S,
A,

Giuse
(Pontificia Universidad Católica de Chile)

- Recent Progre •
  E T H, Zürich • Se

Joint work with:
S. Beckus
J. Bellissard

Source:
arXiv: 1709.00975
arXiv: 1803.03099

FONDECYT
Fondo Nacional de Desarrollo Científico y Tecnológico

§ Outline

1 - How to model aperiodic (quantum) sy

2 - How to construct approximations?

3 - A

4 - How to choo

Bloch's legacy

(1925-1926) Birth of (modern) Quantum Mechanic

W. Heisenberg (matrix mechanic .

(1928) Birth of Quantum Theory of Solids:

F. Bloch (Ph.D the .

(1928 - today) Consequence

- Conductivity pro
- Bethe-Sommerfeld conjecture: proved in many case
- Thermodynamic pro
- Semiclassical model
- To

(1984) Discovery of Quasicry

D. Shechtman *et al.*

- **Cry**

Periodic arrangement $\mathbb{R}^d$. When $d = 3$:

- 230 Fyodorov groups (rotations:, reflections, translations);
- 32 point groups (without translations);
- 11 Laüe groups (X-ray diffraction patterns);
- 5 rotational symmetrie $\equiv$ Cry

Ab

▸ Cry

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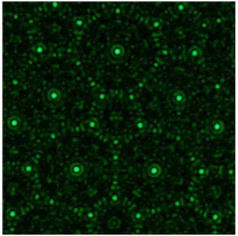
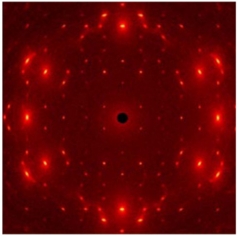
▸ Quasicry

In 1984 a diffraction patterns with a forbidden 10-fold symmetry was ob

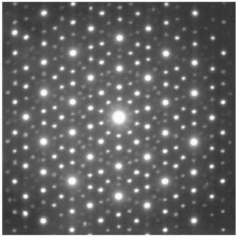
- Pointlike diffraction patterns (like in a perfect cry
- forbidden symmetry (5,8,10,12-fold);
- Long-range order (keyword!).



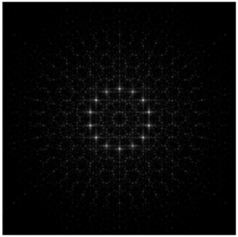
5-fold sym. (arrays of nanoholes)
[F. Huanga et al., Appl. Phys. Lett., 90, 2007]



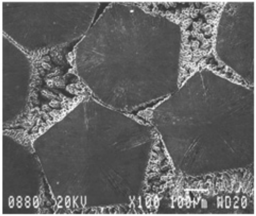
8-fold sym. (Sc-Zn alloy)
[American Physical Society]



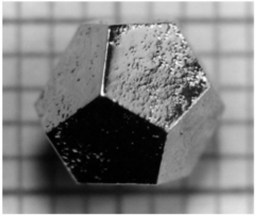
10-fold sym. (Zn-Mg-Ho alloy)
[Wikimedia, Materialscientist]



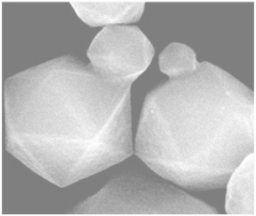
14-fold sym. (simulated patterns, 7 plane waves)
[M. Rule, http://spacecollective.org]



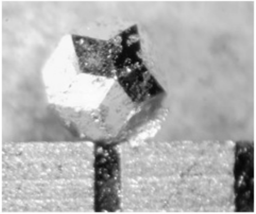
5-fold symmetric-QC (Al-Cu-Ru)
[C. Politis et al., Mod. Phys. Lett. B 3, 1989]



Dodecahedral-QC (Ho-Mg-Zn)
[AMES lab., US Department of Energy]



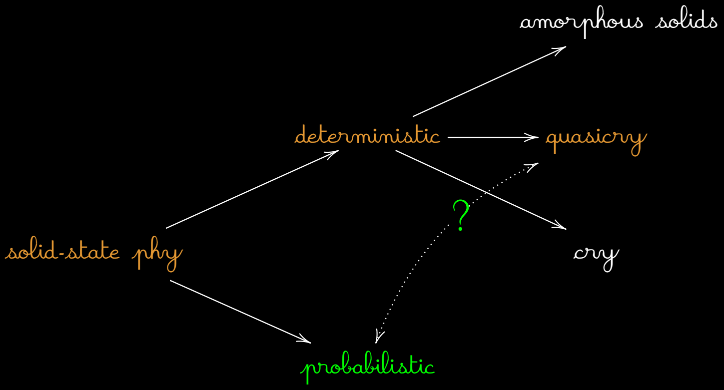
Icosahedral-QC (composite silica spheres)
[A. van Blaaderen, Nature 461, 2009]

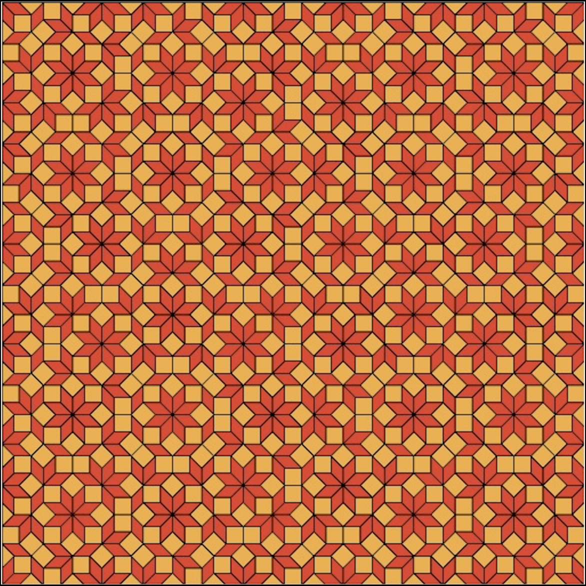


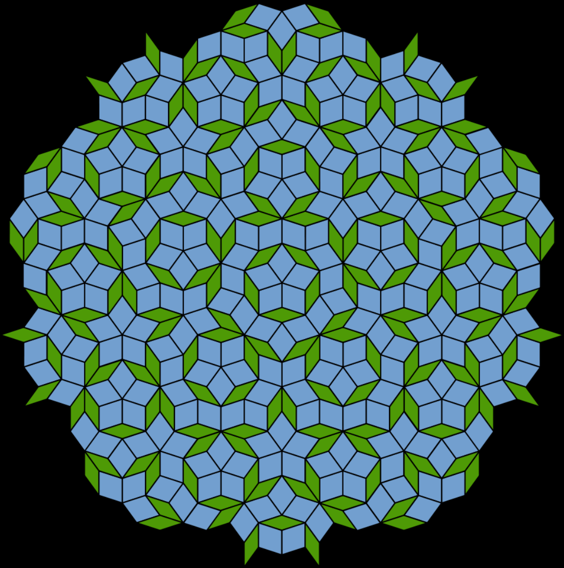
Rhombic triacontahedral-QC (Tb-Mg-Cd)
[T. Huie, JYI 8, 2003]

♦ “Strange” phy

- Insulators at low temperature ... made of good metal
- Mechanically hard and fragile.
- Superplastic transition at high temperature.







♦ The spectral problem

Let $\mathbb{L} \subset \mathbb{R}^d$ be the set of po

The spectral problem

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- Single-particle Hamiltonian

$$H_{\mathbb{L}} := -\frac{\hbar}{2m}\Delta + V_{\mathbb{L}}, \qquad V_{\mathbb{L}} := \sum_{y\in\mathbb{L}} w(\,\cdot\, - y)$$

w is the ty

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- Inde

$$\mathcal{H}_{\mathbb{L}} := \overline{\left\{ U_a H_{\mathbb{L}} U_a{}^{-1} \mid a \in \mathbb{R}^d \right\}}^{\texttt{strong-resolvent}}$$

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U_a unitary (pro

- Computational (very hard!) problem

$$\texttt{Spec}(\mathcal{H}_{\mathbb{L}}) := \overline{\bigcup_{H_\omega \in \mathcal{H}_{\mathbb{L}}} \texttt{Spec}(H_\omega)}\ .$$

Delone set $\mathbb{L} \subset \mathbb{R}^d$

- Discrete and aperiodic

$\mathbb{L} + a = \mathbb{L}$ if and only if $\mathbb{R}^d \ni a = 0$;

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- Delone set

• Uniformly discrete, i.e. there is $r > 0$ such that every o radius r meet $\mathbb{L}$ at mo

• Relatively dense, i.e. there is $R > 0$ such that every clo radius R meet $\mathbb{L}$ at least on one point.

• $\mathtt{Del}_{r,R}(\mathbb{R}^d)$ is the collection of Delone set of ty r, R.

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Finite local complexity

For any $R > 0$ the number of patche $\wp \subset \mathbb{L}$ of radius R is finite (up to translations).

From Delone set

- **The Hull of Delone set $r, R)$**

The set $\Omega := \mathtt{Del}_{r,R}(\mathbb{R}^d)$ can be endowed with a (natural) to

The re Ω is compact, Hausdorff and second countable.

From Delone set

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- The Delone dynamical sy

If $\mathbb{L} \in \Omega$ is a Delone set of ty r, R then it

$$T_a\mathbb{L} := \mathbb{L} + a \in \Omega \,, \qquad \forall\, a \in \mathbb{R}^d$$

is still a Delone set of same ty

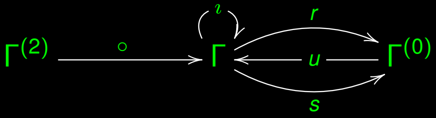
$$\mathbb{R}^d \ni a \overset{T}{\longmapsto} T_a \in \mathbf{Homeo}(\Omega)$$

is an $\mathbb{R}^d$-action and $(\Omega, T, \mathbb{R}^d)$ is a dynamical sy

From Delone set

▸ The (transformation) Delone groupoid

It is de



- $\Gamma^{(0)} := \Omega$ is the unit space;
- $\Gamma := \Omega \times \mathbb{R}^d$ is the arrow space;
- $r(\omega, a) := \omega$ and $s(\omega, a) := T_a^{-1}\omega$ are the range map and source map;
- $u(\omega) := (\omega, 0)$ is the embedding of unit $\Gamma^{(0)} \hookrightarrow \Gamma$;
- $\imath(\omega, a) := (T_a^{-1}\omega, -a)$ is the inverse map;
- compo

$$\Gamma^{(2)} := \left\{ ((\omega_1, a_1), (\omega_2, a_2)) \in \Gamma \times \Gamma \;\middle|\; s(\omega_1, a_1) = r(\omega_2, a_2) \right\}$$

- $(\omega, a) \circ (T_a^{-1}\omega, b) := (\omega, a + b)$ is the multiplication.

From groupoids to ob

- Left-continuous Haar sy

Family of measure $\{\mu^\omega\}_{\omega\in\Omega}$ defined by

$$\mu^\omega(f) := \int_{\mathbb{R}^d} f(\omega, x)dx\ , \qquad f \in C_c(\Gamma) \equiv C_c(\Omega \times \mathbb{R}^d)\ .$$

Pro

i) For each $\omega \in \Gamma^{(0)}$ the support of μ^ω is the r-fiber $\Gamma^\omega := r^{-1}(\omega) \simeq \mathbb{R}^d$;

ii) for each $f \in C_c(\Gamma)$ the map $\Gamma^{(0)} \ni \omega \mapsto \mu^\omega(f) \in \mathbb{C}$ is continuous;

iii) The measure

$$\int_{\Gamma^\omega} f((T_a\omega, a) \circ (\omega, x))\ dx = \int_{\mathbb{R}^d} f(T_a\omega, a + x)\ dx = \int_{\Gamma^{T_a\omega}} f(T_a\omega, y)\ dy$$

♦ From groupoids to ob

▶ $\mathscr{C}^*$- algebraic structure on $C_c(\Gamma)$

- Product (convolution):

$$(f \star g)(\omega, x) \;:=\; \int_{\Gamma^\omega \simeq \mathbb{R}^d} f(\omega, y)\, g(T_{-y}\omega, x - y)\, dy\;.$$

- Adjoint:

$$f^\dagger(\omega, x) \;:=\; \overline{f(T_{-x}\omega, -x)}\;.$$

- Re

$$(\pi_\omega(f)\psi)(x) \;:=\; \int_{\Gamma^\omega} f(T_{-x}\omega, y - x)\, \psi(y)\, dy\;, \qquad \psi \in L^2(\Gamma^\omega, \mu^\omega) \simeq L^2(\mathbb{R}^d)$$

- Reduced-universal norm:

$$|||f||| \;:=\; \sup_{\omega \in \Gamma^{(0)}} ||\pi_\omega(f)|| \;\overset{(*)}{=}\; \sup_{\rho = \texttt{bound. rep.}} ||\rho(f)||$$

(∗) follow

From groupoids to ob

C^*- algebra of ob

$$\mathcal{A} := \overline{C_c(\Gamma)}^{|||\ \ |||}$$

endowed with product $\star$ and adjoint $\dagger$.

From groupoids to ob

- $\mathcal{C}^*$- algebra of ob

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- Affiliation

For each $\lambda \in \mathbb{R}$ there exist $\mathcal{R}_{\lambda,\mathbb{L}} \in \mathcal{A}$ such that

$$\pi_\omega(\mathcal{R}_{\lambda,\mathbb{L}}) := (H_\omega - i\lambda\mathbb{1})^{-1} \quad \text{with} \quad H_\omega \in \mathcal{H}_\mathbb{L} \ .$$

From groupoids to ob

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Conclusions

- The information about $\mathbf{Spec}(\mathcal{H}_\mathbb{L})$ is contained in the Delone groupoiud $(\Gamma, \Gamma^{(0)})$ ... sometime $\Omega \rtimes_T \mathbb{R}^d$.
- An "efficient" approximation scheme for $\mathbf{Spec}(\mathcal{H}_\mathbb{L})$ must be based on an intrinsic approximation scheme of the underlying structural data coded in $\Omega \rtimes_T \mathbb{R}^d$.

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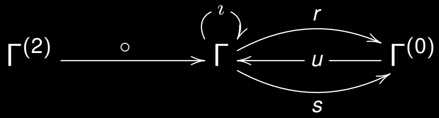
Handy groupoids

- Co



with Γ and $\Gamma^{(0)}$ to $r, s, u, \imath, \circ$ continuous maps.

Handy groupoids

- Co

$$\Gamma^{(2)} \xrightarrow{\ \circ\ } \Gamma \underset{s}{\overset{r}{\rightrightarrows}} \Gamma^{(0)}, \quad u : \Gamma^{(0)} \to \Gamma, \quad \imath : \Gamma \to \Gamma$$

with Γ and $\Gamma^{(0)}$ to $\qquad$ $r, s, u, \imath, \circ$ continuous maps.

- Handy groupoid

i) Γ is locally compact, Hausdorff, second countable;

ii) $\Gamma^{(0)}$ is compact;

iii) r and s are o

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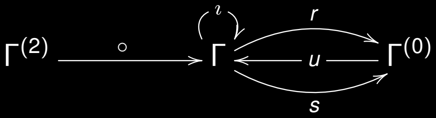

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- Pro

- $\Gamma^{(0)}$ is Hausdorff, and the inclusion $u : \Gamma^{(0)} \hookrightarrow \Gamma$ is clo
- There is a left-continuous Haar sy $\{\mu^\omega\}_{\omega \in \Gamma^{(0)}}$.

Tautological field of groupoids

▶ Invariant set

Let $M \subseteq \Gamma^{(0)}$ and define $[M] := s(r^{-1}(M))$. M is invariant if and only if $M = [M]$. Define

$$\mathtt{Inv}_\Gamma := \left\{ M \subseteq \Gamma^{(0)} \mid \overline{M} = M = [M] \right\}.$$

- Let $\omega \in M \in \mathtt{Inv}_\Gamma$. If $\gamma \in \Gamma$ such that $r(\gamma) = \omega$ then $s(\gamma) \in M$;
- The re $\Gamma_M := \Gamma|_M$ is a well defined groupoid.

Tautological field of groupoids

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Co

Let $\mathbf{Clos}(\Gamma^{(0)})$ the space of clo

$$\mathscr{U}(C, \mathcal{F}) := \left\{ C' \in \mathbf{Clos}(\Gamma^{(0)}) \mid C' \cap C = \emptyset \ \& \ \forall\, O \in \mathcal{F}, C' \cap O \neq \emptyset \right\}.$$

- $\mathbf{Inv}_\Gamma \subseteq \mathbf{Clos}(\Gamma^{(0)})$;
- $\mathbf{Inv}_\Gamma$ is clo

♦ Tautological field of groupoids

▸ Tautological arrow space

$$\mathtt{Taut}_\Gamma := \left\{(M,\gamma) \in \mathtt{Inv}_\Gamma \times \Gamma \mid r(\gamma) \in M \ \& \ s(\gamma) \in M\right\}.$$

• Endowed with the product to $\mathtt{Inv}_\Gamma \times \Gamma$ is clo

compact, Hausdorff and second countable.

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▶ Tautological (handy) groupoid $(\mathtt{Taut}_\Gamma, \mathtt{Taut}_\Gamma^{(0)})$

- $r(M, \gamma) := (M, r(\gamma))$ and $s(M, \gamma) := (M, s(\gamma))$;
- $(M, \gamma) \circ (M, \gamma') := (M, \gamma \circ \gamma')$;
- $(M, \gamma)^{-1} := (M, \gamma^{-1})$.

Tautological field of groupoids

- Continuous Fields of Groupoids

A triple (Γ, T, p) such that:

i) Γ is a to $\Gamma^{(0)} \hookrightarrow \Gamma$;

ii) $p : \Gamma \to T$ is an o

iii) Fiber structure $p = p|_{\Gamma^{(0)}} \circ s = p|_{\Gamma^{(0)}} \circ r$.

- It follow $\Gamma_t := p^{-1}(t) \subseteq \Gamma$ is a sub-groupid for all $t \in T$.

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Theorem 1

Let $(\Gamma, \Gamma^{(0)})$ be a handy groupoid and $(\mathbf{Taut}_\Gamma, \mathbf{Taut}_\Gamma^{(0)})$ the associated tautological groupoid. Consider the map

$$p_\Gamma \ : \ \mathbf{Taut}_\Gamma \longrightarrow \mathbf{Inv}_\Gamma$$

given by $p_\Gamma(M, \gamma) = M$. Then $(\mathbf{Taut}_\Gamma, \mathbf{Inv}_\Gamma, p_\Gamma)$ is a continuous fields of groupoids called the tautological field of Γ.

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Continuous Fields of C^*- algebras

T is a to $\mathcal{A} := \{\mathcal{A}_t\}_{t \in T}$ a collection of C^*- algebras.

▶ Continuous field structure

- There is a collection $\mathcal{Y} := \{\mathcal{Y}_t\}_{t \in T}$ of dense subalgebras;
- For each $A := \{A_t\}$ in $\mathcal{Y}$ the map $t \mapsto \|A_t\|_{\mathcal{A}_t}$ is continuous;
- The family $\mathcal{Y}$ is clo

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Theorem 2

If $(\mathcal{A}, \mathcal{Y})$ is a continuous field of C^*- algebras and if $A \in \mathcal{Y}$ is a continuous self-adjoint field, then:

a) For any $f \in C_0(\mathbb{R})$, the maps $t \mapsto \|f(A_t)\|_{\mathcal{A}_t}$ are continuous;

b) The map

$$T \ni t \longmapsto \mathbf{Spec}(A_t) \in \mathbf{Comp}(\mathbb{R})$$

is continuous with re

Field of groupoids and related algebras

Theorem 3

Let (Γ, T, p) be a continuous field of handy amenable groupoids. Let μ be a Haar sy Γ which induce μ_t on each fiber groupoid Γ_t. Let $A_t := \overline{C_c(\Gamma_t)}$ be the C^*- algebra associated to Γ_t. Then $\mathcal{A} := \{A_t\}_{t \in T}$ is a continuous field of C^*- algebras.

Field of groupoids and related algebras

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- Proved by Landsman & Ramazan and extended to the case of a 2-cocycle by Beckus, Bellissard & D.;
- Theorem 1 + Theorem 3 imply that the tautological field produce a continuous field of $\mathcal{C}^*$- algebras;
- Then Theorem 2 implie

vary continuously with re

Implementing the approximation scheme

Ste $\mathbb{L} \in \mathbf{Del}_{r,R}(\mathbb{R}^d)$.

♦ Implementing the approximation scheme

Ste $\mathbb{L} \in \mathtt{Del}_{r,R}(\mathbb{R}^d)$.

Ste $\Omega := \mathtt{Del}_{r,R}(\mathbb{R}^d)$ one builds the handy groupoid $\Gamma := \Omega \rtimes_T \mathbb{R}^d$ and the associated $\mathcal{C}^*$- algebra $\mathcal{A}$ with the re $\mathcal{R}_\lambda$.

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Ste $\mathtt{Inv}_\Gamma$. Since $M \in \mathtt{Inv}_\Gamma$ if and only if $\omega \in M$ implie $T_a\omega \in M$ for all $a \in \mathbb{R}^d$ one has that the re $\Gamma_M := M \rtimes_T \mathbb{R}^d$ is well defined.

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Ste $(\mathtt{Taut}_\Gamma, \mathtt{Inv}_\Gamma, p_\Gamma)$.

Notice that $p_\Gamma^{-1}(M) \simeq \Gamma_M$ for all $M \in \mathtt{Inv}_\Gamma$.

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Ste *- algebras $\{\mathcal{A}_M\}_{M \in \mathtt{Inv}_\Gamma}$ defined by $\mathcal{A}_M := \overline{C_c(\Gamma_M)}$.

Implementing the approximation scheme

Ste $\Gamma_M \hookrightarrow \Gamma$ provide homomorphism $\mathcal{A} \to \mathcal{A}_M$ wich consist "function" $f \in \mathcal{A}$ to a function $f_M := f|_{\Gamma_M} \in \mathcal{A}_M$. The map $M \to f_M$ is a continuous section of the field $\{\mathcal{A}_M\}_{M \in \mathtt{Inv}_\Gamma}$.

Implementing the approximation scheme

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Ste $\{M_n\}_{n \in \mathbb{N}} \subset \mathtt{Inv}_\Gamma$ such that $M_n \to M_{\mathbb{L}}$ when $n \to \infty$ with re to

♦ Implementing the approximation scheme

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Why the computation of $\mathbf{Spec}(\mathcal{R}_\lambda|_{M_n})$ is ste the computation of $\mathbf{Spec}(\mathcal{R}_{\lambda,\mathbb{L}})$? There is a preferred criterion to select the sequence $\{M_n\}_{n\in\mathbb{N}}$?

§ Outline

1 - How to model aperiodic (quantum) sy

2 - How to construct approximations?

3 - Ho

4 - How to choo

Periodic approximant

Periodicoid unit

- Given $\omega \in \Gamma^{(0)}$ then $[\omega] := s(r^{-1}(\omega)) = s(\Gamma^{\omega})$ is the orbit of ω;
- $\omega \in \Gamma^{(0)}$ is called periodicoid unit if it $[\omega] = \overline{[\omega]}$;
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Periodicoids unit (Delone groupoid)

- Given $\omega \in \Omega$ then $[\omega] = \{T_a\omega \mid a \in \mathbb{R}^d\}$, i.e. the $\mathbb{R}^d$-orbit of ω;
- If $\omega \in \Omega$ is a periodicoid unit the orbit-stabilizer theorem provide

$$[\omega] \simeq \mathbb{R}^d/\mathbf{Stab}_{\omega} := \left\{\mathbf{Stab}_{\omega} + a \mid a \in \mathbb{R}^d\right\}$$

where $\mathbf{Stab}_{\omega} := \{a \in \mathbb{R}^d \mid T_a\omega = \omega\}$ is the stabilizer subgroup;

- $[\omega]$ is compact (clo Ω) and $\mathbf{Stab}_{\omega}$ is co-compact in $\mathbb{R}^d$, i. e. $\mathbf{Stab}_{\omega} \simeq \mathbb{Z}^{d-\ell} \times \mathbb{R}^{\ell}$ for some $0 \leqslant \ell \leqslant d$. However, $\ell = 0$ by discretene
- ω corre $\mathbb{L}_{\omega}$ which is periodic.

♦ Periodic approximant

▶ Conclusions

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- If $M_{\mathbb{L}}$ admit ω_n then the original spectral problem $\mathbf{Spec}(\mathcal{H}_{\mathbb{L}})$ is solved by computing the spectra $\mathbf{Spec}(\mathcal{R}_\lambda|_{[\omega_n]})$ of periodic o

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Main que

When the invariant set $M_{\mathbb{L}} \in \mathtt{Inv}_{\Gamma}$ admit
periodic unit $[\omega_n] \to M_{\mathbb{L}}$ with re
Vietoris to

- Complete characterization in $d = 1$. In this case a combinatorial de
- Work in progre

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Bulk-boundary correspondance for Sturmian Kohmoto like models

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- In this paper (e.g. in Theorem 2.2) the convergence re

Thank you

for

your attention !