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Spectral Study of Schrödinger Operators with Aperiodic Ordered Potentials

JOINT WORK WITH J. BELLISSARD AND G. DE NITTIS

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1. Motivation

We study Schrödinger operators induced by aperiodic solids (e.g. Quasicrystals). In the periodic case the Floquet-Bloch theory is a powerful tool to analyze the spectral properties. A similar tool for the aperiodic case is missing! Here, we investigate the approximation of non-periodic Schrödinger operators by periodic ones.

In general, it is impossible to approximate aperiodic Schrödinger operators by periodic operators in the norm topology. To overcome this difficulty, in [2] we used weaker notions than the convergence in norm. This includes the convergence of the spectrum as well as the strong convergence of the operators. A detailed study of this convergence can be found in [3]. We use C^*-algebra techniques and provide an algorithmic construction of the approximants which will be helpful for concrete computations.

2. One-dimensional systems

Let $\mathcal{A}$ be a finite set and $\mathcal{A}^{\mathbb{Z}} := \{\xi : \mathbb{Z} \to \mathcal{A}\}$ the set of bi-infinite words. Equipped with the product topology the space $\mathcal{A}^{\mathbb{Z}}$ is compact, Hausdorff and metriziable. The action $\mathsf{T} : \mathcal{A}^{\mathbb{Z}} \to \mathcal{A}^{\mathbb{Z}}$ is defined by $(\mathsf{T}\xi)(j) := \xi(j-1)$. A bi-infinite word $\xi \in \mathcal{A}^{\mathbb{Z}}$ is called *periodic* if there exists a $p \in \mathbb{N}$ such that $\xi(j+p) = \xi(j)$ for all $j \in \mathbb{Z}$.

We study closed, T-invariant subsets $\Xi \subseteq \mathcal{A}^{\mathbb{Z}}$ which are called *subshifts*. The pair (Ξ, T) is a topological dynamical system which represents a family of one-dimensional solids. For $\xi \in \mathcal{A}^{\mathbb{Z}}$ the *local pattern* $\mathcal{W}(\xi)$ is the set of all finite subwords of ξ. Then, $\mathcal{W}(\Xi)$ is the collection of all local patterns of elements in Ξ, i.e. $\mathcal{W}(\Xi) := \cup_{\xi\in\Xi}\mathcal{W}(\xi)$.

3. Schrödinger Operator

For a subshift Ξ let $\mathcal{C}^*(\Gamma)$ be the C^*-algebra associated to the groupoid $\Gamma := \Xi \rtimes_{\mathsf{T}} \mathbb{Z}$. Each self-adjoint element $h \in \mathcal{C}^*(\Gamma)$ defines a strongly continuous, covariant family of Schrödinger operators on $\ell^2(\mathbb{Z})$ by the left-regular representation $H_\xi := \pi_\xi(h) : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z}), \xi \in \Xi$. These operators are linear, bounded and self-adjoint.

A typical example for such a family of Schrödinger operators is

$$(H_\xi\psi)(j) := \psi(j-1) + \psi(j+1) + V\left(\mathsf{T}^{-j}\xi\right)\ \psi(j), \quad \psi \in \ell^2(\mathbb{Z}), \qquad (1)$$

where $V : \mathcal{A}^{\mathbb{Z}} \to \mathbb{R}$ is continuous and takes finitely many values (pattern equivariant function).

4. Main Result

Theorem. ([2]) Consider a family of self-adjoint Schrödinger operators $H_\xi : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z}),\ \xi \in \Xi$, associated to a periodically approximable subshift $\Xi \subseteq \mathcal{A}^{\mathbb{Z}}$.
Then, for $\xi \in \Xi$ there exists a sequence of periodic, self-adjoint Schrödinger operators $H_n : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z}),\ n \in \mathbb{N}$, such that:

(i) The sequence $(H_n)_{n\in\mathbb{N}}$ converges strongly to H_ξ for $n \to \infty$.

(ii) The sequence of spectra converges, i.e. $\lim_{n\to\infty}\sigma(H_n) = \bigcup_{\xi\in\Xi}\sigma(H_\xi)$ with respect to the Hausdorff metric on $\mathbb{R}$.

(iii) If Ξ contains at least one non-periodic element the periods of $(H_n)_{n\in\mathbb{N}}$ grow to infinity for $n \to \infty$.

(iv) The approximants are given explicitly by the closed paths that visit all vertices in the Gähler-Anderson-Putnam (De Bruijn) graphs.

5. Periodically approximable

For a subshift Ξ a sequence of oriented, finite graphs $\mathcal{G}_n := (\mathcal{V}_n, \mathcal{E}_n, \partial_r, \partial_s)$, called *Gähler-Anderson-Putnam* [1, 5] (*De Bruijn* [4]) *graphs*, is definded by

$$\mathcal{V}_n := \mathcal{W}(\Xi) \cap \mathcal{A}^n, \qquad \textbf{(vertex set)}$$
$$\mathcal{E}_n := \mathcal{W}(\Xi) \cap \mathcal{A}^{n+1}, \qquad \textbf{(edge set)}$$
$$\partial_s(a_0 \dots a_n) := a_0 \dots a_{n-1}, \qquad \textbf{(source map)}$$
$$\partial_r(a_0 \dots a_n) := a_1 \dots a_n. \qquad \textbf{(range map)}$$

The n-th graph $\mathcal{G}_n$ encodes the local structure of the system Ξ and the possible extensions of the patterns. The subshift is called *periodically approximable* if the graphs $(\mathcal{G}_n)_{n\in\mathbb{N}}$ are strongly connected, i.e. it exists a positively oriented closed path in $(\mathcal{G}_n)_{n\in\mathbb{N}}$ that visit all vertices.

Such paths define a sequence of periodic subshifts Ξ_n tending to Ξ as required in Box 6.

Lemma.(sufficient condition) If the dynamical system (Ξ, T) is minimal, then, the subshift Ξ is periodically approximable.

6. Convergence of the spectrum

It is well-known that for a continuous self-adjoint section of a continuous field of C^*-algebras the spectrum behaves continuously. Since the Schrödinger operators associated to Ξ are elements of $\mathcal{C}^*(\Xi \rtimes_{\mathsf{T}} \mathbb{Z})$ we define a continuous field of C^*-algebras by a sequence of subshifts $(\Xi_n)_{n\in\mathbb{N}}$ tending to Ξ in the Hausdorff-topology. This convergence can be characterized by the convergence of the local patterns:

Lemma. A sequence of subshifts $(\Xi_n)_{n\in\mathbb{N}}$ converge to Ξ, if and only if the local patterns converge, i.e. for all $m \in \mathbb{N}$ exists $n_m \in \mathbb{N}$ such that $\mathcal{W}(\Xi_n) \cap \mathcal{A}^m = \mathcal{W}(\Xi) \cap \mathcal{A}^m, \quad n \geq n_m$ where $\mathcal{A}^m := \{u : \{1, \dots, m\} \to \mathcal{A}\}$.

Let $(\Xi_n)_{n\in\mathbb{N}}$ be a sequence of subshifts tending to $\Xi_\infty := \Xi$ in the Hausdorff-topology. For a given family of Schrödinger operators $(H_\xi)_{\xi\in\Xi}$ the approximating operators are chosen such that they form a continuous section on the related field of C^*-algebras $\pi : \prod_{n\in\overline{\mathbb{N}}}\mathcal{C}^*(\Xi_n \rtimes_{\mathsf{T}} \mathbb{Z}) \to \overline{\mathbb{N}}$.

For instance, let $(H_\xi)_{\xi\in\Xi}$ be defined as in Equation (1) in Box 3 and $\xi \in \Xi$. Then, for $\psi \in \ell^2(\mathbb{Z})$ the approximants are defined by

$$H_n\psi(j) := \psi(j-1) + \psi(j+1) + V(\mathsf{T}^{-j}\eta)\psi(j),$$

where $\eta \in \Xi_n$ is chosen such that $\eta|_{N_n} = \xi|_{N_n}$ the restriction to the set $N_n := \{-\lfloor\frac{n}{2}\rfloor, \dots, \lceil\frac{n}{2}\rceil - 1\}$ around the origin. The last condition is needed to get the strong convergence of H_n to H_ξ.

7. The Fibonacci sequence

Let $\mathcal{A} := \{a, b\}$ and consider the Fibonacci substitution

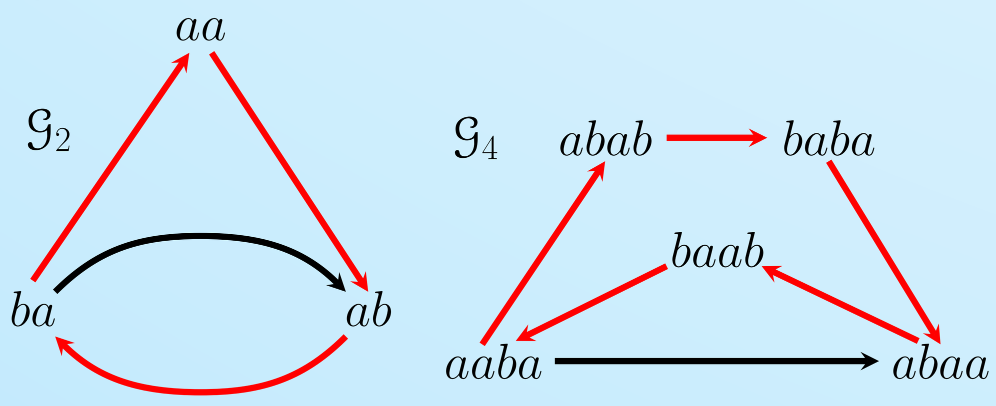
$$a \overset{S}{\mapsto} ab, \qquad b \overset{S}{\mapsto} a.$$

Then, $\xi := \lim_{k\to\infty} S^{2k}(b)|S^{2k}(a)$ defines a fixed point of the substitution and

$$\xi = \dots ababaab|abaabab \dots \in \mathcal{A}^{\mathbb{Z}}.$$

The subshift $\Xi := \overline{\{\mathsf{T}^k\xi \mid k \in \mathbb{Z}\}}$ is minimal and contains no periodic element. Hence, Ξ is periodically approximable and so the main result (Box 4.) applies to any family of Schrödinger operators $(H_\xi)_{\xi\in\Xi}$ associated to the Fibonacci subshift.

The related Gähler-Anderson-Putnam graphs look as follows.



The red paths in $\mathcal{G}_2$ and $\mathcal{G}_4$ are closed paths that visit all vertices and creating the following periodic approximants

Ξ_2 : $\dots aab|aab|aab \dots$ $\qquad$ Ξ_4 : $\dots abab|aabab|aaba \dots$

The substitution rule can be used to compute the other Gähler-Anderson-Putnam graphs.

8. Future projects

(1) Fixing a metric on the space $\mathcal{A}^{\mathbb{Z}}$ the main result can be formulated as follows:
The Hausdorff convergence of subshifts $(\Xi_n)_{n\in\mathbb{N}}$ to Ξ implies the Hausdorff convergence of the spectrum.
Thus, it is natural to ask whether the rate of convergence of the spectrum can be estimated by the Hausdorff distance of Ξ_n to Ξ. In the case of finite range operators we expect an exponentially fast decay.

(2) So far the known techniques are only applicable to one-dimensional systems. Whereas our method could be extended to the higher dimensional case and so will provide a tool to study more complicated systems.

(3) In [3] the continuity of the spectrum is characterized by the continuity of the field of the corresponding C^*-algebra (as in our case). In this sense our result is optimal. In particular, if Ξ_n does not tend to Ξ then the spectrum of the associated Schrödinger operators will not converge in general. Thus, the creation of defects by breaking the convergence of the local patterns should be studied.

References

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