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.

We consider one dimensional Schrödinger operators H defined by

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

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

A *substitution* is a map ξ from a finite alphabet $\mathcal{A}$ to the set $\mathcal{A}^*$ of words on $\mathcal{A}$, which can be naturally extended to a map from $\mathcal{A}^*$ to $\mathcal{A}^*$ and then to a map from $\mathcal{A}^{\mathbb{N}}$ to $\mathcal{A}^{\mathbb{N}}$. We also define the free group $\widehat{\mathcal{A}}^*$, extension of $\mathcal{A}^*$ obtained by addition of the formal inverses of the letters in $\mathcal{A}$ as generators. ξ is said *primitive* if $\exists k \in \mathbb{N}$ s.t. $\forall(\alpha,\beta) \in \mathcal{A}^2$, $\xi^k(\alpha)$ contains β. A *substitution sequence* or *automatic sequence* is a ξ-right fixpoint $u_r = \alpha_r...$ given by indefinite iteration of ξ [1]. By choosing a ξ-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 ξ if the sequence $(V_n)_{n\in\mathbb{Z}}$ is defined by $V_n = v(w_n)$, where v is a map $\mathcal{A} \to \mathbb{R}$.

Such operators have become popular as simple models for electron transport in one-dimensional quasi-crystals [2]. The study of some particular examples, namely the Fibonacci [3-6], Thue-Morse [7,8] and period-doubling [8] 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 [3-5,7,8].

(ii) The spectral gaps are labelled by a countable set of algebraic numbers, depending on the substitution [6-8].

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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 [9], 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 [10].

The basic tool to establish (i) is the transfer-matrix formalism. That is, the study of the properties of solutions of Eq. (1) lead to the analysis of products of two-by two matrices of the form

$$P_n(E) = \prod_{k=1}^{n} T_E(w_{n-k}) \tag{2}$$

where w_k is the k-th letter in the substitution sequence w and $T_E : \mathcal{A} \to SL(2)$ 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 2×2-matrices. This includes in particular the continuous Laplacian with piecewise constant potential of a finite number of different shapes (Kronig-Penney model, see [12]). 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 $\gamma(E) = \lim_{n\uparrow\infty} \frac{1}{n} \log ||T_E^{(n)}||$, known to be of zero Lebesgue measure by a general result in [8] based on a theorem of Kotani [13]. 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 $\omega \in \mathcal{A}^*$

$$T_E(\omega) \equiv \prod_{\alpha\in\omega} T_E(\alpha) \tag{3}$$

and

$$T_E^{(k)}(\omega) \equiv T_E^{(k-1)}(\xi(\omega)), \quad \text{with} \quad T_E^{(0)} \equiv T_E \tag{4}$$

¿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 $\mathcal{B} \subset \mathcal{A}^*$ containing $\mathcal{A}$ for which (4) yields a closed set of recursive polynomial equations for the quantities $x_E^{(k)}(\beta) \equiv \operatorname{tr} T_E^{(k)}(\beta)$, $\beta \in \mathcal{B}$, which is called the *trace map* [14,15,11]. It turns out that to each trace map one can associate a *reduced trace map* that is *monomial* [11], and to this a substitution ϕ on $\mathcal{B}$ whose properties are ultimately crucial for the spectral analysis. We call such a substitution *semi-primitive* if:

(i) There exists $\mathcal{C} \subset \mathcal{B}$ such that $\phi|_{\mathcal{C}}$ is a primitive substitution from $\mathcal{C}$ to $\mathcal{C}^*$;

(ii) There exists k such that for all $\beta \in \mathcal{B}$, $\phi^k(\beta)$ contains at least one letter from $\mathcal{C}$.

With this notation, the main result proven in [11] is the following.

THEOREM [11]: *Let H a one-dimensional Schrödinger operator of type (1) generated by a primitive substitution ξ on a finite alphabet $\mathcal{A}$. Assume that its reduced trace map is associated to a semi-primitive substitution ϕ. Assume also that there is a k such that $\xi^k(0)$ contains $\beta\beta$ for some $\beta \in \mathcal{B}$. 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 $\xi^{n_0}(0) = \xi^m(\gamma_0)\Gamma\omega$, where $\gamma_0 \in \mathcal{C}$, $\Gamma, \omega \in \widehat{\mathcal{A}}^*$, and $\Gamma = \xi^m(\gamma_0)\delta$ for some $\delta \in \widehat{\mathcal{A}}^*$, 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.

The hypothesis of the theorem have been shown to be satisfied in a large number of particular cases in [11]; more recently, in [16] a new class of examples was provided by sequences derived from circle maps with rotation numbers obtained from precious means. The only known example in which even the hypothesis necessary to guarantee the singularity of the spectrum are not satisfied is the Rudin-Shapiro sequence [9].

Let us emphasize that out theorem provides explicit examples of operators with singular continuous spectrum. Complementary results have recently been obtained by Hof et al.[17] 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.

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 [12]. 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 been investigated.

References

[1] M. Queffélec, *Substitution dynamical systems. Spectral analysis*, Springer Lecture Notes in Mathematics **1294** (1987)

[2] D. Schechtman, I. Blech, D. Gratias, J.V. Cahn, Phys. Rev. Lett. **53**, 1951-1953 (1984)

[3] M. Casdagli, Comm. Math. Phys. **107**, 295-318 (1986)

[4] A. Sütő, J. Stat. Phys. **56**, 525-531 (1989)

[5] J. Bellissard, B. Iochum, E. Scoppola, D. Testard, Comm. Math. Phys., **125**, 527-543 (1989)

[6] L. Raymond: *A dynamical approach to the gap-labelling of a quasi-periodic Schrödinger operator* in *Dynamique des systèmes complexes, aspects classique et quantique*, Marseille, 13-17/6/1994

[7] J. Bellissard, in *Number theory and physics*, J.-M. Luck, P.Moussa, M. Waldschmidt, eds., Springer Proceedings in Physics **47**, 140-150 (1990); *see also* F. Axel, J. Peyrière, J. Stat. Phys. **57**, 1013-1047 (1989)

[8] J. Bellissard, A. Bovier, J.-M. Ghez, Comm. Math. Phys. **135**, 379-399 (1991)

[9] J. Bellissard, A. Bovier, J.-M. Ghez, Rev. Math. Phys. **4**, 1-37 (1992)

[10] J.-M. Luck, Phys. Rev **B39**, 5834-5849 (1989)

[11] A. Bovier, J.-M. Ghez, Comm. Math. Phys. **158**, 45-66 (1993) and *erratum*, to appear in Comm. Math. Phys.

[12] A. Bovier, J.-M. Ghez: *Remarks on the spectral properties of tight binding and Kronig-Penney models with substitution sequences*, Preprint CPT-94/P.3003

[13] S. Kotani, Rev. Math. Phys. **1**, 129-133 (1990)

[14] J.-P. Allouche, J. Peyrière, C.R. Acad. Sci. Paris **302**, No 18, série II, 1135-1136 (1986)

[15] M. Kolár, F. Nori, Phys. Rev **B42**, 1062-1065 (1990)

[16] M. Hörnquist, M. Johansson: *Singular continuous electron spectrum for a class of circle sequences*, Preprint Linköping University (1994), to appear in J. Phys. A

[17] A. Hof, O. Knill, B. Simon: *Singular continuous spectrum for palindromic Schrödinger operators*, Preprint Caltech (1994).