On dispersion relations of discrete periodic operators

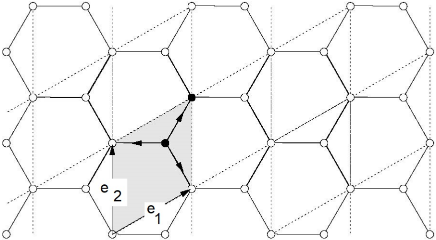
Peter Kuchment
Texas A&M University, USA
Supported by NSF

Workshop on Perturbation of Spectral Bands and Gaps
TU Dortmund, Fakultät für Mathematik
July 29th, 2021

Periodic graphs

Definition

1. Infinite graph Γ –$\mathbb{Z}^n$-**periodic** when equipped with a free and co-compact action of the group $G = \mathbb{Z}^n$, i.e. a mapping $(g, x) \in G \times \Gamma \mapsto gx \in \Gamma$
2. A **fundamental domain** W contains one representative from each orbit.



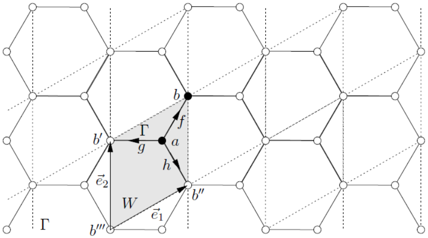
Example: the hexagonal "graphene" Γ with a $\mathbb{Z}^2$-action and a fundamental domain shaded.

Periodic operators

L – **difference operator** Γ. $=$ infinite matrix, rows and columns indexed by vertices.

Assume that L is **periodic w.r.t. the group action** and has **finite order**: each row it has finitely many non-zero entries.

Example: Laplace operator $Lf(v) := \sum_{b \sim a} f(b) - 3f(a)$



Hexagonal lattice Γ and fundamental domain W with its vertices $V(W) = \{a, b\}$ and edges $E(W) = \{f, g, h\}$.

Characters, quasimomenta, multipliers

Characters of $\mathbb{Z}^n$; for any **quasimomentum** $k \in \mathbb{R}^n(\mathbb{C}^n)$, the character

$$\gamma_k(g) = e^{ik\cdot g}, g \in \mathbb{Z}^n$$

$$z = (e^{ik_1}, \dots, e^{ik_n}) \in (\mathbb{C} \setminus \{0\})^n - \textbf{ Floquet multiplier}$$

Then

$$\gamma_k(g) = z^g = z^{g_1} \cdot \dots \cdot z^{g_n}$$

(Laurent polynomials arise)
k- **(or** z-**) automorphic function** $u(x)$ on Γ:

$$u(gx) = \gamma_k(g)u(x) = e^{ik\cdot g}u(x) = z^g u(x)$$

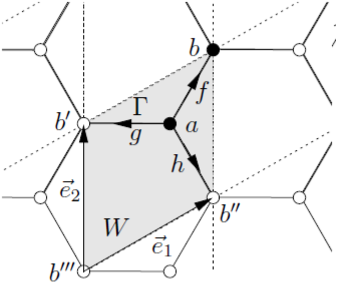
Also called **Floquet function** or **Bloch function** with quasimomentum k.

$$Lf(v) = \sum_{w \sim v} f(w) - 3f(v).$$

Apply L to $z = e^{ik}$-automorphic functions $u : u(gv) = z^g u(v)$.
Values at a, b suffice:

$$u(b') = z_1^{-1} u(b) = e^{-ik_1} u(b), u(b'') = z_2^{-1} u(b) = e^{-ik_2} ub).$$

Values at neighbors of b: $z_1 u(a) = e^{ik_1} u(a), z_2 u(a) = e^{ik_2} u(a)$.



"Symbol" of a periodic difference operator

Thus,

$$(Lu)(a) = -3u(a) + (z_1^{-1} + z_2^{-1} + 1)u(b),$$
$$(Lu)(b) = (z_1 + z_2 + 1)u(a) - 3u(b).$$

"Symbol" of L:

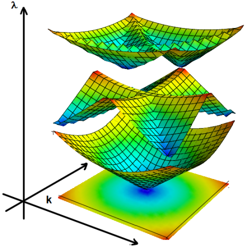
$$L(z) = \begin{pmatrix} -3 & z_1^{-1} + z_2^{-1} + 1 \\ z_1 + z_2 + 1 & -3 \end{pmatrix}$$

$L(z)$ – Laurent polynomial. Multiplying by $z_1 z_2$ becomes polynomial.

Dispersion relation (= Bloch variety)

Definition

- **Real** (**complex**) **dispersion relation** (or **Bloch variety**) B_L of L is the subset $(k, \lambda) \in \mathbb{R}^n_k \times \mathbb{R}_\lambda$ ($\mathbb{C}^n_k \times \mathbb{C}_\lambda$) $Lu = \lambda u$ has a non-zero k- (or z-) automorphic solution $u(x) = e^{ik\cdot x} p(x)$, where $p(x)$ is $\mathbb{Z}^n$-periodic.
- $=$ the graph of the multiple-valued function $k \mapsto \sigma(L(k))$.
- $=$ The set of solutions of $\det\big(L(e^{ik}) - \lambda\big) = 0$.

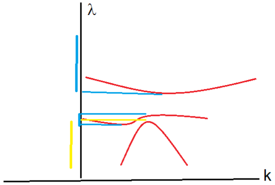


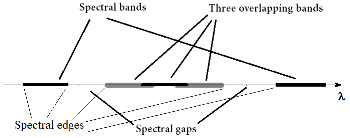
jth eigenvalue branch $\lambda_j(k)$ is j**th band function**.

Spectrum

Theorem

The range of this function (= projection of the dispersion relation to the λ-axis) coincides with the spectrum $\sigma(L)$.





Other roles of the dispersion relation

$$\sigma(L) = \sigma_{ac}(L) \bigcup \sigma_{pp}(L) (\sigma_{sc}(L) = \emptyset)$$

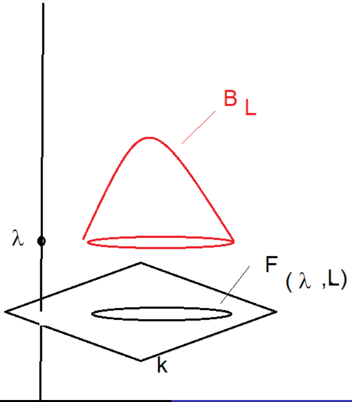
- Absence of *pp* spectrum $\Leftrightarrow$ no flat branches.
- Semi-conducting $\Leftrightarrow$ presence of gaps.
- Effective masses, graphene's properties, topological insulators, Anderson localization, embedded eigenvalues, ...
- Green's function decay, Liouville theorems, Homgenization

Fermi surfaces

Definition

For a fixed $\lambda \in \mathbb{R}$, the **Fermi surface** $F_{\lambda,L}$ is the λ- level set for the multivalued function whose graph is the dispersion curve.
I.e.

$$F_{\lambda,L} := \{k \,|\, (k,\lambda) \in B_L\}$$



Problems. Continuous case

1. **Absolute continuity of spectrum** (= no flat components). Expected for 2nd order periodic elliptic operators with "nice" coefficients. Not completely proven, but many results (Birman, Friedlander, Kuchment, Levendorskiy, Shen, Shterenberg, Sobolev, Suslina, Thomas, ... **Not true for higher order.**
2. **Stronger conjecture:** Bloch variety is irreducible. Proven for 2D Schrödinger operators (Knörrer and Trubowitz, 1990).
3. **Irreducibility of the Fermi surface** for "almost all" energies λ. Proven in the case above. Relation to embedded eigenvalues.
4. **Locations of extrema at symmetry points**. Incorrect in general (Exner, Harrison, Kuchment, Sobolev, Winn). Some positive results (Berkolaiko, Canzani, Cox, Marzuola 2020)

1. *Irreducibility of the Bloch variety.* Does not hold in general, σ_{pp} might be present. Discussion by Kuchment (abelian case, 1989), Veselić (amenable case, 2004), ...
   Theorem: Existence of an L_2 eigenfunction $\Leftrightarrow$ existence of a compactly supported one, and compactly supported ones are complete.
2. In the elliptic PDEcase - superexponential decay.
3. *Irreducibility of the Fermi variety.* For the case when $\Gamma = \mathbb{Z}^2$ - for almost all λ (Gieseker, Knörrer, Trubowitz, book 1991). For all λ except one, and in higher dimensions (Wencai Liu, 2020, arXiv) Reducibility (W. Li, S. Shipman).

IRREDUCIBILITY OF THE BLOCH VARIETY FOR FINITE-RANGE SCHRÖDINGER OPERATORS

JAKE FILLMAN, WENCAI LIU, AND RODRIGO MATOS

Conjectured structure of gap edges (=extrema of the band functions):
generically, extrema are isolated & non-degenerate. Partial: Klopp and Ralston (2000), Colin de Verdiere (1991), Filonov and Kachkovskyi.

Band edge non-degeneracy in discrete case.

Does not hold in some examples (Filonov& Kachkovskiy, 2018)
Discrete Schrödinger operator $H = \Delta + V$ in $l_2(\mathbb{Z}^2)$:

$$(\Delta u)_n = 0.5(u_{n+e_1} + u_{n-e_1} + u_{n+e_2} + u_{n+e_2})$$

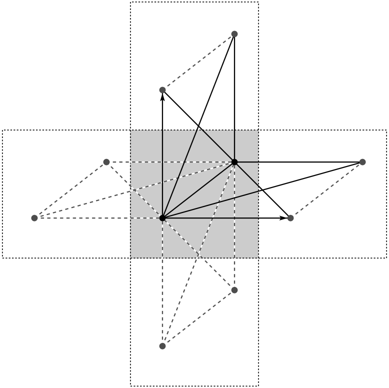
$$(Vu)_n = \begin{cases} v_0 u_n, & \text{if } (n_1+n_2) \text{ even} \\ v_1 u_n, & \text{if } (n_1+n_2) \text{ odd} \end{cases}$$

lattice of two different types of atoms in a chessboard order. V with periods $(2e_1; e_1 + e_2)$.

More freedom is needed?

Do, Kuchment, Sottile, 2020

Γ equipped with a periodic **weight** function α (a metric) that assigns to edges a non-negative numbers.



Fundamental domain W. Periods e_1, e_2. Nine (solid) edges. The dotted edges and other atoms are obtained by shifting. α_j - weights associated with the solid edges.

"Laplace-Beltrami operator"

$$L_\alpha f(u) = \sum_{e=(u,v)\in E} \alpha(e)(f(u) - f(v))$$

Dichotomy (holds for any periodic difference operator of a finite order):

Theorem

The set of vectors α for which there exist non-degenerate critical points of the dispersion relation either belongs to a proper algebraic subset or contains the complement of such a set.

Analog for PDEs has not been proven.

Corollary

If there is an open (or even positive measure) set of αs over which there are no degenerate critical points of the dispersion relation, then this holds true outside of a proper algebraic subset.

The main result

Theorem

The dispersion relation of the operator L_α generically (i.e., outside of an algebraic subset of the parameters α) satisfies all three conditions of conjecture: the critical points are attained by only one band function, are isolated, and non-degenerate.

PDE - countable union of analytic sets?

"Proofs"

Consider the natural projection of the 12-dimensional space of (λ, z, α) onto the 9-dimensional space of αs.

1st "proof"

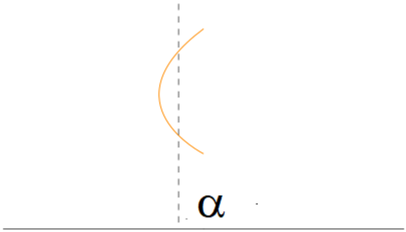
The "bad" subset of the 12-dimensional space is given by 4 algebraic conditions:

- Being on the Bloch variety - one condition.
- Being a critical point - 2 conditions.
- being degenerate - one condition.

Idea: one "expects" the bad set to have dimension 8. Then it projection into the 9-dimensional one would be "small."
Issue: Four equations might have dependencies, and the algebraic "bad" set might have components of dimension ≥ 9.
"Solution": Computational algebraic geometry software finds all components and they are OK.
Concern: This is not a certifiable computation.

More "proofs"

2nd "proof": According to the dichotomy, checking "random" αs would give the correct answer with "probability one."
Works, but not rigorous.
3rd, rigorous proof : Find a "good" value α and check that its neighborhood is "good" and then shut the Corollary.



Works, but involves non-trivial algebraic geometry. Not clear how to generalize.
Recent extensions by M. Faust and F. Sottile

Is having more parameters better?

Conjecture

If the generic non-degeneracy holds for some parameters space α, then allowing more parameters to vary (e.g., adding potentials besides the metric) cannot destroy this feature.

Theorem

The conjecture holds for the example considered.


Спасибо
ありがとうございました
Danke
GRACIAS
TASHAKKUR ATU
SUKSAMA
THANK
YOU
ARIGATO
SHUKURIA
GRAZIE
MEHRBANI
BOLZİN
MERCI
谢谢
Cảm Ơn bạn
Дякую