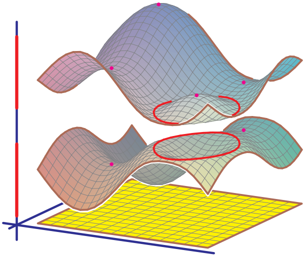
The Critical Point Degree of a Periodic Graph

Computations and Applications of Algebraic Geometry and Commutative Algebra
NZMS-AustMS-AMS Joint International Meeting

13 December 2024



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With Matthew Faust and Jonah Robinson

Supported by NSF grant DMS-2201005

Combinatorial Algebraic Geometry meets Mathematical Physics

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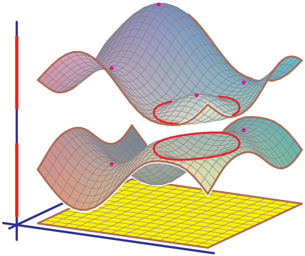

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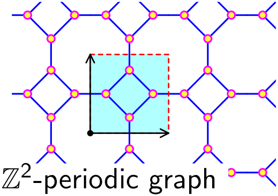
Operators on Periodic Graphs

A locally finite $\mathbb{Z}^d$-periodic graph Γ is a discrete model of a crystal.
Vertices $\mathcal{V} \leftrightarrow$ atoms,
edges $\mathcal{E} \leftrightarrow$ interactions, with
action $\mathcal{V} \times \mathbb{Z}^d \to \mathcal{V} \quad (v, \alpha) \mapsto v + \alpha$.



$\mathbb{Z}^2$-periodic graph

Electron transport is modeled by a Schrödinger operator (on $\ell_2(\mathcal{V})$)

$$H = V + \Delta,$$

where $V\colon \mathcal{V} \to \mathbb{R}$ is a periodic potential and Δ is a weighted graph Laplacian (periodic weights $e\colon \mathcal{E} \to \mathbb{R}$ are interaction strengths)

As H is self-adjoint, its spectrum
$\sigma(H) := \{\lambda \mid H - \lambda \text{ not invertible}\}$ is a subset of $\mathbb{R}$.
It consists of finitely many intervals, representing the familiar structure of electron energy bands and band gaps.

From Fourier (Floquet) Transform to Geometry

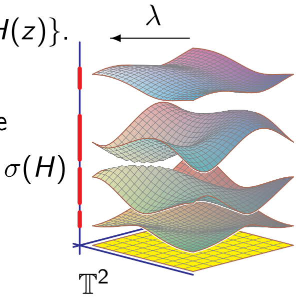
More structure is revealed by Fourier (Floquet) transform.

$\mathbb{T}$: unit complex numbers.
$\mathbb{T}^d$: unitary characters of $\mathbb{Z}^d$: $z \in \mathbb{T}^d$, $\alpha \in \mathbb{Z}^d \longmapsto z^\alpha$.

Fix $W \subset \mathcal{V}$ a fundamental domain for $\mathbb{Z}^d$-action.

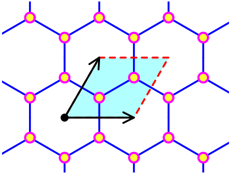
After Fourier transform, H is multiplication by the $W \times W$ *Floquet matrix*, $H(z)$, whose (u, v)-entry is $-\sum_\alpha e_{(u,v+\alpha)} z^\alpha$.

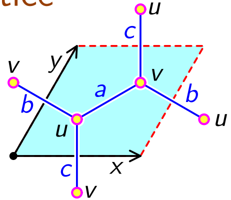
$\sigma(H) = \{\lambda \mid \exists z \in \mathbb{T}^d$ with λ an eigenvalue of $H(z)\}$.

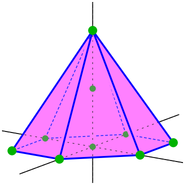


Bloch variety BV $\subset \mathbb{T}^d \times \mathbb{R}$ is the hypersurface defined by $\Phi := \det(\lambda I_W - H(z))$.
The coordinate λ is a function on the Bloch variety, and $\sigma(H) = \lambda(\mathrm{BV})$.

Example: Hexagonal Lattice



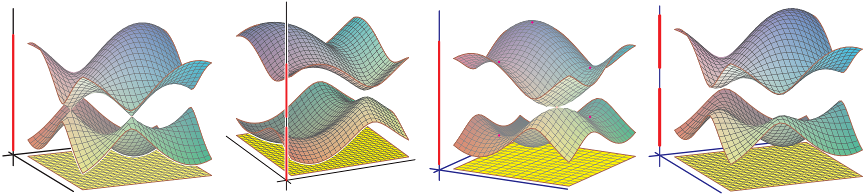




The Floquet matrix is $H(x,y) = \begin{pmatrix} V(u) & -a - bx^{-1} - cy^{-1} \\ -a - bx - cy & V(v) \end{pmatrix}$

and $\Phi = \lambda^2 + \lambda(V(u) + V(v)) + V(u)V(v)$
$- \left(a^2 + b^2 + c^2 + ab(x + x^{-1}) + ac(y + y^{-1}) + bc(xy^{-1} + yx^{-1})\right)$.

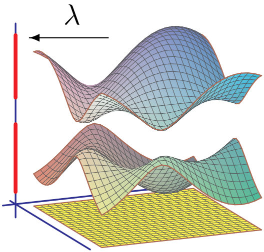
Here are several of its Bloch varieties.



Spectral Edges Nondegeneracy Conjecture

Spectral edges conjecture: For general operators on Γ, critical points of λ on BV above endpoints of spectral bands are nondegenerate extrema.

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



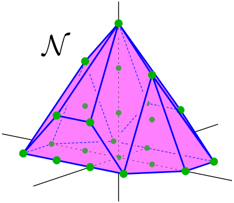
$\rightsquigarrow$ First step: study complex critical points of λ on $\mathrm{BV}_{\mathbb{C}}$.

Lemma. *A point $(z,\lambda) \in (\mathbb{C}^\times)^d \times \mathbb{C}$ is a critical point of λ on $BV_{\mathbb{C}}$ if and only if it is a solution to the system*

$$\Phi(z,\lambda) \;=\; z_i \frac{\partial \Phi}{\partial z_i}(z,\lambda) \;=\; 0 \qquad i = 1, \ldots, d\,.$$

Call these the *critical point equations*.

Critical Points of Discrete Periodic Operators



$\mathrm{supp}\left(\frac{z_i \partial\Phi}{\partial z_i}\right) \subset \mathcal{N}$, the Newton polytope of Φ.

Kushnirenko's Theorem implies

$(*) \qquad \#$ Critical points $\quad \leq$ n-vol$(\mathcal{N})$,

the normalised volume of $\mathcal{N}$.

The projective toric variety X of $\mathcal{N}$ compactifies $(\mathbb{C}^\times)^d \times \mathbb{C}$.
Set $\partial X := X \smallsetminus \left((\mathbb{C}^\times)^d \times \mathbb{C}\right) \ = \ \bigcup_F X_F$, where X_F is the projective toric variety of the face F of $\mathcal{N}$, and F is not its base.

The critical point equations $\longleftrightarrow$ a linear section $\Lambda_\Phi \cap X$.
We have equality in $(*)$ if and only if $\Lambda_\Phi \cap \partial X = \emptyset$.

Faust-S. (1) *if F is vertical then $\Lambda_\Phi \cap X_F \neq \emptyset$.*
(2) *Otherwise $\Lambda_\Phi \cap X_F \neq \emptyset$ implies that BV is singular along F.*

$\Lambda_\Phi \cap \partial X$ consists of *asymptotic critical points*.

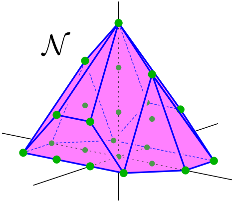
Critical Point Degree

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

w/ Matt Faust, a post doc at Michigan State University and
Jonah Robinson, an undergraduate student,
we identify contributions to the asymptotic critical points.

d_{vert} : Due to vertical faces of $\mathcal{N}$.

d_{sing} : Singularities of BV along faces F when Γ is "asymptotically disconnected", and thus BV is asymptotically reducible.



Theorem: *Let Γ be a $\mathbb{Z}^2$ or $\mathbb{Z}^3$-periodic graph. Then the critical point degree of Γ is at most n-vol$(\mathcal{N}) - d_{\mathrm{vert}} - d_{\mathrm{sing}}$.*

Both contributions arise from structural properties of Γ.

Vertical Faces

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

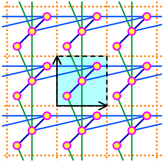
$$\#(\Lambda_\Phi \cap X_F) \;=\; \text{n-vol}(F)\,. \qquad \text{(Kushnirenko's Theorem)}$$

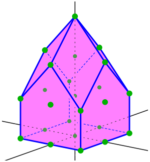
Further: If $F \subset G$ are both vertical, then $\Lambda_\Phi \cap X_F \subset \Lambda_\Phi \cap X_G$.

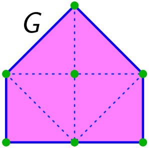
Define: $d_G := \text{n-vol}(G) - \sum_{F\subset G} \text{n-vol}(F) \qquad (F \text{ vertical})$

$d_{\text{vert}} := \sum_{G \text{ is vertical}} d_G$

Example:



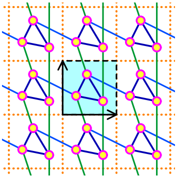


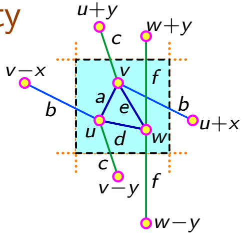


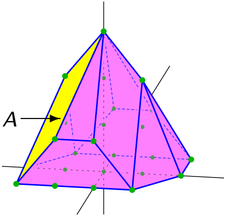
For each vertical facet G, $\text{n-vol}(G) = 6$ and $\text{n-vol}(F) = \text{n-vol}(F') = 1$, so that $d_G = 6 - 2 = 4$.

Then $d_{\text{vert}} = \underbrace{4 \cdot 1}_{\text{(edges)}} + \underbrace{4 \cdot (6-2)}_{\text{(facets)}} = 20.$

Asymptotic Reducibility







The vector $\eta = (-1, 1, -1)$ exposes the face A.
Here is the characteristic matrix with η-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 $\mathrm{BV} \cap X_A$,

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

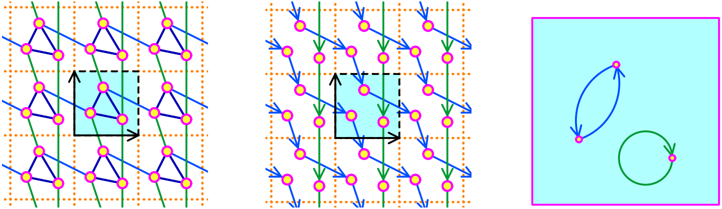
Thus we have two curves with one (singular) point of intersection.

Graph Asymptotically Disconnected

The η-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 BV) of asymptotic critical points is also structural.

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