Periodic Approximants to Aperiodic Hamiltonians

Sponsoring

CRC 701, Bielefeld, Germany

SFB 878, Münster, Germany

Groups, Geometry & Actions

Jean BELLISSARD

Westfälische Wilhelms-Universität, Münster
Department of Mathematics

Georgia Institute of Technology, Atlanta
School of Mathematics & School of Physics
e-mail: jeanbel@math.gatech.edu

Contributors

S. Beckus, *Department of Mathematics*, Technion, Haifa, Israel

G. De Nittis, *Facultad de Matemáticas & Instituto de Física*, Pontificia Universidad Católica, Santiago, Chile

Main References

J. E. Anderson, I. Putnam,
Topological invariants for substitution tilings and their associated C^*-algebras,
Ergodic Theory Dynam. Systems, **18**, (1998), 509-537.

F. Gähler, Talk given at *Aperiodic Order, Dynamical Systems, Operator Algebra and Topology*
Victoria, BC, August 4-8, 2002, *unpublished*.

S. Beckus, J. Bellissard,
Continuity of the spectrum of a field of self-adjoint operators,
Ann. Henri Poincaré, **17**, (2016), 3425-3442.

S. Beckus, J. Bellissard, G. De Nittis,
Spectral Continuity for Aperiodic Quantum Systems I. General Theory,
`arXiv:1709.00975`, August 30, 2017, *to appear in* J. Funct. Anal..

S. Beckus, J. Bellissard, G. De Nittis,
Spectral Continuity for Aperiodic Quantum Systems II. Periodic Approximation in 1D,
`arXiv:1803.03099`, March 8, 2018.

S. Beckus, J. Bellissard, H. Cornean,
Hölder Continuity of Spectra of a Class of Aperiodic Schrödinger Operators,
in preparation.

Content

Warning *This talk is also reporting on unpublished works or under writing.*

1. Motivation
2. Method and Results
3. Approximations
4. Periodic Approximations in $1D$

I - Motivations

Goal

To compute the spectrum and predict the properties of spectral measures of a self-adjoint operator encoding the quantum motion of an electron in $\mathbb{R}^d$ $(d = 1, 2, 3)$ *submitted to an aperiodic but homogeneous potential.*

This should represent the independent electron approximation used to investigate the electronic properties of aperiodic solids or liquids.

By *computing* it is meant both a mathematical method permitting to study it and a potential algorithm liable to compute numerically the results.

Crystals

If the potential is *periodic* with a discrete co-compact period group $G \subset \mathbb{R}^d$, the *translation symmetry* can be used to simultaneously diagonalize the Hamiltonian and the G-action. *(Bloch Theory, 1928))*

Additional *point symmetries* help computing further *(Wigner, Seitz, 1933)*.

Usual Results:

- Band spectrum
- Absolutely continuous spectral measures.

Disordered Systems

An additional potential is added, random in space but time-independent *(quenched disorder)* *(Anderson, 1958)*.

Example: semiconductors at very low temperature.

Results:

- *Strong Localization:* when the kinetic energy is dominated by potential energy.
  Pure point spectrum, only few gaps (proved) *(Pastur, Molcanov 1978, Fröhlich, Spencer 1981, and many others until now)*.
- *Weak Localization:* when the kinetic energy dominates the potential energy.
  Expected (predicted by Physicists, unproved yet): *a.c.* simple spectrum, diffusive quantum motions.

Quasicrystals

Long Range Order, points symmetries, inflation symmetry, algorithmic structure *(cut-and-project method)* *(Schechtman, et al. 1984)*

Expected Results:

- Cantor spectrum at low energy, no gap at high energy in $d \geq 2$.
- *s.c.* spectrum in the gapped region
- *a.c.* simple spectrum at high energy, with level repulsion
- sub-diffusive motion at high energy, in $d \geq 3$ *(insulating phase)*.

In real Materials:

- Additional weak disorder, from structural origin *(phason modes)* or structural defects *(flip-flops)*.
- Implies weak or strong localization at very low temperature *(observed in few experiments)*.

II - Methods, Results

Specific Models

- *d = 1 systems:* $\psi(n+1)+\psi(n-1+V(n)\psi(n) = E\psi(n)$ use the transfer matrix method *(dynamical cocycles)*.
  - *Almost Mathieu:* $V(n) = 2\lambda\cos 2\pi(x-n\alpha)\ \alpha \notin \mathbb{Q}$

    (Hofstadter 1976, Jitomirskaya 1998 and many others)
  - *Fibonacci:* $V(n) = \chi_{[0,\alpha)}(x-n\alpha)\ \alpha = (\sqrt{5}-1)/2$

    (Damanik, Gorodetzki, et al 1992-2016)
  - *Automatic sequences:* Thue-Morse *(JB 1988, 1993; Liu, Qu 2015, many others)*. Calculation of spectral gap edges, gap labeling, Hausdorff dimension. Spectral type of the spectral measure
- *Cluster Approximation:* numerical method *(Khomoto et al, 1985-86)* strong boundary effects.
- *Periodic Approximation :* *(Hofstader 1976, Benza-Sire 1992)*, exponentially small error in the period *(Prodan 2012)*, level repulsion *(U. Grimm et al, 1998)*.

- *Conclusion:*
  - Small number of results except in specific examples, mostly $d = 1$ models with nearest neighbor influence, using transfer matrix and dynamical systems.
  - No systematic method for $d \geq 2$. Only accurate numerical methods.
  - Need of new mathematical approach.

III - Approximations

S. Beckus, J. Bellissard,
Continuity of the spectrum of a field of self-adjoint operators,
Ann. Henri Poincaré, **17**, (2016), 3425-3442.

S. Beckus, J. Bellissard, G. De Nittis,
Spectral Continuity for Aperiodic Quantum Systems I. General Theory,
`arXiv:1709.00975`, August 30, 2017.
to appear in J. Funct. Anal..

Examples

- Tilings with *finite local complexity (FLC)*, or, equivalently, Delone sets of finite type *(Anderson, Putnam, 1998, Lagarias 1999, Gähler 2002, JB, Benedetti, Gambaudo, 2006)*. Anderson and Putnam have proposed a construction of a sequence of CW-complex, describing accurately the tiling space by inverse limit, and providing an accurate finite volume approximation.

- *Delone sets* used in Condensed Matter Physics, including liquids *(JB, 2015)*. Use the time-scale separation between electronic and atomic movements. The local description through the *Voronoi tiling* and the *Delaunay triangulation*, gives predictions observed in numerical simulations. A realistic simplified model for viscosity in liquids can be derived then *(JB, Egami, 2018)*.

Approximation of Subshifts

- For $\mathcal{A}$ a finite set *(alphabet)*, and $d \in \mathbb{N}$, the full d-shift is the compact metrizable Hausdorff space $\Omega = \mathcal{A}^{\mathbb{Z}^d}$ equipped with the $\mathbb{Z}^d$-action by translation $(\tau^a \xi)_m = \xi_{m-a}$.
- The space $\mathfrak{J}$ of all *closed $\mathbb{Z}^d$-invariant subsets* is equipped with the *Hausdorff topology*. It is itself compact, metrizable and Hausdorff.
- A *pattern* of radius $R > 0$ in $M \in \mathfrak{J}$, is the restriction of $\tau^a \xi$ to the ball $\{m \in \mathbb{Z}^d\,;\, |m| \leq R\}$ for some $a \in \mathbb{Z}^d$ and some $\xi \in M$.

Theorem *Given $M \in \mathfrak{J}$, a sequence $(M_n)_{n \in \mathbb{N}}$ in $\mathfrak{J}$ converges to M if and only for any $R > 0$, there is $N \in \mathbb{N}$ such that for any $n > N$, M_n and M share the same patterns of radius R.*

Groupoid Approach

(Ramsay '76, Connes, 79, Renault '80)

In most practical situation there is no symmetry group at all. However, the structure and the translation action, can always be expressed in terms of a *groupoid*.

A *groupoid* G is a category the object of which G_0 and the morphism of which G make up two sets.

Groupoid Approach

More precisely

- there are two maps $r, s : G \to G_0$ (*range* and *source*)
- $(\gamma, \gamma') \in G_2$ are *compatible* whenever $s(\gamma) = r(\gamma')$
- there is an associative *composition law* $(\gamma, \gamma') \in G_2 \mapsto \gamma \circ \gamma' \in G$, such that $r(\gamma \circ \gamma') = r(\gamma)$ and $s(\gamma \circ \gamma') = s(\gamma')$
- a *unit* e is an element of G such that $e \circ \gamma = \gamma$ and $\gamma' \circ e = \gamma'$ whenever compatibility holds; then $r(e) = s(e)$ and the map $e \to x = r(e) = s(e) \in G_0$ is a *bijection* between units and objects;
- each $\gamma \in G$ admits an *inverse* such that $\gamma \circ \gamma^{-1} = r(\gamma) = s(\gamma^{-1})$ and $\gamma^{-1} \circ \gamma = s(\gamma) = r(\gamma^{-1})$

Locally Compact Groupoids

- A groupoid G is *locally compact* whenever
  - G is endowed with a locally compact Hausdorff 2nd countable topology,
  - the maps r, s, the *composition* and the *inverse* are *continuous* functions.

  Then the set of units is a closed subset of G.

- A *Haar system* is a family $\lambda = (\lambda^x)_{x \in G_0}$ of positive Borel measures on the fibers $G^x = r^{-1}(x)$, such that
  - if $\gamma : x \to y$, then $\gamma^* \lambda^x = \lambda^y$
  - if $f \in C_c(G)$ is continuous with compact support, then the map $x \in G_0 \mapsto \lambda^x(f)$ is *continuous*.

Groupoid C*-algebra

Let G be a locally compact groupoid with a Haar system λ. Then

- like with locally compact groups, it is possible to define a *convolution algebra*, endowed with an *adjoint* operation;
- in order to include the influence of magnetic fields (more generally of gauge fields), this convolution algebra must be *twisted*, using a 2-*cocycle*;
- even *a non uniform magnetic fields*, provided it is bounded and uniformly continuous, can be represented this way to the expense of *modifying* the underlying groupoid in a controlled way;
- using the concept of representation, the twisted convolution algebra can be completed to make up a *C*-algebra*;

Groupoid C*-algebra

- like for groups, there is a concept of *amenability* for groupoids *(Anantharam-Delaroche, Renault '99)*; then if non-amenable, the corresponding C*-algebra *may not be unique*, with a minimal one called *reduced*, and a maximum one, called *full*; amenability leads to coincidence of all such C*-algebras;
- in all practical cases met in Condensed Matter Physics, the groupoid used is *amenable* and C*-algebras defined above is the smallest such algebra generated by the *energy (translation in time)* and the action of the *translation in space* twisted by the magnetic field.

Continuous Fields of Groupoids

(N. P. Landsman, B. Ramazan, 2001)

- A *field of groupoid* is a triple (G, T, p), where G is a groupoid, T a set and $p : G \to T$ a map, such that,
  if $p_0 = p \restriction_{G_0}$, then $p = p_0 \circ r = p_0 \circ s$
- Then the subset $G_t = p^{-1}\{t\}$ is a groupoid depending on t.
- If G is *locally compact*, T a *Hausdorff* topological space and p *continuous* and *open*, then $(G, T, P) = (G_t)_{t \in T}$ is called a *continuous field of groupoids*.
- The concept of *continuous field of 2-cocycle* can also be defined *(Rieffel '89, JB, Beckus, De Nittis '18)*.

The Tautological Groupoid

Let G be a locally compact groupoid with G_0 *compact* and a Haar system λ.

- Two units $x, y \in G_0$ are *equivalent*, denoted by $x \sim y$, if there is $\gamma \in G$ such that $r(\gamma) = x$ and $s(\gamma) = y$. This is an equivalence relation.
- A subset $M \subset G_0$ of the unit space is called *invariant* whenever if $x \in M$ and $y \sim x$ implies $y \in M$. Then its closure $\overline{M}$ is also invariant.
- Let $\mathfrak{J}(G)$ be the set of all *closed invariant subsets* of G_0. Equipped with the Hausdorff topology, it is *compact*.

The Tautological Groupoid

- The set $\mathcal{T}(\Gamma)$ of pairs (M, γ) such that both $r(\gamma)$ and $s(\gamma)$ are in M, is a groupoid called the *tautological groupoid* of G.

- The map $p_G : \mathcal{T}(G) \to \mathcal{J}(G)$ defined by $p_G(M, \gamma) = M$ is *continuous* and *open* so that $(\mathcal{T}(G), \mathcal{J}(G), p_G)$ is a continuous field of groupoid, called the *tautological field*.

- If σ is a *continuous 2-cocycle* over $\mathcal{T}(G)$, then it can be restricted to any $M \in \mathcal{J}(G)$ leading to a *continuous field* $(\sigma_M)_{M\in\mathcal{J}(G)}$ of 2-cocycles.

The Main Theorem

Theorem *If G is amenable, then the field $(\mathcal{A}_M)_{M \in \mathfrak{J}(G)}$ of C^*-algebras defined as the algebra of the sub-groupoids $p_G^{-1}(M)$ and the cocyacle σ_M is continuous.*

If $(A_M)_{M \in \mathfrak{J}(G)}$ is a continuous section of self-adjoint elements of this field, then the spectrum Σ_M of A_M is continuous w.r.t. *M in the space $\mathcal{K}(\mathbb{R})$ of compact subspaces of $\mathbb{R}$ equipped with the Hausdorff topology.*

IV - Periodic Approximations in 1D

S. Beckus, J. Bellissard, G. De Nittis,
Spectral Continuity for Aperiodic Quantum Systems II. Periodic Approximation in 1D,
arXiv:1803.03099, March 8, 2018.

Periodic Approximation in 1D

In one dimension, all FLC tiling (or finite type Delone set) are given by a subshift in $\Omega = \mathcal{A}^{\mathbb{Z}}$ for some finite alphabet $\mathcal{A}$. The analogue of the Anderson-Putnam complex is given by a sequence of finite graphs, called here the *GAP-graphs*, encoding the subwords W_n of given length n, interpreted as *collared dots* or *collared letters*.

Subshifts

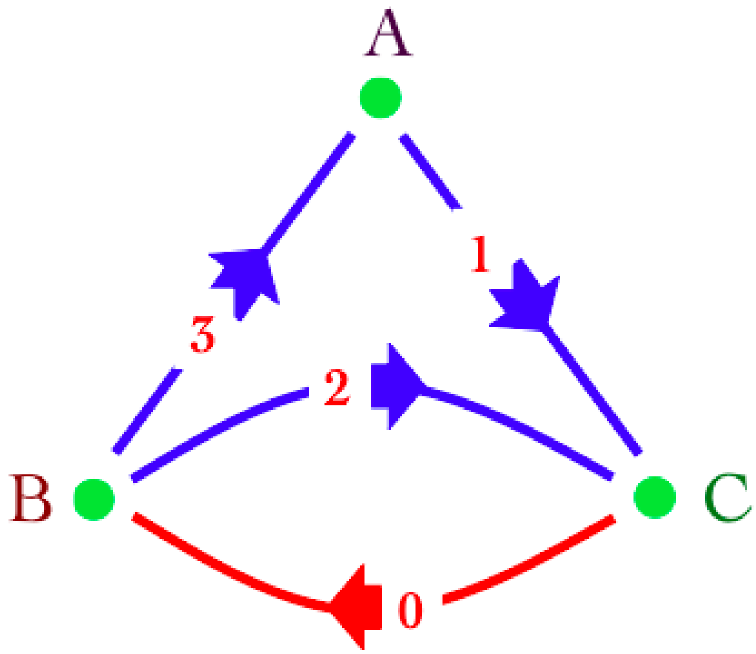
Let $\mathcal{A}$ be a finite *alphabet*, let $\Omega = \mathcal{A}^{\mathbb{Z}}$ be equipped with the shift S. Let $\Sigma \in \mathfrak{I}(\Omega)$ be a subshift. Then

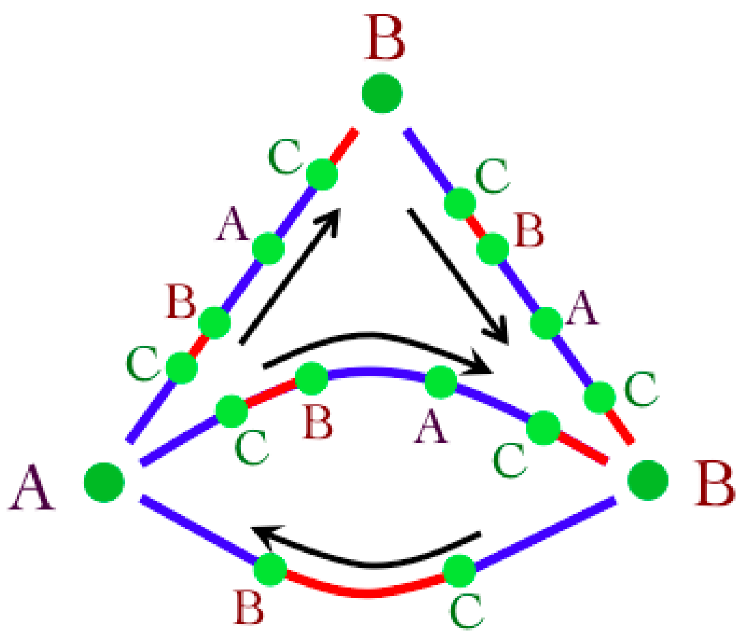
- given $l, r \in \mathbb{N}$ an *(l, r)-collared dot* is a dotted word of the form $u \cdot v$ with u, v being words of length $|u| = l, |v| = r$ such that uv is a *sub-word* of at least one element of Σ
- an *(l, r)-collared letter* is a dotted word of the form $u \cdot a \cdot v$ with $a \in \mathcal{A}$, u, v being words of length $|u| = l, |v| = r$ such that uav is a sub-word of at least one element of Σ: *a collared letter links two collared dots*
- let $\mathcal{V}_{l,r}$ be the set of (l, r)-collared dots, let $\mathcal{E}_{l,r}$ be the set of (l, r)-collared letters: then the pair $\mathcal{G}_{l,r} = (\mathcal{V}_{l,r}, \mathcal{E}_{l,r})$ gives a finite directed graph, which will be called the *GAP-graphs*

(Flye 1894, de Bruijn '46, Good '46, Rauzy '83, Anderson-Putnam '98, Gähler '01)

The Fibonacci Tiling

- **Alphabet:** $\mathcal{A} = \{a, b\}$
- **Fibonacci sequence:** generated by the *substitution* $a \to ab$, $b \to a$ starting from either $a \cdot a$ or $b \cdot a$

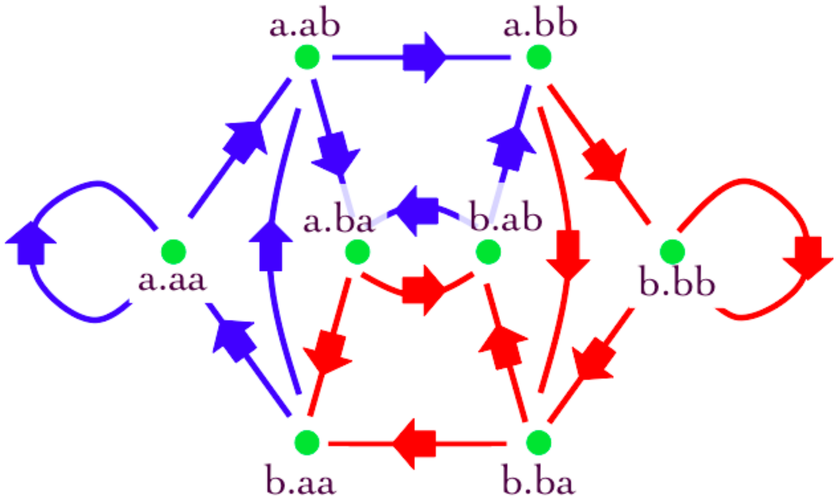




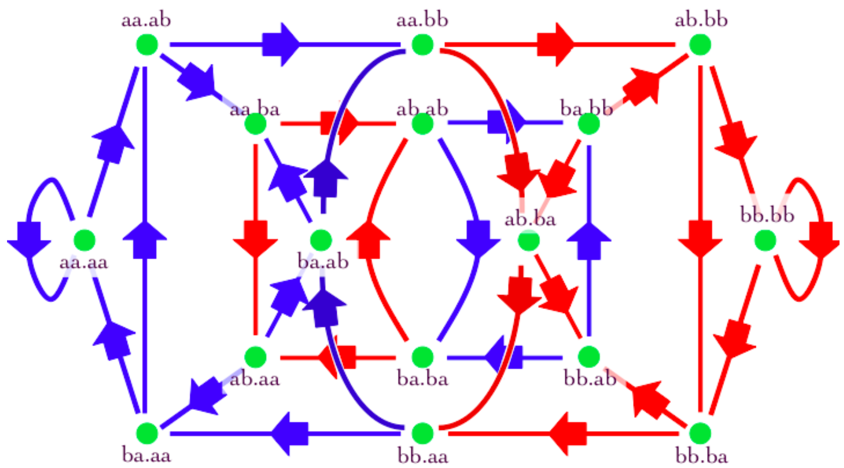
Left: $\mathcal{G}_{1,1}$ *Right:* $\mathcal{G}_{8,8}$

The Full Shift on Two Letters

- **Alphabet:** $\mathcal{A} = \{a, b\}$ all possible word allowed.



$\mathcal{G}_{1,2}$



$\mathcal{G}_{2,2}$

GAP-Graphs

The GAP-graphs are

- *simple:* between two vertices there is at most one edge,
- *connected:* if the sub-shift is *topologically transitive*, (*i.e.* one orbit is dense), then between any two vertices, there is at least one path connected them,
- has *no dandling vertex:* each vertex admits at least one ingoing and one outgoing vertex,
- if $n = l + r = l' + r'$ then the graphs $\mathcal{G}_{l,r}$ and $\mathcal{G}_{l',r'}$ are *isomorphic* and denoted by $\mathcal{G}_n$.

Strongly Connected Graphs

(S. Beckus, PhD Thesis, 2016)

A directed graph is called *strongly connected* if any pair x, y of vertices there is an *oriented path* from x to y and another one from y to x.

Proposition: *If the sub-shift* Σ *is minimal* (i.e. *every orbit is dense), then each of the GAP-graphs is stongly connected.*

Main result:

Theorem: *A subshift* $\Sigma \subset \mathcal{A}^{\mathbb{Z}}$ *can be Hausdorff approximated by a sequence of periodic orbits if and only if it admits is a sequence of strongly connected GAP-graphs.*

V - Lipshitz Continuity

S. Beckus, J. Bellissard, H. Cornean,
Hölder Continuity of Spectra of a Class of Aperiodic Schrödinger Operators,
in preparation.

Lipshitz Continuity

Spectral continuity is insufficient at evaluating the speed of convergence. *Lipshitz continuity* of a continuous field of self-adjoint operators might actually help getting better estimates.

Hamiltonian

- The lattice $\mathcal{L} \subset \mathbb{R}^d$ is a discrete co-compact subgroup. $*$ is a finite alphabet.
- $\Xi = \mathcal{A}^{\mathcal{L}}$ is the full shift, with $\mathcal{L}$-action by the shift operators $\{\mathrm{T}^a\,;\, a \in \mathcal{L}\}$.
- Hilbert space of quantum states $\mathcal{H} = \ell^2(\mathcal{L}) \otimes \mathbb{C}^N$ on which $\mathcal{L}$ acts by

$$(U(a)\psi)(m) = \psi(m-a)\,, \qquad \psi(m) \in \mathbb{C}^N\,,\ \ \psi = (\psi(m))_{m\in\mathcal{L}}$$

Finite Range Hamiltonians

Then $H = (H_\xi)_{\xi \in \Xi}$ is the continuous field of self-adjoint operators

$$(H_\xi \psi)(m) = \sum_{h \in \mathcal{R}} t_h(\mathrm{T}^{-n}\xi)\, \psi(m-n)\,,$$

with $0 \in \mathcal{R}$ *finite* and *invariant* by $h \to -h$. The t_h are continuous functions on Ξ such that $\overline{t_h(\xi)} = t_{-h}(\mathrm{T}^{-h}\xi)$ (for the self-adjointness of H_ξ).

A continuous function $f : \Xi \to \mathbb{C}$ will be called *cylindrical* or *pattern equivariant* if it depends only upon a finite number of components of the point $\xi \in \Xi$ (Kellendonk '03).
H will be called *finite range* if $\mathcal{R}$ is finite and *pattern equivariant* if all the t_h's are pattern equivariant.

Metric

- Let d be a metric on $\mathcal{A}$.
  For $x = (x_1, \cdots, x_d) \in \mathbb{R}^d$ let $|x|_\infty = max_i |x_i|$.
  Then d_Ξ is the metric on Ξ defined by

$$d_\Xi(\xi, \eta) = \min\left\{1, \inf\left\{\frac{1}{r}\,;\, d(\xi(m), \eta(m)) \leq \frac{1}{r}, m \in \mathcal{L}, |m|_\infty \leq r\right\}\right\}$$

- Then d_ξ^H denotes the corresponding *Hausdorff metric* on the space $\mathfrak{J}$ of closed shift invariant subsets of Ξ.
- For $\xi \in \Xi$, its *Hull* is the smallest set $\Xi_\xi \in \mathfrak{J}$ containing ξ.

Main Result

Theorem *Let* $H = (H_\xi)_{\xi \in \Xi}$ *be a continuous field of pattern equivariant self-adjoint operators with finite range. Then there is a constant* C *depending on* H *such that*

$$d_H(\sigma(H_\xi), \sigma(H_\eta)) \leq C\, d_\Xi^H(\Xi_\xi, \Xi_\eta)$$

where $\sigma(A) \subset \mathbb{R}$ *denotes the spectrum of the self-adjoint operator* A *and* d_H *is the Hausdorf metric on the space of compact subset of* $\mathbb{R}$ *defined by the Euclidean metric on* $\mathbb{R}$*.*

UNIVERSITÉ
DE GENÈVE

Thanks for Listening!!