Happy 60th Birthday Jean-Marc!!
Periodic Approximants
to
Aperiodic Hamiltonians

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

Sponsoring

CRC 701, Bielefeld, Germany

SFB 878, Münster, Germany

Groups, Geometry & Actions
Contributors

G. De Nittis, *Department Mathematik*, Friedrich-Alexander Universität, Erlangen-Nürnberg, Germany

S. Beckus, *Mathematisches Institut*, Friedrich-Schiller-Universität Jena, Germany
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I - Continuous Fields
Continuous Fields of Hamiltonians

\( A = (A_t)_{t \in T} \) is a field of self-adjoint operators whenever

1. \( T \) is a topological space,
2. for each \( t \in T \), \( \mathcal{H}_t \) is a Hilbert space,
3. for each \( t \in T \), \( A_t \) is a self-adjoint operator acting on \( \mathcal{H}_t \).

The field \( A = (A_t)_{t \in T} \) is called \textit{p2-continuous} whenever, for every polynomial \( p \in \mathbb{R}(X) \) with degree at most 2, the following norm map is \textit{continuous}

\[
\Phi_p : t \in T \mapsto \|p(A_t)\| \in [0, +\infty)
\]
Theorem: (S. Beckus, J. Bellissard ‘16)

1. A field $A = (A_t)_{t \in T}$ of self-adjoint bounded operators is p2-continuous if and only if the spectrum of $A_t$, seen as a compact subset of $\mathbb{R}$, is a continuous function of $t$ with respect to the Hausdorff metric.

2. Equivalently $A = (A_t)_{t \in T}$ is p2-continuous if and only if the spectral gap edges of $A_t$ are continuous functions of $t$. 
Continuous Fields of Hamiltonians

The field $A = (A_t)_{t \in T}$ is called $p2$-$\alpha$-Hölder continuous whenever, for every polynomial $p \in \mathbb{R}(X)$ with degree at most 2, the following norm map is $\alpha$-Hölder continuous

$$\Phi_p : t \in T \mapsto \|p(A_t)\| \in [0, +\infty)$$

uniformly w.r.t. $p(X) = p_0 + p_1 X + p_2 X^2 \in \mathbb{R}(X)$ such that $|p_0| + |p_1| + |p_2| \leq M$, for some $M > 0$. 
Continuous Fields of Hamiltonians

**Theorem:** (S. Beckus, J. Bellissard ‘16)

1. A field $A = (A_t)_{t \in T}$ of self-adjoint bounded operators is $p2\alpha$-Hölder continuous then the spectrum of $A_t$, seen as a compact subset of $\mathbb{R}$, is an $\alpha/2$-Hölder continuous function of $t$ with respect to the Hausdorff metric.

2. In such a case, the edges of a spectral gap of $A_t$ are $\alpha$-Hölder continuous functions of $t$ at each point $t$ where the gap is open.

3. At any point $t_0$ for which a spectral gap of $A_t$ is closing, if the tip of the gap is isolated from other gaps, then its edges are $\alpha/2$-Hölder continuous functions of $t$ at $t_0$.

4. Conversely if the gap edges are $\alpha$-Hölder continuous, then the field $A$ is $p2\alpha$-Hölder continuous.
Continuous Fields of Hamiltonians

(J. B. 1994)

The spectrum of the Harper model
the Hamiltonian is p2-Lipshitz continuous

\( H = U + U^{-1} + V + V^{-1} \)

A gap closing (enlargement)
Proving Continuity

• Prove that the field $A = (A_t)_{t \in T}$ is a continuous section of a continuous field $\mathcal{A} = (\mathcal{A}_t)_{t \in T}$ of $C^*$-algebras ((Kaplansky ’51, Tomyama ’58, Dixmier-Douady ’62).

• Use groupoid $C^*$-algebras (Renault ’80).

• Use a continuous field of groupoids (Landsman, Ramazan ’01).

• Due to possible presence of a magnetic field, use also a continuous field of 2-cycles (Rieffel ’89).

• Build the tautological groupoid (Beckus, JB, De Nittis ’17) through the set of closed invariant subsets and the Hausdorff topology (Hausdorff ‘14, Vietoris ’22, Chabauty ’50, Fell ’62).
**Theorem** Let $\Gamma$ be a locally compact, Hausdorff, amenable groupoid, with a Haar system and compact set of unit. Let $\mathcal{J}(\Gamma)$ denote its set of invariant subspaces equipped with the Hausdorff topology. Let $\theta$ denote a continuous field of 2-cocycles of $\Gamma$, continuous over $\mathcal{J}(\Gamma)$.

If $f \in C^*(\Gamma, \theta)$, and if $F$ is a closed invariant subset of the unit space of $\Gamma$, let $f_F$ denotes the restriction of $f$ on the sub-groupoid restricted to $F$. Let $\sigma(f)$ denotes the spectrum of $f$.

Then, if $f$ is self-adjoint, the map $F \in \mathcal{J}(\Gamma) \mapsto \sigma(f_F) \in \mathcal{K}(\mathbb{R})$ is continuous.

In particular, such a vector field is $p2$-continuous.
II - Approximations
Finite Clusters

- The earliest numerical calculation on quasicrystals were made on *finite clusters*, reducing the Hamiltonian to a finite dimensional matrix (see for instance Kohmoto, Sutherland, PRL 56, 2740, 1986).

- Boundary effects can be huge, representing *up to 20%* of the *Density of States (DOS)* in some cases. Using symmetries and inflation rules, algebraic arguments, it is possible to reduce the computational time and to increase tremendously the accuracy of numerical results (Kohmoto, Sutherland, loc. cit.).

- It is how *molecular states* were discovered: these are eigenstates localized on a finite cluster. Such eigenstates have a nonzero DOS and lead to a *discontinuity* in the *Integrated DOS*. It was proved later (Lenz, Stollmann ‘03), that such discontinuity can only come from molecular state.
Periodic approximations were used for quasicrystal as those materials admits periodic phases (*Mackay phases*) close to the aperiodic one in the phase diagram.

For the **2D-octagonal tiling** such approximations where theoretically calculated in *(Dumeau, Mossery, Oguey ‘89)*

The numerical calculation of periodic approximation benefits from software using the Bloch theory to calculate the band structure. The **2D-octagonal tiling** was resolved in this way *(Benza, Sire ‘91)*

It was later proved that errors are *exponentially small in the period* of the approximation *(see for instance Prodan ‘12)*, which gives a computational advantage over other methods
Building a Groupoid: methodology

- Let $\Gamma_\infty$ denote the groupoid associated with the aperiodic system under study.
- Let $\Gamma_n$ denote an approximate groupoid used in the approximation scheme.
- Take the disjoint union of all of them $\Gamma = \bigsqcup_{n\in\mathbb{N}\cup\{\infty\}} \Gamma_n$
- Define a topology on $\Gamma$ making it a continuous field over $\mathbb{N} \cup \{\infty\}$, namely a convergent sequence.
III - One-Dimensional FLC Tilings
GAP-graphs
(also called de Bruijn graphs, Rauzy graphs, Anderson-Putnam complex)

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

- 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 $\Sigma$: 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 $G_{l,r} = (\mathcal{V}_{l,r}, \mathcal{E}_{l,r})$ gives a finite *directed graph* (Flye 1894, de Bruijn ‘46, Good ‘46, Rauzy ‘83, Anderson-Putnam ‘98, Gähler, ‘01)
These graphs will be called GAP, in reference to the Gäbler version of the Anderson-Putnam complexes for tilings with Finite Local Complexity (FLC) in any dimensions.
The Fibonacci Tiling

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

*Left:* \( \mathcal{G}_{1,1} \)

*Right:* \( \mathcal{G}_{8,8} \)
The Thue-Morse Tiling

- **Alphabet:** \( A = \{a, b\} \)
- **Thue-Morse sequences:** generated by the substitution \( a \rightarrow ab, b \rightarrow ba \) starting from either \( a \cdot a \) or \( b \cdot a \)

![Diagram](image.png)
The Rudin-Shapiro Tiling

- **Alphabet:** \( A = \{a, b, c, d\} \)

- **Rudin-Shapiro sequences:** generated by the substitution \( a \rightarrow ab, \ b \rightarrow ac, \ c \rightarrow db, \ d \rightarrow dc \) starting from either \( b \cdot a, \ c \cdot a \) or \( b \cdot d, \ c \cdot d \)
The Full Shift on Two Letters

- **Alphabet:** $\mathcal{A} = \{a, b\}$ all possible word allowed.
Strongly Connected 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 dangling vertex**: each vertex admits at least one ingoing and one outgoing vertex,
- if \( n = l + r = l' + r' \) then the graphs \( G_{l,r} \) and \( G_{l',r'} \) are *isomorphic* and denoted by \( G_n \).
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 $\Sigma$ is minimal (i.e. every orbit is dense), then each of the GAP graph is strongly 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.
VI - To Conclude
Lipshitz Continuity

1. **Theorem:** An aperiodic system with disorder described by a subshift of finite type (finite alphabet) on the lattice $\mathbb{Z}^d$ and a Hamiltonian with finite range has a spectrum Lipshitz continuous with respect to the subshift expressed as a closed invariant subset of the full shift.
   
   (Beckus, JB, Cornean, 2018, in preparation)

2. **Theorem:** An aperiodic system describing a 1D-quasicrystal, described by cut-and-projection from $\mathbb{Z}^2$ onto $\mathbb{R}$, described by a line of slope $\alpha$, by a Hamiltonian with finite range and pattern equivariant coefficients, has a spectrum Lipshitz continuous with respect to $\alpha$ once the real line is equipped with a suitable ultrametric inducing a Cantor set topology.
   
   (Beckus, JB, 2018, in preparation)
Open Problems: extend the two results on either FLC tilings in any dimension or on quasicrystals in any cut-and-project situation.

(Beckus, JB, De Nittis, in project)
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