Critical Points of Discrete Periodic Operators

AMS Special Session on Polynomial Systems,
Homotopy Continuation, and Applications.

JMM Boston, 4 January 2023

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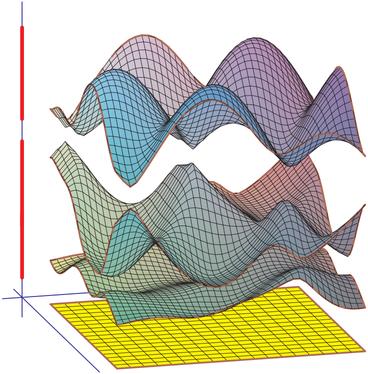
Work with Matthew Faust
arXiv/2206.13469



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 $\mathbb{R}^d$.

This models the evolution (e.g. the quantum wave function) of a free electron under the influence of a potential V.

Solid-state physics compels us to consider this in a crystal, where the Laplace-Beltrami operator Δ and potential are $\mathbb{Z}^d$-periodic.

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

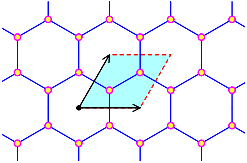
While spectral theory is typically approached via analysis, discretizing brings it into the realm of algebraic geometry.

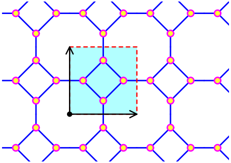
I believe this is an interesting new-ish application of our perspective and tools.

Discrete Periodic Schrödinger Operator

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 $f\colon \mathcal{V}(\Gamma) \to \mathbb{C}$, 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

Let $\mathbb{T} \subset \mathbb{C}$ be the unit circle. After Fourier transform, the operator L_c acts on functions $\hat{f}\colon \mathcal{V}(\Gamma) \times \mathbb{T}^d \to \mathbb{R}$ that satisfy

$$\hat{f}(a+v, z) \;=\; z^a \hat{f}(v, z), \quad \text{for} \quad a \in \mathbb{Z}^d .$$

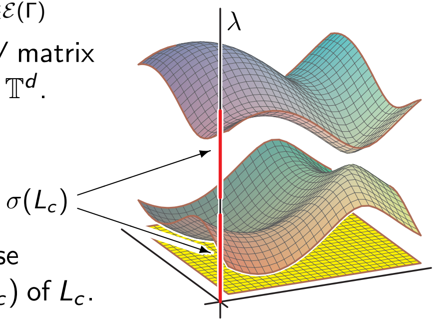
$\hat{f}$ is determined by $\hat{f}(v,z)$ for $v \in W$, the fundamental domain. This is a vector of functions, $\hat{f}(v)\colon \mathbb{T}^d \to \mathbb{R}$, for $v \in W$. Then

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

Thus L_c is multiplication by a $W \times W$ matrix $L_c(z)$ of Laurent polynomials in $z \in \mathbb{T}^d$. The *Bloch variety* is defined by

$$0 = \det(L_c(z) - \lambda I_W) .$$

A hypersurface in $\mathbb{T}^d \times \mathbb{R}_\lambda$, it is a $|W|$-sheeted cover of $\mathbb{T}^d$ whose projection to $\mathbb{R}_\lambda$ is the spectrum $\sigma(L_c)$ of L_c.



Questions From Physics for Algebraic Geometers

- The level set at λ of the Bloch variety is a *Fermi variety*. Natural physical questions ask for the irreducibility of Fermi varieties and of the Bloch variety.
- *Spectral Edges Conjecture*: For general operators on Γ, points on the Bloch variety above endpoints of spectral bands are nondegenerate extrema of λ.

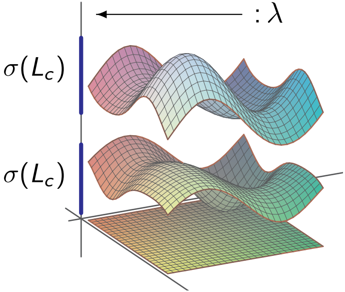
  Many physical properties rely upon this assumption, but it is unknown in most cases, even for discrete periodic operators.
- This is only a selection. ICERM Hot Topics Workshop

For this, we complexify, allowing complex parameters (c, V) and extending z to $(\mathbb{C}^\times)^d$, and then use algebraic geometry.

We will focus on the Spectral Edges Conjecture. For more, see the talks of Matthew Faust (earlier), Lopez Garcia (5:00 200 Hynes), or poster of Jonah Robinson (Friday 3:30 Hynes Auditorium).

Spectral Edges to Critical Points

Each spectral edge is the image of a critical point of λ on the Bloch variety. A first step is to study all critical points.



Implicit differentiation of
$0 = D(z, \lambda) := \det(L_c(z) - \lambda I_W)$
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 $\leq \mathrm{vol}(\mathcal{N}(D))$.

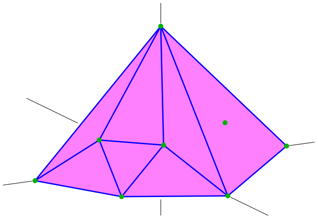
* Monotonicity and $(\mathbb{C}^\times)^d \times \mathbb{C}_\lambda$.

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 $X_{\mathcal{N}(D)}$ in its natural projetive ebedding.



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

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

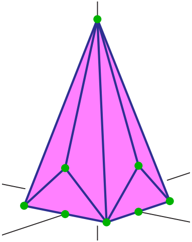
Let BV be the compactified Bloch variety in $X_{\mathcal{N}(D)}$.

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 $(\mathbb{C}^\times)^d \times \mathbb{C}$.

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

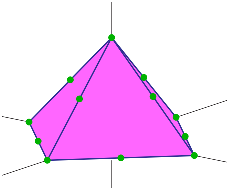
Theorem. *$\#$ critical points $=$ vol$(\mathcal{N}(D)) \Longleftrightarrow \mathcal{N}(D)$ has no vertical faces and $BV \cap \partial X_{\mathcal{N}(D)}$ is smooth.*

Dense Periodic Graphs

A $\mathbb{Z}^d$-periodic graph Γ is *dense* if it has maximally many edges, given its combinatorial structure,
$\mathcal{A}(\Gamma) := \{a \in \mathbb{Z}^d \mid \exists \text{ an edge with endpoints in } W \text{ and } a + W\}$.

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

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

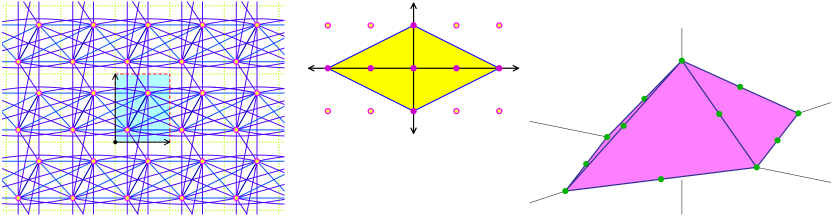


For $d = 2, 3$ *we may choose* U *such that for* $c \in U$*, the Bloch variety is smooth at infinity, and*
$\#$ *critical points* $= vol(\mathcal{N}(\Gamma)) = |W|^{d+1} vol(conv(\mathcal{A}(\Gamma)))$.

One Example

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

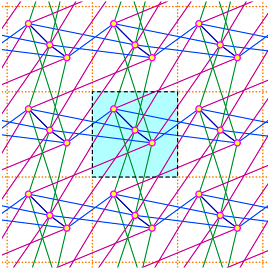
Consider the $\mathbb{Z}^2$-periodic dense graph Γ shown below with $\mathcal{A}(\Gamma)$ and Newton polytope.

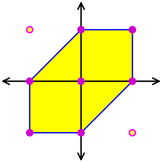


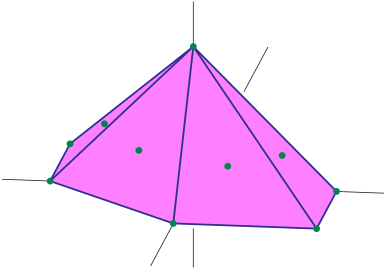
Independent Macaulay2 and Singular calculations at (random) parameters $c = (c, V)$ find a Bloch variety with $64 = 2^3 \cdot 8 = \mathrm{vol}(\mathcal{N}(\Gamma))$ regular critical points, which implies the spectral edges conjecture for Γ. (I can explain, if you want.)

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, W.

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

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Dense Periodic Graphs (Reprise)

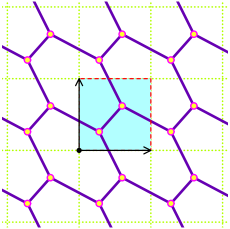
A $\mathbb{Z}^d$-periodic graph Γ is *dense* if it has maximally many edges, given its combinatorial structure.

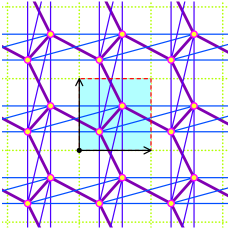
Fix a fundamental domain W for Γ. Its *support* of Γ is the set $\mathcal{A}(\Gamma) := \{a \in \mathbb{Z}^d \mid \exists \text{ an edge with endpoints in } W \text{ and } a + W\}$.

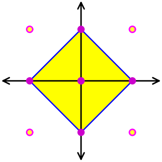
$\rightsquigarrow$ This contains the support of entries in $L_c(z)$.

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

Every graph embedds into a minimal dense graph







$\mathcal{A}(\Gamma)$