SCHRÖDINGER OPERATORS
GENERATED BY SUBSTITUTIONS

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ABSTRACT

Schrödinger operators with potentials generated by primitive substitutions are simple models for one dimensional quasi-crystals. We review recent results on their spectral properties. These include in particular an algorithmically verifiable sufficient condition for their spectrum to be singular continuous and supported on a Cantor set of zero Lebesgue measure. Applications to specific examples are discussed.

1. Introduction

We consider one dimensional Schrödinger operators $H$ defined by

$$H\psi_n = \psi_{n+1} + \psi_{n-1} + V_n \psi_n, \quad \psi \in l^2(\mathbb{Z})$$

where $(V_n)_{n \in \mathbb{Z}}$ is an aperiodic sequence generated by a substitution.

A substitution is a map $\xi$ from a finite alphabet $A$ to the set $A^*$ of words on $A$, which can be naturally extended to a map from $A^*$ to $A^*$ and then to a map from $A^N$ to $A^N$. We also define the free group $\hat{A}^*$, extension of $A^*$ obtained by addition of the formal inverses of the letters in $A$ as generators. $\xi$ is said primitive if $\exists k \in \mathbb{N}$ s.t. $\forall (\alpha, \beta) \in A^2, \xi^k(\alpha)$ contains $\beta$. A substitution sequence or automatic sequence is a $\xi$-right fixpoint $u_r = \alpha_r...$ given by indefinite iteration of $\xi$. By choosing a $\xi$-left fixpoint $u_l = ...\alpha_l$ such that the word $\alpha_l \alpha_r$ is contained in $u_r$, we define by concatenation a doubly infinite word $w = u_l u_r$. We say that a Schrödinger operator of type (1) is generated by $\xi$ if the sequence $(V_n)_{n \in \mathbb{Z}}$ is defined by $V_n = v(w_n)$, where $v$ is a map $A \to \mathbb{R}$.

Such an operator, with the Fibonacci sequence, has become popular as a simple model for electron transport in one-dimensional quasi-crystals (cut-and-project method). The study of this particular example and others, namely the Thue-Morse and period-doubling sequences, has led to the following common expectations for this type of operators:

(i) Their spectrum is purely singular continuous and supported on a Cantor set of zero Lebesgue measure.

(ii) The spectral gaps are labelled by a countable set of algebraic numbers, depending on the substitution.$^*$

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By means of the K-theory of $C^*$-algebras, (ii) has been proven to be correct for all operators generated by primitive substitutions $\xi$, with the limitation that in general one cannot exclude that some gaps are closed. A general perturbative approach to compute the opening of gaps has been proposed in [1].

2. Cantor spectrum

The basic tool to establish (i) is the transfer-matrix formalism. That is, the study of the properties of solutions of Eq. (1) leads to the analysis of products of two-by-two matrices of the form $P_n(E) = \prod_{k=1}^{n} T_E(w_n, w_{n-k})$, where $w_k$ is the $k$-th letter in the substitution sequence $w$ and $T_E : A \rightarrow SL(2)$ is a map that assigns, for fixed energy $E$, to each letter in the alphabet a unimodular two-by-two matrix. In the case of Eq. (1), $T_E(w_n) = \begin{pmatrix} E - v(w_n) & -1 \\ 1 & 0 \end{pmatrix}$, but the precise form of this map is not important, and therefore the same results hold for all types of second order equations that can be reduced to a problem of products of unimodular $2 \times 2$-matrices. This includes in particular the continuous Laplacian with piecewise constant potential of a finite number of different shapes (Kronig-Penney model, see [2-3]). The main idea of the proof of the singularity of the spectrum $\sigma(H)$ of $H$ is its identification with the set $\mathcal{O}$ of zero Lyapunov exponents $\gamma(E) = \text{lim}_{n \uparrow \infty} \frac{1}{n} \log \| T_E^{(n)} \|$, known to be of zero Lebesgue measure by a general result in [4] based on a theorem of Kotani [5]. To do this requires a rather careful analysis of the asymptotic properties of $P_n(E)$, which is made possible by the self-similar structure of the potential. Let, for any word $\omega \in A^*$, $T_E(\omega) = \prod_{\alpha \in \omega} T_E(\alpha)$ and

$$ T_E^{(k)}(\omega) \equiv T_E^{(k-1)}(\xi(\omega)) \quad \text{with} \quad T_E^{(0)} \equiv T_E $$

From this recursion one can obtain an even more useful system of recursive equations for the traces of these transfer matrices. In general there exists a finite subset of words $B \subset A^*$ containing $A$ for which Eq. (2) yields a closed set of recursive polynomial equations for the quantities $x_E^{(k)}(\beta) \equiv \text{tr} T_E^{(k)}(\beta)$, $\beta \in B$, which is called the trace map $[6-8]$. It turns out that to each trace map one can associate, keeping only the term of highest degree in each polynomial, a reduced trace map which is monomial $[9]$, that one can consider as a substitution $\phi$ on the set of traces of transfer matrices of elements of $B$, identified with $B$ in the following, whose properties are ultimately crucial for the spectral analysis. We call such a substitution semi-primitive if:

(i) There exists $C \subset B$ such that $\phi|_C$ is a primitive substitution from $C$ to $C^*$;
(ii) There exists $k$ such that for all $\beta \in B$, $\phi^k(\beta)$ contains at least one letter from $C$.

With this notation, the main result proven in [9] is the following.

**THEOREM [9]:** Let $H$ a one-dimensional Schrödinger operator of type (1) generated by a primitive substitution $\xi$ on a finite alphabet $A$. Assume that its reduced trace map is associated to a semi-primitive substitution $\phi$. Assume also that there is a $k$ such that $\xi^k(0)$ contains $\beta \beta$ for some $\beta \in B$. Then the spectrum of $H$ is singular and supported on a set of zero Lebesgue measure. If moreover there exist $n_0, m < \infty$ such that $\xi^{nm}(0) = \xi^m(\gamma_0) \Gamma \omega$, where $\gamma_0 \in C$, $\Gamma, \omega \in \hat{A}^*$, and $\Gamma = \xi^m(\gamma_0) \delta$ for some $\delta \in \hat{A}^*$, then $H$ has no eigenvalues. Therefore, the spectrum of $H$ is purely singular continuous and supported on a Cantor set of zero Lebesgue measure.

This is in fact an algorithmic procedure to prove the singularity or the singular continuity...
of the spectrum of $H$. Note that the supplementary hypothesis for the second result is probably not necessary, since there is at least one example (Thue-Morse) for which it is not satisfied although $\sigma(H)$ is singular continuous.

3. Examples

The hypothesis of the theorem have been shown to be satisfied in a large number of particular cases in [11].

(i) The Fibonacci sequence: $\xi(a) = ab, \xi(b) = a$: $\sigma(H)$ is singular continuous, as already proven in [4, 5].

(ii) The Thue-Morse sequence: $\xi(a) = ab, \xi(b) = ba$: $\sigma(H)$ is singular as already proven in [8], where we proved that it is in fact singular continuous;

(iii) The period-doubling sequence: $\xi(a) = ab, \xi(b) = aa$: $\sigma(H)$ is singular continuous, as already proven in [8];

(iv) The circle sequence: $\xi(a) = cac, \xi(b) = accac, \xi(c) = abcac$: $\sigma(H)$ is singular continuous, as

(v) The binary non-Pisot sequence: $\xi(a) = ab, \xi(b) = aaa$: $\sigma(H)$ is singular. We can only conjecture that it is singular continuous;

(vi) The ternary non-Pisot sequence: $\xi(a) = c, \xi(b) = a, \xi(c) = bab$: $\sigma(H)$ is singular continuous;

(vii) The Rudin-Shapiro sequence: $\xi(a) = ac, \xi(b) = dc, \xi(c) = ab, \xi(d) = db$: in this case, $\phi$ is not semi-primitive and thus, presently, we cannot even prove the singularity of the spectrum, which is not so surprising if one recalls that it is the ‘most random’ of all these sequences [9, 10].

Let us emphasize that our theorem provides explicit examples of operators with singular continuous spectrum. Complementary results have recently been obtained by Hof et al. [18] in which for certain types of so-called “palindromic” substitutions it was shown that there exists an infinite number of unspecified translates of the original sequence for which the corresponding operator has singular continuous spectrum.

4. Concluding remarks

We end this note with some remarks on the nature of the solutions of the Schrödinger equation (1). The proof of the theorem shows in fact that for energies in the spectrum, no solution tends to zero at infinity, but these leaves room for a variety of behaviours. However, in most cases, there are countable subsets of energies in the spectrum, characterized by the fact that the transfer matrices $T_E^{(n)}(\alpha)$, for given $n$, commute for all $\alpha \in \mathcal{A}$, at which the solutions are extended in a very regular way in that they consist of pieces of repeating patterns arranged according to the substitution $\mathcal{A}$. Such solutions have actually been discovered already in [7 and 8], but they have been recently re-discovered in numerical investigations several times and have given rise to erroneous claims of coexisting absolutely continuous spectrum. While this is nonsense, it is not unlikely that these states will be quite important for the transport properties of systems with singular continuous spectrum,
a problem that still has not been satisfactorily investigated.

5. References

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