The Critical Point Degree of a Periodic Graph

Applied and Computational Algebra
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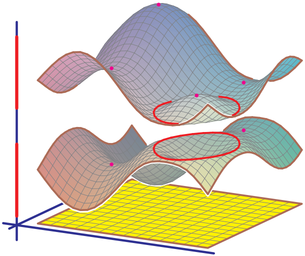
With Matt Faust and Jonah Robinson



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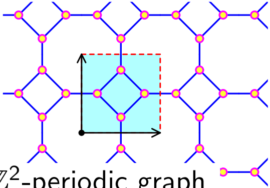
Operators on Periodic Graphs

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



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

Consider 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 (given by periodic weights $e\colon \mathcal{E} \to \mathbb{R}$).

As H is self-adjoint, its spectrum $\sigma(H) \subset \mathbb{R}$ consists of finitely many intervals, representing the familiar structure of electron energy bands and band gaps.

From Floquet Transform to Geometry

More structure is revealed by Floquet (Fourier) transform.

$\mathbb{T}$: unit complex numbers.
$\mathbb{T}^d$: unitary characters of $\mathbb{Z}^d$:

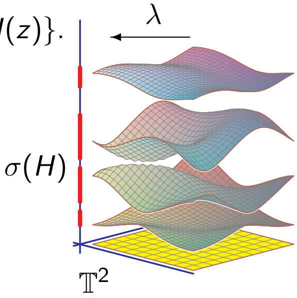
$$z \in \mathbb{T}^d,\ \alpha \in \mathbb{Z}^d \longmapsto z^\alpha := z_1^{\alpha_1} \cdots z_d^{\alpha_d}.$$

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

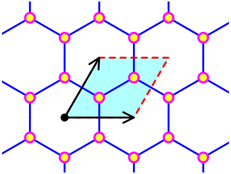
After Floquet transform, H is multiplication by the $W \times W$ matrix $H(z)$ whose (u, v)-entry is $\quad -\sum_\alpha e_{(u,v+\alpha)} z^\alpha$, and

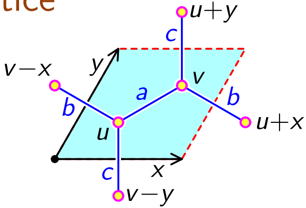
$\sigma(H) = \{\lambda \mid \exists z \in \mathbb{T}^d$ with λ an eigenvalue of $H(z)\}$.

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



Example: Hexagonal Lattice

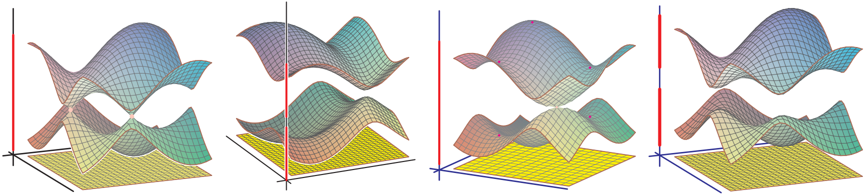




The Floquet matrix is $H(x,y) = \begin{pmatrix} V(u) & -a - bx^{-1} - cy^{-1} \\ -a - bx - cy & V(v) \end{pmatrix}$

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

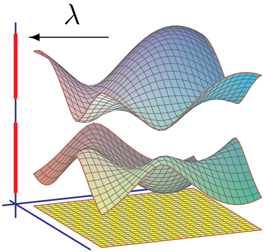
Here are several of its Bloch varieties for different a, b, c, V.



Spectral Edges Nondegeneracy Conjecture

Kuchment made the *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.



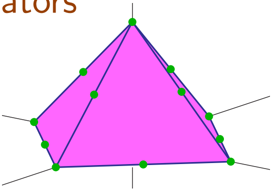
$\rightsquigarrow$ A first step: study critical points of λ on the complexified Bloch variety, $BV_{\mathbb{C}} \subset (\mathbb{C}^\times)^d \times \mathbb{C}$.

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 of equations*

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

These are highly structured polynomial equations.

Critical Points of Discrete Periodic Operators

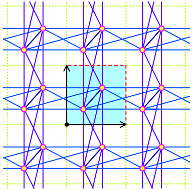


The *Newton polytope $\mathcal{N}$* of the dispersion polynomial Φ is

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

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

Kushnirenko (mostly)
$(*)$ *# Critical points $\leq$ n-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 $32 = \text{n-vol}(\mathcal{N})$.

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

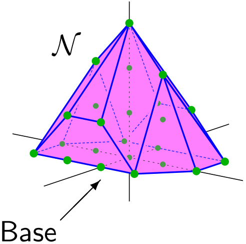
Breiding, S., Woodcock
EDD for hypersurfaces is Bernstein-general.

Asymptotic Critical Points

$\mathrm{BV}_{\mathbb{C}}$ is compactified in a toric variety X, whose geometry is encoded by the polytope $\mathcal{N}$.
Each face F of $\mathcal{N} \longleftrightarrow$ a toric subvariety X_F of X, and

$$\partial X := X \smallsetminus \left((\mathbb{C}^\times)^d \times \mathbb{C}\right) \;=\; \bigcup_F X_F\,,$$

the union over proper, non-base faces F.



The critical point equations (CPE) are a system of linear equations on X, expressed geometrically as $\Lambda_\Phi \cap X$.

We have $\#\big(\Lambda_\Phi \cap X\big) = \text{n-vol}(\mathcal{N})$.

Consequently, 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 X_F.*

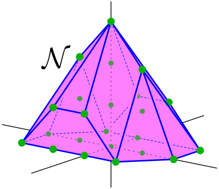
$\Lambda_\Phi \cap \partial X$ consists of *asymptotic critical points*.

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.

With Matt Faust and Jonah Robinson,
we identify contributions from 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.*

$\rightsquigarrow$ Like earlier work, this suggests possibilities for algebraic optimization.

Vertical Faces

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

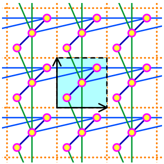
$$\#(\Lambda_\Phi \cap X_F) \;=\; \text{n-vol}(F)\,. \qquad \text{(Kushnirenko's Theorem)}$$

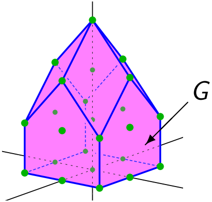
Easier: If $F \subset G$ are both vertical, then $\Lambda_\Phi \cap X_F \subset \Lambda_\Phi \cap X_G$.

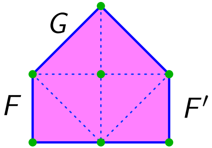
Define: $d_G := \text{n-vol}(G) - \sum_{F \subset G} \text{n-vol}(F) \qquad (F \text{ vertical})$

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

Example:



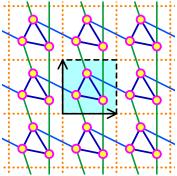


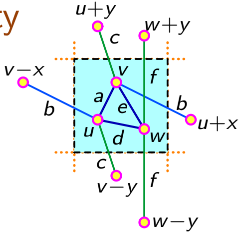


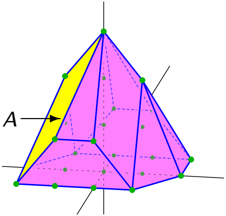
For each vertical facet G, $\text{n-vol}(G) = 6$ and $\text{n-vol}(F) = \text{n-vol}(F') = 1$, so that $d_G = 6 - 2 = 4$.

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

Asymptotic Reducibility







The linear function given by $\eta = (-1, 1, -1)$ is minimized on A.
Characteristic matrix with η-minimal terms underlined

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

Determinant of the η-initial matrix defines $\overline{\mathrm{BV}} \cap X_A$,

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

two curves with one (singular) point of intersection.

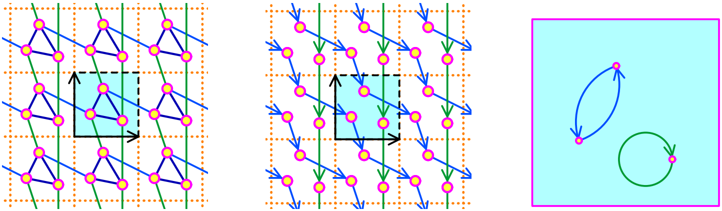
Asymptotically Disconnected Graph

The η-minimal terms in the matrix

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

correspond to directed edges of the η-initial graph.

This has disconnected quotient by $\mathbb{Z}^2$.



Disconnected initial graph $\Longrightarrow$ singularity along X_A.