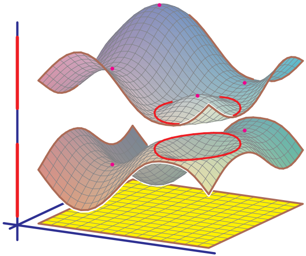
Toric Geometry of Periodic Operators

Computational Algebra, Algebraic Geometry and Applications II

Frank Sottile

Texas A&M University
sottile@tamu.edu



Work with Ngoc Do, Matthew Faust, Peter Kuchment, Jordy Lopez, Jonah Robinson, and Stephen Shipman.

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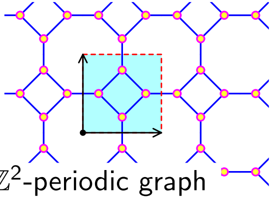
Operators on Periodic Graphs

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 $\mathbb{Z}^d \times \mathcal{V} \to \mathcal{V} \quad (\alpha, v) \mapsto \alpha + v$.


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

Given periodic functions $V\colon \mathcal{V} \to \mathbb{R}$ (potential) and $e\colon \mathcal{E} \to \mathbb{R}^\times$ (edge weights), the Schrödinger operator H acts on functions $\psi\colon \mathcal{V} \to \mathbb{C}$. For $v \in \mathcal{V}$, the value of $H\psi$ at v is

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

H is self-adjoint (on $\ell_2(\mathcal{V})$), and its spectrum $\sigma(H) \subset \mathbb{R}$ consists of finitely many intervals, representing the familiar structure of electron energy bands and band gaps.

Quasi-periodic functions

The representation theory of $\mathbb{Z}^d$ turns this spectral problem into an algebraic family of eigenvalue problems.

Let $z \in (\mathbb{C}^\times)^d$, a character of $\mathbb{Z}^d$. A function $\psi\colon \mathcal{V} \to \mathbb{C}$ is *z-quasi-periodic* ($\psi \in \mathcal{Q}_z$) if for $v \in \mathcal{V}$ and $\alpha \in \mathbb{Z}^d$,

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

Let $W \subset \mathcal{V}$ be a set of orbit representatives. The map $\psi \mapsto \psi|_W$ identifies $\mathcal{Q}_z$ with the vector space $\mathbb{C}^W$ of functions $W \to \mathbb{C}$. The action of the Schrödinger operator H on $\psi \in \mathcal{Q}_z$ is

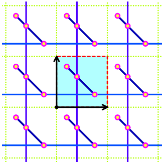
$$(H\psi)(v) \;=\; V(v)\psi(v) - \sum_{v \sim \alpha + u} e_{(v,\alpha_u)} z^\alpha \psi(u) \qquad v, u \in W\,.$$

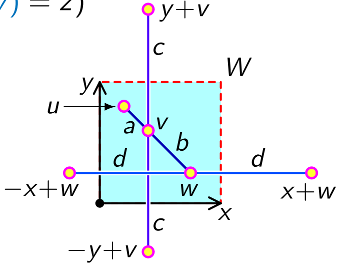
For $z \in (\mathbb{C}^\times)^d$, this is multiplication by a $W \times W$ matrix $H(z)$ of Laurent polynomials, which is a map of free $\mathbb{C}[z^\pm]$-modules.

(This is an algebraic version of Fourier transform.)

Example

For the graph on the left, we show a labeling in a neighborhood of a fundamental domain W. $((x, y) = z)$





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 $v \sim \alpha + u \iff u \sim -\alpha + v$, and by periodicity both edges have the same label.

Bloch varieties

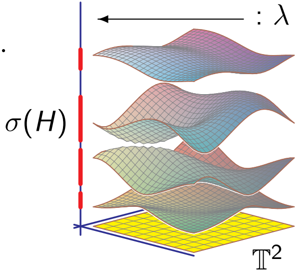
$\mathbb{T} \subset \mathbb{C}^\times$: unit complex numbers & $\mathbb{T}^d$ = unitary characters of $\mathbb{Z}^d$.
The reason we introduced quasi-periodic functions is the

Floquet Theorem.

$$\sigma(H) \;=\; \{\lambda \in \mathbb{R} \mid \exists z \in \mathbb{T}^d \text{ and } \psi \in \mathcal{Q}_z \text{ s.t. } H\psi = \lambda\psi\}$$

The *(real) Bloch variety* $\mathrm{BV}_{\mathbb{R}} \subset \mathbb{R} \times \mathbb{T}^d$ is

$$\mathrm{BV}_{\mathbb{R}} \;:=\; \mathrm{Var}(\det(\lambda I - H(z)))\,.$$



By the Floquet Theorem, its projection to the λ-axis is $\sigma(H)$.

For $z \in \mathbb{T}^d$, $H(z)^T = H(z^{-1}) = H(\overline{z})$, so $H(z)$ is hermitian, and $\mathrm{BV}_{\mathbb{R}} \twoheadrightarrow \mathbb{T}^d$ is a $|W|$-sheeted cover.

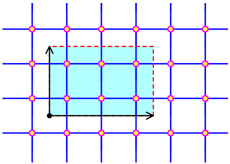
The *Bloch variety*, $\mathrm{BV} \subset \mathbb{C} \times (\mathbb{C}^\times)^d$, is

$\mathrm{BV} \;:=\; \mathrm{Var}(\lambda I - \det(H(z)))$, the complexification of $\mathrm{BV}_{\mathbb{R}}$.

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, and 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.

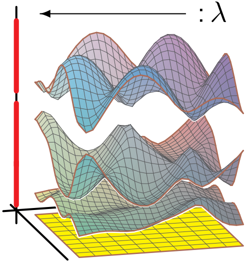
Their methods involved a compactification and modern results on algebraic curves.

Presented in a Bourbaki Lecture by Peters in 1992.

Bättig provided a more appealing toric compactification, including compactifying the operator. (More later.)

Critical Points of λ

Assumptions and open problems from mathematical physics and quantum graphs provide a strong motivation to understand the critical points of λ.

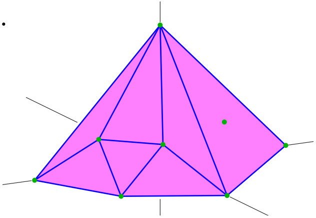


Write $\Phi := \det(\lambda I - H(z))$, which is called the *dispersion polynomial*.

The critical points satisfy the *critical point equations*:

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

These are formulated as toric derivatives so that all equations have the same Newton polytope.



Let $\mathcal{N}$ be the Newton polytope of Φ.

Bounds on the number of critical points

Easy: $2^d|W| \leq \#$ critical points $\leq \text{n-vol}(\mathcal{N})$

$2^d|W|$: comes from the symmetry $H(z)^T = H(z^{-1})$.

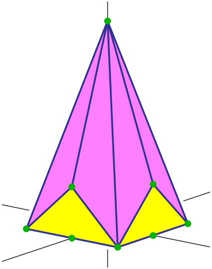
$\text{n-vol}(\mathcal{N})$: Kushnirenko's Theorem

$\overline{\text{BV}}$: compactification of BV in the toric variety $X_{\mathcal{N}}$ of $\mathcal{N}$.

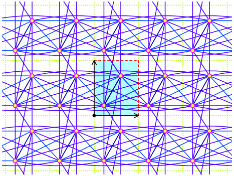
Faust-S.: $\#$ critical points $<$ $\text{n-vol}(\mathcal{N})$ $\Rightarrow$

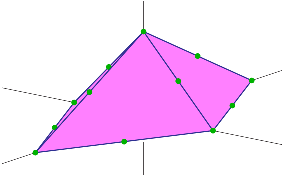
$*$ Newton polytope $\mathcal{N}$ has vertical faces, or

$*$ $\overline{\text{BV}}$ is singular along a toric orbit of $X_{\mathcal{N}}$.



Faust-S.: Have equality if graph is dense:





Bernstein-generality and beyond

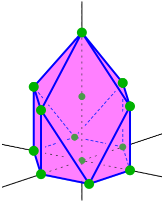
The critical point equations are not general given their support, yet they can have the expected (BKK) number of solutions.

Such a system is *Bernstein-general*. This work inspired:

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

With Faust and Robinson, we identify asymptotic contributions to the critical points.

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



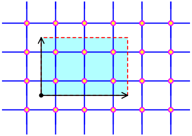
Faust, et al.

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

Both contributions arise from structural properties of graph Γ.

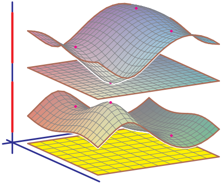
Toric Compactification of Bloch variety

Many recent results in spectral theory used the compactification $\overline{\mathrm{BV}}$ of the Bloch variety and its boundary $\overline{\mathrm{BV}} \smallsetminus \mathrm{BV}$.



Filman, Liu, Matos: Proved irreducibility of BV for d-dimensional versions the grid graph (changing the period):

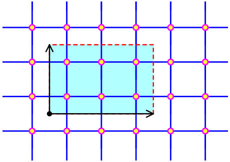
Faust, Lopez-Garcia: Used the boundary and geometric combinatorics to prove irreducibility when changing the period of general graphs.



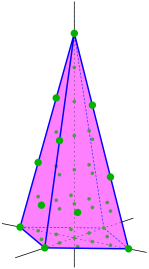
Faust, Liu: Showed that flat bands (eigenvalues of the operator) are not generic.

Faust, S.: Gave a criterion based on Newton polytopes to establish when λ is a perfect Morse function.

Bättig's compactification



1992: Bättig studied $H\colon \ell_2(\mathbb{Z}^2) \to \ell_2(\mathbb{Z}^2)$,
with periodic action of $a\mathbb{Z} \oplus b\mathbb{Z}$.
$\rightsquigarrow H(z)\colon \mathbb{C}[z^{\pm}]^{ab} \to \mathbb{C}[z^{\pm}]^{ab}$,
with Bloch variety BV.
The Newton polytope $\mathcal{N}$ is below.



To each face $\mathcal{F} = \mathrm{conv}\{ab\lambda, \pm bx, \pm ay\}$,
he constructs an $ab\mathbb{Z}$-periodic operator
$H_{\mathcal{F}}\colon \ell_2(\mathbb{Z}) \to \ell_2(\mathbb{Z})$,
and $H_{\mathcal{F}}(\zeta)\colon \mathbb{C}[\zeta^{\pm}]^{ab} \to \mathbb{C}[\zeta^{\pm}]^{ab}$ for $\zeta \in \mathbb{C}^{\times}$.
Set $\xi := \lambda x^{-a}$. Its Bloch variety,
$\mathrm{BV}_{\mathcal{F}} := \mathrm{Var}(\det(\xi I - H(\zeta)))$,
is the component of the boundary $\overline{\mathrm{BV}} \smallsetminus \mathrm{BV}$ corresponding to $\mathcal{F}$.

How much of this can be done in general?

Toric compactification of periodic operators

Given a $\mathbb{Z}^d$-periodic graph, we have algebraic quasi-periodic functions $\mathcal{Q} := \{\psi \in \mathbb{C}[z^\pm]^{\mathcal{V}} \mid \psi(\alpha + v) = z^\alpha \psi(v)\}$.

Choosing a fundamental domain W, we have $\mathcal{Q} \simeq \mathbb{C}[z^\pm]^W$.

Then the map $H(z)\colon \mathbb{C}[z^\pm]^W \to \mathbb{C}[z^\pm]^W$ of free modules is a map $H(z)\colon \mathcal{Q} \to \mathcal{Q}$.

Faust, Lopez-Garcia, Shipman, S.: Suppose that X is a toric variety compactification of $(\mathbb{C}^\times)^d$ or of $\mathbb{C} \times (\mathbb{C}^\times)^d$.

There is a natural sheaf of quasi-periodic functions $\mathcal{Q}_X \subset \mathcal{O}_X^{\mathcal{V}}$ with $\mathcal{Q}_X \simeq \mathcal{O}_X^W$.

This toric variety version of Fourier transform is a first step towards extending the operator $H(z)$ to a toric compactification.

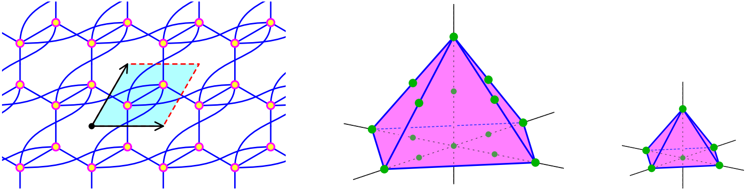
Full graphs

Let $\mathcal{A} := \mathcal{N}(\lambda I - H(z))$ be the Newton polytope of the entries.

A graph is *full* if $\mathcal{N} = |W|\mathcal{A}$.

Bättig's graph is not full. A dense graph is full.

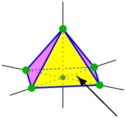
Here is another, with $\mathcal{N}$ and $\mathcal{A}$.



Its characteristic matrix $\lambda I - H(x,y)$ is

$$\begin{pmatrix} \lambda - u & a + bx^{-1} + cy^{-1} + dx + ey \\ a + bx + cy + dx^{-1} + ey^{-1} & \lambda - v \end{pmatrix} .$$

Graceful restriction for full graphs



Faces $\mathcal{F}$ of $\mathcal{A}$ correspond to faces of $\mathcal{N}$, and to charts $X_{\mathcal{F}}$ of the toric variety $X_{\mathcal{N}}$.

The indicated face of $\mathcal{A}$ contains the monomial x^{-1}.

Mutiply $\lambda I - H(x,y)$ by $m^{-1} = x$ to obtain

$$\begin{pmatrix} \lambda x - ux & ax + b + cxy^{-1} + dx^2 + exy \\ ax + bx^2 + cxy + d + exy^{-1} & \lambda x - vx \end{pmatrix} .$$

All terms lie in the coordinate ring of $X_{\mathcal{F}}$ and give an operator on the sheaf $\mathcal{Q}_{\mathcal{F}}$ of quasi-periodic functions on $X_{\mathcal{F}}$, whose determinant defines $\overline{\mathrm{BV}} \cap X_{\mathcal{F}}$.

(This comes from a spectral problem on a directed graph.)

In this way, the original characteristic matrix $\lambda I - H(z)$ extends to an operator on the sheaf $\mathcal{Q}_{\mathcal{N}}$ of quasi-periodic functions on $X_{\mathcal{N}}$.

Extending Bättig?

A toric chart $X_{\mathcal{F}}$ is a neighborhood of the orbit $O_{\mathcal{F}}$ corresponding to $\mathcal{F}$, whose ideal is generated by monomials not in $x + \mathcal{F}$.

We had $x(\lambda I - H(x, y))$:

$$\begin{pmatrix} \lambda x - ux & ax + b + cxy^{-1} + dx^2 + exy \\ ax + bx^2 + cxy + d + exy^{-1} & \lambda x - vx \end{pmatrix} .$$

The highlighted terms lie on $x + \mathcal{F}$ and give the matrix

$$\lambda x I_2 - \begin{pmatrix} 0 & b + cxy^{-1} \\ d + exy^{-1} & 0 \end{pmatrix} \;=\; \lambda x I_2 - H_{\mathcal{F}}(xy^{-1})\,.$$

The matrix $H_{\mathcal{F}}(\zeta^{\pm})$ corresponds to a Schrödinger operator on a periodic directed graph, the initial graph along the face $\mathcal{F}$.

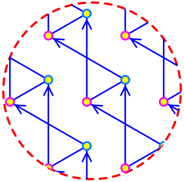
The initial graph

We have

$$\lambda x I_2 - \begin{pmatrix} 0 & b + cxy^{-1} \\ d + exy^{-1} & 0 \end{pmatrix} \;=\; \lambda x I_2 - H_{\mathcal{F}}(xy^{-1})\,.$$

The initial graph has the same vertices, with directed edges (and labeling) corresponding to entries in $H_{\mathcal{F}}$.

It is periodic with respect to a subgroup of $\mathbb{Z}^d$ corresponding to $\mathcal{F}$.



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