Analytic properties of dispersion relations and spectra of periodic operators - a survey

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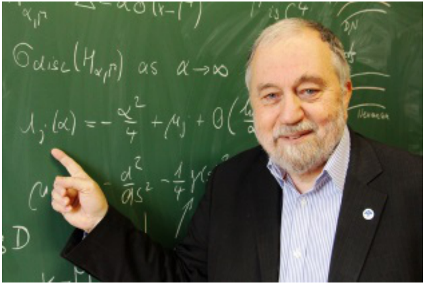
QMath13, Atlanta, October 8 - 11, 2016

Joint works with N. Do, P. Exner, J. Harrison, Minh Kha, Y. Pinchover, A. Raich, A. Sobolev, F. Sottile, B. Vainberg, B. Winn

Supported by the BSF and NSF

First things first



70 corresponds to the totality of an evolution, an evolutionary cycle being fully completed, according to Saint Augustin.

It's official: you are a totally evolved creature, Pavel!

Greetings from the under-evolved, dear friend! Looking up to you!

Related works by

S. Agmon, M. Aizenman & J. Schenker, M. Avellaneda & F.-H. Lin, Y. Avron & B. Simon, M. Babillot, M. Birman & T. Suslina, Y. Colin de Verdiere, A. Figotin, N. Filonov & I. Krachkovski, C. Gerard, M. Gromov & M. Shubin, V. Lin, V. Lin & Y. Pinchover, V. Lin & M. Zaidenberg, J. Moser & M. Struwe, M. Murata & T. Tsuchida, S. Novikov, Y. Pinchover, R. Pinsky, W. Woess

Content

- Dispersion relations (=Bloch varieties) of periodic operators.Band-gap structure of the spectrum.Fermi surfaces.
- Analyticity of Bloch and Fermi Varieties.
- Irreducibility and its role
- Spectral edges and extrema: location and non-degeneracy.
- Threshold effects (i.e., those depending upon spectral structure at and near a spectral edge):
  - Condensed matter – effective masses.
  - Homogenization.
  - Green's function behavior.
  - Liouville-Riemann-Roch theorems.
  - Impurity states.

Periodic Schrödinger operator

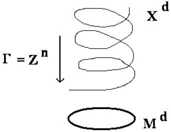
Main example:

$$H = -\Delta + V(x),$$

where V is $\mathbb{Z}^n$-periodic real function of appropriate class (e.g., $V \in L_\infty(\mathbb{R}^n)$).
H -self-adjoint in $L_2(\mathbb{R}^n)$ with domain $H^2(\mathbb{R}^n)$.

More general periodic elliptic operators

More generally, $X \mapsto M$ - normal covering with the deck group $\mathbb{Z}^n$ and compact base M.



X and M can be Riemannian manifolds, analytic manifolds, graphs, or quantum graphs.
H - a periodic operator on X, **elliptic**, i.e. Fredholm on M.
Overdetermined problems: $\overline{\partial}$-operator, Maxwell.

Dispersion relation = Bloch variety

Bloch functions

$$u(x) = e^{ik\cdot x} p(x)$$

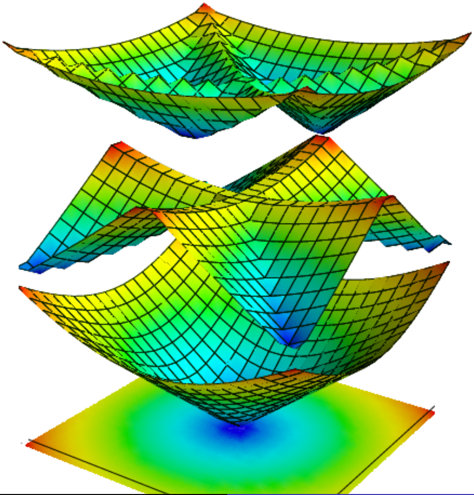
with $p(x)$ being $\mathbb{Z}^n$-periodic, **quasi-momentum** $k \in \mathbb{R}^n$.
Dispersion relation = Bloch variety =

$$\{(k, \lambda) \in \mathbb{R}^{n+1} \,|\, Hu = \lambda u, u \neq 0 \text{ Bloch solution, quasi-momentum } k\}$$

ComplexBloch variety =

$$\{(k, \lambda) \in \mathbb{C}^{n+1} \,|\, Hu = \lambda u, u \neq 0 \text{ Bloch solution, quasi-momentum } k\}$$

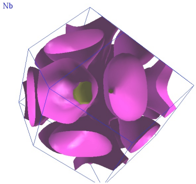
A picture



Fermi surface

Fermi surface at the energy level $\lambda =$ level set of dispersion relation

$$:= \{k \in \mathbb{R}^n (\text{ or } \mathbb{C}^n) \mid Hu = \lambda u, u \neq 0 \text{ Bloch sol'n, quasi-momentum } k\}$$



Fermi surface of Niobium

Dispersion branches (bands)

Dispersion relation is the graph of a multi-valued function $k \mapsto \lambda(k)$.
Single-valued, continuous, piecewise analytic **band functions**

$$\lambda_1(k) < \lambda_2(k) \leq \lambda_3(k) \leq \dots$$

Spectrum

$$H = \int_{\mathcal{B}}^{\oplus} H(k)dk.$$

The direct integral decomposition represents the operator as a "pseudo-differential operator with the miltiple-valued symbol $\lambda(k)$"

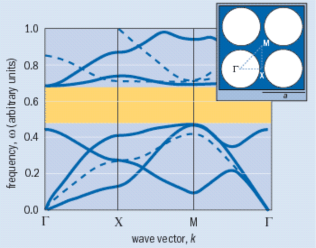
Theorem: *The spectrum of H is equal to the range of $\lambda(k)$, i.e. to the projection of the Bloch variety onto the λ-axis.*

Band-gap structure

Range of $\lambda_j(k)$ (a closed interval) - the j**th spectral band** I_j.

$$\sigma(H) = \bigcup_j I_j.$$

Band may overlap. They may also open unfilled **spectral gaps.**



Analyticity

Theorem

The complex Bloch (Fermi) variety is a codimension 1 *analytic sub-variety of* $\mathbb{C}^{n+1}$ $(\mathbb{C}^n)$.

In fact, it is the set of all zeros of an entire function of some exponential order.

Bloch variety irreducibility

Conjecture *For any periodic Schrödinger operator (or maybe more general periodic elliptic operator of second order) the Complex Bloch variety is irreducible.*

- I.e., any small open piece of dispersion relation determines the whole Bloch variety completely.
- Stronger than absolute continuty
- Holds in $1D$, W. Kohn '59, Avron & Simon '78
- Proven in $2D$ by Knörrer and Trubowitz '90
- Does not hold for higher order operators.

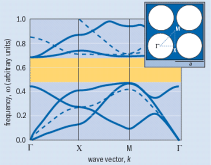
Fermi variety irreducibility

Conjecture *For any periodic Schrödinger operator (or maybe more general periodic elliptic operator of second order) the Complex Fermi variety is irreducible for almost all spectral levels.*

- I.e., any its small open piece determines the whole
- Its role: Irreducibility of the Fermi surface at some level λ in the continuous spectrum implies that localized perturbations cannot create embedded eigenvalues at λ (P.K. and B. Vainberg '98)
- Proven in $2D$ **discrete** case (Gieseker, Knörrer, and Trubowitz '93 book). Easy to prove for separable potentials and some other simple cases (P.K. and Vainberg).

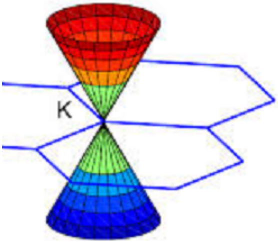
General understanding

• The direct integral decomposition represents the operator as a "pseudo-differential operator with the miltiple-valued symbol $\lambda(k)$"
• The behaviour of wave packets with energy close to a value λ is governed by the structure of the dispersion relation near this level.
• Near a parabolic extremum the behavior should be "Laplacian-like"



Local structure: Conic singularities

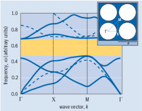
Graphene, etc.
Dirac cones ("Diabolic points")



At the cone's apex behaviour as of solutions of Dirac's equation$\Rightarrow$ graphene marvels.
Wallace '47 (discrete case), P. K. and Post '7 (quantum graph case), Fefferman and Weinstein '12+ , Berkolaiko and Comech '14.

Spectral edges location

Spectral edges occur at some extrema of dispersion relation.
At which values of k can the band edges occur?
Frequent response: at some points of symmetry.



Disproved:
Harrison, P.K., Sobolev, Winn '07
Exner, P.K., Winn '10.

Generic non-degeneracy?

Bad things that can happen:

the same extremal value attained by two or more band functions;

a non-isolated extremum of one band function;

isolated, but degenerate extremum.

Conjecture (stated by many): *generically (with respect to the parameters of the operator, say potential)*

A: *only a single band function reaches the extremal value.*

B: *the extremum is isolated.*

C: *the extremum is non=degenerate (i.e., of parabolic shape).*

What is known?

A proven by Klopp and Ralston '00.

B proven for 2D Schrödinger, Filonov & Krachkovski, '15.

Not just generic!

The whole conjecture proven for

- the bottom of the spectrum (Kirsch & Simon '87)
- in 2D, small C^{∞} potentials, Y. Colin de Verdiere '91
- $\mathbb{Z}^2$-periodic graphs with two atoms (vertices) per a unit cell, N. Do, P.K., F. Sottile, '14.

Transversality approaches???

Why would one care?

"**Threshold effects**" (coined by Birman & Suslina):
Effective masses of electrons
Homogenization
Liouville and Liouville-Riemann-Roch theorems
Green's function asymptotics

Green's function asymptotics at a generic edge

Theorem (P.K. and A. Raich, '12) Let $n \geq 3$, $R_{-\epsilon} = (L+\epsilon)^{-1}$ for $0 < \epsilon \ll 1$ – resolvent of H near the spectral edge $\lambda = 0$.
Let also $R : L^2_{comp}(\mathbb{R}^n) \mapsto L^2_{loc}(\mathbb{R}^n)$ be such, that $\forall$ $\phi, \psi \in L^2_{comp}(\mathbb{R}^d)$,

$$\langle R_{-\epsilon}\phi\,\psi\rangle = \lim_{\epsilon\to 0}\langle R\phi\,\psi\rangle.$$

Then, the Schwartz kernel $G(x,y)$ of R (**the Green's function of** H), has the following asymptotics when $|x-y| \to \infty$:

$$G(x,y) = \frac{\pi^{-n/2}\Gamma(\frac{n-2}{2})e^{i(x-y)\cdot k_0}}{2(\det\mathcal{H})^{1/2}|\mathcal{H}^{-1/2}(x-y)|^{n-2}}\frac{\varphi(k_0,x)\overline{\varphi(k_0,y)}}{\|\varphi(k_0)\|^2_{L^2(\mathbb{T})}}\left(1+O\left(\frac{1}{|x-y|}\right)\right)+r(x,y),$$

where $r(x,y) = O(|x-y|^{-N})$ for any $N>0$, $\mathcal{H}$ - Hessian of the dispersion relation at k_0.

Green's function asymptotics inside the gap

Theorem (Minh Kha, P.K., A. Reich, '15)
For $\lambda < 0, |\lambda| \ll 1$, Green's function G_λ of H admits the following asymptotics as $|x-y| \to \infty$:

$$G_\lambda(x,y) = \frac{e^{(x-y)\cdot(ik_0-\beta_s)}}{(2\pi|x-y|)^{(n-1)/2}} \times \frac{|\nabla E(\beta_s)|^{(n-3)/2}}{\det\left(-\mathcal{P}_s HessE(\beta_s)\mathcal{P}_s\right)^{1/2}} \times \frac{\phi_{k_0+i\beta_s}(x)\overline{\phi_{k_0-i\beta_s}(y)}}{(\phi_{k_0+i\beta_s},\phi_{k_0-i\beta_s})_{L^2(\mathbb{T})}} + e^{(y-x)\cdot\beta_s} r(x,y).$$

Here $s = (x-y)/|x-y|$, $\mathcal{P}_s$ – orthogonal projection from $\mathbb{R}^n$ onto the tangent space at the point s of the unit sphere $\mathbb{S}^{n-1}$, and $r(x,y) = O(|x-y|^{-n/2})$.

Previously known and generalizations

• Both results had been known at (and near) the bottom of the spectrum: M. Babillot '97, 98, M. Murata & T. Tsuchida '03, 06, W. Woess '00.

• Generalization of both to abelian coverings, Minh Kha '15. Some quirks of this case.

Lioville theorems: assumptions and notations

$\lambda = 0$

$V_N(H) := \{u \,|\, Hu = 0, |u(x) \leq C(1 + |x|)^N\}$

$F_H := \{k \,|\,$ exists $U \neq 0, H(k)u = \lambda u\}$ – Fermi surface.

$dim V_N(H) < \infty$ S. T. Yau '75. Colding & Minicozzi '97

Liouville theorems, P.K. & Pinchover, '01, '07

P.K. & Pinchover, '01, '07, partial result by P. Li
Triggered by work s of Avellaneda & F.-H. Lin and J. Moser & M. Struwe '92

Theorem (Liouville)
The following statements are equivalent:

1. $dim\, V_N(H) < \infty$ for some $N \geq 0$
2. $dim\, V_N(H) < \infty$ for all $N \geq 0$
3. $\#F_H < \infty$

Overdetermined

This holds for overdetermined elliptic systems as well. E.g.,
Theorem (holomorphic Liouville)
On abelian covering of a compact complex manifold
$dim\, V_N(\overline{\partial}) < \infty$ for all $N \geq 0$.
Proof:
Indeed, if $u(\gamma z) = e^{ik\cdot\gamma}u(z)$, then $|u(z)|$ is periodic and thus, by maximum principle, $u(z)$ constant. Hence, $F_{\overline{\partial}} = \{0\}$.

Dimension count

At edge of the spectrum – 0 is a simple eigenvalue and $F_L = k_0$.
Taylor expansion $\lambda(k) = \sum\limits_{l \geq l_0} \lambda_l (k - k_0)$.

Theorem (quantitative Liouville)

$$dim\, V_N(L) = \begin{pmatrix} n+N \\ N \end{pmatrix} - \begin{pmatrix} n+N-l_0 \\ N-l_0 \end{pmatrix}.$$

Liouville-Riemann-Roch theorem

- Gromov & Shubin '92 – '94 - Riemann-Roch theorems for elliptic operators with prescribed compact divisor of zeros/poles.
- Minh Kha & P.K. '16 - Liouville-Riemann-Roch theorems for elliptic operators on co-compact abelian coverings with a compact divisor.

A survey

More detailed survey in
P. K., An overview of periodic elliptic operators, *Bulletin of the AMS*, **53** (2016), No. 3, 343–414.

Thanks

Till 120, Pavel!

Thank you