

Critical Points of Discrete Periodic Operators

Widely Applied Mathematics Seminar

SEAS, Harvard U, 26 October 2023



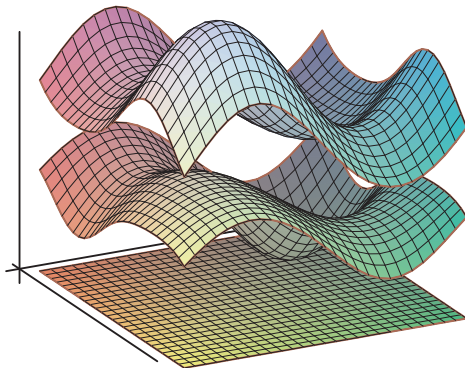
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[arXiv/2206.13469](https://arxiv.org/abs/2206.13469)



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 $V: \mathbb{R}^d \rightarrow \mathbb{R}$ is a potential.)

L is a selfadjoint operator on $L^2(\mathbb{R}^d)$, and $\sigma(L) \subset \mathbb{R}$.

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

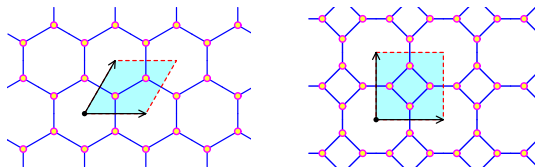
Then $\sigma(L)$ is a union of intervals in \mathbb{R} , giving the familiar structure of energy bands and band gaps.

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

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

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

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

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

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

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

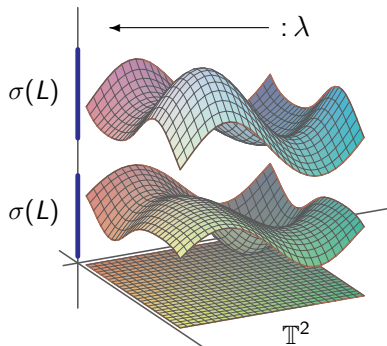
This is multiplication by a $W \times W$ -matrix $L_c(z)$ of Laurent polynomials.

Bloch Variety

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

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: $\{\text{eigenfunctions at energy } \lambda\}$ 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, but it is largely unknown, even for discrete periodic operators.
- There are inverse problems and identifiability, and

Complexify!

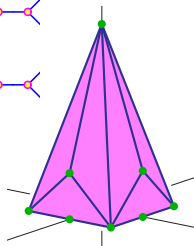
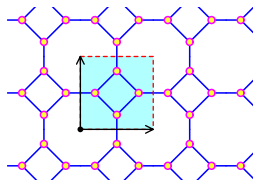
A first step is the algebraic relaxation of complexifying.

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

$$V: \mathcal{V}(\Gamma) \rightarrow \mathbb{C} \quad e: \mathcal{E}(\Gamma) \rightarrow \mathbb{C}$$

- Replace $z \in \mathbb{T}^d$ by $z \in (\mathbb{C}^\times)^d$.
- $z \mapsto \bar{z}^{-1}$ is a non-standard (twisted) complex structure on $(\mathbb{C}^\times)^d$. (an antiholomorphic involution).

As $L(z)^T = L(z^{-1})$,
when (V, e) are real, the dispersion
polynomial is stable under $z \mapsto \bar{z}^{-1}$.

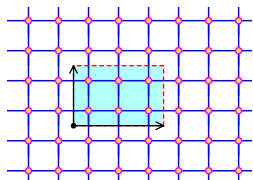


Thus the real Bloch variety is the real locus
of the complex Bloch variety.

The Newton polytope of $D_c(z, \lambda)$ is centrally symmetric in z .

Everything Old is New Again

Gieseke, Knörrer, Trubowitz (1993) studied the Schrödinger operator with $e_{(u,v)} = 1$ 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:

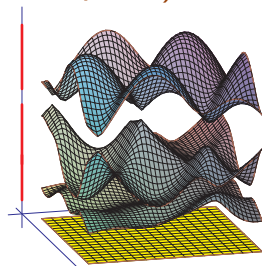
- Density of states (gave a formula).
- Irreducibility of Bloch and Fermi varieties.
- Smoothness of Bloch and Fermi varieties.
- Used a toric compactification and the Torelli Theorem.

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.

First step: 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:

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

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

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

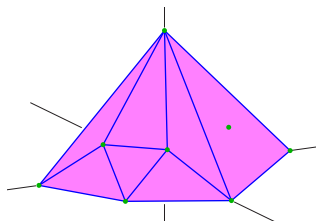
* Monotonicity and $(\mathbb{C}^\times)^d \times \mathbb{C}_\lambda$.

Toric Compactification

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

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

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

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

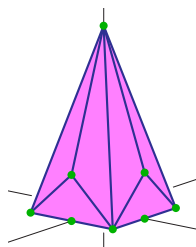
Faces of $X_{\mathcal{N}(D)}$

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 \implies 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
 $\iff BV \cap \mathcal{O}_F$ is singular.
(Quasi-homogeneity of facial form D_F .)



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

Dense Periodic Graphs

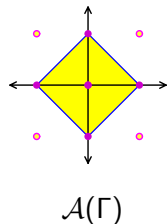
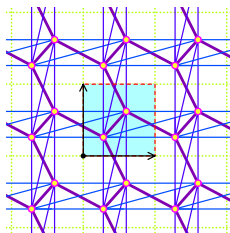
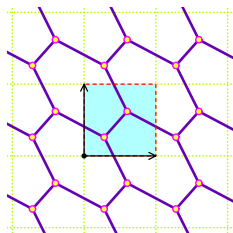
A \mathbb{Z}^d -periodic graph Γ is dense if it has maximally many edges, given its combinatorial structure.

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

\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 embeds 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 .

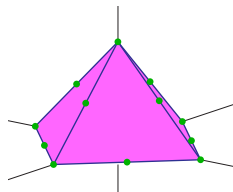
For any graph Γ , we define a polytope $\mathcal{N}(\Gamma)$.

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

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

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

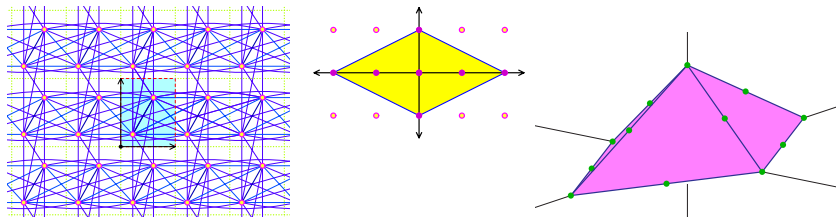
$\# \text{ critical points} = \text{vol}(\mathcal{N}(\Gamma)) = |W|^{d+1} \text{vol}(\text{conv}(\mathcal{A}(\Gamma)))$.



One Example

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

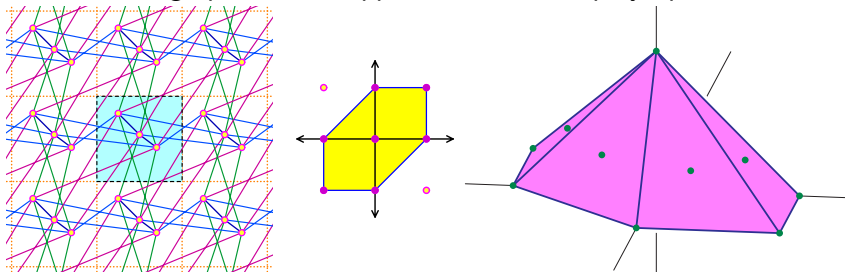
Consider the \mathbb{Z}^2 -periodic dense graph Γ shown below with its support and Newton polytope.



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

2¹⁹ Examples

Consider the graph Γ with support and Newton polytope



Calculations find a Bloch variety with $162 = 3^3 \cdot 6 = \text{vol}(\mathcal{N}(\Gamma))$ 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 2¹⁹ graphs lying between Γ and its corresponding dense graph.

Future Directions

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

- 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 (e, V) ?
- Spectral edges conjecture in dimensions 2 and 3; treating singularities.

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