# Periodic graph operators for algebraic geometers

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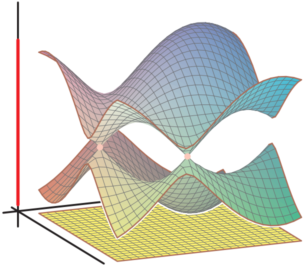

Work with Paul Breiding, Ngoc Do, Matthew Faust, Peter Kuchment, Jordy Lopez, Jonah Robinson, and James Woodcock.

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# Algebraic Geometry in Spectral Theory

While spectral theory comes from mathematical physics and analysis, it affords many opportunities for algebra, geometry, and geometric combinatorics.

The minisymposium "Algebraic Geometry in Spectral Theory", involved the following conference themes:

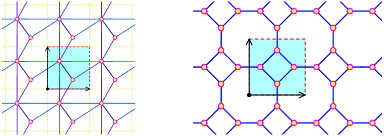
Critical points from algebraic optimization,
Parameter identification,
Stability and real algebraic geometry,
Stratified Morse theory,
Structure of Newton polytopes,
Factorization of matrices of polynomials,
Toric varieties,
and large-scale symbolic computation.

I will illustrate some algebraic aspects while discussing recent work with implications for algebraic optimization.

# Periodic Graph Operators

A discrete model of a crystal is provided by a periodic graph $\Gamma$ with vertices $\mathcal{V}$, edges $\mathcal{E}$, and a free cocompact action of $\mathbb{Z}^d$.

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



Parameters of the *tight binding model* are $\mathbb{Z}^d$-invariant functions: a potential $V\colon \mathcal{V} \to \mathbb{R}$ and edge (interaction) weights $e\colon \mathcal{E} \to \mathbb{R}^\times$.

The Schrödinger operator $H$ acts on functions $\psi\colon \mathcal{V} \to \mathbb{C}$:
For a function $\psi$, $H\psi$ is defined by its value at $v \in \mathcal{V}$,

$$(H\psi)(v) \;=\; V(v)\psi(v) \;-\sum_{v\sim u} e_{(v,u)}\psi(u)\,.$$

$H$ is self-adjoint (on $\ell_2(\mathcal{V})$), and its spectrum $\sigma(H) \subset \mathbb{R}$ corresponds to energy levels electron transport in the crystal.

# Quasi-Periodic Functions (aka Floquet Transform)

Write $\mathbb{T}$ for the unit complex numbers.
Each $z \in \mathbb{T}^d$ is a unitary character for $\mathbb{Z}^d$: $(z, \alpha) \mapsto z^\alpha$.

A function $\psi_z \colon \mathcal{V} \to \mathbb{C}$ is *z-quasi-periodic* if for $v \in \mathcal{V}$ and $\alpha \in \mathbb{Z}^d$,

$$\psi_z(v + \alpha) \;=\; z^\alpha \psi_z(v)\,.$$

A quasi-periodic function depends only on its restriction to a fundamental domain $W \subset \mathcal{V}$ for the $\mathbb{Z}^d$-action.

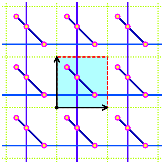
The Schrödinger operator acts on $z$-quasi-periodic functions $\psi_z$

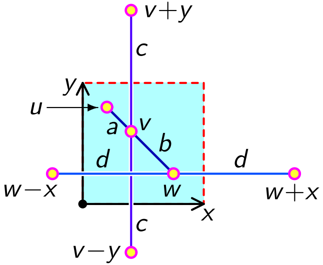
$$(H\psi_z)(v) \;=\; V(v)\psi_z(v) - \sum_{v \sim u+\alpha} e_{(v,u+\alpha)} z^\alpha \psi_z(u) \qquad v, u \in W\,.$$

Letting $z$ vary (and ignoring what $\psi_z$ is), this is multiplication by a $W \times W$ matrix $H(z)$ of Laurent polynomials; a map of free modules over the Laurent ring $\mathbb{C}[z^\pm]$.

# Example

For the graph on the left, we show a labeling in a neighborhood of a fundamental domain $W$.






We have

$$H(z) \;=\; \begin{pmatrix} u & -a & 0 \\ -a & v - c(y + y^{-1}) & -b \\ 0 & -b & w - d(x + x^{-1}) \end{pmatrix} \;.$$

Note that $H(x, y)^T = H(x^{-1}, y^{-1})$.

This is true in general as $v \sim u + \alpha \iff u \sim v - \alpha$, and by periodicity both edges have the same label.

# Bloch varieties

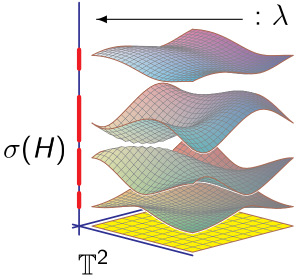
**Theorem.** (Why we introduced quasi-periodic functions.)

$$\begin{aligned}\sigma(H) &= \{\lambda \in \mathbb{R} \mid \exists z \in \mathbb{T}^d \text{ and } \psi_z \text{ s.t. } H\psi_z = \lambda\psi_z\} \\ &= \{\lambda \in \mathbb{R} \mid \exists z \in \mathbb{T}^d \text{ s.t. } \det(H(z) - \lambda I) = 0\}\end{aligned}$$

The *Bloch variety* is defined by the *dispersion polynomial* $D(z, \lambda) := \det(H(z) - \lambda I)$. Its projection to the $\lambda$-axis is $\sigma(H)$.

As $H(z)^T = H(z^{-1})$, for $z \in \mathbb{T}^d$, $H(z)$ is hermitian, so the Bloch variety is a $|W|$-sheeted cover of $\mathbb{T}^d$.

A *Fermi variety* is a slice at a fixed $\lambda$.

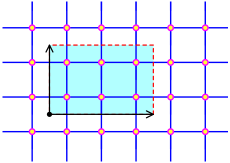



From a matrix of Laurent polynomials to an algebraic variety lying over the spectrum, spectral theory of discrete periodic operators may be studied through the lens of commutative algebra and algebraic geometry.

# Some history

1979: van Moerbeke and Mumford considered $\mathbb{Z}$-periodic *directed graphs*, showing an equivalence between the operators and curves with certain divisors. (The curves are the Bloch varieties).

1993: Gieseker, Knörrer, Trubowitz studied the pure Schrödinger operator 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 determined many properties, including density of states and the irreducibility and smoothness of Bloch and Fermi varieties.

Their methods involved a compactification and the Torelli Theorem.

Presented in a Bourbaki Lecture by Peters in 1992.

Bättig provided a more appealing toric compactification, including compactifying the operator.

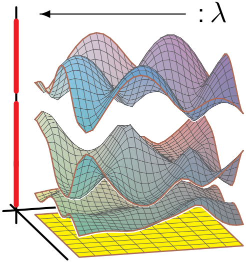
# Spectral edges nondegeneracy conjecture

I now focus on one property from physics.

Each edge of the spectrum is the image of a critical point of $\lambda$ on the Bloch variety.

A common assumption is that those critical points are nondegenerate.

This is needed for effective masses in solid state physics, and many other properties.




Kuchment noted that most physicists assume this, but it is largely unknown, even for discrete periodic operators. He formulated the *Spectral Edges Conjecture*: For general operators on a graph, points on the Bloch variety above endpoints of spectral bands are nondegenerate extrema of $\lambda$.

A first step (for me) is to understand the critical points of $\lambda$ on the complexified Bloch variety.

# Scientific arbitrage

Critical points of $\lambda$ satisfy the *critical points equations*:

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

*Critical Points Property (CPP)*: All critical points are nondegenerate.

**Do, et al.**[1] *Given a family of periodic operators, either almost all or almost none of the operators in the family satisfy the CPP.*

**Proof:** Nondegeneracy of a critical point is an algebraic relation; it is equivalent to the Hessian having full rank. □

$\rightsquigarrow$ This bit of scientific arbitrage is what the journal liked most 🙂.

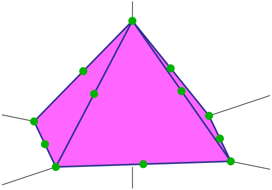
$\Rightarrow$ for a given graph $\Gamma$, presenting *one* parameter value with the maximum number of critical points *and* which satisfes the CPP, implies the Spectral Edges Conjecture for $\Gamma$.

[1] Do, Kuchment, S., J. Math. Phys., 61, (2020).

# Doubling down on arbitrage

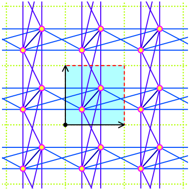
The *Newton polytope* $\mathcal{N}$ of the dispersion polynomial $D(z,\lambda)$ is

$\mathcal{N} \ := \ \mathrm{conv}\{(\alpha, j) \mid z^\alpha\lambda^j \text{ appears in } D\}\,.$



Critical point equations involve $D$ and the $z_i\partial D/\partial z_i$. All have support in $\mathcal{N}$.

**Kushnirenko** (mostly)
*# Critical points* $\leq \mathrm{n\text{-}vol}(\mathcal{N})$.



Do, et al. proved the Spectral Edges Conjecture for this graph whose Newton polytope is above by computing one instance (over a finite field) with $32 = \mathrm{n\text{-}vol}(\mathcal{N})$.

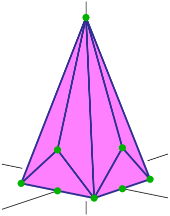
Aside: While not general, the system was *Bernstein-general* in that it had the expected number of solutions. This example inspired:

**Breiding, S., Woodcock**
*EDD for hypersurfaces is Bernstein-general.*

# Toric Compactification

The projective toric variety $X \subset \mathbb{P}$ given by $\mathcal{N}$ compactifies $(\mathbb{C}^\times)^d \times \mathbb{C}$. Let $\mathrm{BV} \subset X$ be the closure of the Bloch variety.

Faces $F$ of $\mathcal{N}$ correspond to toric subvarieties $X_F$ of $X$.



The Critical Point Equations $\longleftrightarrow$ a linear section $\Lambda \cap X$ of $X$.

**Faust-S.** *If $F$ is vertical then $\Lambda \cap X_F \neq \emptyset$. Otherwise, $\Lambda \cap X_F \neq \emptyset$ implies that $\mathrm{BV}$ is singular along $X_F$.*

The union of $X_F$ over non-base faces of $\mathcal{N}$ is the *boundary* $\partial X := X \smallsetminus (\mathbb{C}^\times)^d \times \mathbb{C}$ of $X$.

$\#$ Critical points $= \mathrm{n\text{-}vol}(\mathcal{N})$ if and only if $\Lambda \cap \partial X = \emptyset$.

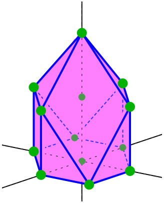
**Corollary.** *$\#$ Critical points $= \mathrm{n\text{-}vol}(\mathcal{N}) \Longleftrightarrow \mathcal{N}$ has no vertical faces and $\mathrm{BV}$ is smooth along each $X_F$.*

Points of $\Lambda \cap \partial X$ are *asymptotic critical points*.

# Critical Point Degree (w/ Faust & Robinson)

The *critical point degree* (*CPD*) of Γ is the number of critical points, counted with multiplicity, on a generic Bloch variety for Γ.

We identify contributions from the asymptotic critical points.



$d_{\mathrm{vert}}$ : Due to vertical faces of $\mathcal{N}$.
$d_{\mathrm{sing}}$ : Singularities of $\mathrm{BV}$ along faces $F$ when Γ is "asymptotically disconnected", and thus $BV$ is asymptotically reducible.

**Faust, et al.** *Let Γ be a periodic graph. Then the critical point degree of Γ satisfies*

$$2^d|W| \;\leq\; \mathrm{CPD} \;\leq\; \text{n-vol}(\mathcal{N}) - d_{\mathrm{vert}} - d_{\mathrm{sing}}\,.$$

Both contributions arise from structural properties of Γ.

$\rightsquigarrow$ Should have implications for algebraic optimization.

(The $2^d|W|$ comes from the symmetry $H(z) = H(1/z)$.)

# Corner points

We noted that $H(z)^T = H(z^{-1})$, which implies that the dispersion polynomial $D(z,\lambda) := \det(H(z) - \lambda I)$ satisfies

$$\overline{D(z,\lambda)} \;=\; \overline{D(1/z,\lambda)} \;=\; D(1/\overline{z},\overline{\lambda})\,.$$

Thus the (real) Bloch variety is the set of real points of the complex Bloch variety under the nonstandard real structure induced from

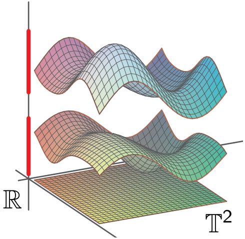
$$(\mathbb{C}^\times)^d \times \mathbb{C} \ni (z,\lambda) \;\longmapsto\; (1/\overline{z},\overline{\lambda}) \in (\mathbb{C}^\times)^d \times \mathbb{C}\,.$$

Either this, or the symmetry $D(z,\lambda) = D(1/z,\lambda)$ implies that whenever $z^2 = 1$, there is a critical point.

These $2^d$ points $\{\pm 1\}^d$, are *corner points*.

At a corner point $z^*$, $H(z^*)$ is a $|W| \times |W|$ symmetric matrix.

This gives $2^d|W|$ critical points of $\lambda$.



# Vertical faces

Observation: If $F \subset \mathcal{N}$ is a vertical face, then

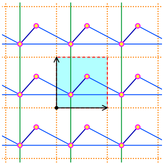
$$\#(\Lambda \cap X_F) \;=\; \text{n-vol}(F)\,. \qquad \text{(Kushnirenko's Theorem)}$$

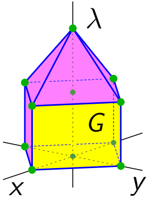
Further: If $F \subset G$ are both vertical, then $\Lambda \cap X_F \subset \Lambda \cap X_G$.

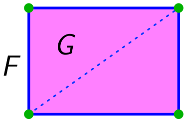
Define: $d_G := \text{n-vol}(G) - \sum_{F\subset G} d_F \cdot \text{mult}_{X_F} X_G$

$$d_{\text{vert}} := \sum_{G \text{ is vertical}} d_G \cdot \text{mult}_{X_G} X$$

Example:





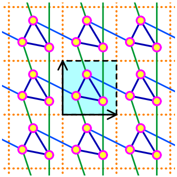



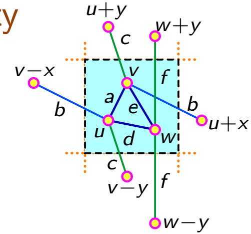

$\text{n-vol}(G) = 2$, $\text{n-vol}(F) = 1$, and $\text{mult}_{X_F} X = 2$.

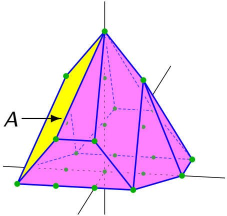
Then $d_{\text{vert}} = 4\cdot(2-2) \;+\; 4\cdot 2 \;=\; 8$.

$\text{n-vol}(\mathcal{N}) = 16$ and $16 - 8 = 2^2|W|$ (+ a little more) $\Longrightarrow$ Spectral Edges Nondegeneracy Conjecture.

# Asymptotic reducibility






The vector $\eta = (-1, 1, -1)$ exposes the face $A$.
Characteristic matrix with $\eta$-initial terms underlined

$$\begin{pmatrix} \underline{\lambda} - u & a + bx^{-1} + \underline{cy^{-1}} & d \\ a + \underline{bx} + cy & \underline{\lambda} - v & e \\ d & e & \underline{\lambda} - w + fy + \underline{fy^{-1}} \end{pmatrix} .$$

The determinant of the initial matrix defines $\mathrm{BV} \cap X_A$,

$$\det \begin{pmatrix} \lambda & cy^{-1} & 0 \\ bx & \lambda & 0 \\ 0 & 0 & \lambda + fy^{-1} \end{pmatrix} = (\lambda^2 - bcxy^{-1})(\lambda + fy^{-1}) .$$

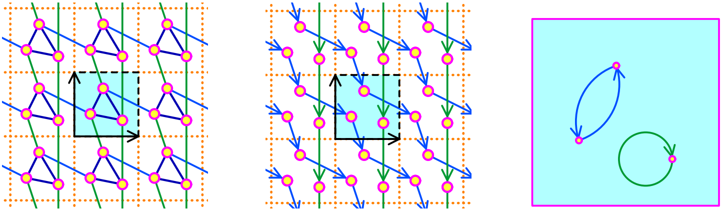
Thus we have two curves with one (singular) point of intersection.

# Graph asymptotically disconnected

The $\eta$-initial terms in the Floquet matrix

$$\begin{pmatrix} \underline{\lambda} - u & a + bx^{-1} + \underline{cy^{-1}} & d \\ a + \underline{bx} + cy & \underline{\lambda} - v & e \\ d & e & \underline{\lambda} - w + fy + \underline{fy^{-1}} \end{pmatrix}$$

determine directed edges of the *initial graph*, with quotient by $\mathbb{Z}^2$.



The singularity (in $\mathrm{BV}$) of asymptotic critical points is also structural.

In well over $10^6$ graphs—all observed generic asymptotic critical points arose from these structures.

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