Algebraic Aspects of Periodic Operators

Applications of Commutative Algebra
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W/ Matthew Faust and
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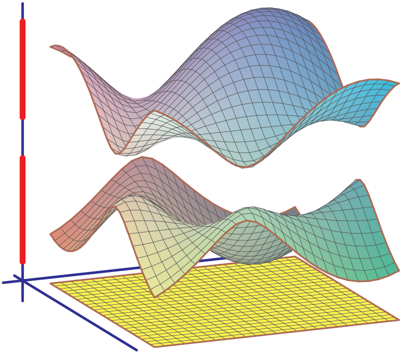

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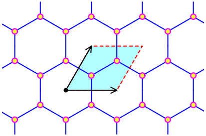
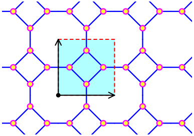
Tight Binding Model

A discrete model of a crystal is provided by a periodic graph Γ 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 $e\colon \mathcal{E} \to \mathbb{R}$.

The Schrödinger operator $H = H_{e,V}$ acts on $\ell_2(\mathcal{V})$:
For $\psi \in \ell_2(\mathcal{V})$, $H\psi$ 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, and its spectrum $\sigma(H) \subset \mathbb{R}$ corresponds to possible energy levels of electrons in the crystal.

Quasi-periodic functions

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 ψ_z

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

Floquet Theorem

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

(Fourier transform on $\ell^2(\mathcal{V})$ also arrives at this formulation.)

Bloch Variety

Floquet Theorem

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

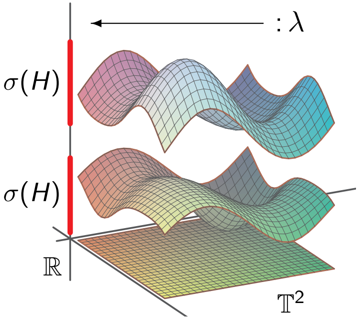
Letting z vary, $\psi\colon \mathbb{T}^d \times \mathcal{V} \to \mathbb{C}$ is *quasi-periodic* if $\psi(v+\alpha) = z^\alpha \psi(v)$. Then the Schrödinger operator

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

acts as a $W \times W$ matrix $H(z)$ of Laurent polynomials.

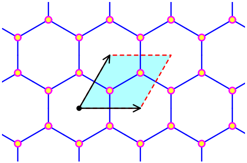
The *dispersion polynomial* $\Phi(z,\lambda) = \det(H(z) - \lambda I_W)$ defines an algebraic hypersurface in $\mathbb{T}^d \times \mathbb{R}$, called the *(real) Bloch variety*.

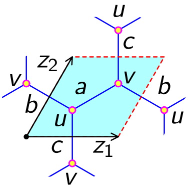
By Floquet Theorem, $\sigma(H)$ is the projection of the Bloch variety to $\mathbb{R}$.

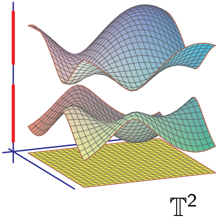


Example: Hexagonal Lattice

The hexagonal lattice underlies the structure of graphene. We show a labeling in a neighboorhood of a fundamental domain W and a Bloch variety with $a = b = c = 1$ and $v \neq u$.







We have

$$H(z) \ = \begin{pmatrix} u & -a - bz_1^{-1} - cz_2^{-1} \\ -a - bz_1 - cz_2 & v \end{pmatrix} \ .$$

Note that $H(z)^T = H(z^{-1})$.

The dispersion polynomial is $\Phi(z, \lambda) = \det(H - \lambda I)$, which is

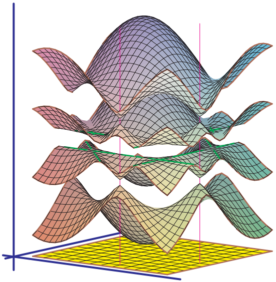
$$(u - \lambda)(v - \lambda) - (a + bz_1^{-1} + cz_2^{-1})(a + bz_1 + cz_2).$$

Some Reality

As $e_{(v,u+\alpha)} = e_{(v-\alpha,u)} = e_{(u,v-\alpha)}$ for all $u, v \in \mathcal{V}$, $\alpha \in \mathbb{Z}^d$,

$$H(z)^T = H(z^{-1})\,. \qquad (*)$$

Consequently, when $z \in \mathbb{T}^d$, $H(z)$ is Hermitian. Thus $H(z)$ has $|W|$ real eigenvalues, and the Bloch variety is a $|W|$-sheeted cover of $\mathbb{T}^d$.

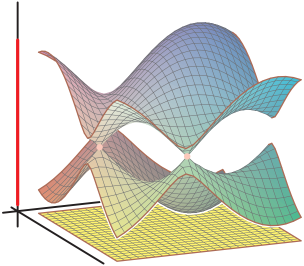


It is (of course) natural to complexify, allowing $(z, \lambda) \in (\mathbb{C}^\times)^d \times \mathbb{C}$.

By $(*)$ $\mathrm{Var}(\Phi(z, \lambda))$ is invariant under the nonstandard complex structure $(z, \lambda) \mapsto (\overline{z}^{-1}, \overline{\lambda})$, so the real Bloch variety is the set of real points of the complex Bloch variety.

$\rightsquigarrow$ This alternate reality is an interesting feature of this subject.

Some Objects, Algebraic



For the hexagonal lattice, if the potentials are equal $V(u) = V(v)$ and the edge weights form a triangle (!) then the real Bloch variety has two ordinary double points, called *Dirac points*.

The matrix $H(z) - \lambda I_W$ is a module endomorphism $\mathbb{C}[z^{\pm}, \lambda]^W$. Its kernel sheaf is called the *Bloch bundle* (by mathematical physicists). It is supported on the Bloch variety.

The level set of the Bloch variety at fixed λ is the *Fermi variety F_λ*.

Many basic objects in this area are algebraic in nature, as are a number of properties that have been studied.

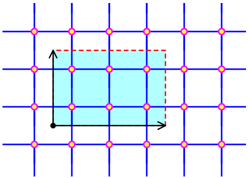
Some Questions From Physics

- Density of states: Spatial density of eigenfunctions at energy λ. This has been studied using free resolutions and by integrating a differential 1-form.
- Natural physical questions ask for the irreducibility of Bloch and Fermi varieties.
- *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 largely unknown, even for discrete periodic operators.
- There is interest in the existence and persistence of Dirac points.
- There is interest in the existence of flat bands.
- There are inverse problems of identifiability (isospectrality).

Everything Old is New Again

Gieseker, Knörrer, and Trubowitz (1993) studied the Schrödinger operator with $e_{(u,v)} = 1$ 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 studied/determined:

- Density of states (gave a formula).
- Irreducibility of Bloch and Fermi varieties.
- Smoothness of Bloch and Fermi varieties.
- Used a toric compactification BV of the Bloch variety and the Torelli Theorem.

This was presented in a Bourbaki Lecture by Peters in 1992.

– Later work compactified the operator on the toric variety.

Example: Integrated Density of States

Write H_n for the restriction of H to $\Gamma/n\mathbb{Z}^d$, a finite graph with $|W|n^d$ vertices.

H_n has $|W|n^d$ eigenvalues/vectors.

Let ρ_n be the discrete measure of point masses at the eigenvectors, normalised to have mass $|W|$.
$\rho := \lim_{n\to\infty} \rho_n$ has support $\sigma(H) \subset \mathbb{R}$.

Its density $d\rho/d\lambda$ with respect to Lebesgue measure is the *integrated density of states*.

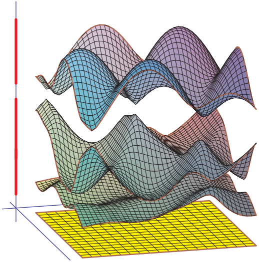
[GKT] : there is a differential form ω_λ on the Fermi variety F_λ (a section of the sheaf of relative differentials $\overline{BV} \to \mathbb{P}^1$) such that

$$\frac{d\rho}{d\lambda} \;=\; \int_{F_\lambda(\mathbb{R})} \omega_\lambda\,.$$

Spectral Edges (Important Physics Assumption)

Each spectral edge is the image of a critical point of λ on the Bloch variety. The spectral edges conjecture posits that generically, these critical points are nondegenerate.

First step: study all critical points.



Equations for the critical points are:

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

All polynomials have support a subset of the Newton polytope $\mathcal{N}(\Phi)$ of the dispersion polynomial $\Phi(z,\lambda)$.

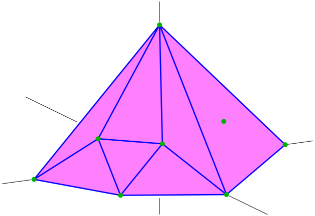
Kushnirenko $\#$ Critical Points $\leq \mathrm{vol}(\mathcal{N}(\Phi))$.

Toric Compactification of Bloch Variety

$\mathcal{N}(\Phi)$: Newton polytope of $\Phi(z, \lambda)$.

Its projective toric variety $X_{\mathcal{N}(\Phi)}$ compactifies the ambient space $(\mathbb{C}^\times)^d \times \mathbb{C}$ of Bloch variety.

The Critical Point Equations (CPE) are a linear section of $X_{\mathcal{N}(\Phi)}$.

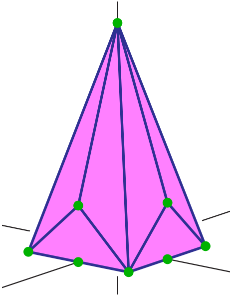


Fact: $\#$ Critical Points $<$ vol($\mathcal{N}(\Phi)$) if and only if there are solutions to (CPE) on boundary

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

a union of orbits $\mathcal{O}_F$ corresponding to non-base faces F of $\mathcal{N}(\Phi)$.

Contribution of Faces of $X_{\mathcal{N}(D)}$



Using homogeneity of facial forms:

- F vertical $\Longrightarrow$ CPE have solutions on $\overline{\mathcal{O}_F}$.
- If F is not vertical, then CPE have solutions on $\mathcal{O}_F \Longleftrightarrow \mathrm{BV} \cap \mathcal{O}_F$ is singular.

Theorem (F.-S. '24). *$\#$ critical points $=$ vol$(\mathcal{N}(D)) \Longleftrightarrow \mathcal{N}(D)$ has no vertical faces and $BV \cap \partial X_{\mathcal{N}(D)}$ is smooth.*

With Faust and Robinson, we give a contribution N_{struct} from vertical faces and from certain oblique facets, determined by the structure of the graph Γ.

Theorem (F.-R.-S.). *$\#$ critical points $\leq$ vol$(\mathcal{N}(D)) \; - \; N_{\mathrm{struct}}$*

($\rightsquigarrow$ interesting theme in polynomial optimisation.)

A Bestiary of Bloch Varieties

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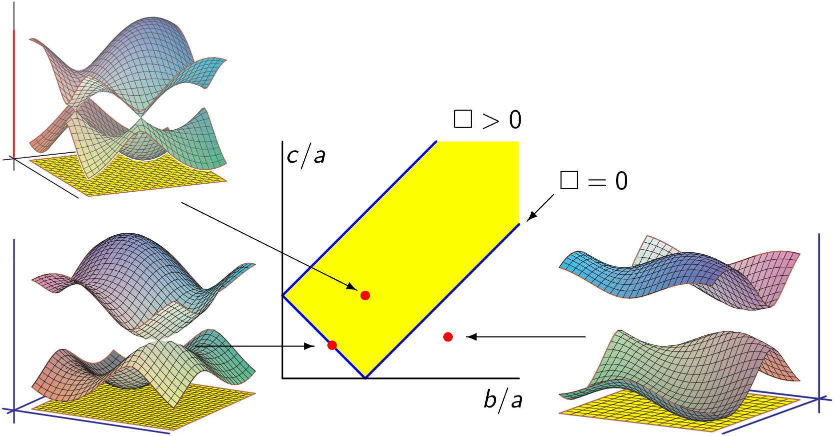
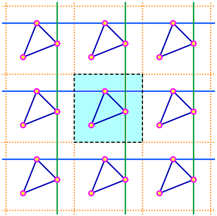
Geography when for $u = v \quad a, b, c > 0$

The location and type of critical points in terms of
$\square = (a+b+c)(a-b+c)(a+b-c)(a-b-c)$.



Robinson's Graph

The graph at right has an extremely fascinating Bloch variety. It has singularities, reality issues, critical points at infinity, etc. It is a deep challenge to study this, in part because of the lack of tools for treating non-standard real structures.



We display two views of its Bloch variety; it has two singular points and the apparent curve of self-intersection is not what it appears.