Algebraic Aspects of Periodic Graph Operators

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Abstract. A periodic linear graph operator acts on states (functions) defined on the vertices of a graph equipped with a free translation action. Fourier transform with respect to the translation group reveals the central spectral objects, Bloch and Fermi varieties. These encode the relation between the eigenvalues of the translation group and the eigenvalues of the operator. As they are algebraic varieties, algebraic methods may be used to study the spectrum of the operator. We establish a framework in which commutative algebra directly comes to bear on the spectral theory of periodic operators, helping to distinguish their algebraic and analytic aspects. We also discuss reducibility of the Fermi variety and non-degeneracy of spectral band edges.

Key words: Periodic operator, graph operator, Bloch variety, Fermi variety, spectral theory, toric variety

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1 Introduction

Periodic operators on graphs serve as "tight-binding" models for the quantum mechanics of electrons in crystalline solids. Their translational symmetry and discrete nature make them naturally amenable to analysis through commutative algebra. By browsing works such as [9, 13, 14, 18, 19], the reader encounters various aspects of the algebraic nature of these operators and the role of algebra in their spectral analysis. This article is a systematic algebraic treatment of periodic graph operators that provides a unifying framework and serves as background material with the hope of benefiting efforts to apply commutative algebra to spectral theory. The article treats only graphs with finite-degree vertices. When reading, it is helpful but not necessary to have familiarity with periodic operators, whether discrete or differential. We refer the reader to introductory sections of the references above, plus an overview focusing on differential operators [24].

First, we develop algebraic aspects of the Fourier transform with respect to a discrete translational symmetry group acting freely on a set of vertices. Upon this, we build the theory of operators that commute with translational symmetries, which are by definition the periodic ones. Then, half of the article is spent on the Bloch and Fermi algebraic varieties, which describe the relation between momentum (eigenvalues of the translation group) and energy (eigenvalues of the operator). The two most salient issues are reducibility and nondegeneracy, both of which impact the spectral theory of the operator. Throughout, we pay attention to identifying algebraic versus analytic aspects of the material. A general background on the algebraic and geometric ideas we use is found in the two books [8, 7] with more specialized background in [6, 38, 39].

2 $\mathbb{Z}^d$ actions and the Fourier transform

The algebraic manipulations of §2.1 set the framework for viewing discrete periodic operators in the context of commutative algebra. They illuminate various points of view and elucidate the roles of algebra and of analysis. Algebraic and analytic points of view of the Fourier transform are discussed in §2.2.

2.1 Algebraic structure

We examine the underlying structure of a set of vertices with a translation group that extends to functions defined on the vertices.

2.1.1 Translation of vertices. Let $\{e_1, \ldots, e_d\}$ be a basis for the group $\mathbb{Z}^d$, with a general element denoted by $n = \sum_{i\in[1,d]} n_i e_i$. A free action of $\mathbb{Z}^d$ on a set $\mathcal{V}$ of "vertices" is denoted by

$$\mathbb{Z}^d \times \mathcal{V} \longrightarrow \mathcal{V} \;::\; (n, x) \longmapsto x \dot{+} n, \tag{2.1}$$

and we will also use the notation $x \dot{-} n := x \dot{+} -n$. A free action by $\mathbb{Z}^d$ is called a group of shifts or translations. Let $W \subset \mathcal{V}$ be a fundamental domain for the action, that is, W contains one vertex from each $\mathbb{Z}^d$ orbit. Because the action is free, each $x \in \mathcal{V}$ has a unique presentation as $x = y \dot{+} n$ with $y \in W$ and $n \in \mathbb{Z}^d$, giving a bijection

$$\mathcal{V} \longleftrightarrow W \times \mathbb{Z}^d \;::\; y \dot{+} n \longleftrightarrow (y, n). \tag{2.2}$$

We assume that W is finite so that the $\mathbb{Z}^d$ action is co-finite. When $|W| = 1$, this is the natural action of $\mathbb{Z}^d$ on itself by addition, $x \dot{+} n = x + n$. We identify $\mathcal{V}$ with the disjoint union of W copies of $\mathbb{Z}^d$, and W with the W copies of $0 \in \mathbb{Z}^d$:

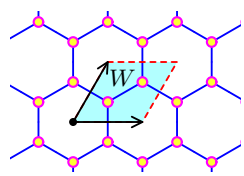
$$\mathcal{V} \longleftrightarrow \bigsqcup_{w\in W} \mathbb{Z}^d \;\cong\; \mathbb{Z}^d \times W, \tag{2.3}$$

with $\mathbb{Z}^d$ acting by addition on each copy of itself.

Concretely, $\mathcal{V}$ could be a periodic set of points in $\mathbb{R}^d$ generated by a finite set of points $W \subset \mathbb{R}^d$ through their shifts by d independent vectors $\{v_j : j \in [1, d]\}$. In this situation, the $\mathbb{Z}^d$ action is actual addition in $\mathbb{R}^d$,

$$x \dot{+} n \;:=\; x + \sum_{j\in[1,d]} n_j v_j. \tag{2.4}$$

A tight-binding model for single-layer graphene has $|W| = 2$ with three repeating edges.



2.1.2 Translation of functions. The group algebra $\mathbb{C}[\mathbb{Z}^d]$ is the complex vector space having $\mathbb{Z}^d$ as a basis, and endowed with the natural multiplication

$$\sum_m a_m m \cdot \sum_n b_n n \;=\; \sum_{m,n} a_m b_n (m + n) \;=\; \sum_\ell \Big(\sum_m a_m b_{\ell - m} \Big) \ell \;=\; \sum_\ell (a * b)_\ell \, \ell\,, \tag{2.5}$$

in which all sums are over $\mathbb{Z}^d$ and have only finitely many nonzero terms. Identifying $\sum a_n n$ with the function $n \mapsto a_n$ identifies $\mathbb{C}[\mathbb{Z}^d]$ with the space $F_0(\mathbb{Z}^d)$ of complex-valued functions on $\mathbb{Z}^d$ having finite support. By (2.5) this identifies the group-algebra multiplication in $\mathbb{C}[\mathbb{Z}^d]$ with convolution in $F_0(\mathbb{Z}^d)$.

We often consider $a = \sum a_n n \in \mathbb{C}[\mathbb{Z}^d]$ as acting on $b = \{b_\ell\}_\ell \in F_0(\mathbb{Z}^d)$. The restriction of this multiplication to the group $\mathbb{Z}^d \subset \mathbb{C}[\mathbb{Z}^d]$ is the shift, or translation, action on $F_0(\mathbb{Z}^d)$,

$$(m \cdot b)_\ell \;=\; b_{\ell - m}, \tag{2.6}$$

and convolution is a linear combination of shift operators. These actions on $F_0(\mathbb{Z}^d)$ extend to the vector space $F(\mathbb{Z}^d) = \mathbb{C}^{\mathbb{Z}^d}$ of all complex-valued functions on $\mathbb{Z}^d$. Restricting to square-summable functions is a unitary representation of $\mathbb{Z}^d$ on $\ell^2(\mathbb{Z}^d)$.

This action is carried to $F(\mathcal{V}) = \mathbb{C}^{\mathcal{V}}$, and the unitary representation is extended to $\ell^2(\mathcal{V})$ by

$$(n \cdot f)(x) \;=\; f(x \dot{-} n). \tag{2.7}$$

The identification (2.3) gives various ways of viewing $F(\mathcal{V})$ or any sub-vector-space; for example,

$$\ell^2(\mathcal{V}) \;\cong\; \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^W \;\cong\; \ell^2(\mathbb{Z}^d, \mathbb{C}^W) \;\cong\; \ell^2(\mathbb{Z}^d)^W. \tag{2.8}$$

The shift operator by the generator e_j of $\mathbb{Z}^d$ is also denoted by S_j,

$$(S_j f)(x) \;=\; f(x \dot{-} e_j). \tag{2.9}$$

2.1.3 Formal Fourier transform. The additive group $\mathbb{Z}^d$ is isomorphic to the multiplicative group of monomials $\mathcal{M}$ in d indeterminates $z = (z_1, \ldots, z_d)$, and the convenient (for our context) isomorphism is

$$\mathbb{Z}^d \longleftrightarrow \mathcal{M} \,:\, n \longleftrightarrow z^{-n}, \tag{2.10}$$

in which $z^n = \prod z_i^{n_i}$. Then one has the identifications

$$F_0(\mathbb{Z}^d) \;\cong\; \mathbb{C}[\mathbb{Z}^d] \;\cong\; \mathbb{C}[\mathcal{M}] \;=\; \mathbb{C}[z^{\pm}], \tag{2.11}$$

with $\mathbb{C}[z^{\pm}]$ the ring of Laurent polynomials in d indeterminates. Therefore we obtain the identifications

$$F_0(\mathcal{V}) \;\cong\; F_0(\mathbb{Z}^d)^W \;\cong\; \mathbb{C}[\mathbb{Z}^d]^W \;\cong\; \mathbb{C}[z^{\pm}]^W, \tag{2.12}$$

in which the last object is a finitely generated free module over $\mathbb{C}[z^{\pm}]$.

The algebraic isomorphism from $F_0(\mathbb{Z}^d)$ (with convolution) to the ring $\mathbb{C}[z^{\pm}]$ of Laurent polynomials in d variables is denoted by $\hat{}$,

$$f \;\longmapsto\; \hat{f} \;=\; \sum_{n\in\mathbb{Z}^d} f(n) z^{-n} \;=\; \sum_{n\in\mathbb{Z}^d} f(-n) z^{n}. \tag{2.13}$$

This is a *formal Fourier transform*, sometimes called the (formal) *Floquet transform* or *z-transform*. It is "formal" as z is an indeterminate rather than a variable to be evaluated at a point. The extension of the Floquet transform to $F(\mathbb{Z}^d)$ yields $\hat{f}$ in the module $\mathbb{C}[[z^{\pm}]]$ of formal Laurent series, and one has

$$f \in F(\mathbb{Z}^d) \text{ has finite support} \;\iff\; \hat{f} \text{ is a Laurent polynomial.} \tag{2.14}$$

To extend this transform to $F(\mathcal{V}) = \mathbb{C}^{\mathcal{V}}$, we fix a fundamental domain W and identify $F(\mathcal{V})$ with $F(\mathbb{Z}, \mathbb{C}^W)$: Consider $f \in F(\mathcal{V})$ as a function of $(n, y) \in \mathbb{Z} \times W$ through the unique presentation $x = y \dot{+} n$; then as a function of the variable n, the object $f(\bullet \dot{+} n)$ is an element of $\mathbb{C}^W$. The formula (2.13) still holds, with the values of f being vector rather than scalar,

$$f \;\longmapsto\; \hat{f} \;=\; \sum_{n\in\mathbb{Z}^d} f(\bullet \dot{+} n) z^{-n} \;=\; \sum_{n\in\mathbb{Z}^d} f(\bullet \dot{-} n) z^{n}. \tag{2.15}$$

This is a Laurent series in the indeterminate z with coefficients in $\mathbb{C}^W$. One can eliminate the need to fix a fundamental domain simply by allowing the argument "$\bullet$" to run over all of $\mathcal{V}$ and not just W. This yields a Laurent series in the indeterminate z with coefficients in $F(\mathcal{V})$,

$$\hat{f}(z, x) \;=\; \sum_{n} f(x \dot{+} n) z^{-n}. \tag{2.16}$$

This is a sum over the $\mathbb{Z}^d$-orbit of the point $x \in \mathcal{V}$. As the coefficients are just shifts of f, the formal Floquet transform on $F(\mathcal{V}) = \mathbb{C}^{\mathcal{V}}$ can be written more compactly as

$$f \;\longmapsto\; \hat{f} \;=\; \sum_{n\in\mathbb{Z}^d} n{\cdot}f\, z^{n}. \tag{2.17}$$

The advantage of retaining x in the Floquet transform is that the action of $n \in \mathbb{Z}^d$ on $\hat{f}(\bullet, z)$ coincides with the action of $z^{-n} \in \mathcal{M}$ on $\hat{f}(\bullet, z)$,

$$n{\cdot}\hat{f} \;=\; z^{-n}\hat{f}. \tag{2.18}$$

2.2 L^2 Floquet transform and Fourier inversion

If the Fourier sum (2.13) converges when evaluated at $z \in (\mathbb{C}^\times)^d$, the symbols $z_1, \ldots, z_d$ become complex variables rather than formal algebraic symbols, and $\hat{f}(z, x)$ becomes a function of two arguments.

2.2.1 Eigenfunctions of the translation group. If (2.13) converges for some $z \in (\mathbb{C}^\times)^d$, then the fundamental property (2.18) of the Floquet transform says that $\hat{f}(z,x)$, viewed as a function of $x \in \mathcal{V}$ is an eigenfunction of the $\mathbb{Z}^d$ action, with n-dependent eigenvalue equal to the homomorphism

$$\mathbb{Z}^d \longrightarrow \mathbb{C}^\times :: n \longmapsto z^{-n}. \tag{2.19}$$

The property can be written equivalently as

$$\hat{f}(z, x\dot{+}n) = z^n \hat{f}(z,x) \qquad \forall n \in \mathbb{Z}^d \quad \forall z \in (\mathbb{C}^\times)^d. \tag{2.20}$$

Often this direction of the shift ($f(x\dot{+}n)$ instead of $f(x \dot{-} n)$) is taken to be the definition of the shift action, so that z^n (instead of z^{-n}) is the eigenvalue of the shift by $n \in \mathbb{Z}^d$.

All homomorphisms from $\mathbb{Z}^d$ to $\mathbb{C}^\times$ form the dual group of *characters* of $\mathbb{Z}^d$. Each character corresponds to a d-tuple $z = (z_1, \ldots, z_d)$ of nonzero complex numbers, called its *weight*. Thus the dual group is isomorphic to the non-compact complex torus $(\mathbb{C}^\times)^d$. The unitary dual group of $\mathbb{Z}^d$ is the group of homomorphisms from $\mathbb{Z}^d$ to the unit circle $\mathbb{T} \subset \mathbb{C}$, which is isomorphic to the compact d-dimensional torus $\mathbb{T}^d \subset (\mathbb{C}^\times)^d$. Reciprocally, $\mathbb{Z}^d$ is the dual group of the torus (continuous homomorphisms from $(\mathbb{C}^\times)^d$ to $\mathbb{C}^\times$). The bihomomorphism z^n captures both directions,

$$\mathbb{Z}^d \times (\mathbb{C}^\times)^d \longrightarrow \mathbb{C}^\times :: (n,z) \longmapsto z^n. \tag{2.21}$$

Denote by $\mathcal{E}_z$ the eigenspace of the $\mathbb{Z}^d$ action on $F(\mathcal{V}) \cong \mathbb{Z}^d \otimes \mathbb{C}^W$ for the weight z^{-1}. Because $f(y\dot{+}n) = z^n f(y)$, each $f \in \mathcal{E}_z$ is determined uniquely by its restriction to W, and thus, as vector spaces,

$$\mathcal{E}_z \cong \mathbb{C}^W. \tag{2.22}$$

Explicitly, an element $g \in \mathbb{C}^W$ corresponds to an element $Q(g,z) \in \mathcal{E}_z$ by

$$Q(g,z)(n) = g z^n, \tag{2.23}$$

considered as an element of $\mathbb{Z}^d \otimes \mathbb{C}^W$ (or as an element of $F(\mathcal{V})$, one would write $Q(g,z)(v) = g(w) z^n$, where $v = n\dot{+}w$ with $w \in W$). The symbol Q stands for "quasi-periodic".

For each $z \in (\mathbb{C}^\times)^d$, let ε_z be a distinguished element of $\mathcal{E}_z$ such that $\varepsilon_z(x) \neq 0$ for all $x \in \mathcal{V}$. Then each $f \in \mathcal{E}_z$ can be written as

$$f(x) = \tilde{f}(x) \varepsilon_z(x). \tag{2.24}$$

The function $\tilde{f}$ is called the *periodic part* of f (with respect to the choice of ε_z). For example, one can take $\varepsilon_z(y) = 1$ for all $y \in W$ so that $\varepsilon_z(y\dot{+}n) = z^n$. When $\mathcal{V}$ is a periodic subset of $\mathbb{R}^d$, as in Equation (2.4), let $q = (q_1, \ldots, q_d)$ be the dual (momentum) variable so that $k_j = q \cdot v_j$ and $z_j = e^{iq \cdot v_j}$. Then, for $x \in \mathbb{R}^d$, one can define $\epsilon_z(x) = e^{iq \cdot x}$, and restrict this function to $\mathcal{V} \subset \mathbb{R}^d$.

2.2.2 Fourier inversion. We have discussed that $F_0(\mathcal{V})$ is isomorphic to $\mathbb{C}[z^\pm]^W$ through the formal Floquet transform. By evaluating $\hat{f}$ at actual points $z \mapsto e^{ik} \in (\mathbb{C}^\times)^d$, it becomes a function whose restriction to the compact torus $\mathbb{T}^d$ is a trigonometric polynomial in $k \in \mathbb{R}^d/(2\pi\mathbb{Z})^d$,

$$\hat{f}(e^{ik}) = \sum_{n \in \mathrm{supp}(f)} f(-n) e^{ik \cdot n} \qquad \text{(finite sum)}. \tag{2.25}$$

After evaluation on $\mathbb{T}^d$, $\mathbb{C}[z^\pm]^W$ becomes the ring of trigonometric polynomial functions $\mathcal{T}(\mathbb{T}^d) \otimes \mathbb{C}^W$ on the compact d-torus, which have the form (2.25). We denote the map from $f \in F_0(\mathcal{V})$ to $\hat{f}(e^{ik})$ by $\mathcal{U}$,

$$\mathcal{U} : F_0(\mathcal{V}) \cong F_0(\mathbb{Z}^d) \otimes \mathbb{C}^W \longrightarrow \mathcal{T}(\mathbb{T}^d) \otimes \mathbb{C}^W. \tag{2.26}$$

$\mathcal{U}f$ could also be denoted by $\hat{f}$, with the understanding that a formal polynomial $\hat{f}(z)$ is being evaluated.

An L^2 norm on $\mathcal{E}_z$ is defined by $\|f\|_2^2 = \sum_{y \in W} |f(y)|^2$. A fundamental theorem of Fourier analysis says that $\mathcal{U}$ is an L^2 isomorphism,

$$\sum_n |f(n)|^2 = \int_{\mathbb{T}^d} \left|\mathcal{U}f(z)\right|^2 d\tilde{V}(z), \tag{2.27}$$

in which $d\tilde{V}(z) = dk_1 \cdots dk_d/(2\pi)^d$, with inverse given by

$$f(n) \;=\; \int_{\mathbb{T}^d} \hat{f}(n,z)\, d\tilde{V}(z). \tag{2.28}$$

In terms of the periodic part $\tilde{f}$ of $\hat{f}$, this is the familiar inverse Fourier transform with kernel $\varepsilon_z(x)$,

$$f(y \dot{+} n) \;=\; \int_{\mathbb{T}^d} \tilde{f}(y,z)\, \varepsilon_z(y \dot{+} n)\, d\tilde{V}(z). \tag{2.29}$$

2.2.3 Completion to L^2. So far, we have defined the formal (algebraic) and analytical Fourier transforms on functions of compact support in $\mathcal{V}$,

$$f \in F_0(\mathcal{V}) \;\longrightarrow\; \hat{f}(z) \in \mathbb{C}[z^{\pm}]^W \;\longrightarrow\; \mathcal{U}f \in \mathcal{T}(\mathbb{T}^d) \otimes \mathbb{C}^W. \tag{2.30}$$

Completion in the root-mean-square norm yields the unitary Fourier transform of Hilbert spaces,

$$\mathcal{U} : \ell^2(\mathcal{V}) \longrightarrow L^2(\mathbb{T}^d) \otimes \mathbb{C}^W. \tag{2.31}$$

The inversion formulas (2.28) and (2.29) state that the formula (2.16) for the Floquet transform produces the components in all the $\mathcal{E}_z$ required to build f. Fourier inversion amounts to writing $\ell^2(\mathcal{V})$ as a direct integral over the torus of simpler spaces [36, §XIII.16],

$$\ell^2(\mathcal{V}) \;=\; \int_{\mathbb{T}^d}^{\otimes} \mathcal{E}_z\, d\tilde{V}(z), \qquad f \;=\; \int_{\mathbb{T}^d}^{\otimes} \hat{f}(\bullet, z)\, d\tilde{V}(z), \tag{2.32}$$

and the transformation $\hat{f} \mapsto \tilde{f}$ is a simple gauge transformation that transforms all the fibers $\mathcal{E}_z$ to $\mathcal{E}_{\mathbf{1}}$.

2.2.4 Spec and spectrum. Evaluation of the formal Floquet transform at values in the torus is analogous to the *Gel'fand transform* for Banach algebras. Evaluation of $\hat{f}(z) \in \mathbb{C}[z^{\pm}]$ at $z \mapsto \zeta = (\zeta_1, \ldots, \zeta_d) \in (\mathbb{C}^{\times})^d$ sends the polynomial $\hat{f}(z)$ to the complex number $\hat{f}(\zeta)$, which is the representative of the coset $\hat{f}(z) \bmod \langle z - \zeta \rangle$ in the field $\mathbb{C}[z^{\pm}]/\langle z - \zeta \rangle \simeq \mathbb{C}$. Formally, $\hat{f}$ becomes a function on the space of maximal ideals in $\mathbb{C}[z^{\pm}]$, called $\operatorname{Spec} \mathbb{C}[z^{\pm}]$, which is homeomorphic to $(\mathbb{C}^{\times})^d$,

$$(\mathbb{C}^{\times})^d \;\cong\; \operatorname{Spec} \mathbb{C}[z^{\pm}] \;\;::\;\; \zeta \longleftrightarrow \langle z - \zeta \rangle. \tag{2.33}$$

Equivalently, $\operatorname{Spec} \mathbb{C}[z^{\pm}]$ is the set of ring homomorphisms from $\mathbb{C}[z^{\pm}]$ to $\mathbb{C}$. The homomorphism that takes the indeterminate z_j to ζ_j for $j \in [1,d]$ has kernel then ideal $\langle z - \zeta \rangle$ and sends the polynomial $\hat{f}(z)$ to the number $\hat{f}(\zeta)$.

As we have seen, translation of compactly supported functions by n, that is, the operator $S^n = \prod_{j \in [1,d]} S_j^{n_j}$ becomes multiplication of Laurent polynomials by z^{-n}, which in turn becomes multiplication of trigonometric polynomials on $\mathbb{T}^d$ by the function ζ^{-n}. This means that, in the direct integral (2.32), the fiber at $\zeta \in \mathbb{T}^d$ of the operator S^n, acting on the fiber $\mathbb{C}^W$ at ζ is just $\zeta^{-n} I_W$. Particularly, the elementary shift S_j has fiber at ζ equal to the coordinate ζ_j. This is because the spectrum of S_j is the unit circle, being the range of the j-th coordinate function ζ_j on $\mathbb{T}^d$. In this way, the unitary part of $\operatorname{Spec} \mathbb{C}[z^{\pm}]$ gives the spectrum of the shift group. More generally, a polynomial in the elementary shifts, with matrix coefficients,

$$A(S) \;=\; \sum_{n \in \mathbb{Z}^d} A_n S^n \tag{2.34}$$

has spectrum equal to the image of the multi-valued eigenvalue function

$$\sigma(\zeta) \;=\; \{\lambda : \det(A(\zeta) - \lambda) = 0\} \tag{2.35}$$

over the compact torus $\mathbb{T}^d$. The Laurent polynomial $\det(A(\zeta) - \lambda)$ and its zero set predominate the L^2 spectral theory of the operator $A(S)$. An operator that commutes with the shift group is called *periodic*, and these are discussed in the next section.

3 Periodic graph operators

An operator A acting on functions on $\mathcal{V}$ is periodic if it commutes with the shift group; such an operator has translational symmetry. Periodic operators in $\ell^2(\mathcal{V})$ have a dichotomy of spectrum: eigenvalues of infinite multiplicity and bands of continuous spectrum. Eigenvalues are completely described by A as a module endomorphism, while continuous spectrum comes from the Bloch variety, which is the singular set of the matrix $\hat{A}(z)-\lambda I$. An interesting exposition of the module homomorphism point of view with extension from $\mathbb{Z}^d$ to amenable group actions is presented in [23].

3.1 On $F_0(\mathcal{V})$: Module endomorphism

A periodic operator A restricted to functions of compact support is a module endomorphism of $\mathbb{C}[z^{\pm}]^W$.

3.1.1 Definition and notation. Let A be a linear operator on $F_0(\mathcal{V})$, and denote by $\hat{A}$ the corresponding operator on $\mathbb{C}[z^{\pm}]^W$ as a vector space over $\mathbb{C}$, through the Floquet transform. That is, $\hat{A}$ is defined through

$$(\hat{A}\hat{f})(z) \;=\; \widehat{(Af)}(z). \tag{3.36}$$

As $F_0(\mathcal{V}) \cong F_0(\mathbb{Z}^d)\otimes\mathbb{C}^W$ consists of functions of finite support on $\mathbb{Z}^d\times W$, it is convenient to denote the evaluation of $f\in F_0(\mathcal{V})$ at $(n\in\mathbb{Z}^d, v\in W)$ by $f_v(n)$, so that $f(n)$ refers to the vector $(f_v)_{v\in W}$ in $\mathbb{C}^W$. Being linear, A is associated with its kernel, or matrix, $a(m,n)$ through

$$(Af)(m) \;=\; \sum_{n\in\mathbb{Z}^d} a(m,n)f(n). \tag{3.37}$$

For each $m,n\in\mathbb{Z}^d$, $a(m,n)$ is a linear operator on $\mathbb{C}^W$ and is thus represented by a matrix $(a_{vw}(m,n))_{v,w\in W}$ indexed by W. This means

$$(Af)_v(m) \;=\; \sum_{n\in\mathbb{Z}^d}\sum_{w\in W} a_{vw}(m,n)f_w(n). \tag{3.38}$$

The operator A has *finite range* if there exists a number R such that, for all $m,n\in\mathbb{Z}^d$, $a(m,n)=0$ whenever $|m-n|>R$. If $a(n,m)=a(m,n)^*$, then A is self-adjoint. Here, $(\ )^*$ is the adjoint with respect to the standard inner product of $\mathbb{C}^W$.

The linear operator A is *periodic* if, for all $f\in F_0(\mathbb{Z}^d)\otimes\mathbb{C}^W$,

$$(Af)(\bullet\dot{+}n) \;=\; A[f(\bullet\dot{+}n)](x) \qquad \forall n\in\mathbb{Z}^d. \tag{3.39}$$

More compactly, this means that A commutes with the shift group $\mathbb{Z}^d$,

$$n{\cdot}Af \;=\; A(n{\cdot}f) \qquad \forall n\in\mathbb{Z}^d. \tag{3.40}$$

Observe that A is periodic if and only if

$$a(m,n) \;=\; \tilde{a}(m-n) \tag{3.41}$$

for some function $\tilde{a}$, which we will just denote by a. A periodic linear operator of finite range has $a(m)=0$ whenever $|m|>R$; denote by $r(A)$ the minimal such R. The operator is self-adjoint if $a(-m)=a(m)^*$. This means that A is a convolution operator

$$(Af)(m) \;=\; \sum_{n\in\mathbb{Z}^d} a(m-n)f(n) \;=\; \sum_{n\in\mathbb{Z}^d} a(n)f(m-n), \tag{3.42}$$

or, equivalently, a linear combination of translations with matrix coefficients,

$$A \;=\; \sum_{n\in\mathbb{Z}^d} a(n)\,n{\cdot} \;=\; \sum_{n\in\mathbb{Z}^d} a(n)S^n, \tag{3.43}$$

as in (2.34). When W consists of only one vertex, A is an element of the group algebra $\mathbb{C}[\mathbb{Z}^d]$ and is sometimes called a Toeplitz operator. Now identify f with $\sum f(n)n\in\mathbb{C}[\mathbb{Z}^d]^W$ and use (2.5) to obtain

$$\sum a(n)n\cdot\sum f(n)n \;=\; \sum (Af)(n)n. \tag{3.44}$$

Remark 1. A linear operator A on $F_0(\mathcal{V})$ corresponds to a directed, labeled graph $\Gamma = (\mathcal{V}, E)$. Identifying $\mathcal{V}$ with $\mathbb{Z}^d \times W$, there is a directed edge $v\dot{+}m \leftarrow w\dot{+}n$ in E with label $a_{vw}(m,n)$, when $a_{vw}(m,n) \neq 0$. Loops $v\dot{+}m \circlearrowleft$ are removed and their labels $a_{vv}(m,m)$ become a potential function $V\colon \mathcal{V} \to \mathbb{C}$. For an edge $v \leftarrow w$, we will write $a_{v\leftarrow w}$ for the corresponding edge label Then, for $f \in F_0(\mathcal{V})$, $v, w \in \mathcal{V}$ (3.38) becomes

$$(Af)(v) \;=\; V(v)f(v) \;+\; \sum_{v\leftarrow w} a_{v\leftarrow w} f(w). \tag{3.45}$$

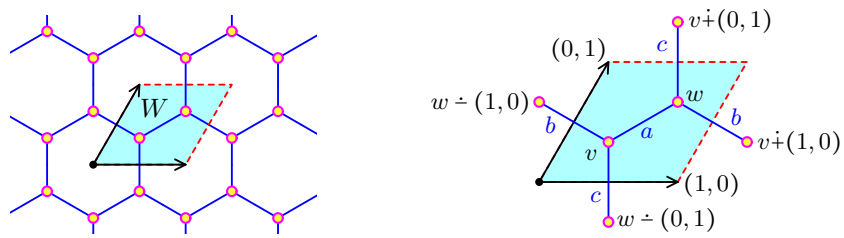
When A has finite range, the graph Γ is locally finite in that each vertex v has finitely many neighbors $\{w \in \mathcal{V} \mid v \leftarrow w\}$. By (3.45), A is a Schrödinger operator: a potential plus weighted graph Laplacian, and it acts on $F(\mathcal{V})$.

If in addition A is $\mathbb{Z}^d$-periodic, then Γ is a $\mathbb{Z}^d$-periodic labeled graph. E.g. the underlying graph is periodic with $V\colon \mathcal{V} \to \mathbb{C}$ and $a\colon E \to \mathbb{C}$ periodic functions. In this case, the operator A commutes with the $\mathbb{Z}^d$-action, it is *periodic*. When $a_{vw}(m,n) = a_{wv}(n,m)^*$, the operator A is self-adjoint, and when $a_{vw}(m,n) = a_{wv}(n,m)$, we may replace the directed graph by a corresponding undirected graph.

3.1.2 Examples. The simplest example is when $\mathcal{V} = \mathbb{Z}$ and there is an (undirected) edge between n and $n \pm 1$ with weight -1, so that Γ is and A becomes

$$(Af)(n) \;=\; -f(n-1) + V(n)f(n) - f(n+1). \tag{3.46}$$

Another example is the $\mathbb{Z}^2$-periodic hexagonal lattice (graphene), in which $W = \{v, w\}$ and there are (undirected) edges connecting $v(= v\dot{+}(0,0))$ to each of w, $w \dot{-} (1,0)$, and $w \dot{-} (0,1)$, and this is extended to all of $\mathbb{Z}^2 \times W$ by periodicity. We show the hexagonal lattice with W shaded and the $\mathbb{Z}^2$-action indicated by the arrows, together with a picture of a labeling of edges in a neighborhood of W.



(3.47)

The operator A for the hexagonal graph with edge-labeling a, b, c as above is

$$\begin{aligned} (Af)(v\dot{+}n) &= V(v)f(v\dot{+}n) \;+\; af(w\dot{+}n) + bf(w\dot{+}n \dot{-} (1,0)) + cf(w\dot{+}n \dot{-} (0,1)) \\ (Af)(w\dot{+}n) &= V(w)f(w\dot{+}n) \;+\; af(v\dot{+}n) + bf(v\dot{+}n\dot{+}(1,0)) + cf(v\dot{+}n\dot{+}(0,1)) \end{aligned} \quad . \tag{3.48}$$

3.1.3 Formal Fourier transform. Under the formal Fourier (or Floquet) transform $n \mapsto z^{-n}$, translation by n becomes multiplication by z^{-n}, and periodicity becomes ring homomorphism. More precisely, with

$$\hat{A}(z) = \sum a(n) z^{-n}, \qquad \hat{f}(z) = \sum f(n) z^{-n}, \qquad \widehat{Af}(z) = \sum (Af)(n) z^{-n}, \tag{3.49}$$

formula (3.44) becomes $\hat{A}(z)\hat{f}(z) = (\widehat{Af})(z)$. This is an algebraic form of the general principal that an operator commuting with a group action becomes a multiplication operator under (formal) Fourier transform.

In summary: The space $F_0(\mathbb{Z}^d)$, identified with $R := \mathbb{C}[z^{\pm}]$ through the formal Floquet transform, is a vector space over $\mathbb{C}$ and also a ring (convolution of functions = multiplication of polynomials). Thus $F_0(\mathcal{V}) = R^W$ is a free R-module. Consequently, one can study general $\mathbb{C}$-linear operators on R^W, or specialized ones that are also R-module endomorphisms of R^W. The operator A, when pulled over to R^W, is written $\hat{A}$. The periodicity property (3.40) means that $\hat{A}$ commutes with multiplication by z^n for all $n \in \mathbb{Z}^d$. This happens if and only if $\hat{A}$ commutes with multiplication by any $\hat{f}(z) \in R$; and this is simply the statement that $\hat{A}$ is a module endomorphism of R^W. This amounts to the following (un)remarkable result.

Theorem 2. *A $\mathbb{C}$-linear operator A on $F_0(\mathcal{V})$ is periodic if and only if $\hat{A}$ is a module endomorphism of $\mathbb{C}[z^{\pm}]^W$.*

Any endomorphism $\hat{A} : R^W \to R^W$ is given by a matrix $\hat{a}_{vw}(z)$ of elements of R indexed by W, that is

$$(\hat{A}p(z))_v \;=\; \sum_{w\in W} \hat{a}_{vw}(z)p_w(z), \tag{3.50}$$

and one can identify $\hat{A}$ with its matrix $(\hat{a}_{vw}(z))_{v,w\in W}$. For the hexagonal graph, the matrix $\hat{A}(z)$ becomes

$$\begin{pmatrix} V(v) & a + bx^{-1} + cy^{-1} \\ a + bx + cy & V(w) \end{pmatrix}, \tag{3.51}$$

where $z = (x, y)$ with x corresponding to $(1, 0)$ and y to $(0, 1)$, where v indexes the first row and column and w the second row and column, and with the labeling of (3.47).

3.1.4 Eigenvalues. For $\lambda \in \mathbb{R}$, the equation $(A - \lambda)f = 0$ for $f \in F_0(\mathcal{V})$ is equivalent to $(\hat{A}(z) - \lambda)\hat{f}(z) = 0$, where $\hat{f}(z) \in \mathbb{C}[z^{\pm}]$. Thus λ is an eigenvalue of $\hat{A}(z)$. For all $n \in \mathbb{Z}^d$, we have $(\hat{A}(z) - \lambda)z^n f(z) = 0$, so that all shifts of f are also eigenvectors of A and thus λ is an eigenvalue of infinite multiplicity.

3.2 On $F(\mathcal{V})$: Floquet eigenspaces

An operator A of finite range can be applied to functions of infinite support. Equivalently, if $\hat{A}(z)$ is a Laurent polynomial in $z = (z_1, \ldots, z_d)$ with coefficients that are $W \times W$ matrices with entries in $\mathbb{C}$, $\hat{A}(z)$ can be applied to Laurent series with vector coefficients, that is, to elements of $\mathbb{C}[[z^{\pm}]]^W$.

3.2.1 Action of A on $\mathcal{E}_\zeta$. For $\zeta \in (\mathbb{C}^\times)^d$, nonzero elements of the space $\mathcal{E}_\zeta$ of quasi-periodic functions have infinite support. A periodic operator A is invariant on $\mathcal{E}_\zeta$, so via the isomorphism $\mathcal{E}_\zeta \cong \mathbb{C}^W$ (2.22), the restriction of A to $\mathcal{E}_\zeta$ induces an operator on $\mathbb{C}^W$. This operator is just $\hat{A}(\zeta)$, the evaluation of $\hat{A}(z)$ at $z = \zeta$. For a function $f \in F(\mathcal{V})$, denote $\hat{f}(z)$ also by $\mathcal{F}(f)(z)$.

Theorem 3. *Let A be a periodic operator of finite range, and let $g \in \mathbb{C}^W$ and $\zeta \in (\mathbb{C}^\times)^d$. Then*

$$\hat{A}(z)[\mathcal{F}Q(g, \zeta)] \;=\; \mathcal{F}Q(\hat{A}(\zeta)g, \zeta). \tag{3.52}$$

Equivalently, $A[Q(g, \zeta)] = Q(\hat{A}(\zeta)g, \zeta)$.

Proof. By definition, one has

$$Q(g, \zeta)(n) = g\,\zeta^n, \qquad \mathcal{F}Q(g, \zeta)(z) = \sum_{n\in\mathbb{Z}^d} g\,\zeta^n\, z^{-n}. \tag{3.53}$$

Let $\hat{A}(z) = \sum_{\ell\in\Lambda} A^\ell z^\ell$ for some finite subset Λ of $\mathbb{Z}^d$. A straightforward sequence of equalities yields

$$\begin{aligned} \hat{A}(z)[\mathcal{F}Q(g, \zeta)] \;&=\; \hat{A}(z)\Big(\sum_{n\in\mathbb{Z}^d} g\zeta^n z^{-n}\Big) \;=\; \sum_{n\in\mathbb{Z}^d} \zeta^n \hat{A}(z) g z^{-n} \;=\; \sum_{n\in\mathbb{Z}^d} \zeta^n \sum_{\ell\in\Lambda} A^\ell g z^{\ell-n} \\ &=\; \sum_{\ell\in\Lambda} A^\ell g \sum_{n\in\mathbb{Z}^d} \zeta^n z^{\ell-n} \;=\; \sum_{\ell\in\Lambda} A^\ell g \sum_{n\in\mathbb{Z}^d} \zeta^{n+\ell} z^{-n} \\ &=\; \sum_{n\in\mathbb{Z}^d} z^{-n}\zeta^n \sum_{\ell\in\Lambda} A^\ell \zeta^\ell g \;=\; \sum_{n\in\mathbb{Z}^d} z^{-n}\hat{A}(\zeta) g \zeta^n \;=\; \mathcal{F}Q(\hat{A}(\zeta)g, \zeta)\,. \end{aligned} \tag{3.54}$$

□

3.2.2 Floquet-Bloch theorem. By Theorem 2, operators that are periodic on $\mathcal{V}$ with respect to the free $\mathbb{Z}^d$ action are exactly those that become multiplication operators under the formal Floquet transform. That is, Af becomes $\hat{A}(z)\hat{f}(z)$, which is matrix-vector multiplication of Laurent polynomials. Evaluation of these polynomials at a point $\zeta \in \mathbb{T}^d$ realizes the Fourier transform, that is

$$(\mathcal{U}f)(\zeta) \;=\; \hat{A}(\zeta)\hat{f}(\zeta). \tag{3.55}$$

3.3 On $L^2(\mathcal{V})$: Full spectral resolution

When extended to L^2, the operator A enjoys all the theory of closed operators in Hilbert space.

3.3.1 Floquet-Bloch theorem revisited. In L^2, Equation (3.55) is a discrete version of the classical Floquet-Bloch Theorem [36, Thm XIII.97], which represents A as a decomposable operator through the direct integral (2.32),

$$A \;=\; \int_{\mathbb{T}^d}^{\otimes} \hat{A}(z)\, d\tilde{V}(z), \qquad Af \;=\; \int_{\mathbb{T}^d}^{\otimes} \hat{A}(z)\hat{f}(\bullet, z)\, d\tilde{V}(z). \tag{3.56}$$

The resolvent of A is represented by

$$(A-\lambda)^{-1} f \;=\; \int_{\mathbb{T}^d}^{\otimes} (\hat{A}(z)-\lambda I)^{-1} \hat{f}(\bullet, z)\, d\tilde{V}(z). \tag{3.57}$$

3.3.2 Invertibility and spectrum. We do not expect that $(A-\lambda I)$ is invertible on $F_0(\mathcal{V})$. This is best seen through the Floquet transform: The matrix operator $(\hat{A}(z)-\lambda I_W)$ on $\mathbb{C}[z^{\pm}]^W$ is a Laurent polynomial in z, so it takes polynomials to polynomials, but its inverse does not. Extending A to $\ell^2(\mathcal{V}) \cong \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^W$, or, equivalently, extending $\hat{A}(z)$ to $L^2(\mathbb{T}^d) \otimes \mathbb{C}^W$, the inverse as a bounded linear operator is

$$(\hat{A}(z)-\lambda I)^{-1} \;=\; \frac{A^{\dagger}(z,\lambda)}{D(z,\lambda)}, \tag{3.58}$$

whenever this is regular on $\mathbb{T}^d$. Here, $A^{\dagger}(z,\lambda)$ is the adjugate matrix to $\hat{A}(z)-\lambda I$ and

$$D(z,\lambda) \;=\; \det(\hat{A}(z)-\lambda I). \tag{3.59}$$

The determinant $D(z,\lambda)$ is known as the *dispersion function* for the operator A. For those λ for which $D(z,\lambda)$ is non-vanishing for all $z \in \mathbb{T}^d$, the inverse $(\hat{A}(z)-\lambda I)^{-1}$ exists from $L^2(\mathbb{T}^d) \otimes \mathbb{C}^W$ to $\ell^2(\mathcal{V})$. Thus the resolvent set of A is the open set

$$\rho(A) \;=\; \left\{\lambda \in \mathbb{C} : D(z,\lambda) \neq 0 \;\forall z \in \mathbb{T}^d\right\}, \tag{3.60}$$

and the spectrum of A is its complement $\sigma(A) = \mathbb{C} \setminus \rho(A)$.

Symmetry of the operator A in the sense that, for all $f, g \in F_0(\mathcal{V})$,

$$(Af, g) \;=\; (f, Ag) \tag{3.61}$$

occurs whenever the matrix for A is Hermitian, that is, $a_{vw}(m,n) = (a_{wv}(n,m))^*$. The extension of A to $\ell^2(\mathcal{V})$ is self-adjoint. This implies that the matrix $\hat{A}(z)$ is self-adjoint for all $z \in \mathbb{T}^d$,

$$\hat{A}(z) \;=\; \hat{A}(z)^* \qquad \forall z \in (\mathbb{T}^*)^d, \tag{3.62}$$

and this implies the more general reflection property

$$\hat{A}(\bar{z}^{-1}) \;=\; \hat{A}(z)^* \qquad \forall z \in (\mathbb{C}^{\times})^d, \tag{3.63}$$

which can also be checked directly by the construction $\hat{A}(z)$ from A. In this situation, the spectrum of A is real, $\sigma(A) \subset \mathbb{R}$ and, furthermore, $D(z,\lambda)$ is real-valued whenever $z \in \mathbb{T}^d$ and $\lambda \in \mathbb{R}$.

3.3.3 Spectral bands. When A is self-adjoint, $D(z,\lambda) = 0$ defines a multi-valued real eigenvalue function $\lambda(z)$ on the torus $\mathbb{T}^d$ with real eigenvalue branches $\lambda_j(k)$ $(z = e^{ik})$, $j \in [1, |W|]$. The image of all of these branches constitutes the spectrum $\sigma(A)$ of A, which consists a union of closed intervals called *spectral bands*. The branches of λ are called *band functions*. Spectral bands are discussed in §4.

3.3.4 Density of states. The physical observable known as the density of states can be expressed in terms of the band functions [19, Ch. 11]. If ν is the integrated density of states, the density is

$$\delta(\lambda) \;=\; \frac{d\nu}{d\lambda}(\lambda) \;=\; \frac{1}{|W|} \sum_{j=1}^{|W|} \int_{\lambda-\lambda_j(k)=0} \frac{d\tilde{S}}{|\nabla_k \lambda_j|}, \tag{3.64}$$

in which $d\tilde{S}$ is the Euclidean volume of the Fermi surface in $\mathbb{T}^d$ scaled by $1/(2\pi)^d$.

For periodic operators, there is another formula for the density of states. For a subset $\mathcal{V}' \subset \mathcal{V}$, let $\mathbb{1}_{\mathcal{V}'}$ denote the spatial projection (cutoff) of functions onto $\mathbb{C}^{\mathcal{V}'}$, and for a Borel set $B \subset \mathbb{R}$, let χ_B denote the spectral projection onto B in the spectral resolution of A. For integers ℓ,

$$\Lambda_\ell \;=\; [-\ell,\ell]^d \subset \mathbb{Z}^d, \tag{3.65}$$

which is empty if $\ell < 0$. The density of states of A is the Borel measure

$$\delta(B) \;=\; \lim_{\ell\to\infty} \frac{\operatorname{tr}(\chi_B \mathbb{1}_{W+\Lambda_\ell})}{|W+\Lambda_\ell|}. \tag{3.66}$$

Since A is periodic, χ_B commutes with the shift S^n, and thus $S^n \mathbb{1}_{\mathcal{V}'} S^{-n} = \mathbb{1}_{\mathcal{V}'+n}$, making $\chi_B \mathbb{1}_{\mathcal{V}'}$ unitarily equivalent to $\chi_B \mathbb{1}_{\mathcal{V}'+n}$. Thus $\operatorname{tr}(\chi_B \mathbb{1}_{W+\Lambda_\ell}) = |\Lambda_\ell| \operatorname{tr}(\chi_B \mathbb{1}_W)$, and we obtain

$$\delta(B) \;=\; \frac{\operatorname{tr}(\chi_B \mathbb{1}_W)}{|W|}. \tag{3.67}$$

This is the von Neumann formula for density of states of a periodic operator. A homological formula based on a free resolution of modules is derived in [23].

3.4 Eigenfunctions: Module *vs.* L^2

Recall the dichotomy mentioned at the beginning of §3. This section shows how A as a module endomorphism, that is, A restricted to $F_0(\mathcal{V})$, gives full information on the L^2 eigenspaces of A.

3.4.1 Flat band functions. §3.1.4 showed that eigenvalues of $\hat{A}(z)$ on $\mathbb{C}[z^\pm]^W$ are of infinite multiplicity. Furthermore, for each $\zeta \in (\mathbb{C}^\times)^d$, the sum of shifts $\sum_{n\in\mathbb{Z}^d} f(\bullet \dot{-} n)\zeta^n$ (this is the Floquet transform at $z = \zeta$) is a λ-eigenfunction of A and is ζ-quasi-periodic. Particularly, λ is an eigenvalue of $\hat{A}(\zeta)$ for each $\zeta \in \mathbb{T}^d$. This means that A has a constant, or "flat", spectral band function at λ.

3.4.2 Module eigenfunctions and L^2 eigenfunctions. In fact, the eigenvalues of $\hat{A}(z)$ on $\mathbb{C}[z^\pm]^W$ are exactly all the eigenvalues of A on $\ell^2(\mathcal{V})$.

Theorem 4. *The following statements are equivalent.*

1. *λ_0 is an eigenvalue of $\hat{A}(z)$, that is, there exists nonzero $f(z) \in \mathbb{C}[z^\pm]$ such that $(\hat{A}(z) - \lambda_0) f(z) = 0$ in $\mathbb{C}[z^\pm]$.*
2. *λ_0 is an L^2 eigenvalue for A, that is, there exists $f \in L^2(\mathcal{V})$ such that $(A - \lambda_0) f = 0$.*
3. *$(\lambda - \lambda_0)$ is a factor of $D(z,\lambda)$.*

When these statements hold, λ is an eigenvalue of A of infinite multiplicity and the L^2 eigenspace contains a dense linear subspace of compactly supported eigenfunctions. The set of eigenvalues of A is finite.

We prove (1)⇒(3)⇒(2)⇒(1), although (1)⇒(2) is straightforward.

Statement (1) means that there exists a nonzero Laurent polynomial vector $f(z) \in \mathbb{C}[z^\pm]^W$ such that $(\hat{A}(z) - \lambda_0 I) f(z) = 0$ in $\mathbb{C}[z^\pm]^W$. Let X be the variety on which $f(z)$ vanishes,

$$X \;=\; \{\zeta \in (\mathbb{C}^\times)^d : f_v(\zeta) = 0 \;\forall v \in W\}. \tag{3.68}$$

For all $\zeta \in (\mathbb{C}^\times)^d \smallsetminus X$, $f(\zeta)$ is a nonzero vector in $\mathbb{C}^W$ and $(\hat{A}(\zeta) - \lambda_0 I) f(\zeta) = 0$, so $D(\zeta,\lambda_0) = 0$ as $(\mathbb{C}^\times)^d \smallsetminus X$ is an open dense set. Therefore $D(z,\lambda_0) = 0$ as a Laurent polynomial in z. This means that $D(z,\lambda)$ has $(\lambda - \lambda_0)$ as a factor.

Assuming (3), for each $\zeta \in (\mathbb{C}^\times)^d$ there is a vector $f(\zeta) \in \mathbb{C}^W$ such that $(\hat{A}(\zeta) - \lambda_0) f(\zeta) = 0$, and the function $f(\zeta)$ can be taken to be continuous on $\mathbb{T}^d$. Fourier inversion provides a function $\check{f} \in \ell^2(\mathbb{Z}^d)$ such that $(A - \lambda_0)\check{f} = 0$.

That (2) implies (1) follows from the remarkable fact that the space of compactly supported eigenfunctions is dense in the whole λ-eigenspace, which is proved below. To see that the dimension of the eigenspace is infinite, let f be a nonzero compactly supported λ-eigenfunction, let s be the diameter of the support of f and note that all the shifts of f by $s\mathbb{Z}^d$ have mutually disjoint supports and are therefore orthogonal.

3.4.3 Approximation by compactly supported eigenfunctions. First, let $\mathcal{E}$ be a nontrivial shift-invariant subspace of the λ-eigenspace of A, and we will prove that there exists a compactly supported λ-eigenfunction of A that is not orthogonal to $\mathcal{E}$, a theorem due to Kuchment [26]. The proof is based on those of [26, 20]. A proof for amenable groups is in [23].

Denote by P the orthogonal projection onto $\mathcal{E}$. For any positive integers ℓ and r, set $\Lambda = \Lambda_\ell$ and $\partial = \Lambda_\ell \setminus \Lambda_{\ell-r}$. The argument in §3.3.4 yields

$$\frac{\operatorname{tr}(\mathbb{1}_W P)}{|W|} = \frac{\operatorname{tr}(\mathbb{1}_{W+\Lambda} P)}{|W||\Lambda|}. \tag{3.69}$$

The space $\mathcal{E}$ being nontrivial implies that $\operatorname{tr}(\mathbb{1}_W P) > 0$. Since $\dim(\operatorname{im}\mathbb{1}_{W+\partial}) = |W+\partial| = |W||\partial|$, we obtain

$$\operatorname{rk}(\mathbb{1}_{W+\partial}\mathcal{E}) \le |W||\partial|. \tag{3.70}$$

Equation (3.69) together with $\|\mathbb{1}_{W+\partial}P\| \le 1$ yield

$$|\Lambda| \operatorname{tr}(\mathbb{1}_W P) = \operatorname{tr}(\mathbb{1}_{W+\Lambda} P) \le \operatorname{rk}(\mathbb{1}_{W+\Lambda} P). \tag{3.71}$$

Fix r fixed, observe that $|\partial|/|\Lambda| \to 0$ as $\ell \to \infty$. Since $\operatorname{tr}(\mathbb{1}_W P) > 0$, one can therefore choose ℓ such that

$$|\partial| < |\Lambda| \frac{\operatorname{tr}(\mathbb{1}_W P)}{|W|}. \tag{3.72}$$

Putting (3.70), (3.71), and (3.72) together yields

$$\operatorname{rk}(\mathbb{1}_{W+\partial} P) < \operatorname{rk}(\mathbb{1}_{W+\Lambda} P). \tag{3.73}$$

Consequently, there exists $\phi \in \mathcal{E}$ such that $\phi \notin \ker(\mathbb{1}_{W+\Lambda})$ and $\phi \in \ker(\mathbb{1}_{W+\partial})$.

Now apply this result with $r = 2r(A)$ (see page 6). Then ϕ is a λ-eigenfunction of A, ϕ is not identically zero on Λ, and ϕ vanishes on ∂. It follows from the definition of $r(A)$ that the compactly supported function $\psi = \mathbb{1}_{W+\Lambda}\phi$ is also a λ-eigenfunction of A. Since $(\psi, \phi) = (\psi, \psi) \neq 0$, ψ is not orthogonal to $\mathcal{E}$.

Denote by $\mathcal{F}$ the closure of the span of all compactly supported λ-eigenfunctions of A, and let $\mathcal{E}$ be its orthogonal complement within the λ-eigenspace of A. Since both $\mathcal{F}$ and the λ-eigenspace are shift-invariant, so is $\mathcal{E}$. If $\mathcal{E}$ is nontrivial, we have proved above that there is a compactly supported eigenfunction that is not orthogonal to $\mathcal{E}$, which contradicts the definition of $\mathcal{E}$. We conclude that $\mathcal{F}$ is equal to the λ-eigenspace of A and that therefore this eigenspace contains the compactly supported λ-eigenfunctions as a dense subset.

4 Bloch and Fermi varieties

The relation $D(z, \lambda) = 0$ is the dispersion relation for the periodic operator A. It has two fundamental meanings. One is that if $D(z, \lambda) = 0$ for some $z \in \mathbb{T}^d$, then $\lambda \in \sigma(A)$. The other is that, for any $\lambda \in \mathbb{C}$ and $z \in (\mathbb{C}^\times)^d$, $D(z, \lambda) = 0$ implies that A admits a Floquet mode at energy λ and weight z. It defines the Bloch variety whose cross section at a fixed value of λ is the Fermi variety at energy λ.

4.1 Definitions

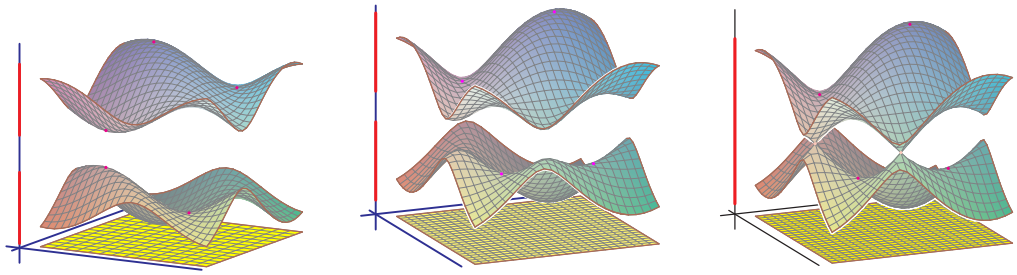
4.1.1 The Bloch variety. The dispersion relation of a periodic graph operator is the zero set of the dispersion function, and it is also known as the *Bloch variety*. The complex Bloch variety is

$$\mathcal{B}_A = \left\{(z, \lambda) \in (\mathbb{C}^\times)^d \times \mathbb{C} : D(z, \lambda) = 0\right\}, \tag{4.74}$$

and the real Bloch variety is

$$\mathbb{R}\mathcal{B}_A = \left\{(z, \lambda) \in \mathbb{T}^d \times \mathbb{R} : D(z, \lambda) = 0\right\}. \tag{4.75}$$

Below are three pictures of real Bloch varieties for the hexagonal lattice (3.47).



$(a,b,c) = (-1,-3,-1)$ $\qquad$ $(a,b,c) = (-1,-1,-1)$ $\qquad$ $(a,b,c) = (-1,-1,-1)$ (4.76)

The third has $V(v) = V(w)$ and is the Bloch variety of the graph Laplacian, later referred to as *graphene*. Its two singular points are called Dirac points, and Figure 1 shows some perturbations of it.

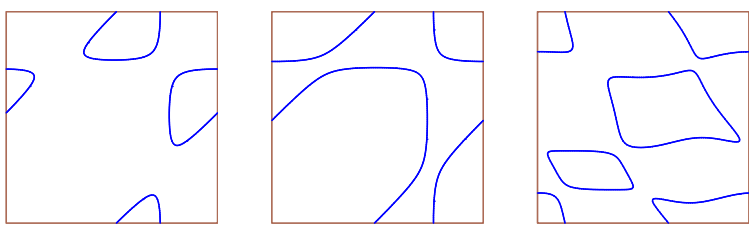
4.1.2 The Fermi variety. The Fermi variety, or Fermi surface, is a cross section of the Bloch variety at a specific energy λ. For $\lambda \in \mathbb{C}$, the complex Fermi surface is

$$\Phi_{A,\lambda} \;=\; \left\{ z \in (\mathbb{C}^\times)^d : D(z,\lambda) = 0 \right\}, \tag{4.77}$$

and for $\lambda \in \mathbb{R}$, the real Fermi surface is

$$\mathbb{R}\Phi_{A,\lambda} \;=\; \left\{ z \in \mathbb{T}^d : D(z,\lambda) = 0 \right\}. \tag{4.78}$$

We show three real Fermi surfaces, which are curves in $\mathbb{T}^2$. The first two are from the middle Bloch variety in (4.76) at $\lambda = 1.5$ and $\lambda = 1.7$, where the potential has been normalized so that $V(v) = 0$ and $V(w) = 1$, so that the three saddle points on the upper branch are at $\lambda = \frac{1}{2}(1+\sqrt{5})$. The third is from a different Bloch variety. They are displayed in the fundamental domain $[-\frac{\pi}{2}, \frac{3\pi}{2}]^2$.



(4.79)

4.2 Spectrum of A

The spectrum of a discrete periodic operator is determined by its Bloch variety annd its projection onto the real λ axis. The spectrum is intimately connected with the Floquet modes of the operator. Recall from §3.3.2 that the spectrum of A is the the closed set

$$\sigma_A \;=\; \left\{ \lambda \in \mathbb{C} : A - \lambda I \text{ does not have a bounded inverse in } \ell^2(\mathcal{V}) \right\}. \tag{4.80}$$

4.2.1 Floquet modes. Floquet modes were introduced in §3.2 as eigenfunctions of the shift group $\mathbb{Z}^d$. Floquet (or Floquet-Bloch) modes for a periodic operator A are simultaneous eigenfunctions of $\mathbb{Z}^d$ and A. For each point (z,λ) on the complex Bloch variety, we have a simultaneous eigenfunction of the shift group $\mathbb{Z}^d$ and the operator A. That is, a function $f : \mathcal{V} \to \mathbb{C}$ such that

$$n{\cdot}f \;=\; z^n f \qquad \text{and} \qquad Af \;=\; \lambda f. \tag{4.81}$$

Such a function is called a *Floquet mode* for energy λ and weight z, or quasi-momentum k, where $z = e^{ik}$. Floquet modes are not in $\ell^2(\mathcal{V})$ because of the first equation.

Theorem 5. *Let $\zeta \in (\mathbb{C}^\times)^d$ and $\lambda \in \mathbb{C}$ be such that $D(\zeta,\lambda) = 0$. Then there exists a Floquet mode for energy λ and weight ζ.*

Proof. Since $D(\zeta,\lambda)=0$, there exists $g\in\mathbb{C}^W$ such that $(\hat{A}(\zeta)-\lambda I_W)g=0$. This makes the right-hand side of (3.52) vanish, with $\hat{A}(z)-\lambda I_W$ in place of $\hat{A}(z)$. Therefore $(\hat{A}(z)-\lambda I_W)[\mathcal{F}Q(g,\zeta)]=0$, so that

$$(A-\lambda I)Q(g,\zeta) \;=\; 0. \tag{4.82}$$

For $f=Q(g,\zeta)$, the second equation of (4.81) is satisfied, and the first is satisfied by definition of Q. □

4.2.2 Spectrum and $D(z,\lambda)$. The spectrum of a periodic operator A has a geometric description:

$$\sigma(A) \;=\; \left\{\lambda\in\mathbb{C} : \Phi_{A,\lambda}\cap\mathbb{T}^d\neq\varnothing\right\}. \tag{4.83}$$

Theorem 6. *A number $\lambda\in\mathbb{C}$ is in the spectrum of A if and only if there exists $\zeta\in\mathbb{T}^d$ such that $D(\zeta,\lambda)=0$.*

Fix $\lambda\in\mathbb{C}$ and suppose $D(\zeta,\lambda)$ is nonzero for all $\zeta\in\mathbb{T}^d$. Then $(\hat{A}(\zeta)-\lambda)^{-1}$ exists as an analytic matrix-valued function on $\mathbb{T}^d$, and therefore is a bounded multiplication operator on $L^2(\mathbb{T}^d)$. By the unitarity of the Fourier transform $\mathcal{U}:\ell^2(\mathcal{V})\to L^2(\mathbb{T}^d)$, the operator $A-\lambda$ is also invertible. Now suppose that there exists $\zeta\in\mathbb{T}^d$ such that $D(\zeta,\lambda)=0$. Then by Theorem 5, there exists a Floquet mode $f:\mathcal{V}\to\mathbb{C}$ for energy λ and weight ζ. For each positive integer ℓ, define the compactly supported function $f_\ell:\mathcal{V}\to\mathbb{C}$ by

$$f_\ell(x) \;=\; \frac{1}{\|f\|_W|\Lambda_\ell|^{1/2}}\mathbb{1}_{W+\Lambda_\ell}(x)f(x), \tag{4.84}$$

in which $\|f\|_W^2=\sum_{x\in W}|f(x)|^2$. Set $r=2r(A)$ and $\partial_\ell=\Lambda_{\ell+r}\smallsetminus\Lambda_{\ell-r}$. For all $x\in\mathcal{V}$,

$$\|[(A-\lambda)f_\ell](x)\| \le \frac{\|A-\lambda\|}{|\Lambda_\ell|^{1/2}}, \tag{4.85}$$

If $x\in\mathcal{V}\smallsetminus(W+\partial_\ell)$, then $[(A-\lambda)f_\ell](x)=0$. Therefore,

$$\|(A-\lambda)f_\ell\|_{\ell^2(\mathcal{V})} \;\le\; \frac{\|A-\lambda\|\sqrt{|W||\partial_\ell|}}{|\Lambda_\ell|^{1/2}} \;\longrightarrow 0 \qquad (\ell\to\infty), \tag{4.86}$$

whereas $\|f_\ell\|_{\ell^2(\mathcal{V})}=1$. This implies that $A-\lambda$ does not have a bounded inverse on $\ell^2(\mathcal{V})$. The sequence $\{f_\ell\}_{\ell\in\mathbb{N}}$ is known as a Weyl sequence for A.

4.2.3 Self-adjointness and real structure. When the operator A is self-adjoint, the real Bloch and Fermi varieties are naturally real algebraic varieties, in a non-standard way. Indeed, complex conjugation $z\mapsto\bar{z}$ is an involution on $\mathbb{C}^n$ that is anti-holomorphic in that the induced map on complex tangent spaces is conjugate-linear. Its fixed points are $\mathbb{R}^n$. More generally, a real structure on a complex space X is an anti-holomorphic involution on X. Its set of fixed points form the real points $X(\mathbb{R})$ of this real structure on X. When they are nonempty and include a smooth point of X, we have that $\dim_{\mathbb{R}}X(\mathbb{R})=\dim_{\mathbb{C}}X$.

Recall from §3.3.2 that when A is self-adjoint, $\hat{A}(z)$ satisfies the reflection principle $\hat{A}(\bar{z}^{-1})=\hat{A}(z)^*$, which implies the corresponding identity of $D(z,\lambda)$,

$$D(\bar{z}^{-1},\bar{\lambda}) \;=\; \overline{D(z,\lambda)}, \tag{4.87}$$

for $z\in(\mathbb{C}^\times)^d$ and $\lambda\in\mathbb{C}$.

The associated involution $(z,\lambda)\mapsto(\bar{z}^{-1},\bar{\lambda})$ is a non-standard real structure on the space $(\mathbb{C}^\times)^d\times\mathbb{C}$ with real points $\mathbb{T}^d\times\mathbb{R}$. It is non-standard as it differs from the usual structure $(z,\lambda)\mapsto(\bar{z},\bar{\lambda})$. By (4.87), this restricts to a real structure on the complex Bloch variety $\mathcal{B}_A$ and for $\lambda\in\mathbb{R}$, on the complex Fermi variety $\Phi_{A,\lambda}$. Their real points are the real Bloch variety $\mathbb{R}\mathcal{B}_A$ and real Fermi variety, respectively.

Thus the real Bloch variety has dimension d in $\mathbb{T}^d\times\mathbb{R}$, and not d–1, which is what one expects from a naïve dimension count: The complex Bloch variety has real codimension 2 in its ambient $(\mathbb{C}^\times)^d\times\mathbb{C}$, implying that the real Bloch variety should have codimension 2 in $\mathbb{T}^d\times\mathbb{R}$, and hence dimension d–1. Similarly, a real Fermi variety has dimension d–1 and not the naïve dimension count of d–2. Moreover, the real Bloch variety determines and is determined by the complex Bloch variety, together with its non-standard real structure.

There are further constraints imposed by A being self-adjoint. The property (4.87) implies that the terms of the polynomial $D(z,\lambda)$ come in pairs of the form $az^n\lambda^m+\bar{a}z^{-n}\lambda^m$ for some $a\in\mathbb{C}$, $n\in\mathbb{Z}^d$, and $m\in\mathbb{N}$. Thus, for fixed $\zeta\in\mathbb{T}^d$, $D(\zeta,\lambda)$ is a polynomial in λ with real coefficients. This only implies that set of roots of $D(\zeta,\lambda)=0$ are stable under complex conjugation. In fact, as $A(\zeta)$ is hermitian, all these roots are real.

4.2.4 Floquet sheaves and modules. Floquet modes of §4.2.1 have an algebraeo-geometric interpretation, The projection map $\mathscr{E} := \big((\mathbb{C}^\times)^d \times \mathbb{C}\big) \times \mathbb{C}^W \to (\mathbb{C}^\times)^d \times \mathbb{C}$ exhibits $\mathscr{E}$ as a (trivial) vector bundle with fiber $\mathbb{C}^W$. The characteristic matrix $\hat{A}(z) - \lambda I_W$ is an endomorphism of $\mathscr{E}$. When $D(z,\lambda) \neq 0$, it is an isomorphism of the fiber $\mathbb{C}^W$ of $\mathscr{E}$ at the point (z,λ), and when $D(z,\lambda) = 0$, Theorem 5 implies that the Floquet modes at (z,λ) are exactly the kernel of $\hat{A}(z) - \lambda I_W$. In the language of algebraic geometry [39], the Floquet modes form the kernel sheaf $\mathscr{F} \subset \mathscr{E}$ of the endomorphism $\hat{A}(z) - \lambda I_W$ of $\mathscr{E}$, and the support of this Floquet sheaf $\mathscr{F}$ is the Bloch variety. In the examples we give, the fibers of $\mathscr{F}$ at smooth points of $\mathcal{B}_A$ are 1-dimensional, and at the singular (Dirac) points in (4.76), they have dimension 2.

The matrix $\hat{A}(z) - \lambda I_W$ of polynomials in $\mathbb{C}[z^\pm, \lambda]$ is also an endomorphism of the free $\mathbb{C}[z^\pm, \lambda]$-module $\mathbb{C}[z^\pm, \lambda]^W$. The counterpart of the Floquet sheaf $\mathscr{F}$ is the kernel of this map $\hat{A}(z) - \lambda I_W$, which is also a module for the ring $\mathbb{C}[z^\pm, \lambda]$ (for more on modules over commutative rings, see [7, Ch. 5]). By the dictionary between affine algebraic varieties and finitely generated commutative $\mathbb{C}$-algebras, these two perspectives, kernel sheaf and kernel module, are equivalent ways to view the same object. This module-theoretic point of view is due to Kravaris [23], who reinterpreted work of Kuchment [26]. Kravaris gave new results on the density of states using free resolutions for general periodic operators, generalizing earlier work of Gieseker, Knörrer, and Trubowitz [19] for the square lattice $\mathbb{Z}^2$.

4.3 Reducibility and defect eigenvalues

The reducibility of the Bloch and Fermi varieties has spectral consequences, notably concerning the existence of embedded eigenvalues caused by local defects, as studied by Kuchment and Vainberg [25].

4.3.1 Components of the Bloch variety. As an element of $\mathbb{C}[z^\pm, \lambda]$, $D(z,\lambda)$ has a decomposition into irreducible elements that are unique up to multiplication by constants and monomials in $\mathbb{C}[z^\pm]$,

$$D(z,\lambda) \;=\; F(\lambda) \prod_{j=1}^{\alpha} \tilde{D}_j(z,\lambda). \tag{4.88}$$

All the factors that are polynomials in λ alone are incorporated into $F(\lambda) = \prod_{\ell=1}^{\gamma} (\lambda - \lambda_\ell)^{p_\ell}$, with the real numbers λ_ℓ being distinct. We do not require the $\tilde{D}_j$ to be distinct. Each factor $\tilde{D}_j(z,\lambda)$ corresponds to a component of the Bloch variety $\mathcal{B}_A$,

$$\mathcal{B}_A^j \;=\; \left\{(z,\lambda) \in (\mathbb{C}^\times)^d \times \mathbb{C} : \tilde{D}_j(z,\lambda) = 0\right\}. \tag{4.89}$$

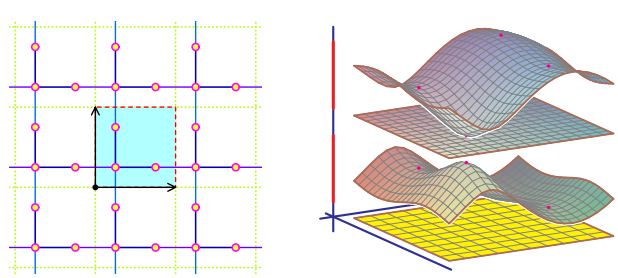
Each of these components contributes a set of spectral bands and gaps to the spectrum of A,

$$\tilde{\sigma}_j(A) = \left\{\lambda \in \mathbb{R} : \exists z \in \mathbb{T}^d,\, (z,\lambda) \in \mathcal{B}_A^j\right\}, \tag{4.90}$$

and each number λ_ℓ is an eigenvalue of A of infinite multiplicity. Thus,

$$\sigma(A) \;=\; \{\lambda_\ell\}_{\ell=1}^{\gamma} \cup \bigcup_{j=1}^{\alpha} \tilde{\sigma}_j(A).$$

Roots λ_ℓ of $F(\lambda)$ are flat bands of the Bloch variety. The Bloch variety of the Lieb lattice (on the left below) has a flat band when the potentials at the vertices of degree 2 are equal.

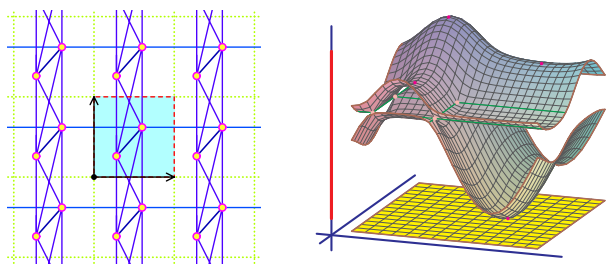


(4.91)

4.3.2 Components of the Fermi variety. Let $\lambda_0 \in \mathbb{C}$ be fixed. The factorization of the z-dependent factors of $D(z,\lambda)$ in (4.88) persists for $D(z,\lambda_0)$ as an element of $\mathbb{C}[z^{\pm}]$, but the factorization may possibly be refined further, as each factor $\tilde{D}_j(z,\lambda_0)$ has its own factorization in $\mathbb{C}[z^{\pm}]$,

$$D(z,\lambda_0) \;=\; F(\lambda_0) \prod_{\ell \in [1,\beta]} D_\ell(z,\lambda_0), \tag{4.92}$$

with $\beta \geq \alpha$. Each $\tilde{D}_j(z,\lambda_0)$ is a product of some of the $D_\ell(z,\lambda_0)$. Note that the number β of factors is taken to be independent of λ_0, and that this factorization is meaningful even if $F(\lambda_0) = 0$. One can prove that either $D(z,\lambda_0)$ is reducible for all $\lambda_0 \in \mathbb{C}$ or it is reducible for only a finite set of values of λ_0 (this is known as Hilbert's Irreducibility Theorem). For example, the pure Schrödinger operator on the graph below has an irreducible Bloch variety, but its Fermi variety at the energy of its Dirac points is highly reducible and is situated on the Bloch variety in a very interesting way.



(4.93)

Each factor $D_j(z,\lambda)$ corresponds to a component of the Fermi variety Φ_{A,λ_0},

$$\Phi^j_{A,\lambda_0} \;=\; \left\{ z \in (\mathbb{C}^\times)^d : D_j(z,\lambda_0) = 0 \right\}. \tag{4.94}$$

Each of these components contributes a set of spectral bands and gaps to the spectrum of A, which refine the bands $\tilde{\sigma}_j(A)$,

$$\sigma_j(A) = \left\{ \lambda_0 \in \mathbb{R} : \mathbb{T}^d \cap \Phi^j_{A,\lambda_0} \neq \varnothing \right\}. \tag{4.95}$$

4.3.3 L^2 response to source in the continuum. We may view $\hat{A}(z)$ as a self-adjoint analytic family over $\mathbb{T}^d$ of operators on $\mathbb{C}^W$. Fix $\lambda \in \mathbb{R}$, and consider the equation

$$(A - \lambda)u \;=\; f \qquad \text{in } \ell^2(\mathcal{V}). \tag{4.96}$$

Under the Fourier transform, this becomes $(\hat{A}(z) - \lambda I)\hat{u}(z) = \hat{f}(z)$ on $L^2(\mathbb{T}^d, \mathbb{C}^W)$, and hence

$$\hat{u}(z) \;=\; \frac{R(z,\lambda)\hat{f}(z)}{D(z,\lambda)}, \tag{4.97}$$

in which $R(z,\lambda)$ is the adjugate of $(\hat{A}(z) - \lambda I)$, a Laurent polynomial in z with coefficients in $\mathbb{C}^{W\times W}$. Note that $u \in \ell^2(\mathcal{V})$ if and only if $\hat{u} \in L^2(\mathbb{T}^d, \mathbb{C}^W)$, and this happens when the right-hand side of (4.97) is regular on $\mathbb{T}^d$, that is, the numerator cancels the zero set of the denominator.

Let $D(z,\lambda) = D_{\mathrm{g}}(z,\lambda) D_{\mathrm{s}}(z,\lambda)$, where $D_{\mathrm{g}}(z,\lambda)$ is the product of all factors D_j of D whose zero sets do not intersect $\mathbb{T}^d$ and $D_{\mathrm{s}}(z,\lambda)$ has the rest of the factors in (4.92). The real variety of D_{g} in $\mathbb{T}^d$ is therefore empty. The subscripts refer to "gap" and "spectrum". The key observation is that, in order for for $R(z,\lambda)\hat{f}(z)$ to cancel the zero set of $D_{\mathrm{s}}(z,\lambda)$ on $\mathbb{T}^d$, it must cancel $D_{\mathrm{s}}(z,\lambda)$ identically as a Laurent polynomial in z. The proof of the following theorem is contained in the proof of [25, Theorem 6].

Theorem 7. *In order for $R(z,\lambda)\hat{f}(z)/D(z,\lambda)$ to be regular on $\mathbb{T}^d$, each vector component of $R(z,\lambda)\hat{f}(z)$ must have $D_{\mathrm{s}}(z,\lambda)$ as a factor.*

Naïvely, this factorization is accomplished if $\hat{f}(z) = D_{\mathrm{s}}(z,\lambda)\hat{f}_0(z)$ for some $f_0(z) \in \mathbb{C}[z^{\pm}]^W$. But additional structure may allow $\hat{f}(z)$ to be chosen so that $R(z,\lambda)\hat{f}(z)$ has D_{s} as a factor even if $\hat{f}(z)$ does not.

4.3.4 Reducibility of $\mathcal{B}_A$ by symmetry. This section is a generalization of a construction in [40]. A finite symmetry of A that commutes with $\mathbb{Z}^d$ yields reducibility of the Bloch variety. Denote a free action $G \times W \to W$ of a finite group G on W by $(g,x) \mapsto g{\cdot}x$. Thus $\mathbb{Z}^d \times G$ acts on $\mathbb{Z}^d \times W$ and therefore also on $\ell^2(\mathcal{V}) = \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^W$ by

$$[(n,g)f](m,y) \;=\; f(m \dot{-} n, g^{-1}y), \tag{4.98}$$

for all $m \in \mathbb{Z}^d$, $y \in W$ and $n \in \mathbb{Z}^d$, $g \in G$. The vector space $\mathbb{C}^W$, as a representation of G, admits a decomposition $\mathbb{C}^W = \bigoplus_{j\in[1,r]} X_j$, in which X_j is a direct sum of s_j copies of one of the m irreducible representations of G. This induces an orthogonal decomposition

$$\ell^2(\mathcal{V}) \;=\; \ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^W \;=\; \bigoplus_{j\in[1,r]} \ell^2(\mathbb{Z}^d) \otimes X_j. \tag{4.99}$$

Now let A commute also with the G action. Thus A is invariant on each component of the decomposition (4.99) and may be further decomposable within each of the components $\ell^2(\mathbb{Z}^d) \otimes X_j$. A can be conceived as a graph operator as follows. Let W_j be an orthonormal basis for X_j as a vector space over $\mathbb{C}$, and, for each $j \in [1,r]$, define a vertex set

$$\mathcal{V}_j \;=\; \mathbb{Z}^d \times W_j. \tag{4.100}$$

The set W_j serves as a fundamental domain of the $\mathbb{Z}^d$ action on $\mathcal{V}_j$, and (4.99) becomes

$$\ell^2(\mathcal{V}) \;=\; \bigoplus_{j\in[1,r]} \ell^2(\mathcal{V}_j). \tag{4.101}$$

The operator A is decomposed into its projections onto these subspaces, that is $A = \sum_{j\in[1,r]} A_j$, where A_j is the restriction of A to $\ell^2(\mathcal{V}_j)$. Under the Floquet transform, we obtain $\hat{A}(z) = \bigoplus \hat{A}_j(z)$, and ultimately

$$D(z,\lambda) \;=\; \prod_{j\in[1,r]} P_j(z,\lambda)^{s_j}, \tag{4.102}$$

in which $P_j(z,\lambda)^{s_j} := \det(\hat{A}_j(z) - \lambda)$. Possible further factorizations of the P_j yield the $\tilde{D}_j$ above.

4.3.5 Generalized symmetries. Begin with an operator $\mathring{A}$ on $\ell^2(\mathring{\mathcal{V}})$, with dispersion function $\mathring{D}(z,\lambda)$. Create a new vertex set consisting of s copies (layers) of $\mathring{\mathcal{V}}$, that is, $\mathcal{V} = \sqcup_{j\in[1,s]} \mathring{\mathcal{V}}$. We will create a "multilayer" operator A on

$$\ell^2(\mathcal{V}) \;=\; \mathbb{C}^s \otimes \ell^2(\mathring{\mathcal{V}}). \tag{4.103}$$

Let $\{P_j\}_{j\in[1,r]}$ $(r \le s)$ be orthogonal projectors onto subspaces of $\mathbb{C}^s$. These subspaces generalize the spaces X_j above, as they are not necessarily coming from an underlying symmetry of W. Define A by

$$A \;=\; I_s \otimes \mathring{A} + \sum_{j\in[1,r]} P_j \otimes L_j \;=\; \sum_{j\in[1,r]} P_j \otimes (\mathring{A} + L_j), \tag{4.104}$$

in which the L_j are periodic graph operators on $\mathring{\mathcal{V}}$. The image of the projector $P_j \otimes I$ is an invariant space of "hybrid states" for A, and A acts on this space by $A + L_j$, as if it were a "single-layer" operator on $\ell^2(\mathring{\mathcal{V}})$, possibly with multiplicity. Now $D(z,\lambda)$ has factors $P_j(z,\lambda) = \det(\hat{A}(z) + \hat{L}_j(z) - \lambda I)$.

A simple case of this construction (see [40]) occurs when all m layers are coupled by one self-adjoint $m \times m$ matrix $K = \sum_{j\in[1,r]} \lambda_j P_j$ and $L_j = I$,

$$A \;=\; I_s \otimes \mathring{A} + K \otimes I \;=\; \sum_{j\in[1,r]} P_j \otimes (\mathring{A} + \lambda_j I). \tag{4.105}$$

The dispersion function is $D(z,\lambda) = \prod_{j\in[1,r]} \mathring{D}_j(z, \lambda - \lambda_j)^{s_j}$, so $\sigma(A)$ is a union of shifts of $\sigma(\mathring{A})$.

4.3.6 Example: AA-stacked bi-layer graphene. The simplest model of AA-stacked graphene is two copies of single-layer graphene H_0 coupled by a 2×2 interlayer hermitian matrix Γ. Let $\mathcal{V}_0$ be the vertex set for the single layer and $D_0(z,\lambda)$ its dispersion function. Then the AA-stacked model $H_{\rm AA}$ acts in $\mathbb{C}^2\otimes\ell^2(\mathcal{V}_0)$,

$$H_{\rm AA} = I_2\otimes H_0 + \Gamma\otimes I. \tag{4.106}$$

Let $\Gamma = U\Lambda U^{-1}$ with U unitary and $\Lambda = \mathrm{diag}(\mu_1,\mu_2)$. Then $\mathcal{U} = U\otimes I$ block-diagonalizes $H_{\rm AA}$, with the blocks being spectrally shifted copies $H_0+\mu_j I$ of the single layer. Thus the dispersion function for $H_{\rm AA}$ is reducible,

$$D(z,\lambda) = D_0(z,\lambda+\mu_1)D_0(z,\lambda+\mu_2). \tag{4.107}$$

This may be seen in the Bloch variety on the right in Figure 1 (on the next page).

4.3.7 Reducibility of $\Phi_{A,\lambda}$ by contracting edges. The coupling of multiple layers in §4.3.5 can be generalized to more elaborate coupling graphs, which results in the shifts λ_j in (4.105) being λ dependent. This has been worked out for quantum graphs, where the edges are endowed with an ordinary differential operator in [41, 5] and then for discrete graphs in [42].

Two decoupled layers of $\mathring{A}$ on $\ell^2(\mathring{\mathcal{V}})$ yield the operator $I_2\otimes\mathring{A}$ on $\mathbb{C}^2\otimes\ell^2(\mathring{\mathcal{V}})$, with vertex set $\mathring{\mathcal{V}}\sqcup\mathring{\mathcal{V}} = \{1,2\}\times\mathring{\mathcal{V}}$. Now, for each pair of "aligned" vertices, say $(1,v)$ and $(2,v)$, create a vertex set $\mathcal{V}_v$ containing these two vertices, and a self-adjoint coupling operator K_v on $\mathcal{V}_v$, ensuring periodicity $K_{v\dotplus n} = K_v$. Then merge these connecting operators with $I_2\otimes\mathring{A}$ to obtain a periodic "bilayer" operator with vertex set $\sqcup_{v\in\mathring{\mathcal{V}}}\mathcal{V}_v$.

Consider now the equation $(A-\lambda)u = f$, where f is supported on the vertices $\mathring{\mathcal{V}}\sqcup\mathring{\mathcal{V}}$. This equation can be written equivalently by eliminating the extra vertices in $\mathcal{V}_v$, for each $v\in\mathring{\mathcal{V}}$, by replacing K_v with its Schur complement. This is a 2×2 matrix indexed by the vertices $(1,v)$ and $(2,v)$ and is a rational function of λ. Explicitly, write the matrix for $K_v-\lambda$ in block form, with $(1,v)$ and $(2,v)$ coming first in the ordering,

$$K_v \;=\; \begin{bmatrix} A_v-\lambda & B_v \\ B_v^* & C_v-\lambda \end{bmatrix}. \tag{4.108}$$

The Schur complement is $S_v = A_v-\lambda - B_v(C_v-\lambda)^{-1}B_v^*$. If the K_v are the same for all $v\in\mathring{\mathcal{V}}$, the resulting contracted operator has the form of (4.105) with $m=2$ and S_v taking the place of K. More generally, if the K_v all commute with each other, then they admit common spectral projections P_1 and P_2, but the eigenvalues depend on v periodically; denote them by μ_j^v for $j\in\{1,2\}$ and $v\in\mathring{\mathcal{V}}$. The resulting contracted operator is λ dependent,

$$\tilde{A}(\lambda) \;=\; \sum_{j\in[1,2]} P_j\otimes\big(\mathring{A} + \sum_{v\in\mathring{\mathcal{V}}}\mu_j^v(\lambda)\big), \tag{4.109}$$

in which $\mu_j^v(\lambda)$ is treated as a function of v and acts as an onsite potential. It generalizes λ_j in (4.105), which is independent of λ and v.

The Fermi dispersion function can be factored as $D(z,\lambda) \;=\; D_1(z,\lambda)D_2(z,\lambda)$, with $D_j(z,\lambda) = \det(\hat{\mathring{A}}(z) + \mathrm{diag}_v\{\mu_j^v(\lambda)\})$. Since these factors are polynomial in z and rational functions of λ, the factorization yields reducibility of the Fermi variety, for each λ that is not a pole, but not for the Bloch variety.

This construction can be done essentially verbatim with m layers.

4.3.8 Reducibility by reduction to one variable. For certain multi-layer graphs not possessing any symmetry, the Fermi surface may still be reducible. Another mechanism for this occurs when the dispersion function is a polynomial $P(\xi,\lambda)$ in a single composite momentum variable $\xi = g(z)\in\mathbb{C}$ and energy λ, with $g(z)\in\mathbb{C}[z^{\pm}]$. This means that the Bloch variety factors through the Riemann surface $\mathcal{R} = \{(\xi,\lambda)\in\mathbb{C}^2 : P(\xi,\lambda)=0\}$. For $\lambda_0\in\mathbb{C}$, let $\mathcal{R}_{\lambda_0}$ denote the finite set of roots ξ of $P(\xi,\lambda_0)$.

$$\begin{array}{ccccc} (\mathbb{C}^\times)^d\times\mathbb{C} & \xrightarrow{z\mapsto\xi} & \mathbb{C}^2 & \xrightarrow{P} & \mathbb{C} \\ \mathcal{B} & \longrightarrow & \mathcal{R} & \longrightarrow & 0 \\ \Phi_{\lambda_0} & \longrightarrow & \mathcal{R}_{\lambda_0} & \longrightarrow & 0 \end{array} \tag{4.110}$$

The Fermi surface at energy λ_0 is the zero set of

$$P(\xi,\lambda_0) \;=\; \prod_j\big(\xi-\xi_j(\lambda_0)\big), \qquad \xi = g(z). \tag{4.111}$$

In this way, the Fermi surface Φ_{λ_0} has components $\Phi^j_{\lambda_0} = \{z \in (\mathbb{C}^\times)^d : g(z) = \xi_j(\lambda_0)\}$, which depend on λ_0 algebraically, through a multi-valued function on $\mathcal{R}$.

Two types of multi-layer quantum graphs that are reducible by reduction to one variable are introduced in [18], and the discrete graph version is treated in [42]. The first type relies on a calculus for computing the dispersion function for the joining of two periodic graphs by merging pairs of vertices, with one vertex per fundamental domain in each graph. The second relies on the bipartiteness of the layers, each having $|W| = 2$. One deduces, for example, that very general stacking of multiple layers of graphene with arbitrary shifts, results in a Fermi surface with as many components as the number of layers.

4.3.9 Example: AB-stacked bi-layer graphene. Bi-layer graphene with one layer shifted relative to the other is called AB-stacked, or Bernal-stacked, graphene. It lies within the class of both types discussed in §4.3.8. The Fermi surface for the Hamiltonian

$$A(z) \;=\; \left[\begin{array}{cc|cc} \Delta & \zeta' & \gamma_4\zeta' & 0 \\ \zeta & \Delta & \gamma_1 & \gamma_4\zeta' \\ \hline \gamma_4\zeta & \gamma_1 & -\Delta & \zeta' \\ 0 & \gamma_4\zeta & \zeta & -\Delta \end{array}\right]. \tag{4.112}$$

(written with respect to the basis (1A, 1B, 2A, 2B)) is reducible into two components, coming from the factorization $D(z,E) = D_1(z,E)D_2(z,E)$ in $\mathbb{C}[z^\pm]$ for each $E \in \mathbb{C}$. Each factor $D_\ell(z,E)$ is a polynomial in $\xi = \zeta\zeta'$, with $\zeta = 1 + z_1 + z_2$ and $\zeta' = 1 + z_1^{-1} + z_2^{-1}$. Physical implications of this reducibility are studied in [33].

Figure 1 shows Bloch varieties for both AB- and AA- stacked bi-layer graphene. They are pertubations of the doubling of the Bloch variety of graphene (on the right in Equation (4.76)). In the first, the Dirac points

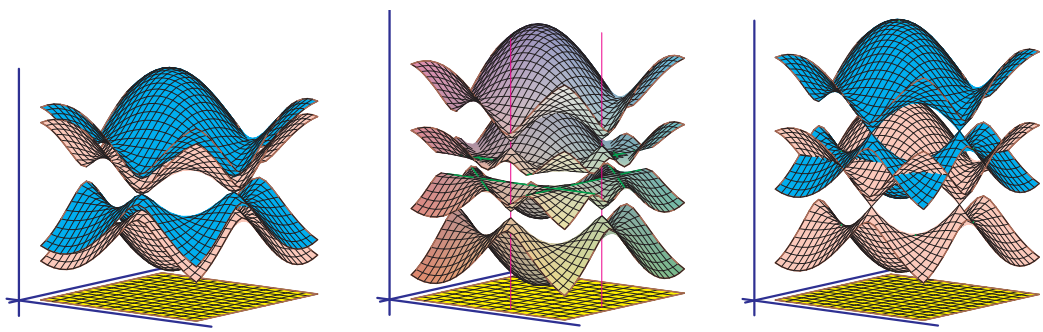


Figure 1: Some Bloch varieties of AB- and AA- stacked bi-layer graphene.

of graphene remain double points, but they are smoothed. For this, the operator is (4.112) with $\Delta = \gamma_4 = 0$ and $\gamma_1 = 1/2$. The second is (4.112) with $\Delta = 1$, $\gamma_4 = 0$, and $\gamma_1 = 2/3$. In it, the Dirac points are smoothed and slightly pulled apart (the faint vertical lines are to help show this). Curiously, the Fermi curve at the endpoints of the band gap are reducible curves of critical points (see §5.1). The third is AA stacked bi-layer graphene, and it consists of two shifted copies of the Bloch variety of graphene.

4.3.10 Defect modes in the continuum. A consequence of reducibility of the Fermi surface is the ability to create a defect state at an energy in the continuous spectrum supported by a local defect, where the state is exponentially decaying and not compactly supported. This is essentially a converse of [25, Theorem 6]. The equation is

$$(A + V - \lambda)u \;=\; 0, \tag{4.113}$$

in which V is a potential operator with finite support, $u \in \ell^2(\mathcal{V})$, and $\lambda \in \sigma(A)$.

To create such a defect mode, first solve the local-source equation $(A - \lambda)u = f$ (4.96). Consider the example of AB-stacked graphene. Recall from §4.3.3 that, to ensure $\lambda \in \sigma(A)$, λ has to be chosen such that one of the factors $D_\ell(z,\lambda)$, say D_2, vanishes at some $z \in \mathbb{T}^2$. To satisfy $u \in \ell^2(\mathcal{V})$, the vector $R(z,\lambda)\hat{f}(z)$ must have $D_2(z,\lambda)$ as a factor in each component. In order to satisfy the additional requirement that u does not have compact support, D_1 must not vanish anywhere on $\mathbb{T}^2$ and $R(z,\lambda)\hat{f}(z)$ cannot have D_1 as a factor

in each component. Thus $\hat{u}$ is a smooth rational function on $\mathbb{T}^2$ so that u is properly exponentially decaying. Then put $f = -Vu$ to obtain (4.113). Since f has compact support, this amounts to a finite-dimensional system for V. If u vanishes at some $x \in \mathcal{V}$, then V cannot be purely on-site; however generally one can find a local potential operator V that works, as demonstrated in [18, 33]. Embedded eigenvalues created by non-compactly supported potentials require other techniques; see [28, 21] for results in one dimension.

4.3.11 Localization of the defect. Let us continue the AB-stacked graphene example. As described at the end of §4.3.3, having a factor of $D_2(z, E)$ in each component of the vector $R(z, \lambda)\hat{f}(z)$ can be achieved naïvely if $\hat{f}(z) = D_2(z, \lambda)\hat{f}_0(z)$ for some $f_0(z) \in \mathbb{C}[z^{\pm}]^W$. This means that f and therefore V generically would be nonzero on 28 vertices (D_2 has seven monomial terms and there are four vertices in a fundamental domain W). However, it is desirable to seek $\hat{f}(z)$ with the minimal number of monomial terms in all components. This corresponds to a source f having minimal support.

For the Hamiltonian 4.112, it is shown in [33] there is a non-obvious matrix factorization $U(\hat{A}(z) - \lambda I)L = \Lambda$, with U and L being block upper and lower matrices in an appropriate basis, and Λ being essentially a 2×2 matrix with a special form. Remarkably, the eigenvectors ϕ_ℓ of Λ are independent of z and its eigenvalues happen to be D_ℓ. Furthermore, ϕ_ℓ and $U\phi_\ell$ have nonzero components only in the aligned pair of A and B vertices of W. Therefore, taking $\hat{f} = \phi_1$ results in $\hat{u} = (\hat{A}(z) - \lambda I)^{-1}\hat{f} = L\Lambda^{-1}U\hat{f}$ having poles on $D_1(z, \lambda) = 0$, which by assumption does not intersect $\mathbb{T}^2$. Since $\hat{f}$ is independent of z and has two non-zero components, f is supported on two vertices. The details are in [33], including a formula for the values of V on the two aligned AB vertices.

4.3.12 Irreducible Fermi varieties. Although naïvely the Fermi variety of a discrete periodic operator (with $d \geq 2$) should be generically irreducible, proving irreducibility is not straightforward. Compared with proving reducibility, the techniques are different; this is because reducibility arises constructively by creating graphs, typically through multiple layers, that are explicitly designed to be algebraically reducible.

Although there may be no crisp way to define when a periodic graph has multiple layers, for $d = 2$ it is reasonable to consider a planar graph to be a single layer. When $|W| = 2$ and the graph is planar, reducibility of the Fermi variety occurs only for the tetrakis grid, and positivity of the matrix elements of the operator always prohibits reducibility. This is proved by computational means [27].

Liu [29] proved irreducibility of the discrete Laplacian plus a periodic potential at every energy (except one when $d = 2$), from which is inferred generic reduction of the dimension of the Fermi variety at band edges. More generally, let A be a $\mathbb{Z}^d$ periodic operator on $\mathbb{Z}^d$ so that $\hat{A}(z)$ is scalar, and let $V : \mathbb{Z}^d \to \mathbb{C}$ be a potential function that is periodic with respect to a sublattice $q_1\mathbb{Z} \times \cdots \times q_d\mathbb{Z}$. Irreducibility of the Bloch variety, but not necessarily the Fermi varieties, of $A + V$ occurs under a condition connecting $\hat{A}(z)$ and the periods q_j [14]. By bounding the number of irreducible components in terms of certain asymptotics of $D(z, \lambda)$, irreducibility can be established for a wider swath of examples [15].

4.3.13 Isospectrality. There are some results about the information that the Bloch and Fermi varieties contain. For Schrödinger operators on $\mathbb{Z}^d$ equal to the discrete Laplacian plus a potential that is periodic with a rectangular fundamental domain, the density of states determines the Bloch variety [3]. Liu introduces Fermi isospectrality [31, 32] of two such potentials when the associated Schrödinger operators have the same Fermi variety for some energy λ. For $d \geq 3$, if two potentials are Fermi-isospectral either both are additively separable or neither is. In the former case, the one-variable summands are essentially Fermi-isospectral, which also holds for $d = 2$. There exist complex potentials that are Floquet-isospectral to the zero potential [10].

5 Nondegeneracy of band edges and beyond

A property of the spectrum revealed by the Bloch variety is its behavior near edges of spectral bands. The spectral edges conjecture about this behavior leads to a deeper study of Bloch varieties.

5.1 Spectral edges nondegeneracy conjecture

The real Bloch variety $\mathbb{R}\mathcal{B}_A \subset \mathbb{T}^d \times \mathbb{R}$ of a periodic graph operator A encodes the relation between the characters $z \in \mathbb{T}^d$ of the $\mathbb{Z}^d$-action and the spectrum $\lambda \in \mathbb{R}$ of the operator (*cf.* §4). Its projection to $\mathbb{R}$ is the spectrum $\sigma(A)$ of A which consists of intervals (spectral bands) each of which is an image of one of the $|W|$ branches (band functions) of $\mathbb{R}\mathcal{B}_A$ over $\mathbb{T}^d$. Endpoints (spectral edges) of spectral bands are the images of extrema of the corresponding band function of $\mathbb{R}\mathcal{B}_A$. Many important notions in physics, including effective mass in solid state physics, the Liouville property, Green's function asymptotics, Anderson localization, and homogenization, require that those extrema are nondegenerate in that the Hessian matrix has full rank. Kuchment noted that this assumption is largely unproven and posed the *spectral edges conjecture* [24, Conj. 5.25]. This posits that for generic parameters (potential and edge labels), each extreme value is attained by a single band function and the extrema are all isolated and nondegenerate. It is stated and disucssed when $d = 2$ for continuous operators in [34].

While posed for all periodic operators (discrete and *continuous*), it remains largely open, even for discrete operators. In this setting, "generic" means avoiding an algebraic subset of the parameters. This conjecture does not always hold. We have already seen an instgance of this in Figure 1. The simplest nontrivial counterexample is due to Filonov and Kachkovskiy in [16, §7]. We give a slightly more involed example. Figure 2 shows a $\mathbb{Z}^2$-periodic graph with five (orbits of) edges, a labeling, and a Bloch variety when the potential is not constant, but $b = d$ and $c = e$. This has eight isolated critical points and two curves of

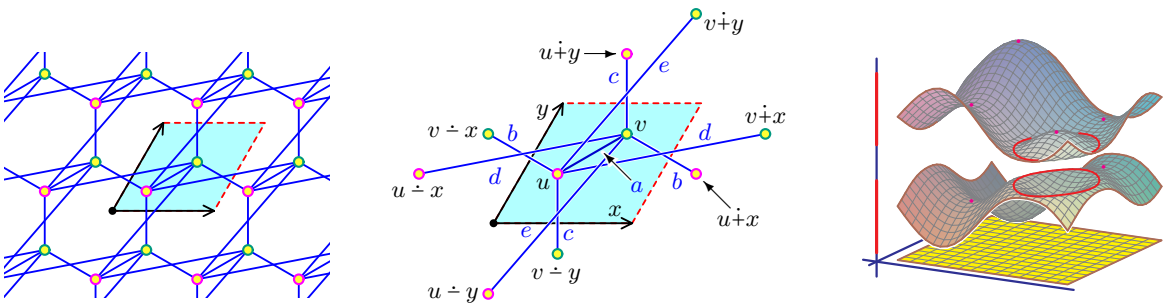


Figure 2: Filonov-Kachkovskiy Bloch variety with a curve of critical points.

critical points (the corresponding Fermi variety is defined by $a + b(x + x^{-1}) + c(y + y^{-1})$), each lying over the edges of the spectral gap. In particular, for pure Schrödinger operators ($a = \cdots = e = 1$) the spectral edges nondegeneracy conjecture fails. When $b \neq d$ or $c \neq e$, all critical points are isolated.

About the same time as [16], Parnovski and Shterenberg found higher-dimensional examples [34, Rem. 4.1], as did Filanov and Kachkovskiy [17]. Flat bands (e.g. the Lieb lattice (4.91)) give other examples with non-isolated critical points. These examples all involve algebraic subsets of the full set of parameters. For general values of the parameters, all critical points are isolated and nondegenerate. A more subtle counterexample is the middle Bloch variety of (4.76)—over each edge of the gap there are two nondegenerate critical points. (A version of the spectral edges conjecture posits that each extrema is attained at a unique point on the Bloch variety.) This occurs whenever the parameters a, b, c (see (3.47)) are the sides of a triangle [37].

For a positive result, Liu [30] proved that the extrema are isolated for the Schrödinger operator acting on the square lattice.

5.2 Nondegeneracy of critical points

The Spectral Edges Conjecture is discussed in [9], which introduces a computational method to study it. Extrema of bands of the real Bloch variety are some (but not all) of the critical points of the coordinate function λ on the complex Bloch variety $\mathcal{B}_A$. A strengthening of the spectral edges conjecture is the *nondegeneracy conjecture*—that every critical point of λ on $\mathcal{B}_A$ is nondegenerate. We have the following dichotomy.

Theorem 8 ([9, Thm. 12])**.** *For a given graph Γ, there is a dense open subset U in the space of parameters for*

Γ *with the property that either all operators on* Γ *with parameters in* U *have all critical points nondegenerate, or every such operator has degenerate critical points.*

This is because there is a system of polynomial equations (5.114) involving the parameters that define the critical points (the critical point equations) and a further equation (determinant of the Hessian) that defines the degenerate critical points. Consequently, the set V of of parameters whose corresponding Bloch variety has a degenerate critical point is constructable. If V is not dense, then U is an open subset of its complement and operators in U have all critical points nondegenerate. If V is dense, then U is an open subset of V and generic operators have degenerate critical points.

5.3 Critical point degree

The algebraic nature of the set of critical points and standard facts in algebraic geometry imply that given a graph Γ, there is a number $N(\Gamma)$ and a open dense subset U of the parameters for Γ with the following properties: Every operator on Γ has at most $N(\Gamma)$ isolate critical points, and if the operator has parameters from U, then it has has exactly $N(\Gamma)$ critical points. This number $N(\Gamma)$ is called the *critical point degree* of Γ [12].

As explained in [9, §5], if there exists one operator on Γ with $N(\Gamma)$ nondegenerate critical points, then the nondegeneracy conjecture holds for Γ. Consequently, if $N(\Gamma)$ is known, then a single computation can establish the nondegeneracy conjecture for Γ. This is used to prove [9, Thm. 16] and to establish the nondegeneracy conjecture for over 2^{19} graphs in [13].

The paper [13] studies the critical points of a periodic operator, giving bounds and conditions which imply the bounds are met. A standard formulation of critical points of implicit functions from algebraic optimization gives the following system of equations for the critical points of λ on the Bloch variety,

$$D(z,\lambda) \;=\; z_1\frac{\partial D}{\partial z_1}(z,\lambda) \;=\; \cdots \;=\; z_d\frac{\partial D}{\partial z_d}(z,\lambda) \;=\; 0\,. \tag{5.114}$$

(As $z \in (\mathbb{C}^\times)^d$, multiplying by z_i does not add solutions.) A monomial $z^n\lambda^j$ is an eigenvector for the Euler operator $z_i\frac{\partial}{\partial z_i}$ with eigenvalue n_i. Thus, the exponents (n,j) of monomials $z^n\lambda^j$ that occur in each of the *Critical Point Equations* (5.114) are a subset of those that occur in $D(z,\lambda)$, called its *support*.

5.4 Toric compactification

Let $\mathcal{N}(A) \subset \mathbb{R}^{d+1}$ be the convex hull of the support of the dispersion function $D(z,\lambda)$ for the operator A. This is the Newton polytope of $D(z,\lambda)$. Figure 3 shows Newton polytopes of general operators on the hexagonal and Lieb lattices, the graph of Figure 2, and another graph with $|W| = 3$. A classical result of

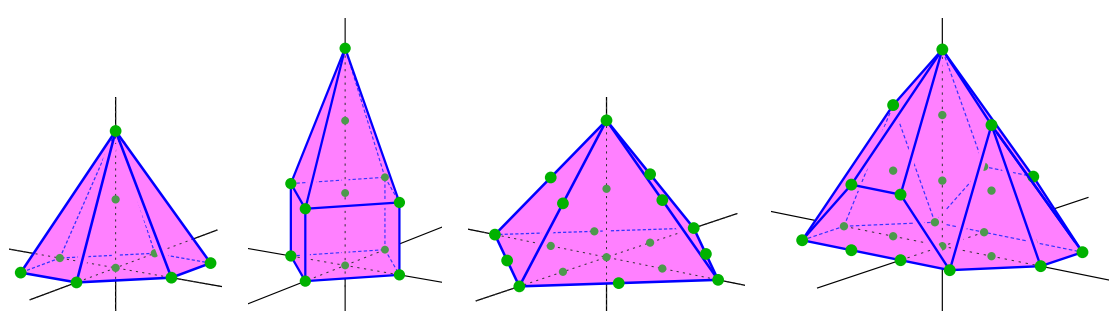


Figure 3: Four Newton polytopes

Kushnirenko [22] gives the following bound for the number of critical points.

Theorem 9 ([13, Cor. 2.5])**.** *The number of isolated critical points of the function* λ *on the Bloch variety* $\mathcal{B}_A$ *is at most* $(d+1)!vol(\mathcal{N}(A))$.

An analysis of the proof (or of [4, Thm. B]) gives conditions for this bound to be sharp. Given a face F of the Newton polytope $\mathcal{N}(A)$, the (sum of) the terms of $D(z,\lambda)$ whose monomials lie on F is the *facial form* $D_F(z,\lambda)$—this is a strict generalization of the notion of terms of highest degree. Similarly, the *facial subsystem* $(\mathrm{CPE})_F$ of the Critical Point Equations (5.114) is the collection of facial forms of the equations in (5.114). The following is a consequence of [13, Cor. 3.5].

Theorem 10. *The inequality in Theorem 9 is an equality if and only if for every face F of $\mathcal{N}(A)$ that is not its base, the facial subsystem $(CPE)_F$ has no solutions.*

Solutions to a facial subsystem $(\mathrm{CPE})_F$ are *asymptotic critical points*. These are studied in [12, 13]. If a face F is vertical (as in the second and fourth polytopes in Figure 3, then $(\mathrm{CPE})_F$ has solutions. For a face F that is not vertical, there are asymptotic critical points if and only if the variety defined by $D_F(z,\lambda)$ is singular. In [12] such asymptotic critical points for general operators on a graph Γ are shown to arise from structural properties of Γ.

5.5 More on toric compactification

The introduction and use of facial forms and subsystems in [12, 13], as well as the use of the component of $D(z,\lambda)$ of lowest degree in [14], are all algebraic manifestations of a natural toric compactification of $\mathcal{B}_A \subset (\mathbb{C}^\times)^d \times \mathbb{C}$. This notion was introduced by Gieseker, Knörrer, and Trubowitz [19] (see also [35]) in their study of the square lattice $\mathbb{Z}^2$ under the free action of $a\mathbb{Z} \oplus b\mathbb{Z}$, and extended by Bättig [1, 2]. We sketch a modern view developed in [11].

Given a polytope $\mathcal{N} \subset \mathbb{R}^r$ with vertices in $\mathbb{Z}^r$, there is a projective toric variety [6] $X_\mathcal{N}$ lying in a projective space $\mathbb{P}(\mathcal{N})$ whose coordinates correspond to the integer points in $\mathcal{A} := \mathcal{N} \cap \mathbb{Z}^r$. (The space $\mathbb{P}(\mathcal{N})$ is the quotient of $\mathbb{C}^\mathcal{A} \smallsetminus \{0\}$ by scalars. It is a compact complex manifold.) There is a map $\varphi\colon (\mathbb{C}^\times)^r \to \mathbb{P}(\mathcal{N})$ that sends a point $x \in (\mathbb{C}^\times)^r$ to the vector $(x^a \mid a \in \mathcal{A})$ of monomials, and $X_\mathcal{N}$ is the closure of its image. This has the important geometric consequence (which is the idea behind Kushnirenko's Theorem) that under φ, linear functions on $\mathbb{P}(\mathcal{N})$ correspond to polynomials on $(\mathbb{C}^\times)^r$ with support in $\mathcal{N}$, and the degree of $X_\mathcal{N}$ is $r!\mathrm{vol}(\mathcal{N})$. Lastly, the difference $X_\mathcal{N} \smallsetminus \varphi((\mathbb{C}^\times)^r)$ is a union of toric subvarieties X_F, one for each face F of $\mathcal{N}$.

In our context, let $\overline{\mathcal{B}_A}$ be the closure of $\varphi(\mathcal{B}_A)$ in $X_{\mathcal{N}(A)}$. Then for each face F of $\mathcal{N}(A)$, the facial form $D_F(z,\lambda)$ defines $\overline{\mathcal{B}_A} \cap X_F$, which we regard as the asymptotic Bloch variety along X_F. Similarly, asymptotic critical points are those that lie along some X_F, for F not the base of $\mathcal{N}(A)$ (the base corresponds to $\lambda = 0$).

A first step to generalize [1, 2, 19] is to extend the vector bundle $\mathscr{E}$ to $X_{\mathcal{N}(A)}$—it remains a trivial bundle. The endomorphism $\hat{A}(z) - \lambda I_W$ similarly extends to the bundle $\mathscr{E}$ over $X_{\mathcal{N}(A)}$ with kernel the Floquet sheaf $\mathscr{F}$ on $X_{\mathcal{N}(A)}$ whose support is the compactified Bloch variety $\overline{\mathcal{B}_A}$. This may always be done.

In his work on the square lattice, Bättig [1, 2] does more. For every face F of $\mathcal{N}(A)$ he associates a periodic, labeled, directed graph Γ_F whose operator A_F has Bloch variety equal to $\overline{\mathcal{B}_A} \cap X_F$. The paper [11] investigates to what extent this may be done for a general graph Γ. When $\mathcal{N}(A)$ is the pyramid $|W| \cdot P$, where P is the convex hull of all entries in the matrix $\hat{A}(z) - \lambda I_W$, then the full package of Bättig—asymptotic spectral problems for each face of $\mathcal{N}(A)$—holds. Only the third Newton polytope in Figure 3 has this form.

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