Critical Points of Discrete Periodic Operators

Combinatorial, Computational, and
Applied Algebraic Geometry

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Work with Matthew Faust
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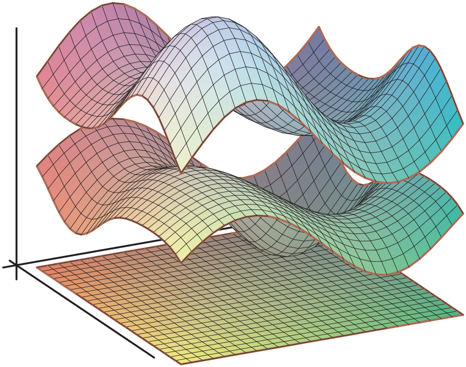


Spectra of Schrödinger Operators

A fundamental problem in mathematical physics is to understand the spectrum $\sigma(L)$ of a Schrödinger operator $L := -\Delta + V$ acting on complex-valued functions on $\mathbb{R}^d$.

($\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}$ is the Laplacian and $V \colon \mathbb{R}^d \to \mathbb{R}$ is a potential.)

L is a selfadjoint operator on $L^2(\mathbb{R}^d)$, $\sigma(L)$ is a union of intervals in $\mathbb{R}$, giving the familiar structure of energy bands and band gaps.

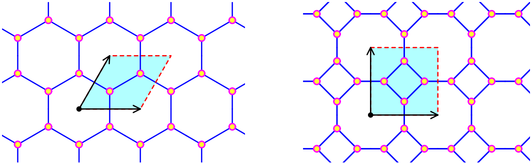
Solid-state physics compels us to consider this in a crystal, where Δ is perturbed to reflect a periodic anisotropy and V is periodic in that $V(x+a) = V(x)$ for $x \in \mathbb{R}^d$ and $a \in \mathbb{Z}^d$.

While spectral theory is typically approached via analysis, discretizing brings it into the realm of algebraic geometry.

Discretizing

Replace $\mathbb{R}^d$ by a graph Γ with vertices $\mathcal{V}(\Gamma)$ and edges $\mathcal{E}(\Gamma)$ having a free action of $\mathbb{Z}^d$ with finitely many orbits.

Two $\mathbb{Z}^2$-periodic graphs with fundamental domains shaded.



The potential $V\colon \mathcal{V}(\Gamma) \to \mathbb{R}$ is $\mathbb{Z}^d$-invariant and we have $\mathbb{Z}^d$-invariant edge weights $c\colon \mathcal{E}(\Gamma) \to \mathbb{R}$. Write c for (V, c).

The Schrödinger operator L_c acts on functions $f\colon \mathcal{V}(\Gamma) \to \mathbb{R}$, as a potential plus a perturbed graph Laplacian.

$$L_c f(u) \ := \ V(u)f(u) + \sum_{(u,v)\in\mathcal{E}(\Gamma)} c_{(u,v)}(f(u) - f(v))\,.$$

Floquet (Fourier) Transform

L_c is self-adjoint on $\ell_2(\mathcal{V}(\Gamma), \mathbb{C})$ and commutes with the $\mathbb{Z}^d$-action, so we may apply the Fourier transform.

$\mathbb{T}$: unit complex numbers. $\mathbb{T}^d$: unitary characters for $\mathbb{Z}^d$.
For $z \in \mathbb{T}^d$, we have $\mathbb{Z}^d \ni a \longmapsto z^a$.

Fourier transform, $f \mapsto \widehat{f}$, where $\widehat{f}(a+u) = z^a \widehat{f}(u)$, is a linear isomorphism $\ell_2(\mathcal{V}(\Gamma)) \xrightarrow{\sim} L^2(\mathbb{T}^d)^{\oplus W}$, where $W \subset \mathcal{V}(\Gamma)$ be a fundamental domain for the $\mathbb{Z}^d$-action.

The operator L_c retains its simple expression. For $u \in W$,

$$L_c \widehat{f}(u) \;=\; V(u)\widehat{f}(u) + \sum_{(u,a+v)\in\mathcal{E}(\Gamma)} c_{(u,a+v)} \left(\widehat{f}(u) - z^a \widehat{f}(v)\right).$$

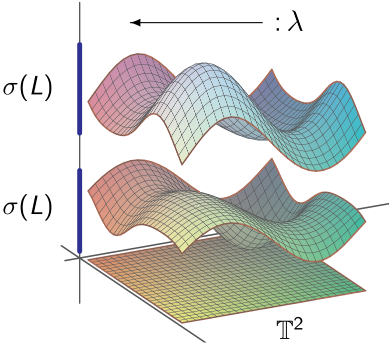
This is multiplication by a $W \times W$-matrix $L_c(z)$ of Laurent polynomials.

Bloch Variety

The *Bloch variety* is the variety defined by the *dispersion relation* $D_c(z,\lambda) := \det(L_c(z) - \lambda I)$.

As $L_c(z)^T = L_c(z^{-1})$,
for $z \in \mathbb{T}^d$, $L_c(z)$ is hermitian.

Thus the Bloch variety is a $|W|$-sheeted cover of $\mathbb{T}^d$.



The spectrum $\sigma(L_c)$ is the projection of Bloch variety to the λ-axis.

From a matrix of Laurent polynomials to an algebraic variety lying over the spectrum, spectral theory of discrete periodic operators may be studied through the lens of algebraic geometry.

I discuss some early results in this program.

Some Questions From Physics

- Density of states: Spatial density of eigenfunctions at energy λ.
  Kravaris: $\{$eigenfunctions at energy $\lambda\}$ is a finitely generated $\mathbb{C}[\mathbb{Z}^d]$-module and may be studied using free resolutions.

- Level set at λ of the Bloch Variety is a *Fermi variety*.
  Natural physical questions ask for the irreducibility of Bloch and Fermi varieties.

- *Spectral edges conjecture*: For general operators on Γ, points on the Bloch Variety above endpoints of spectral bands are nondegenerate extrema of λ.

  Many physical properties rely upon this assumption (made by all physicists), but it is largely unknown, even for operators on discrete graphs.

- There are inverse problems and identifiability, and ....

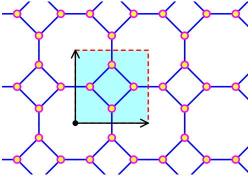
Complexify!

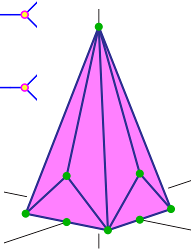
A first step is the algebraic relaxation of complexifying.

- Replace (V, c) by complex-valued functions:

$$V\colon \mathcal{V}(\Gamma) \to \mathbb{C} \qquad c\colon \mathcal{E}(\Gamma) \to \mathbb{C}$$

- Replace $z \in \mathbb{T}^d$ by $z \in (\mathbb{C}^\times)^d$.
- $z \mapsto \overline{z}^{-1}$ is a non-standard (twisted) complex structure on $(\mathbb{C}^\times)^d$. (an antiholomorphic involution).
  As $L(z)^T = L(z^{-1})$,
  when (V, c) are real, the dispersion relation is stable under $z \mapsto \overline{z}^{-1}$.

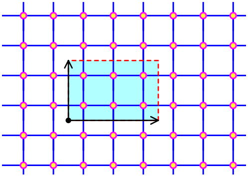




Thus the real Bloch variety is the real locus of the complex Bloch variety.
The Newton polytope of $D_c(z, \lambda)$ is centrally symmetric in z.

Everything Old is New Again

Gieseker, Knörrer, Trubowitz (1993) studied Schrödinger operator with $c_{(u,v)} = 1$ on the grid graph $\mathbb{Z}^2$ where $\mathbb{Z}^2$ acts via $a\mathbb{Z} \oplus b\mathbb{Z}$, with $\gcd(a, b) = 1$. We show this with $a = 3$ and $b = 2$.



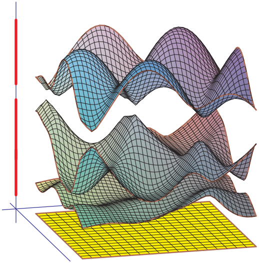
They studied/determined:

- Density of states (gave a formula).
- Irreducibility of Bloch and Fermi varieties.
- Smoothness of Bloch and Fermi varieties.
- Used a toric compactification and the Torelli Theorem.

This was presented in a Bourbaki Lecture by Peters in 1992.

Spectral Edges (Important Physics Assumption)

Each spectral edge is the image of a critical point of λ on the Bloch variety. The spectral edges conjecture posits that generically, these critical points are nondegenerate. A first step is to study all critical points.



Implicit differentiation of $0 = D(z, \lambda)$ gives $0 = \frac{\partial D}{\partial z_i} + \frac{\partial D}{\partial \lambda}\frac{\partial \lambda}{\partial z_i}$. Thus equations for the critical points are:

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

All polynomials have support a subset of the Newton polytope $\mathcal{N}(D)$ of the dispersion relation $D(z, \lambda)$.

Kushnirenko* # Critical Points $\leq \mathrm{vol}(\mathcal{N}(D))$.

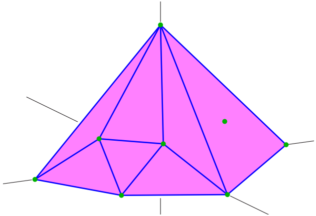
* Monotonicity and $(\mathbb{C}^\times)^d \times \mathbb{C}_\lambda$.

Toric Compactification

Let $\mathcal{N}(D)$ be the Newton polytope of the dispersion relation $D(z, \lambda)$.

Ambient space $(\mathbb{C}^\times)^d \times \mathbb{C}$ of Bloch variety is compactified by $X_{\mathcal{N}(D)}$, the projective toric variety of $\mathcal{N}(D)$.

The Critical Point Equations (CPE) correspond to a linear section of $X_{\mathcal{N}(D)}$



Fact: $\#$ Critical Points $<$ vol$(\mathcal{N}(D))$ if and only if there are solutions to CPE on boundary

$$\partial X_{\mathcal{N}(D)} \ := \ X_{\mathcal{N}(D)} \smallsetminus ((\mathbb{C}^\times)^d \times \mathbb{C})\,.$$

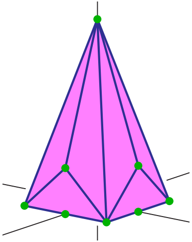
Let BV be the compactified Bloch variety in $X_{\mathcal{N}(D)}$.

Faces of $X_{\mathcal{N}(D)}$

Each face F of $\mathcal{N}(D)$ contributes a torus orbit $\mathcal{O}_F$ to $X_{\mathcal{N}(D)}$.

$\mathcal{N}(D)$ and its base give $(\mathbb{C}^\times)^d \times \mathbb{C}$.

$\partial X_{\mathcal{N}(D)} = \coprod \mathcal{O}_F$, where $F \subsetneq \mathcal{N}(D)$ is not its base.



- F vertical $\Longrightarrow$ CPE have solutions on $\overline{\mathcal{O}_F}$.
  $(z^\eta \nabla_\eta (D|_F) = (\eta \cdot F) D|_F$ for η normal to F.)

- If F is not vertical, then CPE have solutions on $\mathcal{O}_F$
  $\Longleftrightarrow$ BV $\cap\, \mathcal{O}_F$ is singular.
  (Quasi-homogeneity of facial form D_F.)

Theorem. *# critical points = vol($\mathcal{N}(D)$) $\Longleftrightarrow$ $\mathcal{N}(D)$ has no vertical faces and BV $\cap\, \partial X_{\mathcal{N}(D)}$ is smooth.*

Dense Periodic Graphs

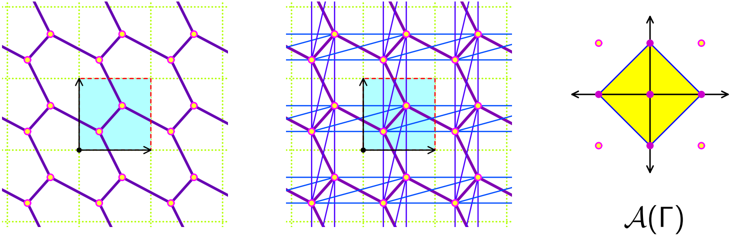
A $\mathbb{Z}^d$-periodic graph Γ is dense if it has maximally many edges, given its combinatorial structure.

Fix a fundamental domain W for Γ. Its *support* of Γ is the set $\mathcal{A}(\Gamma) := \{a \in \mathbb{Z}^d \mid \exists$ an edge with endpoints in W and $a + W\}$.

$\rightsquigarrow$ This contains the support of entries in $L_c(z)$.

Γ is *dense* if for all $a \in \mathcal{A}(\Gamma)$, the restriction to $W \cup (a + W)$ is a complete graph.

Every graph embedds into a minimal dense graph



Critical Points of Dense Periodic Operators

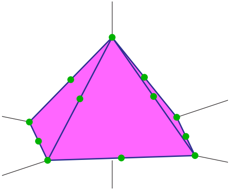
Let E be the set of $\mathbb{Z}^d$-orbits of edges in Γ.

$Y := \mathbb{C}^E \times \mathbb{C}^W$ is the parameter space for operators on Γ.

For any graph Γ, we define a polytope $\mathcal{N}(\Gamma)$.

Theorem. *There is a nonempty open subset $U \subset Y$ consisting of parameters $c = (c, V)$ such that D_c has Newton polytope $\mathcal{N}(\Gamma)$.*

Γ dense $\Rightarrow$ $\mathcal{N}(\Gamma)$ is the pyramid $\mathcal{N}(\Gamma) = |W| \cdot conv(\mathcal{A}(\Gamma) \cup \{(0^d, 1)\})$.



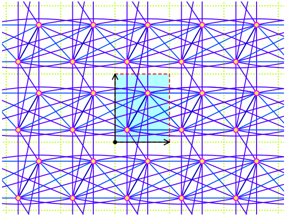
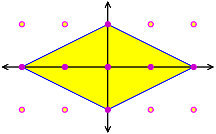
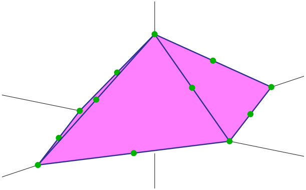
For $d = 2, 3$ we may choose U such that for $c \in U$, the Bloch variety is smooth at infinity, and

$\#$ critical points $= \text{vol}(\mathcal{N}(\Gamma)) = |W|^{d+1}\text{vol}(\text{conv}(\mathcal{A}(\Gamma)))$.

One Example

Easy Fact: A critical point is regular $\iff$ it is a nonsingular point on Bloch variety $\Longrightarrow$ it is nondegenerate.

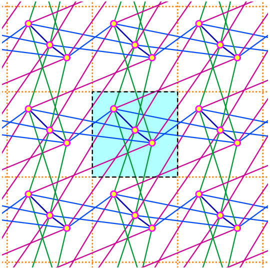
Consider the $\mathbb{Z}^2$-periodic dense graph Γ shown below with its support and Newton polytope.

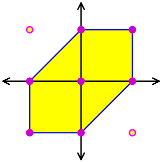




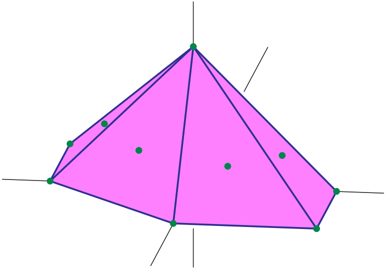
Independent Macaulay2 and Singular calculations at (random) parameters $c = (c, V)$ find a Bloch variety with $64 = 2^3 \cdot 8 = \mathrm{vol}(\mathcal{N}(\Gamma))$ regular critical points, which implies the spectral edges conjecture for Γ. (I can explain, if you want.)

2^{19} Examples

Consider the graph Γ with support and Newton polytope







Calculations find a Bloch variety with $162 = 3^3 \cdot 6 = \mathrm{vol}(\mathcal{N}(\Gamma))$ regular critical points.

Γ is not dense—it is missing 6 edges in each direction $\rightarrow$, $\uparrow$, $\nearrow$, and one in fundamental domain.

$\mathcal{N}(\Gamma)$ equals the Newton polytope of dense graph. Monotonicity implies the spectral edges conjecture for all 2^{19} graphs lying beween Γ and its corresponding dense graph.

Future Directions

(With Faust, García-Lopez, Shipman, Robinson, ...)

- Toric compactifications, desingularizations, extend $L_c(z)$ to boundary, and beyond.
- How do $\mathcal{N}(\Gamma)$, # critical points, etc. depend on Γ?
- Implication of homological invariants of $L_c(z)$ (or its extension) for spectral theory?
- Parameter identification: How much do Bloch and Fermi varieties determine Γ and parameters (c, V)?
- Spectral edges conjecture in dimensions 2 and 3; treating singularities.
- Up coming ICERM Hot Topics Workshop, other workshops in the planning. (Interested?)

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