1$ be the vector space projection associated to this decomposition. We then "average" π_0 over G by defining

$$\pi = \frac{1}{|G|} \sum_{g \in G} g \pi_0 g^{-1}; \tag{2.12}$$

it then immediately follows that π is linear as a sum of products of linear maps. In addition, we claim that π is (1) a map from X to X_1, (2) the identity on X_1, and (3) a G-homomorphism.

(1) To see that $\pi(X) \subset X_1$, let $v \in X$. Then $\pi_0(g^{-1}v) \in X_1$ since $\pi_0(X) \subset X_1$, and consequently $g\pi_0(g^{-1}v) \in X_1$ as well since X_1 is a G-subrepresentation. Thus $\pi(v) \in X_1$ as a sum of vectors in X_1.

[1] This theorem is more generally true for representations over any field $\mathbb{F}$ such that the characteristic of $\mathbb{F}$ does not divide the order of the group G.

(2) To see that $\pi|_{X_1} = \mathrm{Id}_{X_1}$, let $v \in X_1$. Then $g^{-1}v \in X_1$ since X_1 is a subrepresentation, and since π_0 is the identity on X_1 by construction, by plugging in v into (2.12), we get

$$\pi(v) = \frac{1}{|G|}\sum_{g\in G} g\pi_0(g^{-1}v) = \frac{1}{|G|}\sum_{g\in G} gg^{-1}v = \frac{1}{|G|}\sum_{g\in G} v = v.$$

(3) Now let $h \in G$ be arbitrary. Then for any $v \in X$,

$$\begin{aligned}\pi(hv) &= \frac{1}{|G|}\sum_{g\in G} g\pi_0(g^{-1}hv) = \frac{1}{|G|}\sum_{g\in G} h(h^{-1}g)\pi_0((g^{-1}h)v)\\ &= h\frac{1}{|G|}\sum_{g'\in G} g'\pi_0((g')^{-1}v) = h\pi(v).\end{aligned}$$

Therefore π is both a G-homomorphism and a projection onto X_1. □

Lemma 2.4. (Schur's Lemma) *Let X_1, X_2 be irreducible G-representations, and let $T : X_1 \to X_2$ be a homomorphism. Then either T is invertible or $T = 0$.*

Proof. Assume that $T \neq 0$. Since T is a homomorphism, $\ker T$ and $T(x_1)$ are subrepresentations of X_1 and X_2, respectively. Consequently, our assumption that $T \neq 0$ implies that $\ker T$ is a proper subrepresentation, which together with the fact that X_1 is irreducible implies $\ker T = 0$, and so T is injective. Similarly, our assumption that $T \neq 0$ also implies that $T(X_1) \neq 0$, and since X_2 is irreducible, $T(x_1)$ cannot be a proper subrepresentation, so $T(X_1) = X_2$, which tells us that T is surjective. If we then let T^{-1} denote the (set) inverse of T, this map will necessarily be linear and commute with the action of G since T is linear and commutes with the action of G. Therefore T^{-1} is a homomorphism, and so T is invertible (as a G-homomorphism). □

Corollary 2.1. *Let X be an irreducible, finite-dimensional G-representation, and let $T : X \to X$ be a homomorphism. Then $T = \lambda I$ for some $\lambda \in \mathbb{C}$.*

Proof. Let λ be an eigenvalue of T (which necessarily exists since we are assuming all of our representations are over the field $\mathbb{C}$). Then λI is a linear map and, as a scalar multiple of the identity, commutes with g for all $g \in G$, and is therefore a homomorphism. As a result, $T - \lambda I$ is also a homomorphism, and so by Lemma 2.4, $T - \lambda I$ must either be invertible or the zero map. However, if we let $v \in X$ be an eigenvector corresponding to λ, then $(T - \lambda I)v = 0$, and so $T - \lambda I$ cannot be invertible. Therefore $T - \lambda I = 0$, or equivalently $T = \lambda I$, as claimed. □

Using the above results, we can now prove that the representations of abelian groups can be decomposed into subrepresentations of dimension one.

Corollary 2.2. *Let G be a finite abelian group and let X be a finite-dimensional G-representation. Then there exist irreducible, one-dimensional subrepresentations $X_1, \dots, X_n \subset X$ such that*

$$X = \oplus_{j=1}^{n} X_j. \tag{2.13}$$

Remark 2.6. Although we shall not prove it here, Corollary 2.2 is more generally true for unitary representations of compact abelian groups on complex Hilbert spaces, and is a consequence of the Peter-Weyl Theorem [PW27]. In this context, the direct sum (2.13) is a direct sum of Hilbert spaces, and will typically be infinite.

Proof of Corollary 2.2. Let $X_1 \subset X$ be a nontrivial, irreducible subrepresentation (which can be shown to exist by taking the intersection of all subrepresentations containing some nonzero v, for example), and let $g \in G$ be arbitrary. Then G being abelian implies $g : X_1 \to X_1$ is a homomorphism since for all $g' \in G$ and $v \in X_1$:

$$g(g'v) = (gg')v = (g'g)v = g'(gv).$$

Therefore, by Corollary 2.1, $g = \lambda v$ for some $\lambda \in \mathbb{C}$. Since g was arbitrary, this implies that every $g \in G$ is a scalar multiple of the identity. Consequently, if $v \in X_1$ is nonzero, then the one-dimensional subspace spanned by v is a subrepresentation, and so by irreducibility, this must equal X_1.

Now, by Maschke's theorem (Theorem 2.5), there exists a subrepresentation $X_1' \subset X$ such that $X = X_1 \oplus X_1'$. If $X_1' = 0$ we are done; otherwise, X_1' is a nontrivial, finite-dimensional G-representation satisfying $\dim X_1' = \dim X - 1$. Therefore, by an inductive argument, we can construct irreducible, one-dimensional subrepresentations $X_1, X_2, X_3 \dots$ satisfying $X = X_1 \oplus \cdots \oplus X_j \oplus X_j'$ and $\dim X_j' = \dim X - j$. Since X is assumed to be finite-dimensional, eventually this process must terminate, giving us the decomposition (2.13). □

As mentioned in the introduction of this section, we would like to extend the concept of a representation of a group to include both unitary and antiunitary operators. This leads us to the notion of a corepresentation, which we now define. For this definition, if X is a complex inner product space, we let $\mathrm{Isom}(X)$ denote the group of isometries of X viewed as a metric space.

Definition 2.4. *Let G be a group with a subgroup G_0 of index 2 (if G is finite, this is equal to $|G|/|G_0|$), which we call the linear subgroup, and let X be the complexification of some real inner product space (so that the complex conjugate $\overline{v}$ of $v \in X$ is well-defined). A corepresentation of G is a group homomorphism $\rho : G \to \mathrm{Isom}(X)$ such that $\rho|_{G_0}$ is a G_0-representation, and for all $g \in G \setminus G_0$, $v_1, v_2 \in X$ and $z_1, z_2 \in \mathbb{C}$,*

$$\rho(g)(z_1 v_1 + z_2 v_2) = \overline{z_1}\rho(g)v_1 + \overline{z_2}\rho(g)v_2,$$

i.e. $\rho|_{G\setminus G_0}$ *maps into the space of antiunitary operators. Just as we did for representations of G, when the homomorphism is clear we shall typically refer to X as the corepresentation, and denote* $\rho(g)v$ *by* gv.

Given two corepresentations $\rho_1 : G \to Isom(X_1)$, $\rho_2 : G \to Isom(X_2)$, *a G-homomorphism (or simply a homomorphism when the group G is clear) is a linear map* $T : X_1 \to X_2$ *such that for all* $g \in G_0$ *and* $h \in G \setminus G_0$,

$$\rho_2(g)T = T\rho_1(g)$$
$$\rho_2(h)T = \overline{T}\rho_1(h),$$

where $\overline{T}(v) := \overline{T(\overline{v})}$. *We then say that* X_1 *and* X_2 *are isomorphic as corepresentations if there exists a homomorphism* $T : X_1 \to X_2$ *that is also a vector space isomorphism, in which case* T^{-1} *is a homomorphism as well. A sub-corepresentation of a corepresentation X is a vector subspace* $X' \subset X$ *such that* $gv \in X'$ *for all* $g \in G$ *and* $v \in X'$.

Lastly, we say that a corepresentation X is irreducible if it has no proper, nontrivial sub-corepresentations.

To see how we might apply the above theory to the Floquet-Bloch problem (1.3), let Λ be a lattice with point group G, let $K \in \mathcal{B}$, and let μ_0 be an L^2_K-eigenvalue of H with corresponding eigenspace E. If we can then find a subgroup G_0 of G such that E is a G_0-representation, Maschke's Theorem (Theorem 2.5) says that we can decompose E into irreducible subrepresentations. It follows that the multiplicity of the eigenvalue μ_0 is bounded below by the minimal dimension of the irreducible representations of G_0.

To give an explicit example, let Λ be a hexagonal lattice and let K be a vertex of the Brillouin zone $\mathcal{B}$. The L^2_K-eigenspaces of H are then representations of the subgroup G_0 of G generated by a rotation of the plane by $\pi/3$, and since this group is isomorphic to $\mathbb{Z}/3\mathbb{Z}$ and therefore abelian, all of its irreducible representations are one-dimensional (see Corollary 2.2 and Remark 2.6). When V is assumed to be real, however, Theorem 1.3 tells us that there exists an eigenvalue of H which has multiplicity two – what is interesting is that this can likely be explained by the fact that the irreducible corepresentations of G_0 together with complex conjugation are all two-dimensional.

Due to this potential relationship between the multiplicities of L^2_k-eigenvalues of H and the dimensions of irreducible corepresentations, one of our current projects is to compute the irreducible corepresentations of groups whose actions commute with H on L^2_k, so that H restricts to a well-defined operator on these spaces. We therefore finish this section by stating the classification theorem for irreducible corepresentations of G in terms of the irreducible representations of the linear subgroup G_0, and refer the interested reader to [BC09] for a proof.

Theorem 2.7. (Classification of Irreducible Corepresentations) *Let* $\rho : G \to Isom(X)$ *be a corepresentation of some finite group G with linear subgroup* G_0, *and let* $M = \rho(h_0)$

for some arbitrary $h_0 \in G \setminus G_0$. If $\rho_0 : G_0 \to \mathrm{GL}(X_0)$ is a finite-dimensional, irreducible subrepresentation of $\rho|_{G_0} : G_0 \to \mathrm{GL}(X)$ and

$$X_1 := M(X_0) + X_0, \quad \text{and} \quad C := \sum_{h \in G \setminus G_0} \chi_{\rho_0}(h^2),$$

then X_1 is an irreducible sub-corepresentation of X and C must equal either $|G_0|$, $-|G_0|$ or 0. In addition:

(1) If $C = |G_0|$, then $X_1 \cong X_0$ as vector spaces, and for all $g \in G_0$ and $h \in G \setminus G_0$,

$$\begin{aligned} \rho(g) &= \rho_0(g), \\ \rho(h) &= \rho_0(hh_0^{-1})M. \end{aligned}$$

(2) If $C = -|G_0|$, then $X_1 \cong X_0 \oplus X_0$ as vector spaces, and for all $g \in G_0$ and $h \in G \setminus G_0$,

$$\begin{aligned} \rho(g) &= \begin{pmatrix} \rho_0(g) & 0 \\ 0 & \rho_0(g) \end{pmatrix}, \\ \rho(h) &= \begin{pmatrix} 0 & \rho_0(hh_0^{-1})M \\ -\rho_0(hh_0^{-1})M & 0 \end{pmatrix}. \end{aligned}$$

(3) If $C = 0$, then $X_1 \cong X_0 \oplus X_0$ as vector spaces, and for all $g \in G_0$ and $h \in G \setminus G_0$,

$$\begin{aligned} \rho(g) &= \begin{pmatrix} \rho_0(g) & 0 \\ 0 & \rho_0(h_0^{-1} g h_0)^* \end{pmatrix}, \\ \rho(h) &= \begin{pmatrix} 0 & \rho_0(hh_0) \\ \rho_0(h_0^{-1}h)^* & 0 \end{pmatrix}. \end{aligned}$$

2.4 Wavepacket Analysis

As discussed in Chapter 1, the qualitative properties of dispersion surfaces control the effective dynamics of waves. To motivate our interest in this subject, we describe three classes of initial conditions discussed in [FW14; AP05] for the time-dependent Schrödinger equation, where the potential V is periodic with respect to a lattice Λ.

Example 2.8 (Spectral Localization). Let λ be a hexagonal lattice, K be a vertex of the Brillouin zone $\mathcal{B}$, and assume that V is a generic λ-invariant potential, in this case meaning that V is even and invariant under rotations by $2\pi/3$ (this is rigorously defined in Definition 4.2). Then [FW12] showed that K is a Dirac point, as in Definition 1.1, i.e., there is a pair of dispersion surfaces intersecting conically at K. Let $\mu(K)$ denote the value of these dispersion surfaces at K; a consequence of their result is there exist two eigenfunctions ϕ_1, ϕ_2 for $\mu(K)$ which satisfy $\phi_2(x) = \overline{\phi_1(-x)}$. The primary class of initial conditions then studied in [FW14] are those which are *spectrally localized* near K, which are initial conditions of the form

$$\psi(x,0) = \delta\alpha_{10}(\delta x)\phi_1(x) + \delta\alpha_{20}(\delta x)\phi_2(x),$$

with $\alpha_{j0}(x) \in \mathcal{S}(\mathbb{R}^2)$ for $j = 1,2$ and δ small. For such initial conditions, the solution to the time-dependent Schrödinger equation evolves approximately as a slowly modulated superposition of Floquet-Bloch states:

$$\psi^\delta(x,t) \approx e^{-i\mu(K)t}\Big(\delta\alpha_1(\delta x, \delta t)\phi_1(x) + \delta\alpha_2(\delta x, \delta t)\phi_2(x)\Big),$$

where the modulating amplitudes α_1, α_2 satisfy the effective Dirac system

$$\begin{aligned} \partial_t\alpha_1(x,t) &= -\overline{\lambda}(\partial_{x_1} + i\partial_{x_2})\alpha_2(x,t) \\ \partial_t\alpha_2(x,t) &= -\lambda(\partial_{x_1} - i\partial_{x_2})\alpha_1(x,t), \end{aligned} \tag{2.14}$$

where $0 \neq \lambda \in \mathbb{C}$ and with initial data $\alpha(x,0) = \alpha_0(x)$.

Example 2.9 (Localization at a Frequency). Again let $K \in \mathcal{B}$, (not necessarily a vertex), and let $\mu(K)$ be a simple L^2_K-eigenvalue with corresponding eigenfunction $\phi(x)$, such that $\nabla_k\mu(K) \neq 0$. We then consider initial conditions which are *localized at the frequency* $\mu(K)$, which are initial conditions of the form

$$\psi(x,0) = \delta\alpha_0(\delta x)\phi(x),$$

with $\alpha_0(x) \in \mathcal{S}(\mathbb{R}^n)$ and δ small. The solution to the time-dependent Schrödinger equation is then approximately given by

$$\psi(x,t) \approx e^{-i\mu(K)t}\delta\alpha(\delta x, \delta t)\phi(x), \tag{2.15}$$

where the modulating amplitude α satisfies the transport equation

$$\partial_t\alpha(x,t) + \nabla_k\mu(K)\cdot\nabla_x\alpha(x,t) = 0 \tag{2.16}$$

with initial data $\alpha(x,0) = \alpha_0(x)$. Consequently we can rewrite (2.15) as

$$\psi(x,t) \approx e^{-i\mu(K)t}\delta\alpha_0\Big(\delta\big(x - \nabla_k\mu(K)t\big)\Big)\phi(x).$$

That is, the effective transport is ballistic, with speed $\nabla_k\mu(K)$.

Example 2.10 (Localization at a Spectral Band Edge). For our last example, we start with the same assumptions as in Example 2.9, but we now assume that $\mu(K)$ occurs at a spectral band (gap) edge, so that $\nabla_k \mu(K) \neq 0$, and the Hessian $D_k^2 \mu(K)$ is non-degenerate. If we then again consider initial conditions which are *localized at the frequency* $\mu(K)$, the solution to the time-dependent Schrödinger equation is then approximately given by

$$\psi(x,t) \approx e^{-i\mu(K)t} \delta\alpha(\delta x, \delta^2 t)\phi(x),$$

where the modulating amplitude α satisfies the constant coefficient Schrödinger equation

$$i\partial_t \alpha(x,t) = -\frac{1}{2} \nabla_x \cdot D_k^2 \mu(K) \nabla_x \alpha(x,t) \tag{2.17}$$

with initial data $\alpha(x,0) = \alpha_0(x)$. Here, $A := \frac{1}{2} D_k^2 \mu(K)$ is referred to as the inverse of the effective mass tensor.

Each of the results discussed in Examples 2.8 – 2.10 can be proven using the same methods, which we now outline. The initial conditions and can generally be written in the form

$$\psi(x,0) = \sum_{j=1}^{m} \delta\alpha_{j0}(\delta x)\phi_j(x),$$

where $\alpha_{10}, \ldots, \alpha_{m0} \in \mathcal{S}(\mathbb{R}^n)$ and $\phi_1, \ldots, \phi_m$ are eigenfunctions corresponding to the multiplicity m, L_K^2-eigenvalue $\mu_0 := \mu(K)$. We look for solutions of the form

$$\psi(x,t) = e^{-i\mu_0 t} \left(\sum_{j=1}^{m} \delta\alpha_j(\delta x, \delta^r t)\phi_j(x) + E_\delta(x,t) \right) \tag{2.18}$$

for some positive integer r; the goal is then to show that $||E_\delta(x,t)|| \to 0$ as $\delta \to 0$.

Plugging (2.18) into the time-independent Schrödinger equation (1.2), we get

$$\begin{aligned} 0 &= i\partial_t \psi - H\psi \\ &= \mu_0 e^{-i\mu_0 t} \left(\sum_{j=1}^{m} \delta\alpha_j(\delta x, \delta^r t)\phi_j(x) + E_\delta(x,t) \right) \\ &\quad + ie^{-i\mu_0 t} \left(\sum_{j=1}^{m} \delta^{r+1} (\partial_t \alpha_j)(\delta x, \delta^r t)\phi_j(x) + \partial_t E_\delta(x,t) \right) \\ &\quad - e^{-i\mu_0 t} \left(\sum_{j=1}^{m} \mu_0 \delta\alpha_j(\delta x, \delta^r t)\phi_j(x) - \delta^3 (\Delta\alpha_j)(\delta x, \delta^r t)\phi_j(x) \right. \\ &\quad \left. -2\delta^2 (\nabla\alpha_j)(\delta x, \delta^r t) \cdot \nabla\phi_j(x) + HE_\delta(x,t) \right) \end{aligned}$$

Multiplying the first and last expressions by $e^{i\mu_0 t}$ and canceling terms, we get

$$\begin{aligned} i\partial_t E_\delta(x,t) = (H-\mu_0)E_\delta(x,t) \\ - \delta^2 \left(\sum_{j=1}^m \delta^{r-1}(\partial_t \alpha_j)(\delta x, \delta^r t)\phi_j(x) + 2(\nabla\alpha_j)(\delta x, \delta^r t)\cdot\nabla\phi_j(x) \right) \\ - \delta^3 \left(\sum_{j=1}^m (\Delta\alpha_j)(\delta x, \delta^r t)\phi_j(x) \right) \end{aligned}$$

By DuHamel's principle (see [Fri82]), the error term $E_\delta(x,t)$ is then given by

$$\begin{aligned} & E_\delta(x,t) \\ & = i\delta^2 \sum_{j=1}^m \int_0^t e^{-i(H-\mu_0)(t-s)} \left(\delta^{r-1}(\partial_t\alpha_j)(\delta x, \delta^r t)\phi_j(x) + 2(\nabla\alpha_j)(\delta x,\delta^r t)\cdot\nabla\phi_j(x) \right) ds \\ & \quad + i\delta^3 \sum_{j=1}^m \int_0^t e^{-i(H-\mu_0)(t-s)} \left((\Delta\alpha_j)(\delta x, \delta^r t)\phi_j(x) \right) ds \end{aligned}$$

Since $e^{-i(H-\mu_0)(t-s)}$ is a unitary operator on L^2, we are able to bound E_δ by

$$\begin{aligned} ||E_\delta(x,t)|| \le \delta^2 \sum_{j=1}^m \int_0^t \left|\left| \delta^{r-1}(\partial_t\alpha_j)(\delta x,\delta^r t)\phi_j(x) + 2(\nabla\alpha_j)(\delta x,\delta^r t)\cdot\nabla\phi_j(x) \right|\right| ds \\ + \delta^3 \sum_{j=1}^m \int_0^t ||(\Delta\alpha_j)(\delta x,\delta^r t)\phi_j(x)|| \, ds \end{aligned} \tag{2.19}$$

Denote the two integrals in (2.19) by I_1 and I_2, respectively, and consider the integral I_2. Since we are assuming $\alpha \in \mathcal{C}(\mathbb{R}^n)$, so too is $\Delta\alpha$, and thus there exists some $C_1 > 0$ such that $||\Delta\alpha|| \le C_1$. Similarly, since $\phi_j \in L^2_K$, and in particular is quasiperiodic, for $j = 1, \ldots, m$, there exists some $C_2 > 0$ such that $\sup_{x,j} |\phi_j(x)| \le C_2$. Consequently, if we let $C = C_1 C_2$, then for $t \le \delta^{-1}$,

$$I_2 = \int_0^t ||(\Delta\alpha_j)(\delta x,\delta^r t)\phi_j(x)|| \, ds \le C\delta^{-1} \int_0^t ds \le C\delta^{-2},$$

which shows that the second term of the bound given in (2.19) will go to zero as $\delta \to 0$.

Computing a bound for the integral I_1 depends on the initial conditions being studied. In general, however, it requires using the decomposition into Floquet-Bloch modes given by Theorem 2.4 and the corresponding effective equation (2.14), (2.16), or (2.17). One can then show that the integrand is bounded by some C_3, and therefore, for $t \le \delta^{-1}$, $I_1 \le C_3\delta^{-1}$. This then implies that the first term of the bound given in (2.19) will go to zero as $\delta \to 0$ as well, thus proving that $||E_\delta(x,t)|| \to 0$ as $\delta \to 0$.

In conclusion, Examples 2.8 – 2.10 demonstrate why dispersion surfaces and their intersections are of fundamental interest in the study of waves in periodic structures. The general framework we develop in Chapter 4 provides a foundation upon which one can now produce similar results for other lattices and their corresponding band spectrum singularities.

Chapter 3

SPECTRA OF ANALYTIC FAMILIES OF OPERATORS

In order to find interesting dispersion surfaces of the operator H in (1.3), our strategy will be to look at

$$H_z = -\Delta + zV$$

on L^2_k for varying k and generic values of $z \in \mathbb{R}$. In general, we shall use perturbation theory to analyze the spectrum of H_z for z close to 0, and we shall use analyticity to extend our results to large z. We start by analyzing this situation in the finite-dimensional case.

3.1 Analytic Families of Matrices

One of our primary tools is the following theorem:

Theorem 3.1. *Let $\{A_z\}_{z \in U}$ be an analytic family of monic degree n polynomials in $\mathbb{C}[x]$, for some $U \subset \mathbb{C}$ open. Then there is a discrete set D, such that on any simply connected open set $W \subset U \setminus D$, there exists a decomposition*

$$A_z(x) = \prod_{j=1}^{r} (x - \lambda_j(z))^{m_j}, \tag{3.1}$$

where $\lambda_1, \ldots, \lambda_r : W \to \mathbb{C}$ are analytic functions such that $\lambda_1(z), \ldots, \lambda_r(z)$ are distinct roots of A_z and their respective multiplicities $m_1, \ldots, m_r$ are constant on W.

We shall prove this theorem in the following section, but an essentially immediate consequence is the following result, which we shall apply to operators $T(z)$ satisfying A1, restricted to a finite-dimensional subspace:

Theorem 3.2. *Let $M : U \to M_{n \times n}(\mathbb{C})$ be analytic, where $U \subset \mathbb{C}$ open, $U \cap \mathbb{R}$ is non-empty, and $M(z)$ is Hermitian for all $z \in U \cap \mathbb{R}$. Then there exists a discrete set D such that on any simply connected open set $W \subset U \setminus D$, $W \cap \mathbb{R}$ non-empty, $M(z)$ can be decomposed as*

$$M(z) = \sum_{j=1}^{r} \lambda_j(z) \pi_j(z), \qquad \textit{where:} \tag{3.2}$$

- *$\lambda_1, \ldots, \lambda_r : W \to \mathbb{C}$ are analytic functions such that for all $z \in W$, $\lambda_1(z), \ldots, \lambda_r(z)$ are distinct eigenvalues of $M(z)$,*

- *$\pi_1, \ldots, \pi_r : W \to M_{n\times n}(\mathbb{C})$ are eigenprojectors of constant rank corresponding to $\lambda_1, \ldots,$ λ_r, respectively, analytic in z, satisfying $\pi_j(z)\pi_\ell(z) = \delta_{j\ell}\pi_j(z)$ for $j, \ell = 1, \ldots, r$.*

Proof. Let χ_z denote the characteristic polynomial of $M(z)$, using the convention that $\chi_z(\lambda) = \det(\lambda - M(z))$. Then χ_z is a monic degree n polynomial, and so by Theorem 3.1 there exists a discrete set D such that on any simply connected open set $W \subset U \setminus D$, there exist analytic functions $\lambda_1, \ldots, \lambda_r : W \to \mathbb{C}$ such that $\lambda_1(z), \ldots, \lambda_r(z)$ are the distinct eigenvalues of $M(z)$ for all $z \in W$.

For $z \in W$, let $\pi_j(z)$ be the projection onto the generalized eigenspace associated to $\lambda_j(z)$. We then claim that π_j depends analytically on z. Fix some $j \in \{1, \ldots, r\}$ and $z_0 \in W$, and let $\mathcal{C}$ be a simple, closed, positively-oriented contour such that $\lambda_j(z_0)$ is the only eigenvalue of $M(z_0)$ enclosed by $\mathcal{C}$. Since each of the functions λ_ℓ are continuous and there are only finitely many of them, there exists $\varepsilon > 0$ such that $\lambda_j(z)$ is the only eigenvalue of $M(z)$ enclosed by $\mathcal{C}$ for all $|z - z_0| < \varepsilon$. Consequently, from [Kni96, Theorem 3.3], π_j is given on $\mathbb{B}_\varepsilon(z_0)$ by

$$\pi_j(z) = -\frac{1}{2\pi i}\oint_{\mathcal{C}} (M(z) - \zeta)^{-1} d\zeta.$$

Since $z_0 \in W$ was arbitrary, this shows that π_j is analytic on W.

Lastly, observe that for $z \in W \cap \mathbb{R}$ (which is assumed to be non-empty), we can write $M(z)$ as in (3.2) since $M(z)$ is Hermitian on this set, and $\pi_j(z)\pi_\ell(z) = \delta_{j\ell}\pi_j(z)$ for $j, \ell \in \{1, \ldots, r\}$ on this set as well. By the identity theorem, these relations must then hold on all of W. As a result, for all j, π_j is in fact the eigenprojector corresponding to λ_j, and the corresponding eigenspaces are pairwise orthogonal. Since the multiplicities of the eigenvalues $\lambda_1, \ldots, \lambda_r$ are constant on W, we conclude that, for all j, rank $\pi_j(z)$ is constant on W as well. □

Returning to Theorem 3.1, we follow the work of [Kat95] and consider the behavior of the functions $\lambda_1(z), \ldots, \lambda_r(z)$ in a neighborhood of a point $z_0 \in D$. Since the set D is discrete, there exists an open ball B_0 centered at z_0 such that $D \cap B_0 = \{z_0\}$; by this same theorem, if we let $B \subset B_0 \setminus \{z_0\}$ be a smaller open ball, the roots of A_z can be expressed as the analytic functions $\lambda_j(z)$ for $j = 1, \ldots, r$ and for $z \in B$. If we now rotate the ball B around z_0, the functions $\lambda_j(z)$ can be continued analytically, and these extensions will continue to be roots of A_z. It follows that, after exactly one full rotation, the functions $\lambda_1(z), \ldots, \lambda_r(z)$ will have undergone a permutation P; as this is a permutation on a finite set of elements, after potentially reindexing we can partition the set $\{\lambda_j(z)\}_{j=1}^r$ into *cycles*:

$$\{\lambda_1(z), \ldots, \lambda_p(z)\},\ \{\lambda_{p+1}(z), \ldots, \lambda_{p+q}(z)\},\ \ldots, \tag{3.3}$$

meaning that the permutation P acts cyclically on each of the sets in (3.3), so that $P\lambda_j(z) = \lambda_{j+1}(z)$ for $j = 1, \ldots, p-1$, and $P\lambda_p(z) = \lambda_1(z)$. Given a root $\lambda_j(z)$, the *order* of $\lambda_j(z)$ under the permutation P (also often called its *period*) is the length of its corresponding cycle.

Let us now focus on the root $\lambda_1(z)$, and suppose this root has order p as in (3.3); the analysis is identical for any other root. Define

$$f(\omega) = \lambda_1(\omega^p + z_0)$$

with domain consisting of one of the connected components of the set

$$\{\omega \in \mathbb{C} \ : \ \omega^p + z_0 \in B_0\}.$$

By applying the same analytic continuation that defined the permutation P, it follows that f can be extended to an analytic function on $(B_0 - z_0) \setminus \{0\}$ (i.e. the translation of B_0 that it is centered at the origin with the origin removed). As a result, f has a Laurent series expansion of the form

$$f(\omega) = \sum_{\ell=-\infty}^{\infty} a_\ell \omega^\ell. \tag{3.4}$$

However, by continuity of roots, $\lim_{z\to z_0} \lambda_1(z) = \lambda$ for some $\lambda \in \mathbb{C}$ (which is called the *center* of the cycle), and so f is continuous at $\omega = 0$ and is equal to λ. Consequently $a_0 = \lambda$ and $a_\ell = 0$ for $\ell < 0$ in the series (3.4) (we remark that the sum of terms in (3.4) with negative degree is called the *principal part*, and so this latter consequence can be rephrased as saying the principal part of f is equal to 0). Thus we can rewrite f as

$$f(\omega) = \lambda + \sum_{\ell=1}^{\infty} a_\ell \omega^\ell. \tag{3.5}$$

If we now use the substitution $z = \omega^p + z_0$, so that $\omega = (z - z_0)^{1/p}$, then ω is one of p possible roots, and these roots differ by a factor of ζ_p^j, where $\zeta_p = e^{2\pi i/p}$ and $1 \leq j \leq p-1$. Plugging this into (3.5) and letting $(z-z_0)^{1/p}$ denote the principal root, we can then recover the functions $\lambda_1(z), \dots, \lambda_p(z)$ as *Puiseux series* of the form

$$\lambda_j(z) = \lambda + \sum_{\ell=1}^{\infty} a_\ell \zeta_p^{\ell(j-1)} (z-z_0)^{\ell/p}. \tag{3.6}$$

This is summarized by saying that, if $p \geq 2$, then z_0 is a *branch point* of *algebraic order p*. If the length of the cycle were infinite, we would instead say that z_0 is a *logarithmic branch point*; however, such a point is impossible when considering the roots of the polynomial A_z, for as previously noted the permutation P must send each root $\lambda_j(z)$ to one of at most $n = \deg A_z$ roots.

We next perform a similar analysis for the eigenprojectors $\pi_1(z), \dots, \pi_r(z)$ near $x_0 \in D \cap \mathbb{R}$. Just as before, we let B_0 be an open ball centered at x_0 such that $D \cap B_0 = \{x_0\}$, and let $B \subset B_0 \setminus \{z_0\}$ be a smaller open ball centered at some $x_1 \in \mathbb{R}$. Then by Theorem 3.2, $M(z)$ has a decomposition of the form (3.2) on B. In addition, since $\overline{B_0}$ is compact, by continuity of roots, the set

$$\{\zeta \in \mathbb{C} \ : \ \det(M(z) - \zeta) = 0 \text{ for } z \in \overline{B_0}\}$$

is bounded, say by C. Then for fixed $|\zeta| > C$, the resolvent $(M(z) - \zeta)^{-1}$ is necessarily defined and moreover analytic in z on B_0. On the set B, we can write $(M(z) - \zeta)^{-1}$ using (3.2) as

$$(M(z) - \zeta)^{-1} = \sum_{j=1}^{r} \frac{1}{(\lambda_j(z) - \zeta)} \pi_j(z).$$

As a result, if we rotate B around the point x_0, the functions $(M(z) - \zeta)^{-1}, \lambda_j(z)$, and $\pi_j(z)$ for $j = 1, \ldots, r$ can all be continued analytically, and these extensions will continue to be the resolvent, eigenvalues, and eigenprojectors, respectively, of $M(z)$. Just as before, this process induces a permutation P on the eigenvalues and eigenprojectors, but since $(M(z) - \zeta)^{-1}$ is analytic on B_0 it will be left unchanged. We therefore get that

$$\begin{aligned}\sum_{j=1}^{r} \frac{1}{(\lambda_j(z) - \zeta)} \pi_j(z) &= (M(z) - \zeta)^{-1} = P(M(z) - \zeta)^{-1} \\ &= \sum_{j=1}^{r} \frac{1}{(P\lambda_j(z) - \zeta)} P\pi_j(z).\end{aligned} \tag{3.7}$$

We now focus on the eigenprojector $\pi_1(z)$, noting that the analysis for the other eigenprojectors is identical. Again let p denote the order of the corresponding eigenvalue $\lambda_1(z)$ under the permutation P, and assume that both the eigenvalues and eigenprojectors have been indexed corresponding to the cycles of the eigenvalues as in (3.3). Then by the uniqueness of partial fraction decompositions, we deduce from (3.7) that $P\pi_j(z) = \pi_{j+1}(z)$ for $1 \leq j \leq p - 1$, and $P\pi_p(z) = \pi_1(z)$, and so $\pi_1(z)$ has order at most p under the permutation P. To see that $\pi_1(z)$ has order exactly p, recall from Theorem 3.2 that $\pi_j(z)\pi_\ell(z) = \delta_{j\ell}\pi_j(z)$ for $j, \ell = 1, \ldots, r$, and consequently $\pi_1(z), \ldots, \pi_p(z)$ must all be distinct. We therefore conclude that $\pi_1(z)$ has order p.

The following result, due to John Butler [But59], will enable us to prove a stronger version of Theorem 3.2.

Proposition 3.1. *Let $x_0 \in D \cap \mathbb{R}$ be a branch point of order $p \geq 2$. Then for $j = 1, \ldots, p$, $\pi_j(x)$ has a pole at x_0.*

Remark 3.3. This result is more generally true for any branch point $z_0 \in D$ of order $p \geq 2$, not just those in $\mathbb{R}$, although we will only need to consider the case $x_0 \in D \cap \mathbb{R}$ for our purposes.

Proof of Proposition 3.1. First note that, since $\pi_j(z)$ has order p for $j = 1, \dots, p$, we can expand π_j in a Puiseux series around x_0 just as we did for the eigenvalues $\lambda_1(z), \dots, \lambda_p(z)$, and thus there exist matrices $\pi_{j,\ell}$ such that

$$\pi_j(z) = \sum_{\ell=-\infty}^{\infty} \pi_{j,\ell}(z - x_0)^{\ell/p}$$

near x_0. Applying the permutation P to $\pi_j(z)$ we compute that, for $1 \le j \le p-1$

$$\sum_{\ell=-\infty}^{\infty} \pi_{j+1,\ell}(z - x_0)^{\ell/p} = \pi_{j+1}(z) = P\pi_j(z) = \sum_{\ell=-\infty}^{\infty} \pi_{j,\ell}\zeta_p^{\ell}(z - x_0)^{\ell/p}, \tag{3.8}$$

where again $\zeta_p = e^{2\pi i/p}$. Equating coefficients for the first and last expressions in (3.8), we deduce that $\pi_{j,0} = \pi_{j+1,0}$ for $1 \le j \le p-1$. An identical argument shows that $\pi_{p,0} = \pi_{1,0}$ as well.

Now suppose for contradiction that π_j does not have a pole at x_0, so that π_j can be written as

$$\pi_j(z) = \sum_{\ell=0}^{\infty} \pi_{j,\ell}(z - x_0)^{\ell/p}. \tag{3.9}$$

Since we can recover each of the projections $\pi_\ell(z)$ from $\pi_j(z)$ for $\ell \neq j$ by successive applications of the permutation P, this implies that none of the eigenprojectors $\pi_1(z), \dots, \pi_p(z)$ have a pole at x_0, and thus each can be written in the form (3.9). In particular this implies that $\pi_j(z)$ is continuous at x_0 for $j = 1, \dots, p$. Therefore, by Theorem 3.2, we have that, for $j = 1, \dots, p$,

$$\pi_{j,0}\pi_{j+1,0} = \left(\lim_{z\to x_0} \pi_j(z)\right)\left(\lim_{z\to x_0} \pi_{j+1}(z)\right) = \lim_{z\to x_0} \pi_j(z)\pi_{j+1}(z) = 0.$$

A similar argument, using the fact that $\pi_j(z)^2 = \pi_j(z)$, shows that $\pi_{j,0}^2 = \pi_{j,0}$. Putting this all together, we conclude that

$$\pi_{j,0} = \pi_{j,0}\pi_{j,0} = \pi_{j,0}\pi_{j+1,0} = 0.$$

This, however, is a contradiction. A lemma due to Tosio Kato [Kat95, Lemma I.4.10] states that if $\tilde{\pi}_1$, $\tilde{\pi}_2$ are two projectors such that $||\tilde{\pi}_1 - \tilde{\pi}_2|| < 1$, then $\tilde{\pi}_1$ and $\tilde{\pi}_2$ have the same (potentially infinite) rank.[1] It follows that, for sufficiently small z, $\operatorname{rank} \pi_j(z) = \operatorname{rank} 0 = 0$, which contradicts the fact that $\operatorname{rank} \pi_j(z)$ is equal to the multiplicity $m_j > 0$ of $\lambda_j(z)$ for all $z \notin D$. Therefore $\pi_1, \dots, \pi_p$ must all have a pole at $z = x_0$. □

[1] In Kato's book this property is shown for projectors on a finite-dimensional vector space. One can check that the proof applies to infinite-dimensional vector spaces as well.

Theorem 3.4. *Let $M : U \to M_{n\times n}(\mathbb{C})$ be analytic, where $U \subset \mathbb{C}$ open, $I := U \cap \mathbb{R}$ is non-empty, and $M(z)$ is Hermitian for all $z \in U \cap \mathbb{R}$. Then there exists an open neighborhood W of I and a discrete set $D \subset I$ such that on W, $M(z)$ can be decomposed as*

$$M(z) = \sum_{j=1}^{r} \lambda_j(z)\pi_j(z), \qquad \text{where:} \tag{3.10}$$

- *$\lambda_1, \ldots, \lambda_r : W \to \mathbb{C}$ are analytic functions such that for all $z \in W \setminus D$, $\lambda_1(z), \ldots, \lambda_r(z)$ are distinct eigenvalues of $M(z)$,*
- *$\pi_1, \ldots, \pi_r : W \to M_{n\times n}(\mathbb{C})$ are eigenprojectors of constant rank corresponding to $\lambda_1, \ldots,$ λ_r, respectively, analytic in z, satisfying $\pi_j(z)\pi_\ell(z) = \delta_{j\ell}\pi_j(z)$ for $j, \ell = 1, \ldots, r$.*

Proof. This will be an immediate consequence of Theorem 3.2 if we can show that for $x_0 \in D \cap \mathbb{R}$, the functions $\lambda_1, \ldots, \lambda_r$ have order one when analytically continued around each of these points, and therefore can be extended to analytic functions on a neighborhood of these points via equation (3.6). Towards that end, let $x_0 \in D \cap \mathbb{R}$, and let $W \subset U \setminus D$, $W \cap \mathbb{R} \neq \emptyset$ be a simply connected open set such that $x_0 \in \overline{W}$. Then on W, $M(z)$ has a decomposition of the form (3.10). Let $\{x_n\}_{n\in\mathbb{N}} \subset W \cap \mathbb{R}$ such that $x_n \to x_0$; then due to the fact that $M(z)$ is Hermitian for $z \in U \cap \mathbb{R}$, the eigenprojectors $\pi_1, \ldots, \pi_r$ are orthogonal, and therefore satisfy $||\pi_j(x_n)|| = 1$ for $n \in \mathbb{N}$ and $j = 1, \ldots, r$. As a a result, for $j = 1, \ldots, r$

$$\lim_{n\to\infty} ||\pi_j(x_n)|| = 1,$$

and so $\pi_1, \ldots, \pi_r$ cannot have poles at x_0. Thus, by Proposition 3.1, x_0 cannot be a branch point of order $p \geq 2$ for any of the functions $\lambda_1, \ldots, \lambda_r$, and so each of these functions must have order one. □

3.2 *Proof of Theorem 3.1*

To prove Theorem 3.1, we use an extension of the notion of a *Sylvester matrix*.

Definition 3.1. *Let P_j be the vector space of complex polynomials of degree less than or equal to j, and let $A \in P_n$ and $B \in P_m$. Define $\phi_{A,B} : P_{m-1} \times P_{n-1} \to P_{m+n-1}$ by*

$$\phi_{A,B}(Q_1, Q_2) = AQ_1 + BQ_2.$$

Then $\phi_{A,B}$ is a linear map called the Sylvester matrix associated to A and B.

We will generalize the Sylvester matrix as follows. Let $A_1, \ldots, A_m$ be a collection of polynomials for some $m \geq 2$, let $n_j = \deg A_j$, and let $n = n_1 + \cdots + n_m$. We introduce

$$\phi_{A_1,\ldots,A_m} : \prod_{j=1}^{m} P_{n-n_j-1} \to P_{n-1}$$
$$(Q_1, \ldots, Q_m) \mapsto \sum_{j=1}^{m} A_j Q_j$$

Lemma 3.1. *The image of $\phi_{A_1,\ldots,A_m}$ is the intersection of P_{n-1} with the ideal* $(\gcd(A_1, \ldots, A_m))$.

Proof. It is immediate from the definition of $\phi_{A_1,\ldots,A_m}$ that

$$\operatorname{im} \phi_{A_1,\ldots,A_m} \subset P_{n-1} \cap (\gcd(A_1, \ldots, A_m)).$$

To see the reverse containment, by re-indexing the A_j's if necessary, we may assume that $\deg(A_1) \leq \deg(A_j)$ for $j = 2, \ldots, m$. As a result, if $\sum_{j=1}^{m} A_j Q_j$ has degree less than or equal to $n-1$, then we can divide each of $Q_2, \ldots, Q_m$ by A_1, so that there exist polynomials $\widetilde{Q}_j, B_j$ such that

$$Q_j = A_1 B_j + \widetilde{Q}_j \quad \text{and} \quad \deg(\widetilde{Q}_j) < \deg(A_1) = n_1.$$

By our assumptions that $m \geq 2$ and $n_1 = \deg(A_1) \leq \deg(A_j) = n_j$ for $j \neq 1$, we get that $n_1 \leq \sum_{\ell \neq j} n_\ell = n - n_j$ for all $j \neq 1$. Putting this together, we get that $\deg(\widetilde{Q}_j) < n - n_j$, and so $\widetilde{Q}_j \in P_{n-n_j-1}$. In addition, we can now write

$$\sum_{j=1}^{m} A_j Q_j = A_1 Q_1 + \sum_{j=2}^{m} A_i (A_1 B_j + \widetilde{Q}_j) = A_1 \left(Q_1 + \sum_{j=2}^{m} A_j B_j \right) + \sum_{j=2}^{m} A_j \widetilde{Q}_j.$$

From here, observe that since $\widetilde{Q}_j \in P_{n-n_j-1}$ for $j = 2, \ldots, m$, the sum $\sum_{j=2}^{m} A_j \widetilde{Q}_j$ is a polynomial of degree less than or equal to $n-1$. Consequently, we must have that

$$\deg \left(A_1 \left(Q_1 + \sum_{j=2}^{m} A_j B_j \right) \right) \leq n - 1$$

as well, for otherwise the original sum $\sum_{j=1}^{m} A_j Q_j$ would not be a polynomial of degree less than or equal to $n-1$. Therefore, if we let $\widetilde{Q}_1 = Q_1 + \sum_{j=2}^{m} A_j B_j$, then $\widetilde{Q}_1 \in P_{n-n_1-1}$. Thus we get that

$$\sum_{j=1}^{m} A_j Q_j = \sum_{j=1}^{m} A_j \widetilde{Q}_j \in \operatorname{im} \phi_{A_1,\ldots,A_m},$$

and so $\operatorname{im} \phi_{A_1,\ldots,A_m} = P_{n-1} \cap (\gcd(A_1, \ldots, A_m))$, as claimed. $\square$

The reason Lemma 3.1 is important is because if we let $B = \gcd(A_1, \ldots, A_m)$, then

$$\begin{aligned}\operatorname{rank}\phi_{A_1,\ldots,A_m} &= \dim((B) \cap P_{n-1}) \\ &= \dim\{Q \in P_{n-1} \ : \ BQ \in P_{n-1}\} \\ &= \dim\{Q \in P_{n-1} \ : \ \deg Q \leq n - \deg B - 1\} \\ &= n - \deg B.\end{aligned}$$

Lemma 3.2. *Let $M : U \to M_{n\times n}(\mathbb{C})$ be analytic, where $U \subset \mathbb{C}$ is open and connected. The rank of $M(z)$ is constant except possibly at a discrete set of points in U.*

Proof. Pick $z_0 \in U$ such that $\operatorname{rank} M(z_0)$ is maximal, which exists since $\operatorname{rank} M(z)$ can take only integer values from 0 to n, and let $r = \operatorname{rank} M(z_0)$. Then there exists an $r \times r$ submatrix $M_0(z)$ of $M(z)$ such that $M_0(z_0)$ has full-rank. As a result, $\det(M_0(z))$ is an analytic function in z on U, and is nonzero at z_0, and therefore is also nonzero on all of U except possibly at a discrete set of points D. This then implies that $\operatorname{rank} M(z) \geq r$ on $U \setminus D$, which by maximality implies $\operatorname{rank} M(z) = r$ on $U \setminus D$. □

Using this lemma and our generalization of the Sylvester matrix outlined above, we can now prove the following proposition.

Proposition 3.2. *Let $\{A_z\}_{z\in U}$ be an analytic family of monic degree n polynomials in $\mathbb{C}[x]$, for some $U \subset \mathbb{C}$ open. Then there exists a discrete set D such for $j = 1, \ldots, n$,*

$$\rho_j = |\{\lambda \text{ is a root of } A_z \text{ of multiplicity } j\}|$$

is independent of $z \in U \setminus D$

Proof. For simplicity of notation, we define the following maps:

$$\phi_1 = \phi_{A_z, A_z'}, \quad \phi_2 = \phi_{A_z, A_z', A_z''}, \quad \ldots \quad \phi_n = \phi_{A_z, \ldots, A_z^{(n)}}, \tag{3.11}$$

where each of the derivatives in (3.11) is being taken with respect to x (as opposed to z). Similarly, we define:

$$B_1 = \gcd(A_z, A_z'), \quad B_2 = \gcd(A_z, A_z', A_z''), \quad \ldots \quad B_n = \gcd(A_z, \ldots, A_z^{(n)}),$$

and lastly we define $d_j = \deg B_j$ for $j = 1, \ldots, n$.

Let $n_j = \sum_{\ell=0}^{j} \deg A_z^{(\ell)} = \sum_{\ell=0}^{j} n - \ell$; then our arguments preceding this proposition tell us that $\operatorname{rank}\phi_j = n_j - d_j$. In addition, observe that ϕ_k depends analytically on z for $k = 1, \ldots, n$, since the entries of ϕ_k, viewed as a matrix, consist either of the coefficients of A_z and its derivatives or are otherwise zero. Consequently, by Lemma 3.2 there exists a discrete set $D_j \subset U$ such that d_j is constant on $U \setminus D_j$. Letting $D = \cup_{j=1}^{n} D_j$, D is then also discrete as a finite union of discrete sets, and by construction d_j is constant on $U \setminus D$ for $j = 1, \ldots, n$.

Now let $z_0 \in U \setminus D$; our assumption that A_z is monic implies that we can write

$$A_{z_0}(x) = \prod_{j=1}^{r} (x - \lambda_j)^{m_j},$$

where $\lambda_1, \ldots, \lambda_r$ are the r distinct roots of A_{z_0}, and $m_1, \ldots, m_r$ are the corresponding multiplicities. It then follows that

$$\begin{aligned} B_1 &= \prod_{\ell\,:\,m_\ell > 1} (x - \lambda_\ell)^{m_\ell - 1} \\ B_2 &= \prod_{\ell\,:\,m_\ell > 2} (x - \lambda_\ell)^{m_\ell - 2} \\ &\vdots \\ B_{n-1} &= \prod_{\ell\,:\,m_\ell = n} (x - \lambda_\ell) \\ B_n &= 1. \end{aligned}$$

A consequence of these formulas is that

$$|\{\lambda_\ell \text{ is a root of } A_{z_0} \;:\; m_\ell > j\}| = \deg B_j - \deg B_{j+1} = d_j - d_{j+1}.$$

As a result,

$$\begin{aligned} \rho_j &= |\{\lambda \text{ is a root of } A_{z-0} \text{ of multiplicity } j\}| \\ &= |\{\lambda_\ell \text{ is a root of } A_{z_0} \;:\; m_\ell > j-1\}| - |\{\lambda_\ell \text{ is a root of } A_{z_0} \;:\; m_\ell > j\}| \\ &= (d_{j-1} - d_j) - (d_j - d_{j+1}), \end{aligned}$$

where d_0 is understood to be n and $d_j = 0$ for $j > n$. Since z_0 was arbitrary, this tells us that ρ_j is constant on $U \setminus D$ as a sum of constant functions. Therefore, the number of distinct roots of A_z of any given multiplicity is constant on $U \setminus D$. □

Theorem 3.5. *(Local version) Let $z_* \in U \setminus D$. There exists $\varepsilon > 0$ such that the conclusion of Theorem 3.1 holds on $W = \mathbb{B}_\varepsilon(z_*)$.*

Proof. Let $\lambda_1, \ldots, \lambda_r$ be the distinct roots of A_{z_*}, and let

$$\delta = \frac{1}{2} \min_{j \neq \ell} |\lambda_j - \lambda_\ell|. \tag{3.12}$$

We then say $m \in \{1, \ldots, n\}$ is *ε-good* if for every root λ of A_{z_*} of multiplicity m, $\mathbb{B}_\delta(\lambda)$ contains a root of A_z of multiplicity m for all $z \in \mathbb{B}_\varepsilon(z_*)$.

We claim that for any $m \in \{1, \ldots, n\}$, there exists $\varepsilon > 0$ such that m is ε-good. Suppose for contradiction that m is not ε-good for any $\varepsilon > 0$; without loss of generality, we may assume that m is maximal with respect to this property. Then for every $\varepsilon > 0$, there exists a root λ of A_{z_*} of multiplicity m and a $z \in \mathbb{B}_\varepsilon(z_*)$ such that $\mathbb{B}_\delta(\lambda)$ does not contain a root of A_z of multiplicity m. Therefore, if we let Σ denote the set of roots of A_{z_*} of multiplicity m, we can construct sequences $(z_j)_{j\in\mathbb{N}} \subset U \setminus D$, $z_j \to z_*$ and $(\lambda_j)_{j\in\mathbb{N}} \subset \Sigma$ such that for all j, A_{z_j} does not contain a root of multiplicity m in $\mathbb{B}_\delta(\lambda_j)$. Since A_{z_*} has only finitely many roots, by passing to subsequences if necessary, we may assume that $\lambda_j = \lambda_*$ is independent of j.

From here, note that $\rho := |\Sigma|$ is independent of z by Proposition 3.2, and for all $j \in \mathbb{N}$, none of the ρ roots of A_{z_j} of multiplicity m are contained in $\mathbb{B}_\delta(\lambda_*)$. Therefore, for each j, we must either have that there exists a $\tilde{\lambda}_j$ such that A_{z_j} has two roots in $\mathbb{B}_\delta(\tilde{\lambda}_j)$ of multiplicity m, or there exists a root $\tilde{\lambda}_j$ of A_{z_j} of multiplicity m that is not contained in $\mathbb{B}_\delta(\lambda)$ for any $\lambda \in \Sigma$. Therefore, by again passing to subsequences if necessary, one of two situations must hold:

- there exists $\tilde{\lambda}_* \in \Sigma$ such that for all j, A_{z_j} has two roots of multiplicity m in $\mathbb{B}_\delta(\tilde{\lambda}_*)$,
- for each $j \in \mathbb{N}$, there exists $\lambda_j \notin \cup_{\lambda\in\Sigma}\mathbb{B}_\delta(\lambda)$, λ_j a root of A_{z_j} of multiplicity m.

Assume the first situation holds. Since the set $\partial\mathbb{B}_\delta(\tilde{\lambda}_*)$ is compact, A_{z_j} converges uniformly to A_{z_*} on this set. Because of (3.12), A_{z_*} has no zeroes on $\partial\mathbb{B}_\delta(\tilde{\lambda}_*)$, and therefore uniform convergence tells us that for sufficiently large j and $\zeta \in \partial\mathbb{B}_\delta(\tilde{\lambda}_*)$,

$$|A_{z_j}(\zeta) - A_{z_*}(\zeta)| < \inf_{\partial\mathbb{B}_\delta(\tilde{\lambda}_*)} |A_{z_*}| \leq |A_{z_*}(\zeta)|.$$

By Rouché's theorem, A_{z_j} and A_{z_*} have the same number of zeroes in $\mathbb{B}_\delta(\tilde{\lambda}_*)$, counted with multiplicity. However, this is a contradiction, as A_{z_j} has at least $2m$ zeroes in this set, counted with multiplicity, while A_{z_j} by assumption has precisely m zeroes.

Now assume the second situation holds; we first show that the sequence $(\lambda_j)_{j\in\mathbb{N}}$ is bounded. Note that the sequence (z_i) is bounded by virtue of being convergent, and thus there exists $C > 0$ such that $|z_j - z_*| < C$ for all j. In addition, if we write

$$A_z(x) = x^n + a_{n-1}(z)x^{n-1} + \cdots + a_1(z)x + a_0(z),$$

then by definition of A_z being analytic in z, so too are functions $a_\ell(z)$ for $\ell = 0, \ldots, n-1$. As a result, $a'_\ell(z)$ exists and is bounded on the closed disk $\overline{\mathbb{B}_C(z_*)}$, say by C_ℓ, for $\ell = 0, \ldots, n-1$. This implies that for $\ell = 0, \ldots, n-1$ and positive integers j,

$$|a_\ell(z_j) - a_\ell(z_*)| \leq C_\ell |z_\ell - z_*| \leq C \cdot C_\ell.$$

Lagrange's bound on polynomial roots, together with the reverse triangle inequality, then tells us that for all positive integers j,

$$|\lambda_j| \leq \max\left\{1, \sum_{\ell=0}^{n-1} |a_\ell(z_j)|\right\} \leq \max\left\{1, \sum_{\ell=0}^{n-1} |a_\ell(z_*)| + C \cdot C_\ell\right\}.$$

Consequently the sequence $(\lambda_j)_{j\in\mathbb{N}}$ is bounded.

Since the sequence is bounded, by again passing to a subsequence if necessary, we may assume that λ_j converges to some λ_∞. In addition, since λ_j is a root of A_{z_j} of multiplicity m for all j, it is a root of $A_{z_j}^{(\ell)}$ for $\ell = 0, \dots, m-1$ (where again the derivative is being taken with respect to x, and not z). Therefore, for $\ell = 0, \dots, m-1$,

$$A_{z_*}^{(\ell)}(\lambda_\infty) = A_{\lim_{j\to\infty} z_j}^{(\ell)}\left(\lim_{j\to\infty} \lambda_j\right) = \lim_{j\to\infty} A_{z_j}^{(\ell)}(\lambda_j) = \lim_{j\to\infty} 0 = 0.$$

Therefore λ_∞ is a root of A_{z_*} of multiplicity at least m. However, $d(\lambda_\infty, \Sigma) \geq \delta$ since $\delta(\lambda_j, \Sigma) \geq \delta$ by assumption, and therefore by (3.12), λ_∞ must in fact have multiplicity strictly greater than m, which we denote by m'. Since m is assumed to be the maximal integer that is not ε-good for any ε, it follows that m' is ε-good for some $\varepsilon > 0$. Therefore, for sufficiently large j, $\mathbb{B}_\delta(\lambda_\infty)$ contains both λ_j (which is a root of multiplicity m) and a root of multiplicity m', distinct from λ_j. However, Rouché's theorem implies that λ_∞ is then a root of A_{z_*} of multiplicity $m' + m$, which is a contradiction. Consequently, the set of $m \in \{1, \dots, n\}$ which is not ε-good for any $\varepsilon > 0$ is empty, thus proving the claim.

Hence there exists a $\varepsilon > 0$ such that for all $m \in \{1, \dots, m\}$, m is ε-good, and by shrinking ε if necessary, we may assume that $\mathbb{B}_\varepsilon(z_*) \subset U \setminus D$. That is, if $z \in \mathbb{B}_\varepsilon(z_*)$ and λ_* is a root of A_{z_*} of multiplicity m, then $\mathbb{B}_\delta(\lambda_*)$ contains precisely one root of A_z of multiplicity m, which we denote by $\lambda(z)$. Because this holds for every root λ_* of A_{z_*} and the sum of multiplicities of the roots of A_z equals n, we conclude that $\lambda(z)$ is the only root of A_z contained in $\mathbb{B}_\delta(\lambda_*)$. Therefore, by the residue theorem,

$$\lambda(z) = \frac{1}{2\pi i m} \oint_{\partial\mathbb{B}_\delta(\lambda_*)} \frac{\zeta A_z'(\zeta)}{A_z(\zeta)} d\zeta.$$

Since the integral on the right-hand side is analytic in z, this implies that $\lambda(z)$ is analytic on $\mathbb{B}_\varepsilon(z_*)$. Doing this for each root λ_* of A_{z_*}, we get the decomposition (3.1) on $\mathbb{B}_\varepsilon(z_*)$, as desired. □

We can now prove Theorem 3.1 using a combination of the local version (Theorem 3.5) together with the monodromy theorem.

Proof of Theorem 3.1. Let $W \subset U \setminus D$ be a simply connected open set and let $z_0 \in W$. Then by Theorem 3.5, there exists an open disk $B \subset W$, centered at z_0, such that the decomposition (3.1) holds on B.

Now the monodromy theorem tells us that if there exists an analytic continuation of λ_j along any path contained in W starting at z_0, then there exists an extension of λ_j to all of W. In particular, by an analytic continuation of λ_j along a path $\gamma : [0,1] \to \mathbb{C}$, we mean that, for each $t \in [0,1]$, there exists an open disk B_t, centered at $\gamma(t)$, and an analytic map $\mu_t : B_t \to \mathbb{C}$ satisfying

(1) $B_0 = B$ and $\mu_0 = \lambda_j$

(2) For each $t \in [0,1]$ there exists $\varepsilon > 0$ such that for all $t' \in [0,1]$ with $|t - t'| < \varepsilon$, $\gamma(t') \in B_t$ and $\mu_{t'} = \mu_t$ on $B_{t'} \cap B_t$.

Therefore, to apply this theorem, let $j \in \{1, \ldots, r\}$, and let $\gamma : [0,1] \to W$ be a path satisfying $\gamma(0) = z_0$. To show that there exists an analytic continuation of λ_j along the path γ, we first apply Theorem 3.5 again to $\gamma(t)$ for each $t \in [0,1]$ to get an open disk $\widetilde{B}_t$, centered at $\gamma(t)$, such that the decomposition (3.1) exists on $\widetilde{B}_t$. Then for each t, define I_t to be the connected component of $\gamma^{-1}(\widetilde{B}_t)$ containing t. It follows that $\{I_t\}_{t \in [0,1]}$ is an open cover of $[0,1]$, and since this latter set is compact, there exists a finite subcover, which we denote by $\{I_\ell\}_{\ell=1}^{s}$ for some positive integer s. For each interval I_ℓ, we denote the corresponding t and open disk $\widetilde{B}_t$ by t_ℓ and B_ℓ, respectively. To ensure that our eventual analytic continuation satisfies property (1) above, we also add the connected component of $\gamma^{-1}(B_0)$ containing 0, which we denote by I_0, so that the subcover is now given by $\{I_\ell\}_{\ell=0}^{s}$, and $t_0 = 0$ and $B_0 = B$. Furthermore, by taking a minimal subcover and reindexing and shrinking the sets I_ℓ for $\ell > 0$ if necessary, we may assume that $I_0 = [0, b_0)$, $I_\ell = (a_\ell, b_\ell)$ for $\ell = 1, \ldots, s-1$, and $I_s = (a_s, 1]$, where $0 < a_1 < \cdots < a_s$ and $b_0 < \cdots < b_{s-1} < 1$.

For each of the open disks B_ℓ we now need analytic maps $\mu_\ell : B_\ell \to \mathbb{C}$ for $0 \leq \ell \leq s$, which we pick inductively. For the base case, simply let $\mu_0 = \lambda_j$. For the inductive case, assume that there exists an analytic map $\mu_\ell : B_\ell \to \mathbb{C}$ for some $0 < \ell < s$ such that μ_ℓ is a root of A_z for all $z \in B_\ell$. Then $B_\ell \cap B_{\ell+1}$ must be both nonempty, as it contains $\gamma(I_\ell \cap I_{\ell+1}) = \gamma((a_{\ell+1}, b_\ell))$, and connected, as it is the intersection of two disks, and so on $B_\ell \cap B_{\ell+1}$ the map μ_ℓ must equal precisely one of the roots of the decomposition (3.1) on $B_{\ell+1}$. Thus we can let $\mu_{\ell+1}$ be this root.

To finish the proof of the existence of an analytic continuation of λ_j along γ, now let $t \in [0,1]$ be arbitrary. Then $t \in I_i$ for some i, and consequently there exists an open disk $B_t \subset B_\ell$ centered at $\gamma(t)$, and we can let $\mu_t = \mu_\ell|_{B_t}$. In addition, since I_ℓ is open, there exists $\varepsilon > 0$ such that $(t \pm \varepsilon) \subset I_\ell$. As a result, for all $t' \in [0,1]$ satisfying $|t' - t| < \varepsilon$, $\gamma(t') \in B_t \subset B_\ell$, from which it follows by construction of the pairs (B_ℓ, μ_ℓ) for $\ell = 0, \ldots, s$, that $\mu_{t'} = \mu_\ell = \mu_t$ on $B_{t'} \cap B_t$. Thus there exists an analytic continuation of λ_j along γ, and since $j \in \{1, \ldots, r\}$ was arbitrary, the monodromy theorem tells us that there exist extensions of $\lambda_1, \ldots, \lambda_r$ to all of W. Moreover, these functions must still be roots of A_z on W, as they are roots along any path in W.

To conclude, we note that the functions $z \mapsto \text{mult}(\lambda_j(z))$ are locally constant on W, and since W is assumed to be simply connected, and thus also connected, it follows that these functions are in fact constant on W. In particular, this means that the multiplicities of the roots $\lambda_1, \ldots, \lambda_r$ are constant on W. This in turn implies that these roots must be distinct for all $z \in W$, for otherwise their multiplicities would not be constant. $\square$

3.3 Perturbation Theory

In addition to the above tools, the proof of our main theorem also requires some techniques from perturbation theory and variation of eigenvalues. In particular, given an operator T, we will focus on an analysis of the resolvent $(T - \lambda)^{-1}$, our primary tools for which will be the Schur complement formula and Cauchy's integral formula.

Definition 3.2. *Let T be an operator on a vector space $V = V_1 \oplus V_2$ such that, with respect to this decomposition:*

$$T = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

When the block D is invertible, the operator $A - BD^{-1}C$ is called the Schur complement of D, and is denoted by T/D.

This definition is helpful because if both D and its Schur complement T/D are invertible, then so too is T itself, as the following proposition shows. It is easily proven via a direct computation, and its derivation can be found in [Zha05].

Proposition 3.3. (Schur Complement Formula) *Let T be as above, and assume that both D and T/D are invertible. Then T is invertible, and its inverse is:*

$$T^{-1} = \begin{pmatrix} (T/D)^{-1} & -(T/D)^{-1}BD^{-1} \\ -D^{-1}C(T/D)^{-1} & D^{-1} + D^{-1}C(T/D)^{-1}BD^{-1} \end{pmatrix}^{2}.$$

Theorem 3.6. (Cauchy's Integral Formula) *Let f be analytic in the simply connected domain D and let $\mathcal{C}$ be a simple, closed, positively oriented contour in D. Then if z_0 is a point that lies in the region enclosed by $\mathcal{C}$,*

$$f(z_0) = \frac{1}{2\pi i} \oint_{\mathcal{C}} \frac{f(z)}{z - z_0} dz.$$

[2] A similar formula holds when A and $D - CA^{-1}B$ are assumed to be invertible, but we will not use it here.

Note that the above formula applies to Banach-valued functions, and not just complex-valued functions [Kat95]. In particular, given an operator T and a simple, closed, positive-oriented contour $\mathcal{C}$ contained in the resolvent set of T, we define the *spectral (or Riesz) projector* corresponding to $\mathcal{C}$ to be

$$\pi = -\frac{1}{2\pi i}\oint_{\mathcal{C}} (T-\lambda)^{-1} d\lambda. \tag{3.13}$$

By evaluating this operator on an eigenvector corresponding to an eigenvalue μ of $T(z)$ contained in $\mathbb{B}_\delta(\mu_0)$ and using Theorem 3.6, one can check that this operator restricts to the identity on the corresponding eigenspace, and in particular the image of this operator contains all eigenspaces corresponding to eigenvalues μ of $T(z)$ contained in $\mathbb{B}_\delta(\mu_0)$. More generally, π is in fact a projector, as the following lemma shows.

Lemma 3.3. *Let T be an operator and let $\mathcal{C}$ be a simple, closed, positive-oriented contour $\mathcal{C}$ contained in the resolvent set of T. Then the operator π defined in* (3.13) *is a projector.*

Proof. Let $\mathcal{C}_0$ be a simple, closed, positively-oriented contour contained in both the interior of $\mathcal{C}$ and the resolvent set of T (which exists since the resolvent set of T is open). By the residue theorem, π is equal to the integral in (3.13), but with $\mathcal{C}$ replaced with $\mathcal{C}_0$. Then by the first resolvent identity,

$$\begin{aligned}
\pi^2 &= \frac{1}{(2\pi i)^2}\oint_{\mathcal{C}_0}(T-\mu)^{-1}d\mu \oint_{\mathcal{C}}(T-\lambda)^{-1}d\lambda \\
&= \frac{1}{(2\pi i)^2}\oint_{\mathcal{C}_0}\oint_{\mathcal{C}}\frac{(T-\mu)^{-1}-(T-\lambda)^{-1}}{\mu-\lambda}d\lambda d\mu \\
&= \frac{1}{(2\pi i)^2}\left(\oint_{\mathcal{C}_0}(T-\mu)^{-1}\oint_{\mathcal{C}}\frac{1}{\mu-\lambda}d\lambda d\mu - \oint_{\mathcal{C}}(T-\lambda)^{-1}\oint_{\mathcal{C}_0}\frac{1}{\mu-\lambda}d\mu d\lambda\right) \\
&= \frac{1}{(2\pi i)^2}\left(\oint_{\mathcal{C}_0}(T-\mu)^{-1}(-2\pi i)d\mu - \oint_{\mathcal{C}}(T-\lambda)^{-1}(0)d\lambda\right) \\
&= -\frac{1}{2\pi i}\oint_{\mathcal{C}_0}(T-\mu)^{-1}d\mu = \pi.
\end{aligned}$$

□

For the rest of the current and the following sections, we restrict our attention to analytic families of closed operators $T(z)$ satisfying A1, and a corresponding eigenvalue $\mu : (a,b) \to \mathbb{R}$ satisfying A2.

Lemma 3.4. *Let $z_0, \mu_0 \in \mathbb{C}$ such that μ_0 is an eigenvalue of $T(z_0)$. There exist $\varepsilon, \delta > 0$ such that:*

(1) μ_0 is the only eigenvalue of $T(z_0)$ in $\mathbb{B}_\delta(\mu_0)$,

(2) *for every* $z \in \mathbb{B}_\varepsilon(z_0)$*,* $T(z)$ *has no eigenvalue on* $\partial\mathbb{B}_\delta(\mu_0)$*,*

(3) *for every* $z \in \mathbb{B}_\varepsilon(z_0)$*, the operator*

$$\pi(z) := -\frac{1}{2\pi i}\oint_{\partial\mathbb{B}_\delta(\mu_0)}(T(z)-\lambda)^{-1}d\lambda \tag{3.14}$$

is an analytic family of projectors, whose rank is independent of z.

Proof. (1)+(2): Since the spectrum of $T(z_0)$ is discrete, there exists a $\delta > 0$ such that μ_0 is the only eigenvalue of $T(z_0)$ contained in $\overline{\mathbb{B}_\delta(\mu(z_0))}$ (so that (1) automatically holds). To prove (2), fix some $\lambda_0 \in \partial\mathbb{B}_\delta(\mu_0)$; then, for any $\lambda \in \partial\mathbb{B}_\delta(\mu_0)$, we can write

$$\begin{aligned} T(z)-\lambda &= (T(z_0)-\lambda)\cdot(I+K_\lambda(z)), \quad \text{where} \\ K_\lambda(z) &= (T(z_0)-\lambda)^{-1}(T(z)-T(z_0)) = (T(z_0)-\lambda)^{-1}\int_{z_0}^{z}T'(\zeta)d\zeta. \end{aligned} \tag{3.15}$$

Therefore we seek $\varepsilon > 0$ such that for $|z-z_0| < \varepsilon$, the operator $K_\lambda(z)$ is bounded and has norm less than 1 for all $\lambda \in \partial\mathbb{B}_\delta(\mu_0)$, from which the claim follows.

Since $\partial\mathbb{B}_\delta(\mu_0)$ is compact and $(T(z_0)-\lambda)^{-1}$ is analytic, and thus continuous, in λ for all $\lambda \in \mathcal{C}$, there exists $M > 0$ such that

$$||(T(z_0)-\lambda)^{-1}|| \le M$$

for all such λ. Therefore, by the ML inequality,

$$||K_\lambda(z)|| \le ||(T(z_0)-\lambda)^{-1}||\left|\left|\int_{z_0}^{z}T'(\zeta)d\zeta\right|\right| \le CM|z-z_0|,$$

for all $\lambda \in \partial\mathbb{B}_\delta(\mu_0)$. Let

$$\varepsilon = \frac{1}{CM};$$

then $||K_\lambda(z)|| < 1$ for all $|z-z_0| < \varepsilon$, and consequently $I+K_\lambda(z)$ is invertible. Since $T(z_0)-\lambda$ is also invertible, we deduce that $T(z)-\lambda$ is invertible as well, thus proving the claim.

(3) This justifies that the operator $\pi(z)$ in (3.14) is well-defined. In addition, it is analytic since its integrand is analytic for all $z \in \mathbb{B}_\varepsilon(z_0)$, and it is a projector for all such z by Lemma 3.3. Lastly, we can again use [Kat95, Lemma I.4.10] together with analyticity to conclude that the rank of $\pi(z)$ is constant on $\mathbb{B}_\varepsilon(z_0)$. □

We will later use the following corollary:

Corollary 3.1. *Let $\mu_0, z_0 \in \mathbb{R}$ such that μ_0 is eigenvalue of $T(z_0)$ of multiplicity 1, let ϕ_0 be a normalized eigenvector of $T(z_0)$ for the eigenvalue μ_0, and let ε, δ be the quantities produced by Lemma 3.4. For every $z \in (z_0 \pm \varepsilon)$, $T(z)$ has a single eigenvalue $\mu(z)$ in $[\mu_0 \pm \delta]$:*

$$\mu(z) = \mu_0 + (z - z_0) \cdot \langle \phi_0, T'(z_0)\phi_0 \rangle + O(|z - z_0|^2).$$

Proof. For $z \in (z_0 - \varepsilon, z_0 + \varepsilon)$, $T(z)$ is a self-adjoint operator with discrete spectrum. We can therefore diagonalize it: there exist eigenvalues $\mu_k(z)$ and eigenprojectors $\pi_k(z)$ such that:

$$T(z) = \sum_{j=1}^{\infty} \lambda_k(z)\pi_k(z).$$

In particular, by the residue theorem, the projector $\pi(z)$ from (3.14) is given by:

$$\pi(z) = \sum_{k\colon\ |\mu_k(z) - \mu_0| < \varepsilon} \pi_k(z). \tag{3.16}$$

We note that $\pi(z_0)$ has rank one, because μ_0 is the only eigenvalue of $T(z_0)$ in $\mathbb{B}_\delta(z_0)$. Therefore, $\pi(z)$ has rank one as well. We deduce from (3.16) that for every $z \in (z_0 \pm \varepsilon)$, $T(z)$ has a single eigenvalue $\mu(z)$ in $\mathbb{B}_\delta(\mu_0)$, and $\pi(z)$ is its corresponding eigenprojector. Moreover, since $T(z)$ is self-adjoint for $z \in (z_0 \pm \varepsilon)$, we deduce that in fact $\mu(z) \in (\mu_0 \pm \delta)$.

Consequently, for all $z \in (z_0 - \varepsilon, z_0 + \varepsilon)$, we have the following identities:

$$(T(z) - \mu(z))\pi(z) = 0 \quad \text{and} \quad \pi(z)(T(z) - \mu(z)) = 0. \tag{3.17}$$

Taking the trace of the first identity in (3.17) gives us the formula $\mu(z) = \mathrm{Tr}(\pi(z)T(z)\pi(z))$, and so μ is analytic. Therefore, we can take the derivative of the first identity in (3.17), multiple by $\pi(z)$ on the left, and apply the second identity to obtain, after some rearrangement, that

$$\mu'(z)\pi(z) = \pi(z)T'(z)\pi(z). \tag{3.18}$$

Taking the trace of (3.18) evaluated at z_0 and using the formula $\pi(z_0) = \phi_0 \otimes \phi_0$, we obtain

$$\mu'(z_0) = \mathrm{Tr}(\pi(z_0)T'(z_0)\pi(z_0)) = \langle \phi_0, T'(z_0)\phi_0 \rangle.$$

We conclude using a Taylor expansion of μ that:

$$\mu(z) = \mu_0 + (z - z_0)\langle \phi_0, T'(z_0)\phi_0 \rangle + O(|z - z_0|^2).$$

□

3.4 *Proof of Theorems 1.1 and 1.2*

We prove our first two main results: Theorems 1.1 and 1.2, which predict that the eigenvalues and eigenprojectors of analytic families of operators are also analytic on a neighborhood of the real line. While these theorems are directly inspired by [FW12], the technical core of their proofs relies on different arguments. Both approaches consider maximal extensions of μ until a critical threshold b_* of z, at which point they face the same challenge: how to continue μ beyond b_*. Fefferman and Weinstein construct a vector-valued analytic function F, specific to the honeycomb setup, whose zeroes characterize where the multiplicity of μ is no longer m. Because the zeroes of F are discrete, this allows them to continue μ beyond b_*. We rely instead on a Schur-complement reduction (Proposition 3.3) of H_{b_*} near the energy $\mu(b_*)$. This produces a matrix $M(z)$ defined near b_*, which allows us to apply Theorem 3.4 to diagonalize $M(z)$ on a "disk minus one ray" centered at b_*. This allows us to continue μ analytically around b_*.

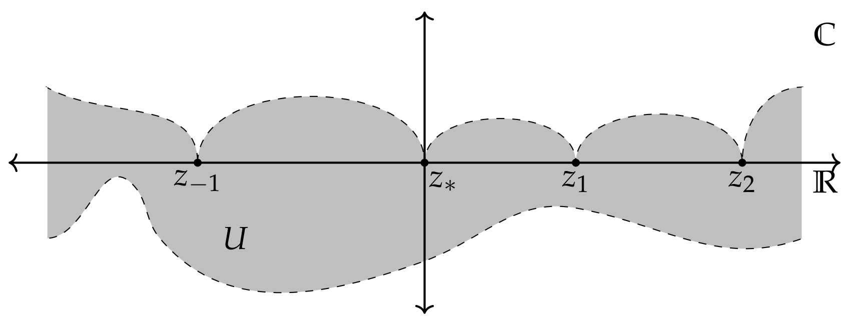


Figure 3.1: A possible configuration of the sets U and D (where in this figure $D = \{z_{-1}, z_*, z_1, z_2\}$) whose existences are guaranteed by Theorem 1.1.

Let $\mathbb{P}_\varepsilon(z)$ denote the disk $\mathbb{B}_\varepsilon(z)$ with the ray starting at z and pointing in the direction of the positive imaginary axis removed, i.e.

$$\mathbb{P}_\varepsilon(z) := \mathbb{B}_\varepsilon(z) \setminus \{z' \,:\, \Re(z') = z, \Im(z') \geq 0\}. \tag{3.19}$$

To prove Theorem 1.1, we first reformulate it using the following definition:

Definition 3.3. *A value $b_* \in [b, +\infty]$ is good (respectively admissible) if there exist sets*

(1) $D \subset (b, b_*)$ finite (respectively of the form $\{z_j\}_{j\in\mathbb{N}}$ with z_j increasing and converging to b_*),

(2) $U \subset \mathbb{C}$ a connected neighborhood of $(a, b_*) \setminus D$ equal to a union of disks $\mathbb{B}_{\varepsilon_z}(z)$ centered at points $z \in (a, b_*) \setminus D$ and sets of the form $\mathbb{P}_{\varepsilon_j}(z_j)$ (as in (3.19)) centered at $z_j \in D$:

$$U = \bigcup_{z \in (a,b_*) \setminus D} \mathbb{B}_{\varepsilon_z}(z) \cup \bigcup_{z_j \in D} \mathbb{P}_{\varepsilon_j}(z_j), \tag{3.20}$$

such that μ extends to a continuous function on $U \cup D$, and for all $z \in U$:

(a) $\mu(z)$ is analytic and an eigenvalue of $T(z)$ of multiplicity m,

(b) the associated eigenprojector $\pi(z)$ is analytic.

Good and admissible values in $[-\infty, a]$ are defined analogously.

Using this terminology, we then prove a slightly stronger statement, of which Theorem 1.1 is a consequence.

Theorem 3.7. *$\pm\infty$ are both admissible.*

We shall prove that $+\infty$ is admissible; the proof for $-\infty$ is identical.

Lemma 3.5. *b is good.*

Proof. Let $\pi(z)$ denote the eigenprojector corresponding to $\mu(z)$, and let $z_0 \in (a, b)$ be arbitrary. Then by Lemma 3.4, there exist $\varepsilon, \delta > 0$ such that $\mu(z_0)$ is the only eigenvalue of $T(z_0)$ in $\mathbb{B}_\delta(\mu(z_0))$ and for every $z \in \mathbb{B}_\varepsilon(z_0)$, $T(z)$ has no eigenvalue on $\partial\mathbb{B}_\delta(\mu(z_0))$. By shrinking ε if necessary, we may also assume $(z_0 \pm \varepsilon) \subset (a, b)$. Since μ is assumed to be continuous, we then must have that $\mu((z_0 \pm \varepsilon)) \subset \mathbb{B}_\delta(\mu(z_0))$, for otherwise there would exist $z \in (z_0 \pm \varepsilon)$ such that $\mu(z) \in \partial\mathbb{B}_\delta(\mu(z_0))$, contradicting Lemma 3.4 (2).

Let $\widetilde{\pi}(z)$ be the operator defined in (3.14), so that $\widetilde{\pi}(z)$ is the spectral projector corresponding to $\partial\mathbb{B}_\delta(\mu(z_0))$. Since $T(z_0)$ is self-adjoint, $\widetilde{\pi}(z_0)$ is precisely the eigenprojector corresponding to $\mu(z_0)$, and therefore has rank m. Consequently, $\pi(z)$ has rank m for all $z \in (z_0 \pm \varepsilon)$. Since $\mu(z)$ has multiplicity m on this set, we deduce that $\widetilde{\pi}(z)$ is in fact the eigenprojector corresponding to μ on $(z_0 \pm \varepsilon)$, and thus equal to $\pi(z)$ on this set. Since the integrand of (3.14) is analytic in z, this implies $\pi(z)$ is real analytic on $(z_0 \pm \varepsilon)$, and since $z_0 \in (a, b)$ was arbitrary, this in fact implies that $\pi(z)$ is real analytic on all of (a, b).

This also justifies that μ can be locally expressed as

$$\mu(z) = \frac{1}{m} \operatorname{Tr} \left(-\frac{1}{2\pi i} \int_{\mathcal{C}} \lambda (T(z) - \lambda)^{-1} d\lambda \right),$$

and since the multiplicity m is assumed to be constant, this tells us that $\mu(z)$ is real analytic on (a, b) as well. Now, since μ and π are both real analytic on (a, b), there exists a connected neighborhood $W \subset \mathbb{C}$ of (a, b) such that both π and μ have analytic extensions to U. It then will follow that b is good with $D = \emptyset$ if we can find a subset $U \subset W$ of the form (3.20) such that $\mu(z)$ is an eigenvalue of $T(z)$ of multiplicity m and π is its associated eigenprojector for all $z \in U$.

Note that, for $z \in (a, b)$,

$$\pi(z)^2 - \pi(z) = 0 \quad \text{and} \quad (T(z) - \mu(z))\pi(z) = 0. \tag{3.21}$$

By the identity theorem, the identities in (3.21) must be true for all $z \in W$. The first identity tells us that $\pi(z)$ is a projector for all $z \in W$, which, together with the second identity, tells us that $\mu(z)$ is an eigenvalue and the image of $\pi(z)$ is contained in its corresponding eigenspace. Moreover, since $\pi(z)$ is analytic, we can again use [Kat95, Lemma I.4.10] to conclude that its rank is constant, and therefore equal to m on all of W. As a result, $\mu(z)$ is an eigenvalue of multiplicity at least m for all $z \in W$.

To finish, recall that for $z_0 \in (a, b)$, there exists $\varepsilon > 0$ such that π is given by (3.14) on $\mathbb{B}_\varepsilon(z_0) \subset U$, and as such, its image contains the eigenspace corresponding to $\mu(z)$, and thus the dimension of this eigenspace is bounded above by m. Therefore the multiplicity of $\mu(z)$ must be exactly equal to m on $\mathbb{B}_\varepsilon(z_0)$. Since such a set exists for all $z_0 \in (a, b)$, we can then define U to be the union of these disks, and then μ restricted to U will be the desired extension. Therefore, b is good. □

Lemma 3.6. *Let $b_* \in [b, +\infty]$ be good, and let D, U be the sets associated to b_* through Definition 3.3. Then μ is C-Lipschitz on $U \cup D$.*

Proof. By definition of b_* being good, we have that, for all $z \in U$, μ and $\pi(z)$ are an eigenvalue and corresponding eigenprojector, respectively, of $T(z)$, and as such satisfy the identities in (3.17), and consequently $\mu'(z)\pi(z) = \pi(z)T(z)\pi(z)$. Taking the norm of both sides of this equation, it follows from sub-multiplicativity that, for $z \in (a, b)$

$$|\mu'(z)| \leq ||T'(z)|| \leq C.$$

Therefore μ is C-Lipschitz on U. Since D is finite though, it follows that U is dense in $U \cup D$, and thus we can conclude that μ is in fact C-Lipschitz on $U \cup D$. □

Lemma 3.7. *If $b_0 \in [b, +\infty)$ is good or admissible, then there exists $b_1 > b_0$ good. In particular, all finite admissible values are good.*

Proof. let D, U be the sets associated to b_0 through Definition 3.3. Then by Lemma 3.6, μ is C-Lipschitz on $U \cup D$, and therefore extends to a C-Lipschitz function (which we shall also denote by μ) on $U \cup D \cup \{b_0\}$.

We now apply Lemma 3.4 to $z_0 = b_0$ and $\mu_0 = \mu(b_0)$ (which is an eigenvalue of $T(b_0)$ by continuity of eigenvalues). Let $\widetilde{\pi}(z)$ be the operator defined in (3.14), so that for some

$\varepsilon, \delta > 0$ and for $z \in \mathbb{B}_{\varepsilon_0}(b_0)$), $\widetilde{\pi}(z)$ is the spectral projector corresponding to eigenvalues contained in $\mathbb{B}_\delta(\mu(b_0))$. Let $\mathcal{E}(z) = \operatorname{Im} \widetilde{\pi}(z)$, so that $\mathcal{E}(z)$ is a finite-dimensional vector space of dimension independent of z. Then, since $T(z)$ is assumed to be acting on a Hilbert space $\mathcal{H}$, we can now decompose $T(z)$ with respect to $\mathcal{E}(z) \oplus \mathcal{E}(z)^\perp$:

$$T(z) = \begin{pmatrix} T_{11}(z) & T_{12}(z) \\ T_{21}(z) & T_{22}(z) \end{pmatrix}.$$

Observe that for $z \in (b_0 \pm \varepsilon)$, $T_{12}(z) = T_{21}(z) = 0$ since $T(z)$ is self-adjoint for $z \in \mathbb{R}$. Since these operators are analytic, the identity theorem tells us they must be identically zero on $\mathbb{B}_\varepsilon(b_0)$.

In addition, note that by construction, $T_{22}(b_0) = T(b_0)|_{\mathcal{E}(b_0)^\perp}$ has no eigenvalues in $\mathbb{B}_\delta(\mu(b_0))$, and since $T(b_0)$ is self-adjoint, this implies $T(b_0) - \mu(b_0)$ is invertible, and its norm is bounded by $1/\delta$. By writing

$$\begin{aligned} T_{22}(z) - \lambda &= (T_{22}(b_0) - \mu(b_0)) \cdot (I + K_\lambda(z)), \quad \text{where} \\ K_\lambda(z) &= (T_{22}(b_0) - \mu(b_0))^{-1}(T_{22}(z) - T_{22}(b_0) + \lambda - \mu(b_0)), \end{aligned}$$

we obtain, by a Neumann series argument such as the one following (3.15), that $T_{22}(z) - \lambda$ is invertible for $|z - b_0| < \delta/2C$ and $|\lambda - \mu(b_0)| < \delta/2$.

Let $(\varphi_1, \ldots, \varphi_n)$ be a basis of $\mathcal{E}(b_0)$. For $|z - b_0| < \varepsilon_0 < \min\{\varepsilon, \delta/2C\}$, ε_0 sufficiently small, the set

$$\{\varphi_j(z) := \pi(z)\varphi_j\}_{j=1}^n$$

forms a basis for $\mathcal{E}(z)$. Let $M(z)$ be the matrix of $T_{11}(z)$ with respect to this basis. Then $M(z)$ is Hermitian for $z \in (b_0 \pm \varepsilon_0)$, and its entries are given by

$$(M(z))_{ij} = \frac{\langle T(z)\varphi_i(z), \varphi_j(z)\rangle}{||\varphi_j(z)||^2},$$

from which it follows that $M(z)$ is analytic on $\mathbb{B}_{\varepsilon_0}(b_0)$.

By Theorem 3.2, after possibly shrinking ε_0, we may express $M(z)$ for $z \in P := \mathbb{P}_{\varepsilon_0}(b_0)$ (as in (3.19)) as

$$M(z) = \sum_{j=1}^r \lambda_j(z)\pi_j(z), \quad \text{where:}$$

- $\lambda_1, \ldots, \lambda_r$ are distinct eigenvalues of $M(z)$ with constant multiplicity that depend analytically on z,

- $\pi_1, \ldots, \pi_r$ are distinct eigenprojectors of $M(z)$ that depend analytically on z.

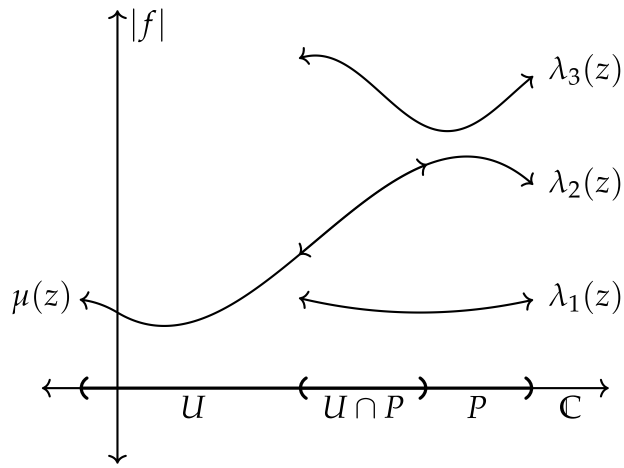


Figure 3.2: A cross section of the dispersion surface μ, and the analytic functions λ_j describing the eigenvalues of $M(z)$ on P. In the situation drawn in this figure, $\mu = \lambda_2$ on $U \cap P$.

Note that by Definition 3.3, and specifically (3.20), $U \cap P$ is connected and contains $(b_0 - \varepsilon_0, b_0)$, and thus is non-empty. Therefore, for $z \in U \cap P$, $\mu(z)$ is an eigenvalue of $T(z)$ in $\mathbb{B}_\delta(\mu(b_0))$, and thus is also an eigenvalue of $M(z)$. As a result, $\mu(z) = \lambda_j(z)$ for some j on $U \cap P$, from which it follows that μ extends to an analytic function on $U \cup P$. This also implies that π and π_j agree on $U \cap P$, and so π extends to an analytic function on $U \cup P$ as well. Thus, for all $z \in U \cup W$,

- $\mu(z)$ is analytic and an eigenvalue of $T(z)$ of multiplicity m,
- $\pi(z)$ is analytic and is the eigenprojector associated to $\mu(z)$.

Let $b_1 = b_0 + \varepsilon_0$. If b_0 is good, observe that $U \cup P$ is a connected neighborhood of $(a, b_1) \setminus (D \cup \{b_0\})$ of the form (3.20), therefore b_1 is good. If on the other hand b_0 is admissible, then write $D = \{z_j\}_{j \in \mathbb{N}}$, with z_j increasing to b_0. Then there exists $J > 0$ such that P contains z_j for all $j \geq J$. Consequently, in the definition of U, we can replace $\mathbb{P}_{\varepsilon_j}(z_j)$ with an open disk $\mathbb{B}_{\varepsilon_j}(z_j) \subset P$ for some potentially new $\varepsilon_j > 0$. Then the resulting set $U \cup P$ is a connected neighborhood of $(a, b_1) \setminus \{z_1, \ldots, z_{J-1}, b_0\}$, also of the form (3.20), and so b_1 is still good. A consequence of this is that b_0 is in fact good, as can be seen by restricting μ back to U (after the relevant replacements). Therefore, all finite admissible values are good. □

Lemma 3.8. *Let $b_j \in [b, +\infty)$ be good values, increasing and converging to $b_* \in [b, +\infty)$. Then b_* is good.*

Proof. By Lemma 3.7, it suffices to prove that b_* is admissible. For $j \in \mathbb{N}$, let D_j, U_j be the sets associated to b_j through Definition 3.3, let μ_j denote the corresponding extension of μ, and let π_j denote the associated eigenprojector. To show that b_* is admissible, we then want to construct sets D, U and extensions μ_* of μ and π_* of π as in Definition 3.3.

Towards that end, we construct new sets $\widetilde{U}_j, \widetilde{D}_j$ for $j \in \mathbb{N}$ recursively. First, let $\widetilde{U}_1 = U_1$ and $\widetilde{D}_1 = D_1$. Then, for $j \geq 1$, by Definition 3.3 we can write U_{j+1} as

$$U_{j+1} = \bigcup_{z \in (a, b_{j+1}) \setminus D_{j+1}} \mathbb{B}_{\varepsilon_z}(z) \cup \bigcup_{z_\ell \in D_{j+1}} \mathbb{P}_{\varepsilon_\ell}(z_\ell).$$

Let W_{j+1} denote the sub-union consisting of the disks and sets of the form $\mathbb{P}_\varepsilon(z)$ centered at $z \geq b_j$:

$$W_{j+1} = \bigcup_{z \in [b_j, b_{j+1}) \setminus D_{j+1}} \mathbb{B}_{\varepsilon_z}(z) \cup \bigcup_{z_\ell \in D_{j+1} \cap [b_j, b_{j+1})} \mathbb{P}_{\varepsilon_\ell}(z_\ell).$$

We then define $\widetilde{U}_{j+1} := \widetilde{U}_j \cup W_{j+1}$, from which it follows that $\widetilde{U}_{j+1}$ is of the form (3.20). In addition, $\widetilde{U}_j \cap W_{j+1}$ is necessarily connected, and μ_j and μ_{j+1} agree on this set since $\widetilde{U}_j \cap W_{j+1} \subset \widetilde{U}_j \cap U_{j+1}$, which is an open and connected set containing (a, b), and therefore μ_j and μ_{j+1} agree on this latter set by the identity theorem. Thus we get a well-defined extension of μ_j to $\widetilde{U}_{j+1}$, which we now denote by μ_{j+1}. It then follows that $\mu_j(z)$ is an eigenvalue of $T(z)$ of multiplicity m for all $z \in \widetilde{U}_{j+1}$ since it satisfies these properties on both $\widetilde{U}_j$ and W_{j+1}. An identical argument tells us that there exists an analytic extension π_{j+1} of π_j to $\widetilde{U}_{j+1}$ such that $\pi_{j+1}(z)$ is the eigenprojector associated with $\mu_{j+1}(z)$. Lastly, we define $\widetilde{D}_{j+1} = \widetilde{D}_j \cup (D_{j+1} \cap [b_j, b_{j+1}))$; then this set is finite since both $\widetilde{D}_j$ and D_{j+1} are finite. Since μ_j is C-Lipschitz by Lemma 3.6, μ_{j+1} extends to a continuous function on $\widetilde{U}_{j+1} \cup \widetilde{D}_{j+1}$.

Now let

$$U = \bigcup_{j \in \mathbb{N}} \widetilde{U}_j, \quad D = \bigcup_{j \in \mathbb{N}} \widetilde{U}_j.$$

Since $\widetilde{U}_j \cup \widetilde{D}_j \subset \widetilde{U}_{j+1} \cup \widetilde{D}_{j+1}$ for all $j \in \mathbb{N}$, we can then define $\mu_* : U \cup D \to \mathbb{C}$ and $\pi_* : U \cup D \to \mathbb{C}$ as the direct limit of the extensions μ_j to the sets $\widetilde{U}_j \cup \widetilde{D}_j$, and π_j to the sets $\widetilde{U}_j$, respectively. As such, it follows that the sets U and D (where D is possibly infinite) together with the extensions μ_* and π_* satisfy the conditions of Definition 3.3, and so b_* is admissible. However, by Lemma 3.7, this implies that b_* is good. □

Proof of Theorem 1.1. Assume that $+\infty$ is not admissible and consider

$$b_+ = \sup\{b_* \in [b, +\infty) \ : \ b_* \text{ admissible}\}.$$

Then by Lemma 3.5, this supremum is being taken over a non-empty set, and so it is well-defined. Let b_j be an increasing sequence of admissible values converging to b_+. By Lemma 3.7, b_j is good for all j, and so by Lemma 3.8, b_+ is good and therefore also admissible. However, this then implies by Lemma 3.7 that there exists $b_* > b_+$ that is also good, contradicting maximality of b_+. Therefore, $+\infty$ must be admissible. □

We formulated the above proof of Theorem 1.1 before becoming aware of Rellich's similar result [Rel40] discussed in Section 1.1. In particular, note that in the proof of Theorem 1.1 and the preceding lemmas, we only used Theorem 3.2 – which gave us a decomposition of the analytic family of matrices $M(z)$ on $\mathbb{P}_{\varepsilon_0}(b_0)$ for $b_0 \in D \cap \mathbb{R}$ – instead of the stronger result, Theorem 3.4 – which would give us the same decomposition, but on $\mathbb{B}_{\varepsilon_0}(b_0)$. Using this latter result, Theorem 1.2 is essentially an immediate consequence of Theorem 1.1 via the following definition.

Definition 3.4. *A value $b_* \in [b, +\infty]$ is perfect (respectively almost-perfect) if there exist sets*

(1) $D \subset (b, b_*)$ finite (respectively of the form $\{z_j\}_{j\in\mathbb{N}}$ with z_j increasing and converging to b_*),

(2) $U \subset \mathbb{C}$ a connected neighborhood of (a, b_*) equal to a union of disks $\mathbb{B}_{\varepsilon_z}(z)$ centered at points $z \in (a, b_*)$:

$$U = \bigcup_{z\in(a,b_*)} \mathbb{B}_{\varepsilon_z}(z),$$

such that μ extends to an analytic function on U and

(a) $\mu(z)$ is an eigenvalue of $T(z)$ for all $z \in U$,

(b) $\mu(z)$ has multiplicity m for all $z \in U \setminus D$,

(c) the associated eigenprojector $\pi(z)$ is analytic on U.

Perfect and almost-perfect values in $(-\infty, a]$ are defined analogously.

It follows that to prove Theorem 1.2, it suffices to prove that $\pm\infty$ are both almost perfect.

Proof of Theorem 1.2. First note that the proof of Lemma 3.5 actually shows that b is perfect. In addition, by using Theorem 3.4 instead of Theorem 3.2, Lemmas 3.6 – 3.8 still hold if every occurrence of the adjectives good and admissible are replaced with perfect and almost perfect, respectively. As a result, our proof of Theorem 1.1 then shows, using the appropriately modified lemmas, that $+\infty$ is in fact almost-perfect, and an identical proof shows that $-\infty$ is almost-perfect as well. □

Chapter 4

DISPERSION SURFACES OF SCHRÖDINGER OPERATORS: GENERAL THEORY

Using Theorem 1.2, we now develop a general framework for analyzing the dispersion surfaces of Schrödinger operators $-\Delta + V$ for generic potentials V invariant under a lattice Λ, i.e. periodic with respect to Λ and symmetric with respect to its point group. We start by discussing the spectral theory of $-\Delta$ on L^2_K and defining lattice-invariant potentials. We then state and prove perturbative lemmas on Floquet-Bloch eigenvalues of $H_z = -\Delta + zV$. Brought together, these results outline our strategy to describe the generic structure of the dispersion surfaces of invariant Schrödinger operators. In the following two chapters we then apply this framework to analyze the dispersion surfaces of Schrödinger operators with potentials invariant under a variety of specific two and three-dimensional lattices, respectively.

4.1 Spectral Theory of the Laplacian on L^2_K

Fix some lattice Λ with basis $(v_1, \dots, v_n)$ and reciprocal basis $(k_1, \dots, k_n)$, and fix some $K \in \mathbb{R}^n$. For simplicity of notation, if $m \in \mathbb{Z}^n$ let

$$mk := \sum_{j=1}^{n} m_j k_j.$$

We then claim that $\phi_m(x) = e^{i(K+mk)\cdot x}$ for $m \in \mathbb{Z}^n$ is an orthonormal basis of eigenvectors for $-\Delta$ on L^2_K. Indeed, note that

$$-\Delta\phi_m(x) = ||K + mk||^2 \phi_m(x),$$

and $(\phi_m)_{m\in\mathbb{Z}^n}$ is the image of the orthonormal basis $(\otimes_{j=1}^{n} e^{2\pi i m_j x_j})_{m\in\mathbb{Z}^n}$ of $L^2[0,1]^{\otimes n}$ under the unitary map which first sends $\otimes_{j=1}^{n} e^{2\pi i m_j x_j}$ to $e^{imk\cdot x} \in L^2_0$, and then $e^{imk\cdot x}$ to ϕ_m via multiplication by $e^{iK\cdot x}$. Consequently,

$$\sigma(-\Delta) = \{||K + mk||^2 \ : \ m \in \mathbb{Z}^n\}.$$

and the multiplicity of an eigenvalue $\mu_m := ||K + mk||^2$ is given by

$$m_{-\Delta}(\mu_m) = \left|\left\{k' \in K + \Lambda^* \ : \ ||k'||^2 = ||K + mk||^2\right\}\right|. \tag{4.1}$$

This motivates us to define an equivalence relation between quasi-momenta as follows: let $K_1, K_2 \in \mathbb{R}^n$; then

$$K_1 \sim K_2 \text{ if } ||K_1|| = ||K_2|| \text{ and there exists } k \in \Lambda^* \text{ such that } K_1 = K_2 + k. \tag{4.2}$$

Let $[K]$ denote the equivalence class containing K; then $[K] = \{k \in K + \Lambda^* \ : \ ||k|| = ||K||\}$, and by (4.1),

$$m_{-\Delta}(\mu_0) = \Big|[K]\Big|, \tag{4.3}$$

i.e. the multiplicity of $\mu_0 = ||K||^2$ is equal to the cardinality of the set $[K]$.

From here, recall that the Floquet-Bloch problem (1.3) is periodic with respect to the dual lattice Λ^*, so we focus our analysis on $K \in \mathcal{B}$. For such K, the minimal eigenvalue of $-\Delta$ on L^2_K is then given by μ_0, since by definition of the Brillouin zone $\mathcal{B}$,

$$||K||^2 \leq ||K - k'||^2, \quad \forall k' \in \Lambda^*. \tag{4.4}$$

This also implies that if K is in the interior of $\mathcal{B}$, then the inequality (4.4) is strict, and so the eigenvalue μ_0 is simple.

Conversely, we expect $K \in \partial\mathcal{B}$, particularly the vertices of $\mathcal{B}$, to correspond to eigenvalues of high multiplicity. In fact, by Proposition 2.1, if we let m denote the number of (hyper)faces of $\mathcal{B}$ which contain K, then $m_{-\Delta}(\mu_0) \geq m + 1$. Furthermore, if we let $m' = m_{-\Delta}(\mu_0)$ and assume that K lies on a single (hyper)face of $\mathcal{B}$, then the proof of Proposition 2.1, and specifically (4.1), tells us that there exist vectors $K_1, \ldots, K_{m'} \in \Lambda^*$ such that $||K - K_j||^2 = ||K||^2$ for $j = 1, \ldots, m'$. As a result, (2.8) implies that $K \cdot K_j = \frac{1}{2}||K_j||^2$ for $j = 1, \ldots, m'$, and so K lies on the m' distinct (hyper)planes defined by $x \cdot K_j = \frac{1}{2}||K_j||^2$ for $j = 1, \ldots, m'$. However, since K lies on a single (hyper)face of $\mathcal{B}$, this implies K lies on exactly one of these (hyper)planes, and so $m' = m_{-\Delta}(\mu_0) = 2$. A consequence is that the vertices of $\mathcal{B}$ correspond to eigenvalues of comparatively high multiplicity. As a result, these quasi-momenta are the most likely to have interesting intersections of dispersion surfaces, and we therefore focus our analysis on these points.

Our focus on the vertices of $\mathcal{B}$ conveniently also simplifies our later computations, for if K is a vertex, the corresponding equivalence class $[K]$ is contained in the set of vertices, ensuring that we only have to check a finite number of elements of $K + \Lambda^*$ to determine $[K]$.

Proposition 4.1. *Let $V(\mathcal{B})$ denote the vertices of $\mathcal{B}$ and let $K \in V(\mathcal{B})$. Then*

$$[K] = V(\mathcal{B}) \cap (K + \Lambda^*).$$

Proof. Let $K \in V(\mathcal{B})$ and let $k' \in \Lambda^*$; it then suffices to prove that $||K - k'||^2 = ||K||^2$ if and only if $K - k' \in V(\mathcal{B})$. However, (2.5) implies that $||K - k'||^2 = ||K||^2$ if and only if $K \cdot k' = \frac{1}{2}||k'||^2$, and so by the proof of Proposition 2.1, $K - k'$ lies on the same number of (hyper)faces of $\mathcal{B}$ as K does. Together with the fact that $K \in V(\mathcal{B})$, this implies $K - k' \in V(\mathcal{B})$ as well. $\square$

4.2 Invariant Potentials

Now that we understand the spectral theory of $-\Delta$ on L^2_K, we want to introduce a potential V. Towards that end, fix a lattice Λ with basis $(v_1, \dots, v_n)$, dual basis $(k_1, \dots, k_n)$, and point group G. Observe then that G acts isometrically on scalar-valued functions:

$$g_* f(x) := f(g^\top x).$$

We will later need an induced action of a subgroup G_0 of G on L^2_k for some quasi-momentum k. However, for this action to be well-defined, we need G_0 to satisfy an additional criterion.

Definition 4.1. *We say $g \in G$ is k-invariant if*

$$gk \in k + \Lambda^*.$$

Analogously, we say a subgroup G_0 of G is k-invariant if g is k-invariant for all $g \in G_0$.

To see that k-invariant subgroups give well-defined actions, note that if G_0 is such a subgroup and $g \in G_0$, then by definition there exists $k' \in \Lambda^*$ such that $gk = k + k'$. Then for all $v \in \Lambda$, $g^\top v \in \Lambda$ as well by definition of G, and as a result

$$\begin{aligned} g_*\psi(x+v) &= \psi(g^\top x + g^\top v) = e^{ik\cdot g^\top v}\psi(g^\top x) = e^{igk\cdot v} g_*\psi(x) \\ &= e^{i(k+k')\cdot v} g_*\psi(x) = e^{ik\cdot v} g_*\psi(x). \end{aligned}$$

In particular, this shows that k-invariant group elements map L^2_k to itself.

We now define potentials invariant with respect to Λ.

Definition 4.2. *Let Λ be a lattice with point group G. We say that $V \in C^\infty(\mathbb{R}^n, \mathbb{R})$ is Λ-invariant if:*

1) *V is Λ-periodic, i.e. $V(x+v) = V(x)$ for all $x \in \mathbb{R}^2$ and $v \in \Lambda$,*

2) *V is G-invariant, i.e. $g_*V = V$ for all $g \in G$.*

When the lattice Λ is clear from the context, we will omit it and simply refer to V as an invariant potential.

Example 4.1 ("Atomic" Lattice Potentials). Let Λ be a lattice with symmetry group G, and let V_0 be a smooth, radial, and rapidly decreasing function, which we think of as an "atomic potential". Then the potential given by

$$V(x) := \sum_{v\in\Lambda} V_0(x+v)$$

is an example of a Λ-invariant potential, which we associate with "atoms" at each $v \in \Lambda$. Our assumption that V_0 is rapidly decreasing ensures that V is well-defined. To see that V is Λ-periodic, let $v_0 \in \Lambda$. Then $v_0 + \Lambda = \Lambda$, and conseqeuently

$$V(x+v_0) = \sum_{v\in\Lambda} V_0(x+v_0+v) = \sum_{v\in v_0+\Lambda} V_0(x+v) = V(x).$$

Similarly, to see that V is G-invariant, let $g \in G_0$. Since G is a subgroup of the orthogonal group, our assumption that V_0 is radial implies $g_* V_0(x) = V_0(g^\top x) = V_0(x)$. Consequently,

$$g_* V(x) = \sum_{v\in\Lambda} V_0(g^\top x + v) = \sum_{v'\in\Lambda} V_0(g^\top(x+gv)) = \sum_{v\in g\Lambda} V_0(x+v) = V(x).$$

Therefore, V is indeed a Λ-invariant potential.

When V is an invariant potential, the fact that V is Λ-periodic enables us to expand V as a Fourier series with coefficients $\{V_m\}_{m\in\mathbb{Z}^n}$:

$$V(x) = \sum_{m\in\mathbb{Z}^n} V_m e^{imk\cdot x}$$
$$V_m = \left\langle e^{imk\cdot x}, V \right\rangle.$$

For simplicity of notation, if $k' \in \Lambda^*$ so that $k' = mk$ for some $m \in \mathbb{Z}^n$, we shall also denote V_m by $V_{k'}$. If we then view these coefficients as a function on Λ, they are invariant under an induced action of G:

$$g_* V_k = V_{g^\top k} = \left\langle e^{ig^\top k\cdot x}, V \right\rangle = \left\langle e^{ik\cdot x}, g_* V \right\rangle = \left\langle e^{ik\cdot x}, V \right\rangle = V_k. \tag{4.5}$$

By working with an invariant potential V together with a k-invariant subgroup $G_0 < G$, we are then able to reduce the Floquet-Bloch problem (1.3) using the following proposition.

Lemma 4.1. *Fix some $k \in \mathbb{R}^n$, let V be a Λ-invariant potential, and let $G_0 < G$ be k-invariant. Then $H = -\Delta + V$ and all $g \in G_0$ map a dense subspace of L^2_k to itself. Moreover, restricted to this dense subspace, $[H, g_*] = 0$.*

Proof. Let C^∞_k denote the space of smooth functions satisfying $f(x+v) = e^{-ik\cdot v} f(x)$ for all $x \in \mathbb{R}^n$, $v \in \Lambda$; then all $g \in G_0$ map this space to itself by k-invariance, and so too does H. To see that $[H, g_*] = 0$, first note that by definition of G, g_* is an isometry and therefore commutes with Δ. In addition, by G-invariance of V, we have that for all $f \in C^\infty_k$,

$$g_*(Vf)(x) = (g_* V)(g_* f)(x) = (V(g_* f))(x).$$

Therefore g_* commutes with both Δ and V, and thus commutes with H, as claimed. $\square$

A subset of invariant potentials that has been studied extensively are honeycomb lattice potentials (see [FW12; FW14], for example), which are Λ-invariant potentials for a honeycomb lattice Λ (also often referred to as hexagonal lattices in the context of crystallography). Several consequences of the definition of a honeycomb lattice potential also naturally extend to this more general definition, which we shall later need.

Remark 4.2. The spectral properties of $H_V = -\Delta + V$ are independent of isometries of the potential V, which has a number of implications:

1. If V is the translation of an invariant potential, so that $\widetilde{V}(x) = V(x - x_0)$ is an invariant potential for some $x_0 \in \mathbb{R}^n$, then H_V will have the same spectral properties as $H_{\widetilde{V}}$, and therefore all of the following results apply to such a potential with negligible modification.

2. If U is a orthogonal transformation and V is a Λ-invariant potential, then $V \circ U^*$ is a $U\Lambda$-invariant potential, and the dual lattice satisfies $(U\Lambda)^* = U\Lambda^*$. As a result, the spectral properties of H_V on L^2_k are the same as those of $H_{V\circ U^*}$ on L^2_{Uk}. Therefore, we can always replace the lattice Λ with $U\Lambda$ for some computationally convenient U.

3. Furthermore, our remark about orthogonal transformations implies that the spectral properties of H_V on L^2_k are the same as those of H_V on L^2_{gk} for all $g \in G$. Together with the Λ^*-periodicity of the Floquet-Bloch eigenvalue problem (1.3), this implies that the dispersion surfaces of H near a quasi-momenta $k \in \mathbb{R}^n$ are determined locally by those near gk. Consequently, it suffices to consider quasi-momenta whose orbits under G are distinct.

Remark 4.3. Since all invariant potentials are assumed to be real-valued, if $(\phi(x;k), \mu)$ is an eigenpair of the Floquet-Bloch problem (1.3) with quasi-momentum k, then $(\overline{\phi(x;k)}, \mu)$ is also an eigenpair with quasi-momentum $-k$.

Moreover, every lattice Λ is necessarily invariant under the negative of the identity, which implies that the point group G must always include this matrix; therefore, by G-invariance, every invariant potential V must also be even. This together with our previous observation implies that $(\overline{\phi(-x;k)}, \mu)$ is an eigenpair as well, with quasi-momentum k.

4.3 Decomposing L^2_K via a K-Invariant Subgroup

For the rest of this section, we make the following assumption on K:

Assumption A3: There exists an abelian subgroup G_0 of G such that $G_0K = [K]$ and $|G_0| = |G_0K|$.

Although this might appear to be a restrictive assumption at first glance, we will see in Chapters 5 and 6 that such a subgroup exists in most applications of interest. This assumption is helpful because by construction of $[K]$, G_0 is necessarily K-invariant, and thus has a well-defined action on L^2_K. In addition, by our assumption that V is G-invariant and the fact that g_* is the pushforward by an orthogonal matrix for every $g \in G_0$, H commutes with the action of G_0 on L^2_K. We can therefore reduce the spectral problem for H on L^2_K to spectral problems on the invariant subspaces of G_0, which will be one-dimensional (see Corollary 2.2 and Remark 2.6).

Before we perform this reduction, however, we introduce some notation. By Lemma 2.1, there exists a minimal system of generators $g_1, \ldots, g_\ell$ of G_0 with respective orders $n_1, \ldots, n_\ell$. Since G_0 is assumed to be abelian, it follows that $G_0 \cong \bigoplus_{j=1}^{\ell} \mathbb{Z}_{n_j}$. In addition, if $g \in G_0$ is of order N, then $\sigma_{L^2_K}(g_*)$, the spectrum of g_* viewed as an operator on L^2_K, is contained in the N-th roots of unity U_N (and in fact, we will see in Lemma 4.2 that $\sigma_{L^2_K}(g_*) = U_N$). This follows first from the fact that g_* has finite order, and consequently has pure point spectrum, and if ω is an eigenvalue of g_*, then $g^N = e$ implies $\omega^N = 1$, and so $\omega \in U_N$. With this in mind, we define:

$$\mathbb{J} := \prod_{j=1}^{\ell} \{0, \ldots, n_j - 1\} \quad \text{and} \quad \mathbb{U} := \prod_{j=1}^{\ell} U_{n_j}, \tag{4.6}$$

so that $G_0 = \{g^j \ : \ j \in \mathbb{J}\}$, where we are using the multi-index notation $g^j = g_1^{j_1} \cdots g_\ell^{j_\ell}$.

Again using the fact that G_0 is abelian, we can then simultaneously diagonalize the operators $(g_j)_*$, which leads us to the following decomposition of L^2_K:

$$L^2_K = \bigoplus_{\omega \in \mathbb{U}} L^2_{K,\omega}, \quad L^2_{K,\omega} := \bigcap_{j=1}^{\ell} \ker_{L^2_K}((g_j)_* - \omega_j).$$

It is worth noting that the spaces $L^2_{K,\omega}$ for $\omega \in \mathbb{U}$ are pairwise orthogonal by virtue of the operators $(g_j)_*$ being unitary.

Lastly, it will also simplify our later computations by introducing a convenient method of enumerating elements of $[K]$. Specifically, for each $j \in \mathbb{J}$ we define $m(j) \in \mathbb{Z}^n$ as the n-tuple satisfying

$$g^j K = K + m(j) \cdot (k_1, \ldots, k_n); \tag{4.7}$$

then $m(j)$ exists and is unique by A3.

4.4 Strategy

Our goal is to describe the structure of dispersion relations of H_z near some quasi-momentum $K \in \mathbb{R}^n$ for generic values of z, where we continue to assume that K together with a subgroup G_0 of G satisfy A3. Our strategy relies on the four key lemmas stated below; their proofs are postponed to Section 4.5. We start with a result regarding the spectral theory of $-\Delta$ on $L^2_{K,\omega}$.

Lemma 4.2. *Let $K \in \mathbb{R}^n$ and G_0 of G satisfy A3. For each $\omega \in \mathbb{U}$, $||K||^2$ is an $L^2_{K,\omega}$-eigenvalue of $-\Delta$ of multiplicity 1, with corresponding normalized eigenvector given by*

$$\phi_\omega(x) = \frac{1}{\sqrt{|G_0|}} \sum_{j \in \mathbb{J}} \omega^j e^{ig^{-j}K\cdot x}. \tag{4.8}$$

Lemma 4.2 together with Corollary 3.1 will then help us construct an eigenvalue $\mu(z)$ of H_z satisfying A2.

Lemma 4.3. *Let $K \in \mathbb{R}^n$ and G_0 of G satisfy A3 and let $\omega \in \mathbb{U}$. There exist $\varepsilon, \delta > 0$ such that for $z \in (-\varepsilon, \varepsilon)$, H_z has a unique $L^2_{K,\omega}$-eigenvalue in $(||K||^2 \pm \delta)$, given by*

$$\mu(z) = ||K||^2 + z \cdot \sum_{j \in \mathbb{J}} \omega^j V_{m(j)} + \mathcal{O}(|z|^2),$$

where $m(j)$ is the multi-integer defined in (4.7).

A straightforward application of Theorem 1.3 implies that H_z has an $L^2_{K,\omega}$-eigenvalue $\mu(z)$ splitting from the L^2_K-eigenvalue $||K||^2$ of $H_0 = -\Delta$, which for generic $z \in \mathbb{R}$ is simple and whose eigenprojector can be extended to an analytic map on a neighborhood of the real line.

When K is a vertex of the Brillouin zone, we will be able to compute the generic multiplicities of the L^2_K-eigenvalues of H_z splitting from the eigenvalue $||K||^2$ of $-\Delta$ using symmetry arguments. We will then describe the structure of the corresponding dispersion surfaces near K using the following three results.

Lemma 4.4. *Let $\mu(z)$ be an L^2_K-eigenvalue of H_z for some $z \in \mathbb{R}$, let $\pi(z) : L^2_K \to L^2_K$ be the corresponding eigenprojector, and let $\mathcal{E}(z)$ be the corresponding eigenspace.*

(1) There exist $\varepsilon, \delta > 0$ such that for $||\kappa|| < \varepsilon$, the $L^2_{K+\kappa}$ eigenvalues of H_z in $\mathbb{B}_\delta(\mu(z))$ satisfy

$$\det\left((u(z) - \mu) + M(z,\kappa) + R(\mu,\kappa)\right)|_{\mathcal{E}(z)} = 0,$$

where $M(z,\kappa) = -\pi(z)(2i\kappa \cdot \nabla)\pi(z)$ and $||R(\mu,\kappa)|| \le C_1||\kappa||^2$ for some $C_1 > 0$.

(2) If $\lambda(z,\kappa)$ is a simple eigenvalue of $M(z,\kappa)$, continuous in κ on some open set $U \subset B_\varepsilon(0)$ such that $\sup_{\kappa\in U} |\lambda(z,\kappa)| < \delta$, then there exists a simple eigenvalue $\mu(z,\kappa)$ of H_z on $L^2_{K+\kappa}$ satisfying

$$\mu(z,\kappa) = \mu(z) + \lambda(z,\kappa) + \mathcal{O}(||\kappa||^2). \tag{4.9}$$

(3) If $M(z,\kappa) = 0$, then every $L^2_{K+\kappa}$-eigenvalue $\mu(z,\kappa)$ of H_z satisfies $\mu(z,\kappa) = \mu(z) + \mathcal{O}(||\kappa||^2)$.

For the following lemma, we continue to let $M(z,\kappa) := -\pi(z)(2i\kappa\cdot\nabla)\pi(z)$, although we no longer assume that $z \in \mathbb{R}$, so that we can use this lemma in conjunction with Theorem 1.2.

Lemma 4.5. *Let $\mu(z)$ be an L^2_K-eigenvalue of H_z for some $z \in \mathbb{R}$ such that the corresponding eigenprojector $\pi(z)$ depends analytically on $z \in U$. The characteristic polynomial of $M(z,\kappa)$, acting on the finite-dimensional eigenspace $\mathcal{E}(z)$, depends analytically on $z \in U$.*

Lastly, to compute the characteristic polynomial of $M(z,\kappa)$, we will express this matrix with respect to a basis consisting of one vector from each of the subspaces $L^2_{K,\omega}$ for ω in some subset of $\mathbb{U}$. This final lemma will help us simplify these computations.

Lemma 4.6. *Let $\phi \in L^2_{K,\omega}$ and let $\psi \in L^2_{K,\widetilde{\omega}}$ for $\omega, \widetilde{\omega} \in \mathbb{U}$. Then for all $j \in \mathbb{J}$, $\langle \phi, \nabla\psi\rangle$ is an eigenvector of g^j with corresponding eigenvalue $\omega^{-j}\widetilde{\omega}^j$. Moreover, if K is a vertex of the Brillouin zone $\mathcal{B}$, then $\langle \phi, \nabla\phi\rangle = 0$.*

4.5 *Proofs of Lemmas 4.2 – 4.6*

Proof of Lemma 4.2. We first note that $||K||^2$, as an L^2_K-eigenvalue of $-\Delta$, by A3 has multiplicity $|G_0K| = |G_0|$. Consequently, it suffices to prove that for each $\omega \in \mathbb{U}$, the function ϕ_ω in (4.8) is a normalized $L^2_{K,\omega}$-eigenvector for the eigenvalue $||K||^2$, for then this eigenvalue on $L^2_{K,\omega}$ would necessarily be simple since $|\mathbb{U}| = |G_0|$.

To see that ϕ_ω is normalized, observe that the $|G_0|$ functions $e^{ig^jK\cdot x}$ form an orthonormal system because of A3. Indeed, each of these exponentials is distinct, for if $g^jK = g^{j'}K$, then $g^{j-j'}K = K$, which implies $g^{j-j'} = I$ because $|G_0K| = |G_0|$. Therefore $g^j = g^{j'}$ and $j = j'$.

To show that $\phi_\omega \in L^2_{K,\omega}$, we first note that $\phi_\omega \in L^2_K$ since $g^jK \in K + \Lambda^*$ for every $j \in \mathbb{J}$. In addition, we compute that

$$(g_1)_*\phi_\omega(x) = \frac{1}{\sqrt{|G_0|}}\sum_{j\in\mathbb{J}} \omega^j e^{ig^{-j}K\cdot g^\top x} = \frac{\omega_1}{\sqrt{|G_0|}}\sum_{j\in\mathbb{J}} \omega^{j-e_1} e^{ig^{-j+e_1}K\cdot x} = \omega_1\phi_\omega(x),$$

with similar identities when testing the pushforward operators by $g_2,\ldots,g_\ell$. We conclude by noting that ϕ_ω is an eigenvector of $-\Delta$ with eigenvalue $||K||^2$ since $||g^jK|| = ||K||$ by virtue of g^j being an orthogonal matrix for every $j \in \mathbb{J}$. $\square$

Proof of Lemma 4.3. By Lemma 4.2 and Corollary 3.1, there exist $\varepsilon, \delta > 0$ such that H_z has a single eigenvalue $\mu(z)$ in $(||K||^2 \pm \delta)$ for all $z \in (-\varepsilon, \varepsilon)$, given by:

$$\begin{aligned}\mu(z) &= ||K||^2 + z\langle \phi_\omega, H_z' \phi_\omega \rangle + \mathcal{O}(|z|^2) \\ &= ||K||^2 + z\langle \phi_\omega, V\phi_\omega \rangle + \mathcal{O}(|z|^2).\end{aligned}$$

It therefore suffices to prove that

$$\langle \phi_\omega, V\phi_\omega \rangle = \sum_{j \in \mathbb{J}} \omega^j V_{m(j)}.$$

Towards that end, first recall that V, viewed as a multiplication operator, commutes with g_* for all $g \in G$ due to V being Λ-invariant. Consequently, by expanding ϕ_ω via (4.8), we compute that

$$\begin{aligned}\langle \phi_\omega, V\phi_\omega \rangle &= \frac{1}{\sqrt{|G_0|}} \sum_{j \in \mathbb{J}} \omega^{-j} \left\langle e^{ig^{-j}K\cdot x}, V\phi_\omega \right\rangle = \frac{1}{\sqrt{|G_0|}} \sum_{j \in \mathbb{J}} \omega^{-j} \left\langle e^{iK\cdot x}, V(g_*^j \phi_\omega) \right\rangle \\ &= \frac{1}{\sqrt{|G_0|}} \sum_{j \in \mathbb{J}} \left\langle e^{iK\cdot x}, V\phi_\omega \right\rangle = \sqrt{|G_0|} \left\langle e^{iK\cdot x}, V\phi_\omega \right\rangle \\ &= \sum_{j \in \mathbb{J}} \omega^j \left\langle e^{iK\cdot x}, Ve^{ig^{-j}K\cdot x} \right\rangle = \sum_{j \in \mathbb{J}} \omega^j \left\langle e^{i(K - g^{-j}K)\cdot x}, V \right\rangle = \sum_{j \in \mathbb{J}} \omega^j V_{-m(j)}. \qquad (4.10)\end{aligned}$$

Note that in (4.10), we have used the fact that $K - g^{-j}K = -m(j) \cdot (k_1, \ldots, k_n)$. Lastly, since V is necessarily even, $V_{-m(j)} = V_{m(j)}$ for all $j \in \mathbb{J}$, thus completing the proof. $\square$

Proof of Lemma 4.4. We first prove, using the Schur complement formula (Proposition 3.3), that there exist $\varepsilon, \delta > 0$ such that for $||\kappa|| < \varepsilon$ and $\mu \in \mathbb{B}_\delta(\mu(z))$,

$$\begin{aligned}&H_z - \mu \text{ is invertible on } L^2_{K+\kappa} \\ \Leftrightarrow\ &(u(z) - \mu) + M(z,\kappa) + R(\mu,\kappa) \text{ is invertible on } \mathcal{E}(z), \qquad (4.11)\end{aligned}$$

where $M(z,\kappa) = -\pi(z)(2i\kappa \cdot \nabla)\pi(z)$ and $R(\mu,\kappa) \le C_1||\kappa||^2$ for some $C_1 > 0$. Since $z \in \mathbb{R}$ is assumed to be fixed, for simplicity of notation we suppress the dependence of $\mathcal{E}(z)$ on z, and denote this eigenspace simply by $\mathcal{E}$. We also note that the operators H_z on $L^2_{K+\kappa}$ and $H_{z,\kappa} := e^{-i\kappa\cdot x} H_z e^{i\kappa\cdot x}$ on L^2_K have the same spectrum. Indeed, if $\phi(x) \in L^2_K$, then $\psi(x) := e^{i\kappa\cdot x}\phi(x) \in L^2_{K+\kappa}$. Furthermore, ψ is an $L^2_{K+\kappa}$ eigenvector of H_z with eigenvalue μ if and only if

$$H_{z,\kappa}\phi(x) = e^{-i\kappa\cdot x} H_z \psi(x) = \mu\phi(x),$$

or, in other words, ϕ is an L^2_K eigenvector of $H_{z,\kappa}$ with eigenvalue μ. Therefore, it is equivalent to prove that $H_{z,\kappa} - \mu$ is invertible on L^2_K if and only if $(u(z) - \mu) + M(z,\kappa) + R(\mu,\kappa)$ is invertible on $\mathcal{E}$.

Write $H_{z,\kappa}$ as a 2×2 block operator with respect to the decomposition $L^2_K = \mathcal{E} \oplus \mathcal{E}^\perp$:

$$H_{z,\kappa} = \begin{pmatrix} H^{(11)}_{z,\kappa} & H^{(12)}_{z,\kappa} \\ H^{(21)}_{z,\kappa} & H^{(22)}_{z,\kappa} \end{pmatrix}.$$

Letting $\pi(z)^\perp = I - \pi(z)$, we compute that

$$\begin{aligned} H^{(11)}_{z,\kappa} &= \pi(z)H_{z,\kappa}\pi(z) = \pi(z)e^{-i\kappa\cdot x}(-\Delta + zV(x))e^{i\kappa\cdot x}\pi(z) \\ &= \pi(z)(H_z - 2i\kappa\cdot\nabla + ||\kappa||^2)\pi(z) \\ &= \mu(z) + M(z,\kappa) + ||\kappa||^2, \\ H^{(12)}_{z,\kappa} &= \pi(z)(H_z - 2i\kappa\cdot\nabla + ||\kappa||^2)\pi(z)^\perp \\ &= -\pi(z)(2i\kappa\cdot\nabla)\pi(z)^\perp + \mathcal{O}(||\kappa||^2) = \mathcal{O}(||\kappa||), \\ H^{(21)}_{z,\kappa} &= \left(H^{(12)}_{z,\kappa}\right)^* = \mathcal{O}(||\kappa||). \end{aligned}$$

Next, we claim that there exist $\varepsilon, \delta > 0$ such that for $||\kappa|| < \varepsilon$ and $\mu \in \mathbb{B}_\delta(\mu(z))$, $H^{(22)}_{z,\kappa} - \mu$ is invertible and its inverse is uniformly bounded in μ. To prove this, observe that since H_z has a compact resolvent and is self-adjoint due to our assumption that $z \in \mathbb{R}$, we can order the distinct eigenvalues of H_z so that there exist eigenvalues $\mu_- < \mu(z) < \mu_+$ and the remaining eigenvalues of H_z are all strictly farther away from $\mu(z)$. Consequently, if we let

$$\delta = \frac{1}{2}\min\left\{|\mu(z) - \mu_-|, |\mu(z) - \mu_+|\right\},$$

it then follows that $H_z|_{\mathcal{E}^\perp}$ has no eigenvalues in $\mathbb{B}_\delta(\mu(z))$ since by construction $\mu(z)$ is not an eigenvalue of $H_z|_{\mathcal{E}^\perp}$. Therefore $H_z|_{\mathcal{E}^\perp} - \mu$ is invertible and its norm is bounded by $1/\delta$. In addition, the fact that H_z is self-adjoint implies that $\mathrm{Im}(H_z|_{\mathcal{E}^\perp}) \subset \mathcal{E}^\perp$, and as a result $(H_z - \mu)|^{-1}_{\mathcal{E}^\perp}$ is a well-defined operator from $\mathcal{E}^\perp$ to itself (and in fact is a bijection from $\mathcal{E}^\perp$ to $H^2_K \cap \mathcal{E}^\perp$ by elliptic regularity).

Thus, for all $\mu \in \mathbb{B}_\delta(\mu(z))$, we have

$$\begin{aligned} H^{(22)}_{z,\kappa} - \mu &= \pi(z)^\perp(H_z - \mu - 2i\kappa\cdot\nabla + ||\kappa||^2)\pi(z)^\perp \\ &= (H_z - \mu)|_{\mathcal{E}^\perp} - \pi(z)^\perp(2i\kappa\cdot\nabla)\pi(z)^\perp + ||\kappa||^2 \\ &= (H_z - \mu)|_{\mathcal{E}^\perp}\left(I - T(\mu,\kappa)\right), \end{aligned}$$

where

$$T(\mu,\kappa) = (H_z - \mu)|^{-1}_{\mathcal{E}^\perp}\left(\pi(z)^\perp(2i\kappa\cdot\nabla)\pi(z)^\perp + ||\kappa||^2\right).$$

Again using elliptic regularity, for each $\mu \in \mathbb{B}_\delta(\mu(z))$ there exists some $C_\mu > 0$ such that $||T(\mu,\kappa)|| \le C_\mu ||\kappa||$. In addition, since $\mathbb{B}_\delta(\mu(z))$ is contained in the resolvent set of H_z, $T(z,\kappa)$ is continuous in μ on this set, which together with the fact that $\mathbb{B}_\delta(\mu(z))$ is precompact, means that there exists some $C > 0$, uniform in μ, such that $||T(\mu,\kappa)|| \le C||\kappa||$. Therefore, if we set $\varepsilon = 1/C$, it follows from a Neumann series argument such as the one following (3.15) that $H^{(22)}_{z,\kappa} - \mu$ is invertible and its inverse satisfies

$$(H^{(22)}_{z,\kappa} - \mu)^{-1} = (H_z - \mu)|^{-1}_{\mathcal{E}^\perp} + \mathcal{O}(||\kappa||),$$

uniformly in μ, for $\mu \in \mathbb{B}_\delta(\mu(z))$ and $||\kappa|| < \varepsilon$.

Since $H^{(22)}_{z,\kappa} - \mu$ is invertible for all $\mu \in \mathcal{B}_\delta(\mu(z)$ and $||\kappa|| < \varepsilon$, the Schur complement of the block $H^{(22)}_{z,\kappa} - \mu$ is well-defined for all such μ and κ and is given by:

$$(H^{(11)}_{z,\kappa} - \mu) + H^{(12)}_{z,\kappa}(H^{(22)}_{z,\kappa} - \mu)^{-1} H^{(21)}_{z,\kappa} = (\mu(z) - \mu) + M(z,\kappa) + R(\mu,\kappa), \quad \text{where}$$
$$R(\mu,\kappa) = ||\kappa||^2 + H^{(12)}_{z,\kappa}(H^{(22)}_{z,\kappa} - \mu)^{-1} H^{(21)}_{z,\kappa}.$$

However, since $||(H^{(22)}_{z,\kappa} - \mu)^{-1}|| \le \delta + C||\kappa||$ uniformly in μ, it follows that $||R(\mu,\kappa)|| \le C_1||\kappa||^2$ for some $C_1 > 0$, thus proving (4.11). Using this, we now prove (1), (2), and (3) of Lemma 4.4.

(1) This is immediate from (4.11), since μ is an $L^2_{K+\kappa}$-eigenvalue of H_z if and only if $H_z - \mu$ is not invertible, and $(\mu(z) - \mu) + M(z,\kappa) + R(\mu,\kappa)$ is not invertible on $\mathcal{E}$ if and only if its determinant is zero.

(2) Suppose $\lambda(z,\kappa)$ is a simple eigenvalue of $M(z,\kappa)$, continuous in κ on some open set $U \subset B_\varepsilon(0)$ such that $\sup_{\kappa \in U} |\lambda(z,\kappa)| < \delta$. Then for any $\kappa_0 \in U$, by continuity of λ there exists a neighborhood $U_0 \subset U$ of κ_0 and a $\delta_0 < \delta$ such that $\sup_{\kappa \in U_0} |\lambda(z,\kappa)| < \delta_0$. Thus, by simplicity, there exists a simple, closed, positively-oriented contour $\mathcal{C}$ contained in $\mathbb{B}_\delta(\mu(z))$, such that $\mathcal{C}$ strictly encloses $\mu(z) + \lambda(z,\kappa)$ and no other eigenvalue of $\mu(z) + M(z,\kappa)$ for all $\kappa \in U_0$. In addition, since $\mathcal{C}$ and $\overline{U_0}$ are compact (since $U_0 \subset B_\varepsilon(0)$) and $((\mu(z) - \mu) + M(z,\kappa))^{-1}$ is continuous in μ, κ for all $\mu \in \mathcal{C}$ and $\kappa \in U_0$, there exists $C_2 > 0$ such that

$$||((\mu(z) - \mu) + M(z,\kappa))^{-1}|| \le C_2 \tag{4.12}$$

for all $\mu \in \mathcal{C}$ and $\kappa \in U_0$.

We now want to use Cauchy's integral formula (Theorem 3.6) to relate the eigenvalues of $H_{z,\kappa}$ to those of $M(z,\kappa)$. To do so, we now prove that the operator $(\mu(z) - \mu) + M(z,\kappa) + R(\mu,\kappa)$ is invertible and its inverse is uniformly bounded in μ for all $\mu \in \mathcal{C}$ and $\kappa \in U_0$. First, observe that

$$(\mu(z) - \mu) + M(z,\kappa) + R(\mu,\kappa) = ((\mu(z) - \mu) + M(z,\kappa))\,(I + S(z,\kappa))\,, \quad \text{where}$$
$$S(z,\kappa) = ((\mu(z) - \mu) + M(z,\kappa))^{-1} \cdot \mathcal{O}(||\kappa||^2).$$

By (4.12), after increasing C_2 if necessary, $||S(z,\kappa)|| \leq C_2||\kappa||^2$ for all $\mu \in \mathcal{C}$. Therefore, by replacing ε with the minimum of itself and $1/\sqrt{C_2}$, it follows from another Neumann series argument that $(\mu(z)-\mu)+M(z,\kappa)+R(\mu,\kappa)$ is invertible and its inverse satisfies

$$(((\mu(z)-\mu)+M(z,\kappa)+R(\mu,\kappa)))^{-1} = ((\mu(z)-\mu)+M(z,\kappa))^{-1} + \mathcal{O}(||\kappa||^2)$$

for all $\mu \in \mathcal{C}$ and $\kappa \in U_0$, where again the bound is uniform in μ.

Thus, for all such μ and κ, we can write $(H_{z,\kappa}-\mu)^{-1}$ with respect to the decomposition $L^2_K = \mathcal{E} \oplus \mathcal{E}^\perp$ as

$$(H_{z,\kappa}-\mu)^{-1} = \begin{pmatrix} ((\mu(z)-\mu)+M(z,\kappa))^{-1} + \mathcal{O}(||\kappa||^2) & \mathcal{O}(||\kappa||) \\ \mathcal{O}(||\kappa||) & (H^{(22)}_{z,\kappa}-\mu)^{-1} + \mathcal{O}(||\kappa||^2) \end{pmatrix},$$

where all bounds are uniform in μ. Consequently, by applying Cauchy's integral formula and taking the trace of both sides, we get

$$\begin{aligned} \operatorname{Tr}&\left(\frac{1}{2\pi i}\oint_{\mathcal{C}} \mu(H_{z,\kappa}-\mu)^{-1}d\mu\right) \\ &= \operatorname{Tr}\left(\frac{1}{2\pi i}\oint_{\mathcal{C}} \mu((\mu(z)-\mu)+M(z,\kappa))^{-1}d\mu\right) \\ &\quad + \operatorname{Tr}\left(\frac{1}{2\pi i}\oint_{\mathcal{C}} \mu(H^{(22)}_{z,\kappa}-\mu)^{-1}d\mu\right) + \operatorname{Tr}\left(\frac{1}{2\pi i}\oint_{\mathcal{C}} \mu\cdot\mathcal{O}(||\kappa||^2)d\mu\right) \\ &= \mu(z)+\lambda(z,\kappa)+\mathcal{O}(||\kappa||^2). \end{aligned} \tag{4.13}$$

To compute (4.13), we have used three facts. First, we used that $\lambda(z,\kappa)$ is a simple eigenvalue of $M(z,\kappa)$ and the only eigenvalue contained in $\mathcal{C}$. Second, we used that $\mu(H^{(22)}_{z,\kappa}-\mu)^{-1}$ is analytic in μ on $\mathbb{B}_\delta(\mu(z))$, and so its integral on $\mathcal{C}$ equals zero. Lastly, we used that the integral of $\mu\cdot\mathcal{O}(||\kappa||^2)$ is $\mathcal{O}(||\kappa||^2)$, due to the ML inequality and since the bound is uniform in μ. An identical argument also tells us that

$$\operatorname{Tr}\left(\frac{1}{2\pi i}\oint_{\mathcal{C}}(H_{z,\kappa}-\mu)^{-1}d\mu\right) = \operatorname{Tr}\left(\frac{1}{2\pi i}\oint_{\mathcal{C}}((\mu(z)-\mu)+M(z,\kappa))^{-1}d\mu\right) + \mathcal{O}(||\kappa||^2). \tag{4.14}$$

From here, note that $H_{z,\kappa}$ is self-adjoint since it is unitarily equivalent to H_z, and it is also analytic in κ in the sense of A1(i). Consequently, by the residue theorem, it follows that if we let

$$\pi(\kappa) = \frac{1}{2\pi i}\oint_{\mathcal{C}}(H_{z,\kappa}-\mu)^{-1}d\mu,$$

then $\pi(\kappa)$ is the projection onto the eigenspaces corresponding to eigenvalues of $H_{z,\kappa}$ contained in $\mathcal{C}$, and it is analytic in κ since its integrand is. Therefore (4.14) becomes

$$\operatorname{rank}\pi(\kappa) = 1 + \mathcal{O}(||\kappa||^2).$$

Since $\pi(\kappa)$ is analytic in κ, its rank must be constant, and we therefore deduce that $H_{z,\kappa}$ has a single, simple eigenvalue $\mu(z,\kappa)$ in $\mathcal{C}$. It then follows from (4.13) that

$$\mu(z,\kappa) = \mu(z) + \lambda(z,\kappa)) + \mathcal{O}(||\kappa||^2$$

for all $\kappa \in U_0$. Since this equation holds on a neighborhood of κ_0 for every $\kappa_0 \in U$, we conclude that (4.9) holds on all of U.

(3) Assume that $M(z,\kappa) = 0$; then by (1), for $||\kappa|| < \varepsilon$, the $L^2_{K+\kappa}$-eigenvalues of H_z in $B_\delta(\mu(z))$ are equal to the eigenvalues of $\mu(z) + R(\mu,\kappa)|_{\mathcal{E}}$, which in turn are equal to $\mu(z)$ plus the eigenvalues of $R(\mu,\kappa)$. However, if $\lambda(\kappa)$ is an eigenvalue of $R(\mu,\kappa)|_{\mathcal{E}}$, then

$$|\lambda(\kappa)| \le ||R(\mu,\kappa)|| \le C_1||\kappa||^2.$$

Therefore, for $||\kappa|| < \varepsilon$, the $L^2_{K+\kappa}$-eigenvalues of H_z in $B_\delta(\mu(z))$ satisfy $\mu(z,\kappa) = \mu(z) + \mathcal{O}(||\kappa||^2)$. □

Proof of Lemma 4.5. Let $m = \dim \mathcal{E}(z)$, which is constant by analyticity of $\pi(z)$ and [Kat95, Lemma I.4.10]. As a symmetric function of eigenvalues, the determinant of $M(z,\kappa) - \lambda$ can be expressed as a (universal) polynomial in the traces of its m first powers. This means that $\det_{\mathcal{E}(z)}(M(z,\kappa) - \lambda)$ is polynomial (with coefficients independent of z, κ, and λ) in

$$\mathrm{Tr}_{\mathcal{E}(z)}\left((M(z,\kappa) - \lambda)^j\right) = \mathrm{Tr}_{L^2_K}\left((M(z,\kappa) - \lambda\pi(z))^j\right), \quad \text{for } j = 1,\dots,m.$$

The operator $M(z,\kappa) - \lambda\pi(z)$ is finite-rank and analytic in z; hence its trace is analytic in z. Thus $\det_{\mathcal{E}(z)}\left(M(z,\kappa) - \lambda\right)$ is analytic in z. □

Proof of Lemma 4.6. We start by looking at how the group action of G_0 interacts with the gradient of a function $f \in L^2_K$. Let $g \in G_0$; then

$$\nabla(g_* f)(x) = \nabla(f(g^\top x)) = g(\nabla f)(g^\top x) = g(g_* \nabla f)(x).$$

Multiplying the first and last of these expressions on the right by $g^\top$, we get

$$g_* \nabla f = g^\top \nabla(g_* f). \tag{4.15}$$

Now let $\phi \in L^2_{K,\omega}$ and let $\psi \in L^2_{K,\widetilde{\omega}}$ for $\omega, \widetilde{\omega} \in \mathbb{U}$. To show that $\langle \phi, \nabla\psi\rangle$ is an eigenvector of g^j with corresponding eigenvalue $\omega^{-j}\widetilde{\omega}^j$ for all $j \in \mathbb{J}$, we compute the following, using (4.15) and the fact that $(g^j)^\top = g^{-j}$ since G_0 consists of orthogonal matrices:

$$g^j\langle \phi, \nabla\psi\rangle = g^j\langle g^j_*\phi, g^j_*\nabla\psi\rangle = \langle g^j_*\phi, \nabla(g^j_*\psi)\rangle = \overline{\omega^j}\widetilde{\omega}^j\langle \phi, \nabla\psi\rangle = \omega^{-j}\widetilde{\omega}^j\langle \phi, \nabla\psi\rangle. \tag{4.16}$$

Lastly, to show that $\langle \phi, \nabla\phi \rangle = 0$ when K is a vertex of $\mathcal{B}$, note that (4.16) implies that $\langle \phi, \nabla\phi \rangle$ is an eigenvector of g^j with eigenvalue 1 for all $j \in \mathbb{J}$. However, we claim that the only such vector is the zero vector. Suppose $k \in \mathbb{R}^n$ such that gk for all $g \in G_0$. Then, since K is assumed to be a vertex of $\mathcal{B}$, it necessarily must lie on at least n hyperfaces of $\mathcal{B}$. Therefore, by Proposition 2.1, there exist linearly independent lattice vectors $K_1, \ldots, K_n \in \Lambda^*$ such that $K - K_j$ is also a vertex of $\mathcal{B}$ satisfying $||K - K_j|| = ||K||$, and thus contained in the equivalence class $[K]$. By A3, for $j = 1, \ldots, n$, there exists $h_j \in G_0$ (where the notation here is chosen to differentiate h_j from the generator g_j) such that $h_j K = K - K_j$. Thus we get that, for all j,

$$k \cdot K_j = k \cdot (K - h_j K) = k \cdot K - h_j^\top k \cdot K = k \cdot K - k \cdot K = 0.$$

Since the set $\{K_j\}_{j=1}^n$ is linearly independent, it is a basis for $\mathbb{R}^n$, and it therefore follows that $k = 0$. As a result, we conclude that $\langle \phi, \nabla\phi \rangle = 0$. □

Chapter 5

SCHRÖDINGER OPERATORS INVARIANT UNDER TWO-DIMENSIONAL LATTICES

In this chapter, we apply the general framework developed in Chapter 4 to two-dimensional Bravais lattices. Every such lattice is isometric to one of the lattices generated by the bases listed in the first rows of Tables 5.1 and 5.2; namely the *square*, *hexagonal*, *rectangular*, *centered rectangular*, and *oblique* lattices. Consequently, if V is a Λ-invariant potential for some two-dimensional lattice Λ, by Remark 4.2 we may assume that V is invariant with respect to one of these listed lattices. We shall then show that the dispersion surfaces of Schrödinger operators with potentials invariant under the square and hexagonal lattices generically have unusual dispersion surfaces near vertices of the Brillouin zone, reproducing results due to [Kel+18] and [FW12], respectively, which are also listed in Theorem 1.3. Next, we apply this framework to the rectangular lattice and see that, while the framework works as intended, it does not produce interesting intersections of dispersion surfaces. Lastly, we discuss the centered rectangular and oblique lattices, which have comparatively small symmetry groups and thus we suspect are unlikely to have such intersections.

For the rest of this chapter, $r, \rho_0, \rho, f, f_1, f_2$ shall denote the following matrices:

$$r := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \qquad \rho_0 := \begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & 1/2 \end{pmatrix}, \qquad \rho := \rho_0^2 = \begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}, \tag{5.1}$$
$$f := \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \qquad f_1 := \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad f_2 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Note that r, ρ_0, and ρ are counter-clockwise rotations in the plane by $\pi/4$, $\pi/3$, and $2\pi/3$, respectively.

5.1 *Geometry of Two-Dimensional Lattices.*

Let Λ^S, Λ^H, Λ^R, Λ^{CR}, and Λ^O denote the square, hexagonal, rectangular, centered rectangular, and oblique lattices, respectively, which are generated by the bases given in the first row of Tables 5.1 and 5.2 for $a, a_1, a_2 > 0$, $0 < \theta < \pi/2$. These tables also include some spectral results for $-\Delta$ seen as a Λ^S, Λ^H, Λ^R, Λ^{CR}, and Λ^O invariant operator, respectively, on L^2_K, where K is a vertex of the corresponding Brillouin zone $\mathcal{B}$, as these points exhibit a high degree of symmetry (see Section 4.1). In addition, by Λ^*-periodicity

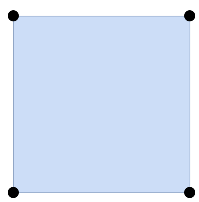
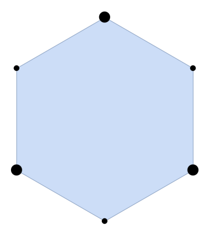
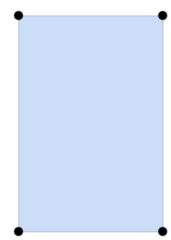
	Λ^R	Λ^S	Λ^H
Basis	$\begin{pmatrix} a \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a \end{pmatrix}$	$\begin{pmatrix} a\sqrt{3}/2 \\ a/2 \end{pmatrix}, \begin{pmatrix} a\sqrt{3}/2 \\ -a/2 \end{pmatrix}$	$\begin{pmatrix} a_1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a_2 \end{pmatrix}$
Dual Basis	$\begin{pmatrix} q \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ q \end{pmatrix}$	$\begin{pmatrix} q\sqrt{3}/3 \\ q \end{pmatrix}, \begin{pmatrix} q\sqrt{3}/3 \\ -q \end{pmatrix}$	$\begin{pmatrix} q_1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ q_2 \end{pmatrix}$
$\mathcal{B}$			
K	$\begin{pmatrix} q/2 \\ q/2 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 2q/3 \end{pmatrix}$	$\begin{pmatrix} q_1/2 \\ q_2/2 \end{pmatrix}$
m	4	3	4
G	$\langle r, f_1 \rangle$	$\langle \rho_0, f_1 \rangle$	$\langle f_1, f_2 \rangle$
G_0	$\langle r \rangle$	$\langle \rho \rangle$	$\langle f_1, f_2 \rangle$
$\mathbb{U}$	U_4	U_3	U_2^2

Table 5.1: Geometry of the square, hexagonal, and rectangular lattices.

of the the Floquet-Bloch problem (1.3) and by Remark 4.2, it suffices to consider vertices K such that the sets $G \cdot [K]$, i.e. the orbits of the equivalence classes $[K]$ (defined in (4.2))

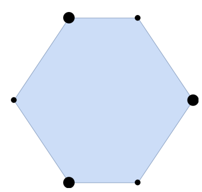
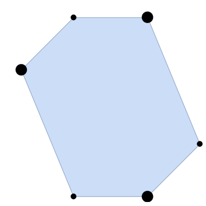
	Λ^{CR}	Λ^{O}
Basis	$\begin{pmatrix} a_1 \\ 0 \end{pmatrix}, \begin{pmatrix} a_1/2 \\ a_2/2 \end{pmatrix}$	$\begin{pmatrix} a_1 \\ 0 \end{pmatrix}, \begin{pmatrix} a_2 \cos\theta \\ a_2 \sin\theta \end{pmatrix}$
Dual Basis	$\begin{pmatrix} q_1 \\ -q_2 \end{pmatrix}, \begin{pmatrix} 0 \\ 2q_2 \end{pmatrix}$	$\begin{pmatrix} q_1 \\ -q_1 \cot\theta \end{pmatrix}, \begin{pmatrix} 0 \\ q_2 \csc\theta \end{pmatrix}$
$\mathcal{B}$		
K	$\begin{pmatrix} (q_1^2 + q_2^2)/2q_1 \\ 0 \end{pmatrix}$	$\begin{pmatrix} (q_1^2 \csc^2\theta + q_1 q_2 \cot\theta \csc\theta)/2 \\ (q_2 \csc\theta)/2 \end{pmatrix}$
m	3	3
G	$\langle f_1, f_2 \rangle$	$\langle f \rangle$

Table 5.2: Geometry of the centered rectangular and oblique lattices.

under the action of the point group G, are distinct.

In both Table 5.1 and Table 5.2, in addition to a basis (v_1, v_2), we list for each of the lattices Λ^R, Λ^{CR}, Λ^S, Λ^H, and Λ^O:

- The corresponding dual basis (k_1, k_2), where $q = \frac{2\pi}{a}$, $q_j = \frac{2\pi}{a_j}$ for $j = 1, 2$ (which by definition satisfies $v_j \cdot k_\ell = 2\pi\delta_{j\ell}$ for $j, \ell = 1, 2$);

- A picture of the Brillouin zone $\mathcal{B}$, where the vertices are sized in reference to the vertex listed in the following row. Specifically, given a vertex K, the set $[K]$ consists of vertices of $\mathcal{B}$ by Proposition 4.1, which are denoted by larger dots. Those vertices which lie in $(G \cdot [K]) \setminus [K]$ have smaller dots. In particular, the vertices of the Brillouin zone of every two-dimensional lattice all lie in a single set of the form $G \cdot [K]$;

- A vertex K of the Brillouin zone;
- The multiplicity m of the L^2_K-eigenvalue $||K||^2$ of $-\Delta$, which by (4.3) is equal to the cardinality of the set $[K]$;
- The point group G, expressed in terms of its generators;

For Table 5.1 we also include:

- An abelian subgroup G_0 of G, which together with the vertex K satisfy A3;
- The corresponding group $\mathbb{U}$ consisting of tuples of roots of unity, as defined in (4.6).

5.2 *Proof Outline for Theorem 1.3*

In Sections 5.3 and 5.4, we shall prove Theorem 1.3 for the lattices Λ^S and Λ^H, respectively, by using the lemmas stated in Section 4.4. In Chapter 6, we shall use the same methods to prove Theorem 1.3 for the simple cubic, the body-centered cubic, the face-centered cubic, and lastly the stacked hexagonal, in Sections 6.2, 6.3 – 6.4, 6.5, and 6.7, respectively. Each of these proofs will require the same three steps, which we now outline.

(1) Upper bound on multiplicity: Let Λ be one of the lattices listed in Table 5.1, and let (k_1, k_2), $\mathcal{B}$, K, m, G_0, and $\mathbb{U}$ be the objects listed in the corresponding column. We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Then for each $\omega \in \mathbb{U}$, Lemma 4.3 describes how the multiplicity m, L^2_K-eigenvalue $||K||^2$ of $H_0 = -\Delta$ splits as z increases into simple $L^2_{K,\omega}$-eigenvalues given by:

$$\mu_\omega(z) = ||K||^2 + z \cdot \sum_{j \in \mathbb{J}} \omega^j V_{m(j)} + \mathcal{O}(|z|^2),$$

In particular, if $\omega, \widetilde{\omega} \in \mathbb{U}$ are such that $\mu'_\omega(0), \mu'_{\widetilde{\omega}}(0)$ are distinct, then the eigenvalues $\mu_\omega(z), \mu_{\widetilde{\omega}}(z)$ clearly split. This test provides an upper bound on possible multiplicities of $\mu_\omega(z)$, viewed as an L^2_K-eigenvalue.

(2) Lower bound on multiplicity: Our argument in step (1) is inconclusive when $\mu'_\omega(0) = \mu'_{\widetilde{\omega}}(0)$, and so in this case we provide a lower bound on the splitting multiplicities using

a symmetry argument. Note that the multiplicity of $\mu_\omega(z)$ as an L^2_K-eigenvalue is at least one, so it suffices to prove a lower bound on the multiplicity of $\mu_\omega(z)$ for those $\omega \in \mathbb{U}$ such that the upper bound computed in (1) is strictly greater than 1. This argument will typically rely on the existence of symmetries S of H_z such that

$$S\big(L^2_{K,\omega}\big) = L^2_{K,\widetilde{\omega}}.$$

This implies that H_z on $L^2_{K,\omega}$ and $L^2_{K,\widetilde{\omega}}$ are conjugated, hence isospectral: $\mu_\omega(z) = \mu_{\widetilde{\omega}}(z)$. In each case, this will provide a lower bound on the multiplicity of $\mu_\omega(z)$ as an L^2_K-eigenvalue equaling the upper bound computed in step (1), and thus we deduce that $\mu_\omega(z)$ has constant multiplicity, which we denote by m_ω, for sufficiently small z. It then follows that $\mu_\omega(z)$ satisfies A2, and so we can apply Theorem 1.2 to conclude that H_z has an L^2_K-eigenvalue $\mu_\omega(z)$ which has multiplicity $m_\omega$for $z \in \mathbb{R}$ away from a discrete set D_1, and whose eigenprojector $\pi_\omega(z)$ is analytic on a open neighborhood U of the real line.

(3) Computation of the characteristic polynomial: Let

$$\mathbb{U}_\omega = \{\widetilde{\omega} \in \mathbb{U} \;:\; \mu'_{\widetilde{\omega}}(0) = \mu'_\omega(0)\},$$

so that $m_\omega = |\mathbb{U}_\omega|$ and $\mu_\omega = \mu_{\widetilde{\omega}}$ for all $\widetilde{\omega} \in \mathbb{U}_\omega$ by steps (1) and (2). Then for all such $\widetilde{\omega}$ and sufficiently small z,

$$\big(H_z - \mu_\omega(z)\pi_\omega(z)\big)|_{L^2_{K,\widetilde{\omega}}} = 0,$$

and by analyticity this must hold for all $z \in U$. Therefore $\mu_\omega(z)$ is an $L^2_{K,\widetilde{\omega}}$-eigenvalue of multiplicity at least one for all $z \in U$, and thus is a simple $L^2_{K,\widetilde{\omega}}$-eigenvalue for all $z \in \mathbb{R} \setminus D_1$. As a result, for all such z there exists a basis $(\phi_1, \ldots, \phi_{m_\omega})$, normalized to have L^2_K-norm 1, of the eigenspace $\mathcal{E}$ corresponding to $\mu_\omega(z)$ consisting of precisely one vector from $L^2_{K,\widetilde{\omega}}$ for each $\widetilde{\omega} \in \mathbb{U}_\omega$.

For $z \in \mathbb{R} \setminus D_1$, Lemma 4.4 then describes the structure of the dispersion surfaces corresponding to $\mu_\omega(z)$ near the vertex K. For each of the lattices we examine, one of two things happens: either all of the eigenvalues of $M(z,\kappa) = -\pi_\omega(z)(2i\kappa \cdot \nabla)\pi_\omega(z)|_{\mathcal{E}}$ are simple on an open set (not necessarily connected) near $\kappa = 0$, or $M(z,\kappa)$ is identically 0. In the first case, if $\lambda(z,\kappa)$ is a simple eigenvalue of $M(z,\kappa)$, then Lemma 4.4(2) tells us there exists a simple eigenvalue $\mu_\omega(z,\kappa)$ of H_z on $L^2_{K+\kappa}$ such that

$$\mu_\omega(z,\kappa) = \mu_\omega(z) + \lambda(z,\kappa) + \mathcal{O}(||\kappa||^2). \tag{5.2}$$

Note that (5.2) also always holds at $\kappa = 0$, since $\lambda(z,0) = 0$ by virtue of $M(z,0) = 0$, although $\mu_\omega(z,\kappa)$ will typically no longer be simple at this point. As a result, in the specific case where the eigenvalues of $M(k)$ are simple on a punctured neighborhood of $\kappa = 0$, the (5.2) in fact holds on a neighborhood of $\kappa = 0$. On the other hand, if $M(z,\kappa)$ is identically zero, then Lemma 4.4(3) tells us that every dispersion surface corresponding to $\mu_\omega(z)$ near the vertex K satisfies

$$\mu_\omega(z,\kappa) = \mu_\omega(z) + \mathcal{O}(||\kappa||^2),$$

which immediately implies that $(K, \mu(z))$ is a quadratic point (as per Definition 1.1).

Using the basis $(\phi_1, \ldots, \phi_{m_\omega})$, we can then compute the entries of $M(z,\kappa)$ with respect to this basis using Lemma 4.6. In particular, this lemma tells us that the diagonal entries of $M(z,\kappa)$ are all zero, and we only need to compute the entries above the diagonal since $M(z,\kappa)$ is Hermitian. Once we have an explicit expression for $M(z,\kappa)$, we can then compute its characteristic polynomial.

We then finish by checking which of the coefficients of this polynomial are nonzero for z sufficiently small, which by Lemma 4.5 will then imply that these coefficients remain nonzero for all $z \in \mathbb{R}$ away from a discrete set D_2 by analyticity. To perform this computation, we will typically use the fact that a normalized eigenvector $\phi_\omega(x;z)$ corresponding to the $L^2_{K,\omega}$-eigenvalue $\mu_\omega(z)$ satisfies

$$\phi_\omega(x;z) = \phi_\omega(x) + \mathcal{O}(|z|), \tag{5.3}$$

where $\phi_\omega(x)$ is the normalized eigenvector corresponding to $\mu_\omega(0)$ given by (4.8). This follows from the observation that $\pi_\omega(z)\phi_\omega$ is an eigenvector corresponding to $\mu_\omega(z)$ for z sufficiently small, and the fact that $\pi_\omega(z) = \pi_\omega(0) + \mathcal{O}(|z|)$ by a Neumann series argument. Letting $D = D_1 \cup D_2$, we then conclude that (5.3) will hold for all $z \in \mathbb{R}$ away from the discrete set D.

5.3 *Proof of Theorem 1.3 for the Square*

Let $\Lambda = \Lambda^S$, and let (k_1, k_2), $\mathcal{B}$, K, m, G_0, and $\mathbb{U}$ be the objects listed in the corresponding column of Table 5.1 (i.e. the first column). We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Lastly, we will again need the matrices r, f_1, f_2 defined in (5.1).

(1) Upper bound on multiplicity: For each $\omega \in \mathbb{U}$, $\mu'_\omega(0)$ is given by:

$$\mu'_\omega(0) = \sum_{j \in \mathbb{J}} \omega^j V_{m(j)}.$$

A quick computation shows that

$$\begin{aligned} r^{-1}K &= K - k_2, \\ r^{-2}K &= K - k_1 - k_2, \\ r^{-3}K &= K - k_1. \end{aligned}$$

It follows from the definition of $m(j)$ (given by (4.7)), together with the fact that $V_{-m(j)} = V_{m(j)}$ (since V is even as noted in Section 3.2), that we can rewrite $\mu'_\omega(0)$ as

$$\mu'_\omega(0) = V_{0,0} + \omega V_{0,1} + \omega^2 V_{1,1} + \omega^3 V_{1,0}.$$

Also note that V is invariant under both r and f_1, and is therefore invariant under the product rf_1, which permutes the coordinate axis. It follows from (4.5) that $V_{1,0} = V_{0,1}$, and consequently

$$\mu'_\omega(0) = V_{0,0} + (\omega + \omega^3)V_{1,0} + \omega^2 V_{1,1}.$$

We then plug ω into this formula for each $\omega \in \mathbb{U}$, which gives us the following:

$$\begin{aligned} \mu'_1(0) &= V_{0,0} + 2V_{1,0} + V_{1,1}, \\ \mu'_i(0) = \mu'_{-i}(0) &= V_{0,0} - V_{1,1}, \\ \mu'_{-1}(0) &= V_{0,0} - 2V_{1,0} + V_{1,1}. \end{aligned}$$

Note that the set where the right-hand sides of any pair of the above three equations are equal describes a hyperplane. Consequently, the set where the right-hand sides of the above three equations fail to be distinct is a union of three hyperplanes. It follows that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into at least two simple eigenvalues and an eigenvalue of multiplicity at most two.

(2) Lower bound on multiplicity: As noted in Section 5.2, it suffices to consider $\mu_\omega(z)$ for $\omega \in \mathbb{U}$ such that the upper bound on the multiplicity computed in (1) is strictly greater than 1. In addition, observe that f_1 is K invariant since $f_1 K = K - k_1$. As a result, if $\phi \in L^2_{K,i}$ is an eigenvector of H_z, then $r_*\phi$ is also an eigenvector of H_z in L^2_K with the same eigenvalue. In addition, since $rf_1 = f_1 r^3$, it follows that

$$r_*(f_1)_*\phi = (f_1)_* r_*^3 \phi = -i(f_1)_*\phi.$$

Hence, $(f_1)_*\phi \in L^2_{K,-i}$, and so $\mu_i(z)$ is an L^2_K-eigenvalue with multiplicity at least 2, which together with step (1) implies that its multiplicity is exactly two. Therefore, H_z has a double L^2_K-eigenvalue for all $z \in \mathbb{R}$ away from a discrete set D_1, and the corresponding eigenprojectors are analytic on some open neighborhood U of $\mathbb{R}$.

(3) Computation of the characteristic polynomial: Fix some $z \in \mathbb{R} \setminus D_1$, and let $\phi_1 \in L^2_{K,i}$ and $\phi_2 \in L^2_{K,-i}$ be normalized eigenvectors for the eigenvalue $\mu_i(z)$ of H_z. The entries of $M(z,\kappa)$ with respect to this basis are given by $-2i\kappa \cdot \langle \phi_j, \nabla \phi_\ell \rangle$. For $j \neq \ell$, $\langle \phi_j, \nabla \phi_\ell \rangle$ is an eigenvector of r with eigenvalue $(-i)(-i) = -1$ by Lemma 4.6, and thus must be the zero vector. It follows that $M(z,\kappa) = 0$ for all z and κ, and thus we conclude that

$$\mu_i(z,\kappa) = \mu_i(z) + \mathcal{O}(||\kappa||^2).$$

By Definition 1.1 this means that $(K, \mu_i(z))$ is a 2-fold quadratic point for all $z \in \mathbb{R} \setminus D_1$. This completes the proof of Theorem 1.3 when Λ is a square lattice.

5.4 *Proof of Theorem 1.3 for the Hexagonal*

Let $\Lambda = \Lambda^H$ and let (k_1, k_2), $\mathcal{B}$, K, m, G_0, and $\mathbb{U}$ be the objects listed in the corresponding column of Table 6.1 (i.e. the second column). We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Lastly we will need the matrices ρ_0, ρ defined in (5.1).

(1) Upper bound on multiplicity: Just as we did in Section 5.3, we start by computing relations among the Fourier coefficients $V_{m(j)}$ for $j \in \mathbb{J}$. In particular, we compute that

$$\rho^{-1}K = K + k_2,$$
$$\rho^{-2}K = K - k_1.$$

Again using the fact that V is even, it follows that for $\omega \in \mathbb{U}$,

$$\mu'_\omega(0) = V_{0,0} + \omega V_{0,1} + \omega^2 V_{1,0}.$$

By (4.5) we also have that

$$V_{k_1} = \rho_* V_{k_1} = V_{\rho^\top k_1} = V_{k_2},$$

which tells us that $V_{1,0} = V_{0,1}$. Therefore we can rewrite $\mu'_\omega(0)$ as

$$\mu'_\omega(0) = V_{0,0} + (\omega + \omega^2) V_{1,0}.$$

We then plug ω into this formula for each $\omega \in \mathbb{U}$ to obtain:

$$\mu'_1(0) = V_{0,0} + 2V_{1,0},$$
$$\mu'_{\zeta_3}(0) = \mu'_{\overline{\zeta_3}}(0) = V_{0,0} - V_{1,0},$$

where ζ_3 is a third root of unity, which we can choose to be the one with positive imaginary part. The set where the right-hand sides of the above two equations fail to be distinct is a single hyperplane (namely, where $V_{1,0} = 0$). Therefore, we conclude that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into at least a simple eigenvalue and an eigenvalue of multiplicity at most two.

(2) Lower bound on multiplicity: Let T be the conjugate-parity operator: $Tf(x) = \overline{f(-x)}$, and let ϕ_1 be a normalized eigenvector of H_z in L^2_{K,ζ_3} for the eigenvalue $\mu_{\zeta_3}(z)$. For $z \in \mathbb{R}$, $\phi_2 := T\phi_1 \in L^2_K$ is also an eigenvector of H_z for the same eigenvalue by 4.3. In addition, observe that

$$\rho_* \phi_2(x) = \overline{\phi_1(-\rho^\top x)} = \overline{\zeta_3 \phi_1(-x)} = \overline{\zeta_3} \phi_2(x).$$

Therefore $\phi_2 \in L^2_{K,\overline{\zeta_3}}$, which implies that H_z has a double L^2_K-eigenvalue for all $z \in \mathbb{R}$ away from a discrete set D_1, and the corresponding eigenprojector is analytic on some open neighborhood U of $\mathbb{R}$.

(3) Computation of the characteristic polynomial: Fix some $z \in \mathbb{R} \setminus D_1$, and let $\phi_1 \in L^2_{K,\zeta_3}$ be a normalized eigenvector of H_z for the eigenvalue $\mu_{\zeta_3}(z)$. Then, as we saw in step (2), $\phi_2 := T\phi_1 \in L^2_{K,\overline{\zeta_3}}$ is an eigenvector of H_z with eigenvalue $\mu_{\zeta_3}(z)$ as well, and thus ϕ_1, ϕ_2 form a basis for the corresponding eigenspace. The entries of $M(z,\kappa)$ with respect to this basis are given by $-2i\kappa \cdot \langle \phi_j, \nabla \phi_\ell \rangle$. Therefore, by Lemma 4.6, the entries of $M(z,\kappa)$ are entirely determined by $\langle \phi_1, \nabla \phi_2 \rangle$.

To compute this entry, note that by Lemma 4.6,

$$\rho \langle \phi_1, \nabla \phi_2 \rangle = \overline{\zeta_3}^2 \langle \phi_1, \nabla \phi_2 \rangle = \zeta_3 \langle \phi_1, \nabla \phi_2 \rangle.$$

Hence, $\langle \phi_1, \nabla \phi_2 \rangle$ is an eigenvector of ρ with eigenvalue ζ_3, and is therefore of the form

$$\langle \phi_1, \nabla \phi_2 \rangle = \alpha \begin{pmatrix} i \\ 1 \end{pmatrix}$$

for some $\alpha \in \mathbb{C}$. Consequently, with respect to the basis (ϕ_1, ϕ_2), $M(z,\kappa)$ is given by:

$$M(z,\kappa) = -2i \begin{pmatrix} 0 & \alpha(\kappa_2 + i\kappa_1) \\ -\overline{\alpha}(\kappa_2 - i\kappa_1) & 0 \end{pmatrix}.$$

A quick computation then gives the characteristic polynomial of $M(z,\kappa)$ (as a polynomial in μ):

$$\mu^2 + |\alpha|^2 ||\kappa||^2.$$

By Lemma 4.5, the coefficient $|\alpha|^2$ is analytic in z, and therefore will be nonzero away from a discrete set if it is nonzero for z sufficiently small. However, by Lemma 4.2 we can assume that, for z sufficiently small, ϕ_1, ϕ_2 are given by:

$$\phi_1(x;z) = \frac{1}{\sqrt{3}} \left(e^{iK\cdot x} + \zeta_3 e^{i\rho^{-1}K\cdot x} + \overline{\zeta_3} e^{i\rho^{-2}K\cdot x} \right) + \mathcal{O}(|z|),$$
$$\phi_2(x;z) = \frac{1}{\sqrt{3}} \left(e^{iK\cdot x} + \overline{\zeta_3} e^{i\rho^{-1}K\cdot x} + \zeta_3 e^{i\rho^{-2}K\cdot x} \right) + \mathcal{O}(|z|).$$

It follows that, for z small,

$$\alpha = e_2 \cdot \langle \phi_1, \nabla \phi_2 \rangle = \frac{i}{3} e_2 \cdot \left(K + \zeta_3 \rho^{-1} K + \overline{\zeta_3} \rho^{-2} K \right) + \mathcal{O}(|z|^2) = -\frac{i\sqrt{3}}{3} q + \mathcal{O}(|z|^2).$$

Therefore $|\alpha|^2$ is nonzero for z sufficiently small, and thus remains nonzero for all $z \in U$ away from another discrete set D_2. It follows that $|\alpha|^2$ is nonzero on $\mathbb{R} \setminus D_2$, and so by Definition 1.1 we conclude that $(K, \mu_{\zeta_3}(z))$ is a Dirac point for all $z \in \mathbb{R} \setminus (D_1 \cup D_2)$.

5.5 A Discussion of the Rectangular

Let $\Lambda = \Lambda^R$, and let (k_1, k_2), $\mathcal{B}$, K, m, G_0, and $\mathbb{U}$ be the objects listed in the corresponding column (i.e., the third column) of Table 5.1. We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Lastly, we will again need the matrices f_1, f_2 defined in (5.1).

(1) Upper bound on multiplicity: We start by computing relations among the Fourier coefficients $V_{m(j)}$ for $j \in \mathbb{J}$. In particular, we compute that, for $j = 1, 2$,

$$f_j^{-1} K = K - k_j.$$

It follows from the definition of $m(j)$ that $m(j) = -j$, which together with the fact that V is even implies that for $\omega \in \mathbb{U}$,

$$\mu_\omega'(0) = \sum_{j \in \mathbb{J}} \omega^j V_j.$$

Thus we can rewrite $\mu_\omega'(0)$ as

$$\mu_\omega'(0) = V_{0,0} + \omega_1 V_{1,0} + \omega_2 V_{0,1} + \omega_1 \omega_2 V_{1,1}.$$

Unlike for Λ^S and Λ^H, we do not expect any relations between the coefficients $\{V_j\}_{j \in \mathbb{J}}$ without making further assumptions about V. This is because $0, ||k_1||, ||k_2||, ||k_1 + k_2||$ must necessarily be distinct, for otherwise Λ would either be isometric to the square lattice or not have full-rank. Consequently, since every element of G is orthogonal, there cannot exist $g \in G$ such that $gk_1 = k_2$, for instance, and therefore generic Λ-invariant potentials would not have Fourier coefficients which satisfy $V_{k_1} = V_{k_2}$.

We now plug ω into the above formula for each $\omega \in \mathbb{U}$, which gives us the following:

$$\begin{aligned}
\mu_{1,1}'(0) &= V_{0,0} + V_{1,0} + V_{0,1} + V_{1,1}, \\
\mu_{1,1}'(0) &= V_{0,0} - V_{1,0} + V_{0,1} - V_{1,1}, \\
\mu_{1,1}'(0) &= V_{0,0} + V_{1,0} - V_{0,1} - V_{1,1}, \\
\mu_{1,1}'(0) &= V_{0,0} - V_{1,0} - V_{0,1} + V_{1,1}.
\end{aligned}$$

Note that the set where the right-hand sides of the above four equations fail to be distinct is a union of six hyperplanes. It follows that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into four simple eigenvalues.

At this point, observe that steps (2) and (3) as described in Section 5.2 only need to be performed if the multiplicity of $\mu_\omega(0)$ is strictly greater than 1. Consequently, in this case $||K||^2$ does not split into eigenvalues $\mu_\omega(z)$ that produce intersections of dispersion surfaces for generic z. Therefore, although the framework developed in Chapter 4 does apply in this case, it does not produce interesting results.

5.6 A Discussion of the Centered Rectangular and Oblique

For these last two lattices in two dimensions, there is no longer a fixed angle between the given basis vectors, and consequently it becomes more difficult to compute the corresponding Brillouin zones and their vertices. However, we can still compute the multiplicity of $\mu_0 = ||K||^2$ for $K \in V(\mathcal{B})$ as an L^2_K-eigenvalue of $-\Delta$, independent of this angle.

To do so, we observe that in both cases $\mathcal{B}$ is a (non-regular) hexagon, and by Proposition 4.1, the equivalence relation defining $[K]$ partitions $V(\mathcal{B})$. In addition, as discussed in Section 4.1, each equivalence class must have cardinality at least three, and therefore the partition must either consist of two classes of cardinality three each, or one class of cardinality six. However, the latter case is not possible, since by Theorem 2.3 there exists a basis $(\tilde{k}_1, \tilde{k}_2)$ of Λ^* consisting of Voronoi relevant vectors, meaning that there are edges of $\mathcal{B}$ which lie on the lines given by $x \cdot \tilde{k}_j = \frac{1}{2}||\tilde{k}_j||^2$ for $j = 1, 2$. Then it is possible that either $K + \tilde{k}_j$ or $K - \tilde{k}_j$ is a vertex of $\mathcal{B}$ for $j = 1, 2$, but not both, because then K would not be a vertex. Consequently, by Proposition 4.1, there can be at most four vertices in a given equivalence class, corresponding to the power set of $\{\tilde{k}_1, \tilde{k}_2\}$. Therefore we conclude that $\mu_0 = ||K||^2$ has multiplicity three for any $K \in V(\mathcal{B})$ and $\Lambda = \Lambda^{CR}, \Lambda^O$.

Herein lies the problem: the symmetry groups of Λ^{CR}, Λ^O have order four and two, respectively, and therefore, by basic group theory, neither has a subgroup of order three. It is consequently impossible to find a subgroup which satisfies A3; thus, the framework established in Chapter 4 does not apply here. That being said, due to their low degree of symmetry, Schrödinger operators with potentials invariant under these lattices are unlikely to have interesting intersections of dispersion surfaces. As we saw in the previous sections, higher multiplicity eigenvalues are typically a result of relations between the Fourier coefficients of V, which in turn are a consequence of the symmetries of the lattice. On the other hand, lattices with fewer symmetries, such as the rectangular lattice discussed in Section 5.5, result in the eigenvalue μ_0 of $H_0 = -\Delta$ splitting completely as z increases. We therefore expect similar results for Λ^{CR} and Λ^O.

Chapter 6

SCHRÖDINGER OPERATORS INVARIANT UNDER THREE-DIMENSIONAL LATTICES

We now perform an analysis similar to the one done in the previous chapter, but for a select number of three-dimensional lattices. In particular, we start by examining Schrödinger operators invariant under *cubic lattices*, which is a lattice system consisting of lattices whose point groups are isomorphic to the *octahedral group*. Every such lattice is isometric to one of the three lattices generated by the bases listed in the first row of Table 6.1, and so by Remark 4.2, if V is a cubic lattice invariant potential, we may assume that V is invariant with respect to one of these listed lattices. In particular, these are the *simple cubic*, *body-centered cubic*, and *face-centered cubic*, respectively. We then finish with an analysis of *stacked hexagonal* lattices due to their relevance to graphene and (two-dimensional) hexagonal lattices; these lattices are isometric to the lattice generated by the basis listed in the first column of Table 6.2.

Using the general framework developed in Chapter 4, we prove that the dispersion surfaces of Schrödinger operators with potentials invariant under these lattices generically have unusual dispersion surfaces near vertices of the Brillouin zone, as listed in Theorem 1.3. Each of these proofs will require the same three steps described in Section 5.2: (1) a computation of an upper bound on the multiplicity of eigenvalues $\mu(z)$ of $H_z = -\Delta + zV$, (2) a computation of a lower bound on these same multiplicities, and (3) a computation of the characteristic polynomial.

For the rest of this chapter,

$$r := \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad s := \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad f := \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad (6.1)$$

$$f_1 := \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad f_2 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \qquad f_3 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$f_{12} := \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad f_{13} := \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \qquad f_{23} := \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix},$$

$$s_0 := \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad \rho_0 := \begin{pmatrix} 1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \rho := \rho_0^2 = \begin{pmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Note that ρ_0 and ρ are counter-clockwise rotations in the x_1x_2-plane by $\pi/3$ and $2\pi/3$, respectively.

6.1 Geometry of Cubic Lattices.

Let G denote the octahedral group with presentation $G \cong \langle r, s, f \rangle$, and let Λ^{SC}, Λ^{BC}, and Λ^{FC} denote the simple cubic, body-centered cubic, and face-centered cubic lattice, respectively, which are generated by the bases given in row 1 of Table 6.1 for some $a > 0$. Just as we did in Section 5.1, we give spectral results for $-\Delta$ seen as a Λ^{SC}, Λ^{BC}, and Λ^{FC} invariant operator on L^2_K, where K is a vertex of the corresponding Brillouin zone $\mathcal{B}$. For each of these lattices, K (and in fact every vertex of the respective Brillouin zones $\mathcal{B}$) has a subgroup G_0 of G satisfying A3, and as a result

$$G \cdot [K] = G \cdot (G_0 \cdot K) = G \cdot K.$$

Therefore, unlike for the two-dimensional lattices discussed in Chapter 5, by Remark 4.2 it suffices to consider vertices K which have distinct orbits under the action of the point group G, as opposed to the equivalence classes $[K]$ having distinct orbits.

Similar to Table 5.1, Table 6.1 includes for each of the lattices Λ^{SC}, Λ^{BC}, and Λ^{FC}:

- A basis (v_1, v_2, v_3);
- The corresponding dual basis (k_1, k_2, k_3), where $q = \frac{2\pi}{a}$;
- A picture of the Brillouin zone $\mathcal{B}$, where the vertices are colored and sized in reference to the vertices listed in the following row. Specifically, given a vertex K, the set $[K]$ consists of vertices of $\mathcal{B}$ by Proposition 4.1, which are colored the same and have larger dots. In comparison, those vertices which lie in $(G \cdot K) \setminus [K]$ are colored the same but have smaller dots. Note that in three dimensions, not every vertex of $\mathcal{B}$ necessarily lies in $G \cdot K$, as can be seen in the Brillouin zone of the body-centered cubic lattice;
- Vertices K of the Brillouin zone, corresponding to distinct orbits under the action of G.

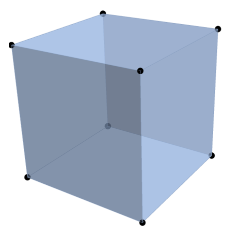
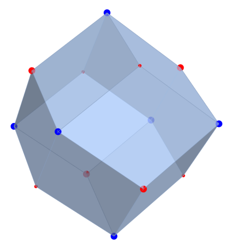
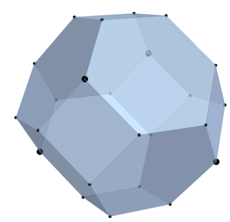
	Λ^{SC}	Λ^{BC}		Λ^{FC}
Basis	$\begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ a \end{pmatrix}$	$\begin{pmatrix} a \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ a \\ 0 \end{pmatrix}, \begin{pmatrix} a/2 \\ a/2 \\ a/2 \end{pmatrix}$		$\begin{pmatrix} a/2 \\ a/2 \\ 0 \end{pmatrix}, \begin{pmatrix} -a/2 \\ a/2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ -a/2 \\ a/2 \end{pmatrix}$
Dual Basis	$\begin{pmatrix} q \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ q \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ q \end{pmatrix}$	$\begin{pmatrix} q \\ 0 \\ -q \end{pmatrix}, \begin{pmatrix} 0 \\ q \\ -q \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 2q \end{pmatrix}$		$\begin{pmatrix} q \\ q \\ q \end{pmatrix}, \begin{pmatrix} -q \\ q \\ q \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 2q \end{pmatrix}$
$\mathcal{B}$				
K	$\begin{pmatrix} q/2 \\ q/2 \\ q/2 \end{pmatrix}$	$\begin{pmatrix} q/2 \\ q/2 \\ q/2 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0 \\ q \end{pmatrix}$	$\begin{pmatrix} 0 \\ q \\ q/2 \end{pmatrix}$
m	8	4	6	4
G_0	$\langle f_1, f_2, f_3 \rangle$	$\langle f_{13}, f_{23} \rangle$	$\langle r, f \rangle$	$\langle s_0 \rangle$
$\mathbb{U}$	U_2^3	U_2^2	$U_3 \times U_2$	U_4

Table 6.1: Geometry of the cubic lattices.

- The multiplicity m of the L^2_K-eigenvalue $||K||^2$ of $-\Delta$, equal to the cardinality of the set $[K]$;

- An abelian subgroup G_0 of G, expressed in terms of its generators, which together with the vertex K satisfy A3;
- The corresponding group $\mathbb{U}$ consisting of tuples of roots of unity, as defined in (4.6).

6.2 *Proof of Theorem 1.3 for the Simple Cubic*

Let $\Lambda = \Lambda^{SC}$, and let (k_1, k_2, k_3), $\mathcal{B}$, K, m, G_0, and $\mathbb{U}$ be the objects listed in corresponding column (i.e. the first column) of Table 6.1. We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Lastly, we will need the matrices r, s, f, f_1, f_2, f_3 defined in (6.1).

(1) Upper bound on multiplicity: Just as we did in Sections 5.3 - 5.5, we start by computing relations among the Fourier coefficients $V_{m(j)}$ for $j \in \mathbb{J}$. To begin, we compute that, for $j = 1, 2, 3$,

$$f_j^{-1} K = K - k_j.$$

It follows from the definition of $m(j)$ (given by (4.7)) that $m(j) = -j$, and since V is even, we also have that $V_{-j} = V_j$. Thus, we arrive at the formula

$$\mu'_\omega(0) = \sum_{j \in \mathbb{J}} \omega^j V_j.$$

In addition, observe that V is invariant under r, which permutes the coordinate axes. Consequently, we have the identities

$$V_{1,0,0} = V_{0,1,0} = V_{0,0,1} \quad \text{and} \quad V_{1,1,0} = V_{1,0,1} = V_{0,1,1}.$$

As a result, we can rewrite $\mu'_\omega(0)$ as

$$\mu'_\omega(0) = V_{0,0,0} + (\omega_1 + \omega_2 + \omega_3) V_{1,0,0} + (\omega_2\omega_3 + \omega_1\omega_3 + \omega_1\omega_2) V_{1,1,0} + \omega_1\omega_2\omega_3 V_{1,1,1}.$$

We then plug ω into this formula for each $\omega \in \mathbb{U}$, which gives us the following:

$$\begin{aligned} \mu'_{1,1,1}(0) &= V_{0,0,0} + 3V_{1,0,0} + 3V_{1,1,0} + V_{1,1,1}, \\ \mu'_{-1,1,1}(0) = \mu'_{1,-1,1}(0) = \mu'_{1,1,-1}(0) &= V_{0,0,0} + V_{1,0,0} - V_{1,1,0} - V_{1,1,1}, \\ \mu'_{1,-1,-1}(0) = \mu'_{-1,1,-1}(0) = \mu'_{-1,-1,1}(0) &= V_{0,0,0} - V_{1,0,0} - V_{1,1,0} + V_{1,1,1}, \\ \mu'_{-1,-1,-1}(0) &= V_{0,0,0} - 3V_{1,0,0} + 3V_{1,1,0} - V_{1,1,1}. \end{aligned}$$

The set where the right-hand sides of the above four equations fail to be distinct is a union of six hyperplanes. It follows that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into at least two simple eigenvalues and two eigenvalues of multiplicity at most three.

(2) Lower bound on multiplicity: Observe that $f_1 r = r f_3$, $f_2 r = r f_1$, and $f_3 r = r f_2$. As a result, if $\phi \in L^2_{K,(-1,1,1)}$ is an eigenvector of H_z, then $r_*\phi$ is also an eigenvector of H_z with the same eigenvalue and

$$\begin{aligned}(f_1)_*(r_*\phi) &= r_*(f_3)_*\phi = r_*\phi \\ (f_2)_*(r_*\phi) &= r_*(f_1)_*\phi = -r_*\phi \\ (f_3)_*(r_*\phi) &= r_*(f_2)_*\phi = r_*\phi.\end{aligned}$$

Hence, $r_*\phi \in L^2_{K,(1,-1,1)}$, and an identical computation shows that $r_*^2\phi$ is an eigenvector of H_z as well, but in $L^2_{K,(1,1,-1)}$. Therefore, $\mu_{(-1,1,1)}(z)$ is an L^2_K-eigenvalue with multiplicity at least 3, which together with step (1) implies that its multiplicity is exactly 3. The same argument applied to an eigenvector ϕ of H_z in $L^2_{K,(1,-1,-1)}$ shows that $\mu_{(-1,1,1)}(z)$ is an L^2_K-eigenvalue with multiplicity 3 as well. Therefore, H_z has two triple L^2_K-eigenvalues for all $z \in \mathbb{R}$ away from a discrete set D_1, and the corresponding eigenprojectors are analytic on some open neighborhood U of $\mathbb{R}$.

(3) Computation of the characteristic polynomial: Fix some $z \in \mathbb{R} \setminus D_1$, and let $\phi_1 \in L^2_{K,(-1,1,1)}$, $\phi_2 \in L^2_{K,(1,-1,1)}$ and $\phi_3 \in L^2_{K,(1,1,-1)}$ be normalized eigenvectors for the eigenvalue $\mu_{(-1,1,1)}(z)$ of H_z. The entries of $M(z,\kappa)$ with respect to this basis are given by $-2i\kappa \cdot \langle \phi_j, \nabla\phi_\ell \rangle$. For $j \neq \ell$, $\langle \phi_j, \nabla\phi_\ell \rangle$ is an eigenvector of both f_j and f_ℓ with eigenvalue -1 by Lemma 4.6, and thus it lies in $\mathbb{C}e_j \cap \mathbb{C}e_\ell = \{0\}$. It follows that $M(z,\kappa) = 0$ for all z and κ, and thus we conclude that

$$\mu_{(-1,1,1)}(z,\kappa) = \mu_{(-1,1,1)}(z) + \mathcal{O}(||\kappa||^2).$$

By Definition 1.1 this means that $(K, \mu_{(-1,1,1)}(z))$ is a 3-fold quadratic point for all $z \in \mathbb{R} \setminus D_1$. The exact same argument shows that $(K, \mu_{(-1,1,1)}(z))$ is a 3-fold quadratic point as well.

6.3 *Proof of Theorem 1.3 for the Body-Centered Cubic at* $K = (q/2, q/2, q/2)$

Let $\Lambda = \Lambda^{BC}$, let $K = (q/2, q/2, q/2)$ and let (k_1, k_2, k_3), $\mathcal{B}$, m, G_0, and $\mathbb{U}$ be the objects listed in the corresponding column of Table 6.1 (i.e. the second of the three columns for the first three rows and the second of the four columns for the remaining rows). We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Lastly we will need the matrices $r, s, f, f_{12}, f_{13}, f_{23}$ defined in (6.1).

(1) Upper bound on multiplicity: As per usual, we start by computing relations among the Fourier coefficients $V_{m(j)}$ for $j \in \mathbb{J}$, noting that:

$$f_{13}^{-1}K = K - k_1 - k_3,$$
$$f_{23}^{-1}K = K - k_2 - k_3,$$
$$f_{12}^{-1}K = K - k_1 - k_2 - k_3.$$

Since V is even, it follows that for $\omega \in \mathbb{U}$,

$$\mu'_\omega(0) = V_{0,0,0} + \omega_1 V_{1,0,1} + \omega_2 V_{0,1,1} + \omega_1\omega_2 V_{1,1,1}.$$

Also note that V being invariant under r implies $V_{1,0,1} = V_{0,1,1}$. In addition, $V_{1,1,1} = V_{1,0,0}$ since

$$V_{k_1+k_3} = r_* V_{k_1+k_3} = V_{r^\top(k_1+k_3)} = V_{k_2+k_3}.$$

Therefore

$$\mu'_\omega(0) = V_{0,0,0} + (\omega_1 + \omega_2 + \omega_1\omega_2)V_{1,1,1}.$$

Plugging ω into this formula for each $\omega \in \mathbb{U}$ gives us:

$$\mu'_{1,1}(0) = V_{0,0,0} + 3V_{1,1,1},$$
$$\mu'_{-1,1}(0) = \mu'_{1,-1}(0) = \mu'_{-1,-1}(0) = V_{0,0,0} - V_{1,1,1}.$$

The set where the right-hand sides of the above two equations fail to be distinct is a single hyperplane. Therefore, we again conclude that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into at least a simple eigenvalue and an eigenvalue of multiplicity at most three.

(2) Lower bound on multiplicity: Observe that $f_{13}r = rf_{23}$ and $f_{23}r = rf_{12}$. As a result, if ϕ is an eigenvector of H_z in $L^2_{K,(-1,1)}$, then $r_*\phi$ and $r_*^2\phi$ are again eigenvectors of H_z with the same eigenvalue on $L^2_{K_{BC},(1,-1)}$ and $L^2_{K_{BC},(-1,-1)}$, respectively. Therefore, H_z has a triple L^2_K-eigenvalue for all $z \in \mathbb{R}$ away from a discrete set D_1, and the corresponding eigenprojector is analytic on some open neighborhood U of $\mathbb{R}$.

(3) Computation of the characteristic polynomial: Fix some $z \in \mathbb{R} \setminus D_1$, and let $\phi_1 \in L^2_{K,(-1,1)}$ be a normalized eigenvector of H_z for the eigenvalue $\mu_{(-1,1)}(z)$. Then, as we saw in step (2), $\phi_2 := r_*\phi \in L^2_{K,(1,-1)}$ and $\phi_3 := r_*^2\phi \in L^2_{K,(-1,-1)}$ are eigenvectors of H_z with eigenvalue $\mu_{(-1,1)}(z)$ as well, and thus form a basis for the corresponding eigenspace. The entries of $M(z,\kappa)$ with respect to this basis are given by $-2i\kappa \cdot \langle \phi_j, \nabla\phi_\ell \rangle$, and we also note that $\langle \phi_2, \nabla\phi_3 \rangle = \langle r_*\phi_1, \nabla(r_*\phi_1) \rangle = r\langle \phi_1, \nabla\phi_2 \rangle$. Therefore, by Lemma 4.6, the entries of $M(z,\kappa)$ are entirely determined by $\langle \phi_1, \nabla\phi_2 \rangle$ and $\langle \phi_1, \nabla\phi_3 \rangle$.

To compute these, note that $f_{12} = f_{13}f_{23}$, and so again by Lemma 4.6,

$$f_{12}\langle \phi_1, \nabla\phi_2 \rangle = (-1)^2 \langle \phi_1, \nabla\phi_2 \rangle = \langle \phi_1, \nabla\phi_2 \rangle.$$

Hence, $\langle \phi_1, \nabla \phi_2 \rangle$ is an eigenvector of f_{12} with eigenvalue 1, and is therefore of the form αe_3 for some $\alpha \in \mathbb{C}$. An identical argument applied to $\langle \phi_1, \nabla \phi_3 \rangle$ and the element $f_{13} \in G$ implies that $\langle \phi_1, \nabla \phi_3 \rangle = \beta e_2$ for some $\beta \in \mathbb{C}$.

Note that $\alpha = -\overline{\beta}$:

$$\begin{aligned}\alpha = e_3 \cdot \langle \phi_1, \nabla \phi_2 \rangle = r e_2 \cdot \langle \phi_1, \nabla \phi_2 \rangle = e_2 \cdot r_*^2 \langle r_*^2 \phi_1, r_*^2 \nabla \phi_2 \rangle \\ = e_2 \cdot \langle \phi_3, \nabla \phi_1 \rangle = -e_2 \cdot \overline{\langle \phi_1, \nabla \phi_3 \rangle} = -\overline{\beta}.\end{aligned}$$

Thus, with respect to the basis (ϕ_1, ϕ_2, ϕ_3), $M(z, \kappa)$ is given by:

$$M(z,\kappa) = -2i \begin{pmatrix} 0 & \alpha\kappa_3 & -\overline{\alpha}\kappa_2 \\ -\overline{\alpha}\kappa_3 & 0 & \alpha\kappa_1 \\ \alpha\kappa_2 & -\overline{\alpha}\kappa_1 & 0 \end{pmatrix}.$$

A quick computation then gives the characteristic polynomial of $M(z, \kappa)$ (as a polynomial in μ):

$$\mu^3 - 4|\alpha|^2 ||\kappa||^2 \mu + 16 \operatorname{Im}(\alpha^3) \kappa_1 \kappa_2 \kappa_3.$$

It follows that the eigenvalues of $M(z, \kappa)$ will be simple away from $\kappa = 0$ as long as the coefficients $|\alpha|^2$ and $\operatorname{Im}(\alpha^3)$ are nonzero.

By Lemma 4.5, $|\alpha|^2$ and $\operatorname{Im}(\alpha^3)$ are analytic in z, and therefore will be nonzero away from a discrete set if they are nonzero for z sufficiently small. However, by Lemma 4.2 we can assume that, for z sufficiently small, ϕ_1, ϕ_2 are given by:

$$\begin{aligned}\phi_1(x;z) &= \frac{1}{2}\left(e^{iK\cdot x} - e^{if_{13}K\cdot x} + e^{if_{23}K\cdot x} - e^{if_{12}K\cdot x}\right) + \mathcal{O}(|z|), \\ \phi_2(x;z) &= \frac{1}{2}\left(e^{iK\cdot x} + e^{if_{13}K\cdot x} - e^{if_{23}K\cdot x} - e^{if_{12}K\cdot x}\right) + \mathcal{O}(|z|).\end{aligned}$$

It follows that, for z small,

$$\alpha = e_3 \cdot \langle \phi_1, \nabla \phi_2 \rangle = \frac{i}{4} e_3 \cdot (K - f_{13}K - f_{13}K + f_{12}K) + \mathcal{O}(|z|^2) = \frac{iq}{2} + \mathcal{O}(|z|^2).$$

Therefore, $|\alpha|^2$ and $\operatorname{Im}(\alpha^3)$ are nonzero for z sufficiently small, and thus remain nonzero for all $z \in U$ away from another discrete set D_2. It follows that they are nonzero on $\mathbb{R} \setminus D_2$, and so by Definition 1.1 we conclude that $(K, \mu_{(-1,1)}(z))$ is a 3-fold Weyl point for all $z \in \mathbb{R} \setminus (D_1 \cup D_2)$.

6.4 *Proof of Theorem 1.3 for the Body-Centered Cubic at* $K = (0, 0, q)$

Let $\Lambda = \Lambda^{BC}$, let $K = (0, 0, q)$ and let (k_1, k_2, k_3), $\mathcal{B}$, m, G_0, and $\mathbb{U}$ be the objects listed in the corresponding column of Table 6.1 (i.e. the second of the three columns for the first three rows and the third of the four columns for the remaining rows). We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Lastly, we will need the group element s_0 defined in (6.1).

(1) Upper bound on multiplicity: First, we observe that

$$\begin{aligned} r^{-1}K &= K + k_2, & r^{-1}fK &= K - k_2 - k_3, \\ r^{-2}K &= K + k_1, & r^{-2}fK &= K - k_1 - k_3 \\ f^{-1}K &= K - k_3. \end{aligned}$$

Since V is even, it follows that for $\omega \in \mathbb{U}$,

$$\mu'_\omega(0) = V_{0,0,0} + \omega_1 V_{0,1,0} + \omega_1^2 V_{1,0,0} + \omega_2 V_{0,0,1} + \omega_1\omega_2 V_{0,1,1} + \omega_1^2\omega_2 V_{1,0,1}.$$

We also have that

$$V_{k_1} = (f_1)_* V_{k_1} = V_{f_1^\top k_1} = V_{k_1+k_3},$$

which tells us that $V_{1,0,0} = V_{1,0,1}$. Furthermore, since V is invariant under r, we obtain $V_{1,0,0} = V_{0,1,0} = V_{1,0,1} = V_{0,1,1}$. Thus we can rewrite $\mu'_\omega(0)$ as

$$\mu'_\omega(0) = V_{0,0,0} + \left(\omega_1 + \omega_1^2 + \omega_1\omega_2 + \omega_1^2\omega_2\right) V_{1,0,0} + \omega_2 V_{0,0,1}.$$

We then plug ω into this formula for each $\omega \in \mathbb{U}$ to obtain:

$$\begin{aligned} \mu'_{1,1}(0) &= V_{0,0,0} + 4V_{1,0,0} + V_{0,0,1}, \\ \mu'_{\zeta_3,1}(0) = \mu'_{\overline{\zeta_3},1}(0) &= V_{0,0,0} - 2V_{1,0,0} + V_{0,0,1}, \\ \mu'_{1,-1}(0) = \mu'_{\zeta_3,-1}(0) = \mu'_{\overline{\zeta_3},-1}(0) &= V_{0,0,0} - V_{0,0,1}. \end{aligned}$$

The set where the right-hand sides of the above three equations fail to be distinct is a union of three hyperplanes. Therefore, we conclude that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into at least a simple eigenvalue, an eigenvalue of multiplicity at most two, and an eigenvalue of multiplicity at most three.

(2) Lower bound on multiplicity: Let T be the conjugate-parity operator: $Tf(x) = \overline{f(-x)}$, and let ϕ_1 be a normalized eigenvector of H_z in $L^2_{K,(\zeta_3,1)}$ for $\mu_{(\zeta_3,1)}(z)$. For $z \in \mathbb{R}$, $\phi_2 = T\phi_1 \in L^2_K$ is also an eigenvector of H_z for the same eigenvalue since V by Remark 4.3. In addition, observe that

$$\begin{aligned} r_*\phi_2(x) &= \overline{\phi_1(-r^\top x)} = \overline{\zeta_3\phi_1(-x)} = \overline{\zeta_3}\phi_2(x) \\ f_*\phi_2(x) &= \overline{\phi_1(-f^\top x)} = \overline{\phi_1(-x)} = \phi_2(x). \end{aligned}$$

Therefore $\phi_2 \in L^2_{K,(\overline{\zeta_3},1)}$.

To give a lower bound on the multiplicity of $\mu_{(1,-1)}(z)$, let $L^2_{K,-1} = \ker_{L^2_K}(f_* + 1)$, i.e. the space of odd functions in L^2_K. By construction of the subspaces $L^2_{K,\omega}$, it follows that

$$L^2_{K,-1} = L^2_{K,(1,-1)} \oplus L^2_{K,(\zeta_3,-1)} \oplus L^2_{K,(\overline{\zeta_3},-1)}.$$

Also note that $s_0 K = K - k_3$, and so s_0 is K-invariant, which together with the fact that s_0 commutes with f, implies that $(s_0)_*$ is a well-defined operator on $L^2_{K,-1}$.

Now let

$$\begin{aligned}\psi_1(x) &= \sin(2\pi x_1) + i \sin(2\pi x_2),\\ \psi_2(x) &= \sin(2\pi x_1) - i \sin(2\pi x_2),\\ \psi_3(x) &= \sqrt{2}\sin(2\pi x_3).\end{aligned}$$

A quick computation confirms that $\psi_j \in L^2_{K,-1}$, $||\psi_j|| = 1$, and $-\Delta\psi_j = (2\pi)^2\psi_j = ||K||^2\psi_j$ for $j = 1,2,3$. In addition, note that $\sigma((s_0)_*) = U_4$, the fourth roots of unity. If we let $\mathcal{E}_\omega = L^2_{K,-1} \cap \ker_{L^2_{K,-1}}((s_0)_* - \omega)$ for $\omega \in U_4$, then $\psi_1 \in \mathcal{E}_{-i}$, $\psi_2 \in \mathcal{E}_i$ and $\phi_3 \in \mathcal{E}_{-1}$. Therefore $||K||^2$ is a simple eigenvalue of $-\Delta$ on $\mathcal{E}_\omega$ for $\omega \in \{-i, i, -1\}$, and so by Corollary 3.1 it follows that, for sufficiently small $z \in \mathbb{R}$, there is a unique eigenvalue $\lambda(z)$ of H_z on $\mathcal{E}_{-i}$ satisfying $\lambda(z) = ||K||^2 + \mathcal{O}(|z|)$. Let $\Psi_z \in \mathcal{E}_{-i}$ denote the normalized eigenvector corresponding to λ_z, and let $\Phi_z \in L^2_{K,(1,-1)}$ denote a normalized eigenvector corresponding to $\mu_{(1,-1)}(z)$, so that

$$\Psi_z = \psi_1 + \mathcal{O}(|z|), \quad \text{and} \quad \Phi_z = \phi + \mathcal{O}(|z|),$$

where ϕ is defined by (4.8) with $\omega = (\zeta_3, -1)$.

Now assume for contradiction that $\mu_{(1,-1)}(z)$ has multiplicity strictly less than 3 for $z \neq 0$. Then $T\Psi_z$ and $T\Phi_z$ are also eigenvectors corresponding to $\lambda(z)$ and $\mu_{(1,-1)}$, respectively, and so both of these eigenvalues must have multiplicity at least two. Since we are assuming that the multiplicity of $\mu_{(1,-1)}$ is strictly less than 3, we deduce that these eigenvalues must in fact be equal, and their multiplicity is exactly two.

As a result, for all $z \in \mathbb{R}$, nonzero and sufficiently small,

$$\operatorname{span}(\Psi_z, T\Psi_z) = \operatorname{span}(\Phi_z, T\Phi_z).$$

Therefore we can express Φ_z with respect to Ψ_z and $T\Psi_z$ as

$$\Phi_z = \langle \Phi_z, \Psi_z \rangle \Psi_z + \langle \Phi_z, T\Psi_z \rangle T\Psi_z, \tag{6.2}$$

where we have used the fact that $T\Psi_z \in \mathcal{E}_i$, and is therefore orthogonal to Ψ_z. Taking the limit of both sides of (6.2) as $z \to 0$, we obtain

$$\phi = \langle \phi, \psi_1 \rangle \psi_1 + \langle \phi, T\psi_1 \rangle T\psi_1.$$

This is not possible: by (4.8), the left-hand side depends on x_3, while the right-hand side depends only on x_1, x_2. We conclude that H_z has a double and a triple L^2_K-eigenvalue for all $z \in \mathbb{R}$ away from a discrete set D_1, and the corresponding eigenprojector is analytic on some open neighborhood U of $\mathbb{R}$.

(3) Computation of the characteristic polynomial: Fix some $z \in \mathbb{R} \setminus D_1$, and let $\phi_1 \in L^2_{K,(\zeta_3,1)}$, $\phi_2 \in L^2_{K,(\overline{\zeta_3},1)}$ be normalized eigenvectors for the eigenvalue $\mu_{(\zeta_3,1)}(z)$ of H_z. The entries of $M(z,\kappa)$ with respect to this basis are given by $-2i\kappa \cdot \langle \phi_j, \nabla \phi_\ell \rangle$, and by Lemma 4.6, the entries of $M(z,\kappa)$ are entirely determined by $\langle \phi_1, \nabla \phi_2 \rangle$. However, this same lemma also tells us that $\langle \phi_1, \nabla \phi_2 \rangle$ is an eigenvector of f with eigenvalue 1, and therefore must be the zero vector. It follows that $M(z,\kappa) = 0$ for all z and κ, and thus we conclude that $(K, \mu_{(\zeta,1)}(z)$ is a 2-fold quadratic point.

Now, let $\phi_1 \in L^2_{K,(1,-1)}$, $\phi_2 \in L^2_{K,(\zeta_3,-1)}$, and $\phi_3 \in L^2_{K,(\overline{\zeta_3},-1)}$ be normalized eigenvectors for the eigenvalue $\mu_{(1,-1)}(z)$ of H_z. Then the same argument implies that, for $j, \ell \in \{1,2,3\}$, $j \ \ell$, $\langle \phi_1, \nabla \phi_2 \rangle$ is again an eigenvector of f with eigenvalue 1 and therefore must be the zero vector. We thus conclude that $(K, \mu_{(1,-1)}(z)$ is a 3-fold quadratic point for all $z \in \mathbb{R} \setminus D_1$.

6.5 *Proof of Theorem 1.3 for the Face-Centered Cubic*

Let $\Lambda = \Lambda^{FC}$, and let (k_1, k_2, k_3), $\mathcal{B}$, K, m, G_0, and $\mathbb{U}$ be the corresponding objects listed in the final column of Table 6.1. We also let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. Lastly, we will need the matrix s_0 defined in (6.1).

(1) Upper bound on multiplicity: First, we observe that

$$\begin{aligned} s_0^{-1}K &= K - k_1, \\ s_0^{-2}K &= K - k_1 - k_2 + k_3, \\ s_0^{-3}K &= K - k_2. \end{aligned}$$

Since V is even and invariant under r, it follows that for $\omega \in \mathbb{U}$,

$$\mu'_\omega(0) = V_{0,0,0} + \omega V_{1,0,0} + \omega^2 V_{1,1,-1} + \omega^3 V_{0,1,0} = V_{0,0,0} + (\omega + \omega^3) V_{1,0,0} + \omega^2 V_{1,1,-1}.$$

We then plug ω into this formula for each $\omega \in \mathbb{U}$ to obtain:

$$\begin{aligned} \mu'_1(0) &= V_{0,0,0} + 2V_{1,0,0} + V_{1,1,-1}, \\ \mu'_i(0) = \mu'_{-i}(0) &= V_{0,0,0} - V_{1,1,-1}, \\ \mu'_{-1}(0) &= V_{0,0,0} - 2V_{1,0,0} + V_{1,1,-1}. \end{aligned}$$

The set where the right-hand sides of the above three equations fail to be distinct is a union of three hyperplanes. Therefore, we conclude that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into at least two simple eigenvalues and an eigenvalue of multiplicity at most two.

(2) Lower bound on multiplicity: Again let T be the conjugate-parity operator and let ϕ_1 be a normalized eigenvector of H_z in $L^2_{K,i}$. For $z \in \mathbb{R}$, $\phi_2 = T\phi_1 \in L^2_K$ is also an eigenvector of H_z for the same eigenvalue, and

$$(s_0)_*\phi_2(x) = \overline{\phi_1(-s_0^\top x)} = \overline{i\phi_1(-x)} = -i\phi_1(x),$$

which implies $\phi_2 \in L^2_{K,-i}$. Therefore, H_z has a double L^2_K-eigenvalue for all $z \in \mathbb{R}$ away from a discrete set D_1, and the corresponding eigenprojector is analytic on some open neighborhood U of $\mathbb{R}$.

(3) Computation of the characteristic polynomial: Fix some $z \in \mathbb{R} \setminus D_1$, and let $\phi_1 \in L^2_{K,i}$, $\phi_2 \in L^2_{K,-i}$ be normalized eigenvectors for the eigenvalue $\mu_i(z)$ of H_z. The entries of $M(z,\kappa)$ with respect to this basis are given by $-2i\kappa \cdot \langle \phi_j, \nabla\phi_\ell \rangle$, and by Lemma 4.6, the entries of $M(z,\kappa)$ are entirely determined by $\langle \phi_1, \nabla\phi_2 \rangle$. This same lemma also tells us that $\langle \phi_1, \nabla\phi_2 \rangle$ is an eigenvector of s_0 with eigenvalue -1, and is therefore of the form αe_3 for some $\alpha \in \mathbb{C}$.

Thus, with respect to the basis (ϕ_1, ϕ_2), $M(z,\kappa)$ is given by

$$M(z,\kappa) = -2i \begin{pmatrix} 0 & \alpha\kappa_3 \\ -\overline{\alpha}\kappa_3 & 0 \end{pmatrix},$$

and its characteristic polynomial is $\mu^2 - 4|\alpha|^2\kappa_3^2$. It follows that the eigenvalues of $M(z,\kappa)$ can be written as $\lambda(z,\kappa) = \pm 2|\alpha\kappa_3|$, and therefore these eigenvalues will be simple for $\kappa_3 \neq 0$ as long as $\alpha \neq 0$.

By Lemma 4.5, the coefficient $|\alpha|^2$ is analytic in z, and therefore will be nonzero away from a discrete set if it is nonzero for z sufficiently small. However, by Lemma 4.2 we can assume that, for z sufficiently small, ϕ_1, ϕ_2 are given by:

$$\phi_1(x) = \frac{1}{2}\left(e^{iK\cdot x} + ie^{iS_0^3K\cdot x} - e^{is_0^2K\cdot x} - ie^{is_0K\cdot x}\right) + \mathcal{O}(|z|),$$
$$\phi_2(x) = \frac{1}{2}\left(e^{iK\cdot x} - ie^{is_0^3K\cdot x} - e^{is_0^2K\cdot x} + ie^{is_0K\cdot x}\right) + \mathcal{O}(|z|).$$

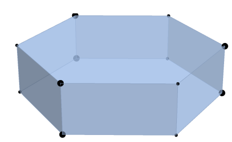
It follows that, for z small,

$$\alpha = e_3 \cdot \langle \phi_1, \nabla\phi_2 \rangle = \frac{i}{4}e_3 \cdot \left(K - s_0^3K + s_0^2K - s_0K\right) + \mathcal{O}(|z|^2) = \frac{iq}{2} + \mathcal{O}(|z|^2).$$

Therefore, $|\alpha|^2$ is nonzero for z sufficiently small, and thus remains nonzero on U away from another discrete set D_2. It follows that $|\alpha|^2$ is nonzero on $\mathbb{R} \setminus D_2$, and so by Definition 1.1 we conclude that $(K, \mu_i(z))$ is a basin point for all $z \in \mathbb{R} \setminus (D_1 \cup D_2)$.

6.6 *Geometry of Stacked Hexagonal Lattices.*

For this section and the next, let $\Lambda = \Lambda^{SH}$ denote the stacked hexagonal lattice which is generated by the basis given in Table 6.2 for $a_1, a_2 > 0$. Just as in Tables 5.1, 5.2, and 6.1, we also also includes some spectral results for $-\Delta$ seen as a Λ invariant operator on L^2_K, where K is a vertex of the corresponding Brillouin zone $\mathcal{B}$. In particular, this table includes the basis (v_1, v_2, v_3) the dual basis (k_1, k_2, k_3) (where $q_j = 2\pi/a_j$ for $j = 1, 2$), a picture of the Brillouin zone $\mathcal{B}$ with vertices sized and colored as in the previous tables, a vertex K, the mutliplicity m of $||K||^2$ as an L^2_K-eigenvalue of $-\Delta$, the point group G and a subgroup G_0 satisfying A3 (which we describe using the matrices ρ_0, ρ, f_1, f_3 from (6.1)), and the corresponding group $\mathbb{U}$.

Basis	Dual Basis	$\mathcal{B}$
$\begin{pmatrix} a_1\sqrt{3}/2 \\ a_1/2 \\ 0 \end{pmatrix}, \begin{pmatrix} a_1\sqrt{3}/2 \\ -a_1/2 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ a_2 \end{pmatrix}$	$\begin{pmatrix} q_1\sqrt{3}/3 \\ q_1 \\ 0 \end{pmatrix}, \begin{pmatrix} q_1\sqrt{3}/3 \\ -q_1 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ q_2 \end{pmatrix}$	

K	m	G	G_0	$\mathbb{U}$
$\begin{pmatrix} 0 \\ 2q_1/3 \\ q_2/2 \end{pmatrix}$	6	$\langle \rho_0, f_1, f_3 \rangle$	$\langle \rho, f_3 \rangle$	$U_3 \times U_2$

Table 6.2: Geometry of the stacked hexagonal lattice Λ^{SH}.

6.7 *Proof of Theorem 1.3 for the Stacked Hexagonal*

Perhaps unsurprisingly, our proof of Theorem 1.3 in this case will not only proceed similarly to those done for the other lattices analyzed in this work, but specifically will closely follow our proof corresponding to the two-dimensional hexagonal lattice in Section 5.4.

(1) Upper bound on multiplicity: Let V be a Λ-invariant potential and let $H_z = -\Delta + zV$. We again start by computing relations among the Fourier coefficients $V_{m(j)}$ for $j \in \mathbb{J}$. In

particular, we compute that

$$\rho^{-1}K = K + k_2, \qquad \rho^{-2}K = K - k_1 \qquad f_3^{-1}K = K - k_3$$
$$f_3^{-1}\rho^{-1}K = K + k_2 - k_3 \qquad f_3^{-1}\rho^{-2}K = K - k_1 - k_3.$$

Since V is even, it follows that for $\omega \in \mathbb{U}$,

$$\mu'_\omega(0) = V_{0,0,0} + \omega_1 V_{0,1,0} + \omega_1^2 V_{1,0,0} + \omega_2 V_{0,0,1} + \omega_1\omega_2 V_{0,1,1} + \omega_1^2\omega_2 V_{1,0,1}.$$

We also have that

$$V_{k_1} = \rho_* V_{k_1} = V_{\rho^\top k_1} = V_{k_2},$$

which tells us that $V_{1,0,0} = V_{0,1,0}$, and an identical argument applied to $V_{k_1+k_3}$ tells us that $V_{1,0,1} = V_{0,1,1}$ as well. Therefore we can rewrite $\mu'_\omega(0)$ as

$$\mu'_\omega(0) = V_{0,0,0} + (\omega_1 + \omega_1^2)V_{1,0,0} + \omega_2 V_{0,0,1} + (\omega_1 + \omega_1^2)\omega_2 V_{1,0,1}.$$

We then plug ω into this formula for each $\omega \in \mathbb{U}$ to obtain:

$$\begin{aligned} \mu'_{1,1}(0) &= V_{0,0,0} + 2V_{1,0,0} + V_{0,0,1} + 2V_{1,0,1}, \\ \mu'_{\zeta_3,1}(0) = \mu'_{\overline{\zeta_3},1}(0) &= V_{0,0,0} - V_{1,0,0} + V_{0,0,1} - V_{1,0,1}, \\ \mu'_{1,-1}(0) &= V_{0,0,0} + 2V_{1,0,0} - V_{0,0,1} - 2V_{1,0,1}, \\ \mu'_{\zeta_3,-1}(0) = \mu'_{\overline{\zeta_3},-1}(0) &= V_{0,0,0} - V_{1,0,0} - V_{0,0,1} + V_{1,0,1}, \end{aligned}$$

where ζ_3 is a third root of unity, which we can again choose to be the one with positive imaginary part, just as in Section 5.4. The set where the right-hand sides of the above four equations fail to be distinct is a union of six hyperplanes. Therefore, we conclude that for V away from a set of codimension 1, the eigenvalue $||K||^2$ of $-\Delta$ splits into at least two simple eigenvalues and two eigenvalues of multiplicity at most two.

(2) Lower bound on multiplicity: Let T again be the conjugate-parity operator, and let ϕ_1 be a normalized eigenvector of H_z in $L^2_{K,(\zeta_3,1)}$ for the eigenvalue $\mu_{\zeta_3,1}(z)$. For $z \in \mathbb{R}$, $\phi_2 := T\phi_1 \in L^2_K$ is also an eigenvector of H_z for the same eigenvalue by Remark 4.3 since V is even and real. In addition, observe that

$$\begin{aligned} \rho_*\phi_2(x) &= \overline{\phi_1(-\rho^\top x)} = \overline{\zeta_3\phi_1(-x)} = \overline{\zeta_3}\phi_2(x) \\ (f_3)_*\phi_2(x) &= \overline{\phi_1(-f_3^\top x)} = \overline{\phi_1(-x)} = \phi_2(x). \end{aligned}$$

Therefore $\phi_2 \in L^2_{K,(\overline{\zeta_3},1)}$, and so $\mu_{\zeta_3,1}(z)$ has multiplicity 2. An identical argument applied to an eigenvector of H_z in $L^2_{K,(\zeta_3,-1)}$ shows that $\mu_{\zeta_3,-1}(z)$ also has multiplicity 2. Therefore, H_z has two double L^2_K-eigenvalue for all $z \in \mathbb{R}$ away from a discrete set D_1, and the corresponding eigenprojectors are analytic on some open neighborhood U of $\mathbb{R}$.

(3) Computation of the characteristic polynomial: Fix some $z \in \mathbb{R} \setminus D_1$, and let $\phi_1 \in L^2_{K,(\zeta_3,1)}$ be a normalized eigenvector of H_z for the eigenvalue $\mu_{\zeta_3,1}(z)$. Then, as we saw in step (2), $\phi_2 := T\phi_1 \in L^2_{K,(\overline{\zeta_3},1)}$ is an eigenvector of H_z with eigenvalue $\mu_{\zeta_3,1}(z)$ as well, and thus ϕ_1, ϕ_2 form a basis for the corresponding eigenspace. The entries of $M(z,\kappa)$ with respect to this basis are given by $-2i\kappa \cdot \langle \phi_j, \nabla\phi_\ell \rangle$. Therefore, by Lemma 4.6, the entries of $M(z,\kappa)$ are entirely determined by $\langle \phi_1, \nabla\phi_2 \rangle$.

To compute this entry, note that by Lemma 4.6,

$$\rho\langle \phi_1, \nabla\phi_2 \rangle = \overline{\zeta_3}^2 \langle \phi_1, \nabla\phi_2 \rangle = \zeta_3 \langle \phi_1, \nabla\phi_2 \rangle.$$

Hence, $\langle \phi_1, \nabla\phi_2 \rangle$ is an eigenvector of ρ with eigenvalue ζ_3, and is therefore of the form

$$\langle \phi_1, \nabla\phi_2 \rangle = \alpha \begin{pmatrix} i \\ 1 \\ 0 \end{pmatrix}$$

for some $\alpha \in \mathbb{C}$. Consequently, with respect to the basis (ϕ_1, ϕ_2), $M(z,\kappa)$ is given by:

$$M(z,\kappa) = -2i \begin{pmatrix} 0 & \alpha(\kappa_2 + i\kappa_1) \\ -\overline{\alpha}(\kappa_2 - i\kappa_1) & 0 \end{pmatrix}.$$

A quick computation then gives the characteristic polynomial of $M(z,\kappa)$:

$$\mu^2 + |\alpha|^2(\kappa_1^2 + \kappa_2^2).$$

It follows that the eigenvalues of $M(z,\kappa)$ can be written as

$$\lambda(z,\kappa) = \pm 2|\alpha|\sqrt{\kappa_1^2 + \kappa_2^2},$$

and therefore these eigenvalues will be simple for $\kappa_1^2 + \kappa_2^2 \neq 0$ as long as $\alpha \neq 0$.

By Lemma 4.5, the coefficient $|\alpha|^2$ is analytic in z, and therefore will be nonzero away from a discrete set if it is nonzero for z sufficiently small. However, by Lemma 4.2 we can assume that, for z sufficiently small, ϕ_1, ϕ_2 are given by:

$$\begin{aligned}
\phi_1(x;z) = \frac{1}{\sqrt{6}} \Big(& e^{iK\cdot x} + \zeta_3 e^{i\rho^{-1}K\cdot x} + \overline{\zeta_3} e^{i\rho^{-2}K\cdot x} \\
& + e^{if_3^{-1}K\cdot x} + \zeta_3 e^{if_3^{-1}\rho^{-1}K\cdot x} + \overline{\zeta_3} e^{if_3^{-1}\rho^{-2}K\cdot x} \Big) + \mathcal{O}(|z|), \\
\phi_2(x;z) = \frac{1}{\sqrt{6}} \Big(& e^{iK\cdot x} + \overline{\zeta_3} e^{i\rho^{-1}K\cdot x} + \zeta_3 e^{i\rho^{-2}K\cdot x} \\
& + e^{if_3^{-1}K\cdot x} + \overline{\zeta_3} e^{if_3^{-1}\rho^{-1}K\cdot x} + \zeta_3 e^{if_3^{-1}\rho^{-2}K\cdot x} \Big) + \mathcal{O}(|z|).
\end{aligned}$$

It follows that, for z small,

$$\begin{aligned}
\alpha =& e_2 \cdot \langle \phi_1, \nabla \phi_2 \rangle \\
=& \frac{i}{6} e_2 \cdot \left(K + \zeta_3 \rho^{-1} K + \overline{\zeta_3} \rho^{-2} K + f_3^{-1} K + \zeta_3 f_3^{-1} \rho^{-1} K + \overline{\zeta_3} f_3^{-1} \rho^{-2} K \right) + \mathcal{O}(|z|^2) \\
=& -\frac{i\sqrt{3}}{3} q + \mathcal{O}(|z|^2).
\end{aligned}$$

Therefore $|\alpha|^2$ is nonzero for z sufficiently small, and thus remains nonzero for all $z \in U$ away from another discrete set D_2. It follows that $|\alpha|^2$ is nonzero on $\mathbb{R} \setminus D_2$. Performing the same computations for the eigenvalue $\mu_{\zeta_3,-1}(z)$ shows that the characteristic polynomial of $M(z, \kappa)$ in this case is also given by $\mu^2 + |\alpha|^2(\kappa_1^2 + \kappa_2^2)$, where $|\alpha|^2$ is again nonzero on $\mathbb{R}$ away from a discrete set. By Definition 1.1, we conclude that both $(K, \mu_{\zeta_3,1}(z))$ and $(K, \mu_{\zeta_3,-1}(z))$ are valley points for all $z \in \mathbb{R}$ away from a discrete set.

BIBLIOGRAPHY

[AP05] Grégoire Allaire and Andrey Piatnitski. "Homogenization of the Schrödinger Equation and Effective Mass Theorems". In: *Communications in Mathematical Physics* 258 (2005), pp. 1–22. DOI: https://doi.org/10.1007/s00220-005-1329-2.

[AK24] Habib Ammari and Thea Kosche. "Topological phenomena in honeycomb Floquet metamaterials". In: *Math. Ann.* 388.3 (2024), pp. 2755–2785. ISSN: 0025-5831,1432-1807. DOI: 10.1007/s00208-023-02583-0. URL: https://doi.org/10.1007/s00208-023-02583-0.

[Amm+20] Habib Ammari et al. "Honeycomb-lattice Minnaert bubbles". In: *SIAM J. Math. Anal.* 52.6 (2020), pp. 5441–5466. ISSN: 0036-1410,1095-7154. DOI: 10.1137/19M1281782. URL: https://doi.org/10.1137/19M1281782.

[Bal24] Guillaume Bal. "Semiclassical propagation along curved domain walls". In: *Multiscale Model. Simul.* 22.1 (2024), pp. 66–105. ISSN: 1540-3459,1540-3467. DOI: 10.1137/23M1545872. URL: https://doi.org/10.1137/23M1545872.

[BBD24] Guillaume Bal, Simon Becker, and Alexis Drouot. "Magnetic slowdown of topological edge states". In: *Comm. Pure Appl. Math.* 77.2 (2024), pp. 1235–1277. ISSN: 0010-3640,1097-0312. DOI: 10.1002/cpa.22154. URL: https://doi.org/10.1002/cpa.22154.

[Bal+23] Guillaume Bal et al. "Edge state dynamics along curved interfaces". In: *SIAM J. Math. Anal.* 55.5 (2023), pp. 4219–4254. ISSN: 0036-1410,1095-7154. DOI: 10.1137/22M1489708. URL: https://doi.org/10.1137/22M1489708.

[BC18] Gregory Berkolaiko and Andrew Comech. "Symmetry and Dirac Points in Graphene Spectrum". In: *Journal of Spectral Theory* 8, No. 3 (2018), pp. 1099–1147. DOI: https://doi.org/10.4171/JST/223.

[BC09] Christopher John Bradley and Arthur P. Cracknell. *The Mathematical Theory Of Symmetry In Solids: Representation theory for point groups and space groups*. Oxford University Press, 2009. ISBN: 9780199582587.

[BBN78] Harold Brown, Rolf Bulow, and Joachim Neubüser. *Crystallographic Groups of Four-Dimensional Space*. Wiley, 1978. ISBN: 9780471030959.

[But59] John Butler. "Perturbation series for eigenvalues of Analytic Non-symmetric Operators". In: *Archiv der Mathematik* 10 (1959), pp. 21–27. DOI: https://doi.org/10.1007/BF01240753.

[CW21] Maxence Cassier and Michael I. Weinstein. "- High contrast elliptic operators in honeycomb structures". In: *Multiscale Model. Simul.* 19 (2021), pp. 1784–1856.

[CW24] Jonah Chaban and Michael I. Weinstein. "Instability of quadratic band degeneracies and the emergence of Dirac points". In: *Preprint, arXiv:2404.05886.* (2024).

[Dro19a] A. Drouot. "Characterization of edge states in perturbed honeycomb structures". In: *Pure Appl. Anal.* 1 (2019), pp. 385–445.

[Dro19b] A. Drouot. "The bulk-edge correspondence for continuous honeycomb lattices". In: *Comm. Partial Differential Equations* 44 (2019), pp. 1406–1430.

[Dro21] A. Drouot. "Ubiquity of conical points in topological insulators". In: *J. Éc. polytech. Math.* 8 (2021), pp. 507–532.

[DW20] A. Drouot and M. I. Weinstein. "Edge states and the valley Hall effect". In: *Adv. Math.* 368 (2020), 51pp.

[Dro22] Alexis Drouot. "Topological insulators in semiclassical regime". In: *Preprint, arXiv:2206.08238* (2022).

[DF03] David S. Dummit and Richard M. Foote. *Abstract Algebra, 3rd Edition*. Wiley, 2003. ISBN: 9780471433347.

[FLW16] C. L. Fefferman, J. P. Lee-Thorp, and M. I. Weinstein. "Edge states in honeycomb structures". In: *Ann. PDE* 2.2 (2016), Art. 12, 80. ISSN: 2524-5317,2199-2576. DOI: 10.1007/s40818-016-0015-3. URL: https://doi.org/10.1007/s40818-016-0015-3.

[FLW18] Charles L. Fefferman, James P. Lee-Thorp, and Michael I. Weinstein. "Honeycomb Schrödinger operators in the strong binding regime". In: *Comm. Pure Appl. Math.* 71.6 (2018), pp. 1178–1270. ISSN: 0010-3640,1097-0312. DOI: 10.1002/cpa.21735. URL: https://doi.org/10.1002/cpa.21735.

[FW12] Charles L. Fefferman and Michael I. Weinstein. "Honeycomb Lattice Potentials and Dirac Points". In: *Journal of the American Mathematical Society* 25 (2012), pp. 1169–1220. DOI: https://doi.org/10.48550/arXiv.1202.3839.

[FW14] Charles L. Fefferman and Michael I. Weinstein. "Wave Packets in Honeycomb Structures and Two-Dimensional Dirac Equations". In: *Communications in Mathematical Physics* 326 (2014), pp. 251–286. DOI: https://doi.org/10.1007/s00220-013-1847-2.

[FMP16] Domenico Fiorenza, Domenico Monaco, and Gianluca Panati. "$\mathbb{Z}_2$ invariants of topological insulators as geometric obstructions". In: *Comm. Math. Phys.* 343.3 (2016), pp. 1115–1157. ISSN: 0010-3616,1432-0916. DOI: 10.1007/s00220-015-2552-0. URL: https://doi.org/10.1007/s00220-015-2552-0.

[Fri82] John Fritz. *Partial Differential Equations*. Applied Mathematical Sciences. Springer New York, 1982. ISBN: 9780387906096.

[GZZ22] Haimo Guo, Meirong Zhang, and Yi Zhu. "Three-Fold Weyl Points for the Schrödinger Operator with Periodic Potentials". In: *SIAM Journal on Mathematical Analysis* 54 (2022). DOI: https://doi.org/10.1137/21M1410464.

[Hel13] Bernard Helffer. *Spectral Theory and its Applications*. Cambridge Studies in Advanced Mathematics. Cambridge University Press, 2013. ISBN: 9781139505727.

[HXZ23] Pipi Hu, Peng Xie, and Yi Zhu. "Traveling edge states in massive Dirac equations along slowly varying edges". In: *IMA J. Appl. Math.* 88.3 (2023), pp. 455–471. ISSN: 0272-4960,1464-3634. DOI: 10.1093/imamat/hxad015. URL: https://doi.org/10.1093/imamat/hxad015.

[HRS20] Christoph Hunkenschröder, Gina Reuland, and Matthias Schymura. "On compact representations of Voronoi cells of lattices". In: *Mathematical Programming* 183 (2020), pp. 337–358. DOI: https://doi.org/10.1007/s10107-019-01463-3.

[Jr72] Willard Miller Jr. *Symmetry groups and their applications*. Pure and Applied Mathematics. Academic Press, 1972. ISBN: 9780124974609.

[Kat95] Tosio Kato. *Perturbation Theory for Linear Operators*. Classics in Mathematics. Springer, 1995. ISBN: 9783540586616.

[Kel+18] R. T. Keller et al. "Spectral Band Degeneracies of $\frac{\pi}{2}$-Rotationally Invariant Periodic Schrödinger Operators". In: *Multiscale Modeling and Simulation* 16 (2018). DOI: https://doi.org/10.1137/18M1171527.

[Kit12] Charles Kittel. *Introduction to Solid State Physics, 8th Edition*. Methods of Mathematical Physics. Academic Press, 2012. ISBN: 9780123958280.

[Kni96] Oliver Knill. *The Residue Theorem and Its Applications*. https://people.math.harvard.edu/~knill/teaching/residues_1996/residue.pdf. 1996.

[LWZ19] J. P. Lee-Thorp, M. I. Weinstein, and Y. Zhu. "Elliptic Operators with Honeycomb Symmetry: Dirac Points, Edge States and Applications to Photonic Graphene". In: *Archive for Rational Mechanics and Analysis* 232 (2019), pp. 1–63. DOI: https://doi.org/10.1007/s00205-018-1315-4.

[LLZ23] Wei Li, Junshan Lin, and Hai Zhang. "Dirac points for the honeycomb lattice with impenetrable obstacles". In: *SIAM J. Appl. Math.* 83.4 (2023), pp. 1546–1571. ISSN: 0036-1399,1095-712X. DOI: 10.1137/22M1505116. URL: https://doi.org/10.1137/22M1505116.

[PW27] Fritz Peter and Hermann Weyl. "Die Vollständigkeit der primitiven Darstellungen einer geschlossenen kontinuierlichen Gruppe". In: *Mathematische Annalen* 97 (1927), pp. 737–755. DOI: https://doi.org/10.1007/BF01447892.

[RS04] Michael Reed and Barry Simon. *Analysis of Operators, Vol. 4*. Wiley, 2004. ISBN: 9780471415268.

[Rel40] Franz Rellich. "Störungstheorie der Spektralzerlegung. V". In: *Mathematische Annalen* 118 (1940), pp. 462–484. DOI: https://doi.org/10.1007/BF01487382.

[Wig59] E. P. Wigner. *Group theory and its applications to the quantum mechanics of atomic spectra*. Academic Press, New York, 1959. ISBN: 9780127505503.

[Wik25] Wikipedia contributors. *Bravais Lattice*. [Online; accessed 01-February-2025]. 2025. URL: https://en.wikipedia.org/wiki/Bravais_lattice.

[Zha05] Fuzhen Zhang, ed. *The Schur Complement and Its Applications*. Numerical Methods and Algorithms. Springer, 2005. ISBN: 9780387242712.