Spectral Calculations for Quasiperiodic Schrödinger Operators

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One dimensional Schrödinger operators

Consider the Hamiltonian H defined pointwise by

$$(H\psi)(n) = \psi(n+1) + \psi(n-1) + V(n)\psi(n)$$

for doubly-infinite square-summable sequences $\psi \in \ell_2(\mathbf{Z})$.

- Here the *potential* $\{V(n)\}$ is a *bounded*, *real-valued* sequence.
- Thus H is a *bounded, self-adjoint operator* with matrix representation

$$H = \begin{bmatrix} \ddots & \ddots & \ddots & & & & \\ & 1 & V(-1) & 1 & & & \\ & & 1 & V(0) & 1 & & \\ & & & 1 & V(1) & 1 & \\ & & & & \ddots & \ddots & \ddots \end{bmatrix}.$$

- We wish to understand how the potential V affects the solution $\psi(t)$ of the Schrödinger equation

$$\psi_t(t) = -\mathrm{i}H\psi(t).$$

- Such an understanding requires knowledge of the spectrum $\sigma(H)$.

Overview

- A ‘rough guide’ to one-dimensional Schrödinger operators
  — periodic, random, and quasi-periodic potentials
- Properties of the Fibonacci Hamiltonian
  — spectral estimates
- Computation of the fractal dimension of the spectrum

Three classes of potential

We shall encounter three classes of potential functions,
each of which give rise to Schrödinger operators
with distinct spectral characteristics.

- Periodic potentials.
  1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, ... (period 1)
  1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, ... (period 2)

- Random potentials.
  0, 1, 1, 1, 1, 1, 0, 0, 1, 0, 0, 0, 0, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 0, ... (Bernoulli)

- Deterministic potentials that are not periodic.
  1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, ... (Fibonacci)

We wish to characterize the spectrum in terms of the potential function.

Spectral Theorem

If H is a self-adjoint, N-dimensional matrix, we can always write

$$H = \sum_{k=1}^{N} \lambda_j P_j,$$

where $P_j = u_j u_j^*$ is an orthogonal projection onto the span of the unit eigenvector u_j. For any function f analytic on the spectrum of H, we have

$$\langle x, f(H)x\rangle = \sum_{k=1}^{N} f(\lambda_j)\langle x, P_j x\rangle.$$

Similarly, if H is a bounded, self-adjoint operator on $\ell_2(\mathbf{Z})$, then for all $\psi \in \ell_2(\mathbf{Z})$ there exists a unique *spectral measure* μ_ψ such that

$$\langle \psi, f(H)\psi\rangle = \int_{\sigma(A)} f(E)\, \mathrm{d}\mu_\psi(E)$$

for all f analytic on $\sigma(H)$.

The measure can be decomposed into its *absolutely continuous*, *singular continuous*, and *pure point* components.

See, e.g., [Reed & Simon 1978; Teschl 1999; Damanik].

Periodic potentials

Let the potential V be periodic with period p.

Let $H^{\pm}$ denote rank-2 updates of the $p \times p$ section:

$$H^{\pm} = \begin{bmatrix} V(1) & 1 & & \\ 1 & V(2) & \ddots & \\ & \ddots & \ddots & 1 \\ & & 1 & V(p) \end{bmatrix} \pm e_1 e_n^* \pm e_n e_1^*$$

with eigenvalues

$$\sigma(H^+) = \{E_1^+, \ldots, E_p^+\}, \qquad \sigma(H^-) = \{E_1^-, \ldots, E_p^-\}.$$

Collect the union of these eigenvalues and sort them in increasing order:

$$E_1 < E_2 \le E_3 < E_4 \le \cdots \le E_{2p-1} < E_{2p}.$$

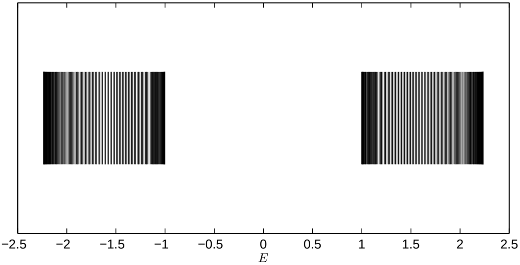
The spectrum of the Hamiltonian is *purely absolutely continuous* and

$$\sigma(H) = \bigcup_{j=1}^{p} [E_{2j-1}, E_{2j}].$$

[Teschl 1999, Ch. 7]

Example of a periodic potential

Spectrum of a 500×500 section: periodic potential with $V(n) = (-1)^n$.



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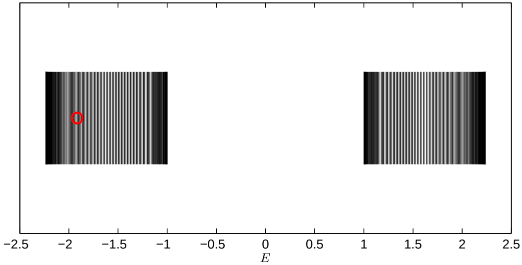
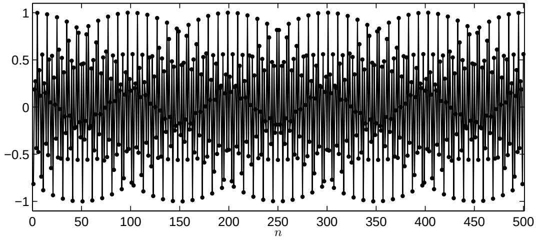


sample eigenvector (linear scale)



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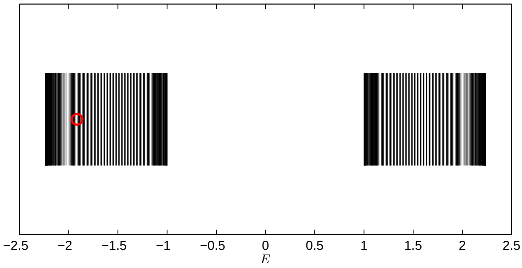

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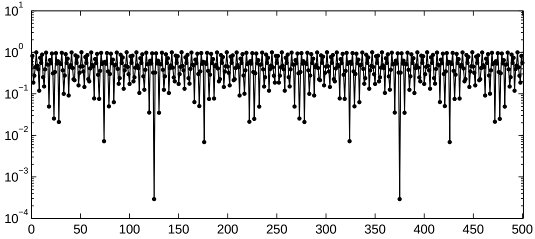

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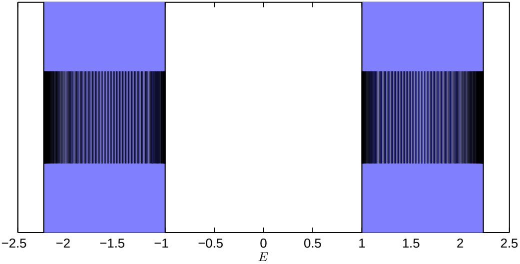
blue bands show $\sigma(H)$



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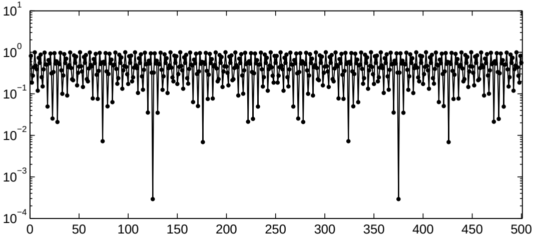

Random potentials

We restrict attention to *Anderson models*, where every entry of the potential is an independent, identically distributed (iid) random variable.

For example, $V(n) = \pm 1$, or $V(n) \in [-2, 2]$, with uniform probability.

There are exceptional ways to sample such distributions (e.g., giving periodic samples), so we can only hope for "almost sure" statements (those that hold with probability 1).

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Summary of results [Teschl 1999, Ch. 5; Damanik] for potentials V drawn from a compact, nontrivial interval of $\mathbf{R}$.

- There exists some bounded set $\mathbf{\Sigma} \subset \mathbf{R}$ such that

$$\sigma(H) = \Sigma, \text{ a.s.}$$

- The spectrum is almost surely pure point.
- The eigenfunctions are almost surely localized (exponentially decaying).

The non-self-adjoint case is also interesting [Hatano and Nelson 1996, ...].

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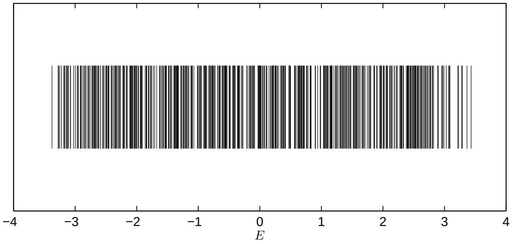

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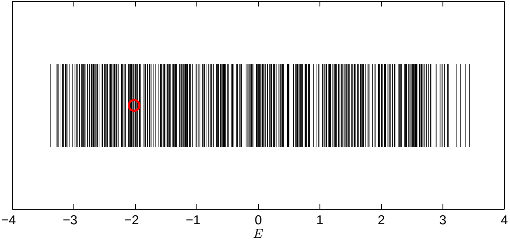

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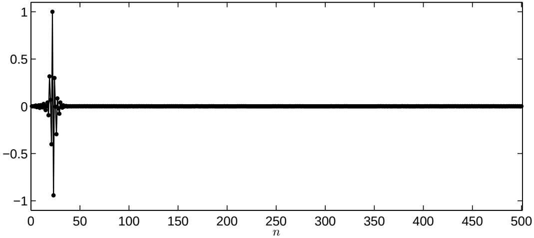

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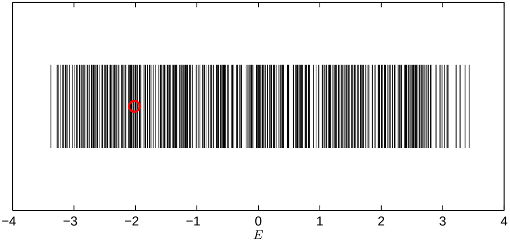

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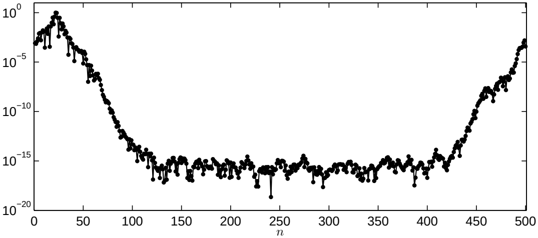


Anderson localization

Deterministic, non-periodic potentials

The periodic and stochastic models are separated by a gulf of deterministic, non-periodic potentials that are of particular interest as models, e.g., of quasicrystals.

Do these more closely resemble the periodic or stochastic case?

To answer to this question, one analyzes details of each particular potential. Three examples, all with $\lambda > 0$:

- Almost Mathieu potential. Let $|\omega| = 1$ and α irrational:

$$V(n) = \lambda \cos(2\pi(\omega + \alpha n))$$

- Period doubling potential. Let α be irrational:

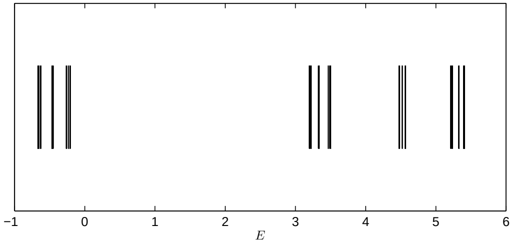
$$V(n) = \lambda \cos(2\pi\alpha 2^n)$$

- Fibonacci potential. Let ϕ denote the golden ratio, $\phi \equiv \frac{1}{2}(\sqrt{5} + 1)$;

$$V(n) = \begin{cases} \lambda, & (n/\phi \bmod 1) \geq 1 - 1/\phi; \\ 0, & \text{otherwise.} \end{cases}$$

Example of a deterministic, non-periodic potential

Spectrum of a 500×500 section: Fibonacci potential with $\lambda = 4.1$.



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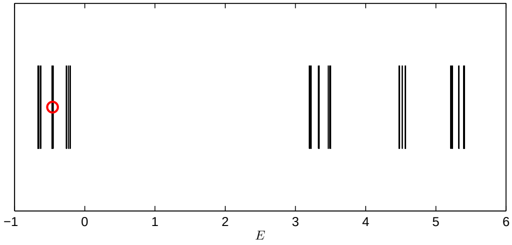

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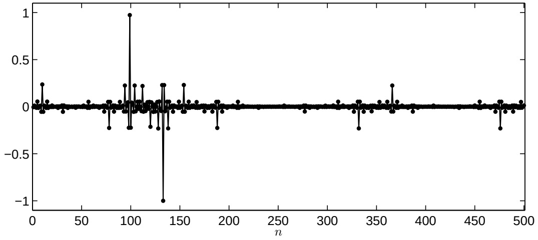

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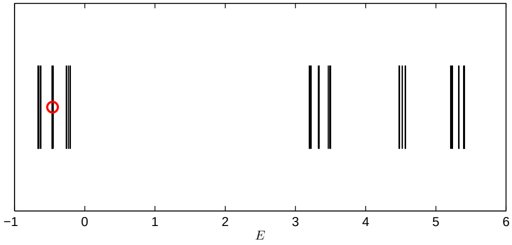

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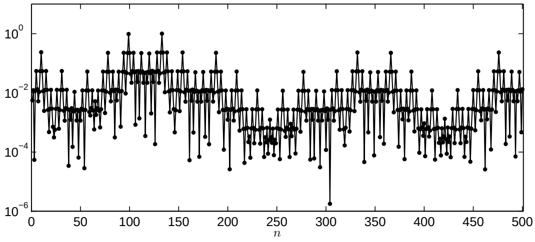
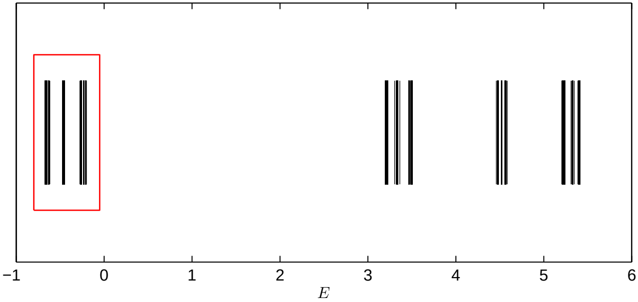


Closer examination of the Fibonacci spectrum

5000×5000 section with Fibonacci potential, $\lambda = 4.1$.

We zoom-in near the left end of the spectrum...



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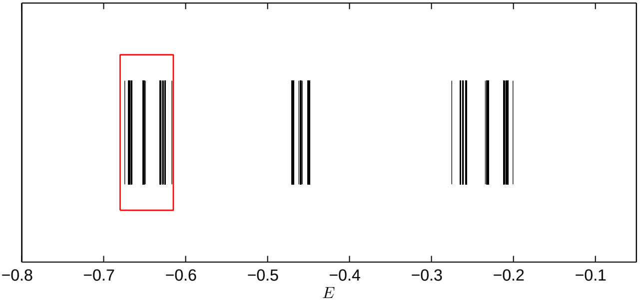

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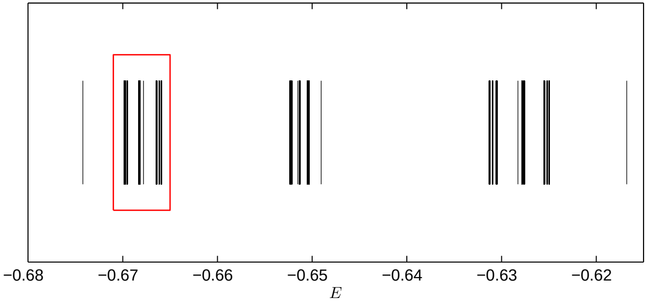

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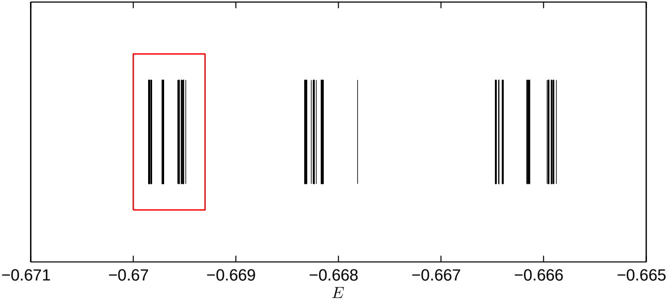

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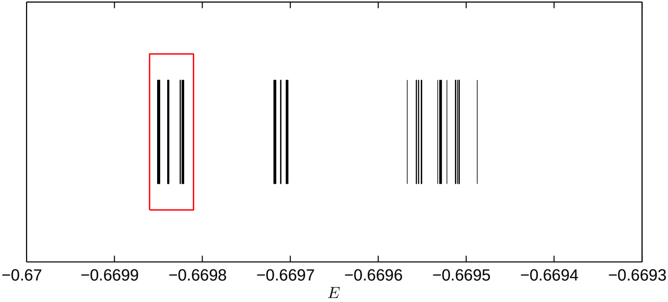

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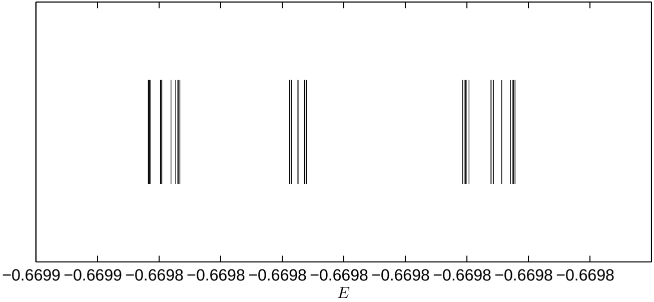

We would like to rigorously explain this phenomenon.

Fibonacci potential

Let Σ_λ denote the spectrum of the Hamilonian with Fibonacci potential

$$V(n) = \begin{cases} \lambda, & (n/\phi \bmod 1) \geq 1 - 1/\phi; \\ 0, & \text{otherwise.} \end{cases}$$

[Kohmoto, Kadanoff, Tang 1983; Ostlund et al. 1983]

Fibonacci potential $V(n)$ for $n = 1, \ldots 75$ with $\lambda = 1$:
101101011011010110101101101011011010110101101101011010110110101101101011010

75 random Bernoulli samples:
101111100100001100101100010000001101001101011111001001110001011000001001001

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Some known facts [Sütő 1989]:

- Σ_λ is a Cantor set, $\text{Leb}(\Sigma_\lambda) = 0$;
- The spectral measures associated with Σ_λ are purely singular continuous.

Box counting dimension

We wish to measure the fractal dimension of the spectrum Σ_λ.
One characterization is the *box counting dimension*.

For fixed $\varepsilon > 0$, count the number of ε-intervals that cover $S \subset \mathbf{R}$:

$$N_S(\varepsilon) = \#\{j \in \mathbf{Z} : [j\varepsilon, (j+1)\varepsilon) \cap S \neq \emptyset\}.$$

We can then define the *lower* and *upper box counting dimension* as

$$\dim_B^-(S) = \liminf_{\varepsilon \to 0} \frac{\log N_S(\varepsilon)}{\log(1/\varepsilon)}, \qquad \dim_B^+(S) = \limsup_{\varepsilon \to 0} \frac{\log N_S(\varepsilon)}{\log(1/\varepsilon)}.$$

When these two values agree, the result is the *box counting dimension*:

$$\dim_B(S) = \dim_B^-(S) = \dim_B^+(S).$$

Box counting dimension

Examples:

- If $S = [a, b]$ with $b > a$, then $N_S(\varepsilon) \approx (b-a)/\varepsilon$ and so

$$\dim_B(S) = \lim_{\varepsilon \to 0} \frac{\log(b-a) + \log(1/\varepsilon)}{\log(1/\varepsilon)} = 1.$$

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- For the Cantor middle-thirds set,

$$\dim_B(S) = \frac{\log(2)}{\log(3)} = 0.6309\ldots.$$

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  Bounds derived from [Liu and Wen 2004] and [Raymond 1997]:

$$0.23104\ldots = \frac{\log 2}{3} \leq \lim_{\lambda \to \infty} \dim_B(\Sigma_\lambda) \log \lambda \leq 2 \log \phi = 0.96242\ldots.$$

Wave packet spreading

Why care about the fractal dimension of the spectrum?

Wave packet spreading

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We wish to measure how fast a localized initial state $\psi(0)$ spreads out under the evolution of the Schrödinger equation

$$\psi'(t) = -\mathrm{i}Ht\psi(t).$$

Let $\delta_n \in \ell_2(\mathbf{Z})$ be zero everywhere except for 1 in the nth entry.

We will take $\psi(0) = \delta_1$.

How much energy is contained in the tails of the solution?

At time T, define

$$P(N,T) = \frac{2}{T} \sum_{|n|>N} \mathrm{e}^{-2t/T} |\langle \mathrm{e}^{-\mathrm{i}Ht}\delta_1, \delta_n\rangle|^2 \, \mathrm{d}t.$$

Decay of wave packet tails

$$P(N,T) = \frac{2}{T} \sum_{|n|>N} \mathrm{e}^{-2t/T} |\langle \mathrm{e}^{-\mathrm{i}Ht} \delta_1, \delta_n \rangle|^2 \, \mathrm{d}t$$

How fast are the tails of the wave packet decaying?

With

$$S^-(\alpha) = -\liminf_{T\to\infty} \frac{\log P(T^\alpha - 2, T)}{\log T}, \qquad S^+(\alpha) = -\limsup_{T\to\infty} \frac{\log P(T^\alpha - 2, T)}{\log T},$$

we have the critical exponent:

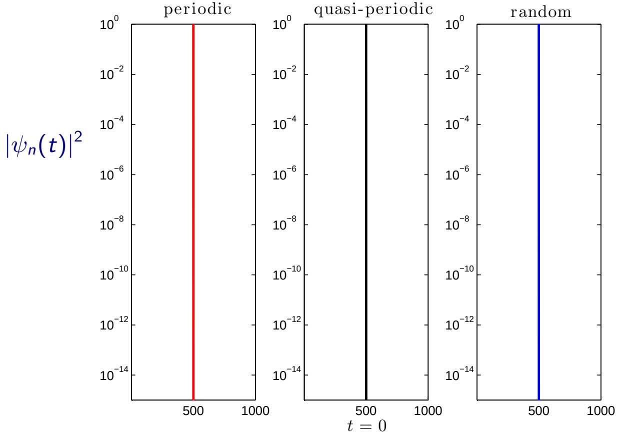
$$\alpha^\pm = \sup\{\alpha \geq 0 : S^\pm(\alpha) < \infty\}.$$

Theorem [DEGT 2008]: For the Fibonacci potential with $\lambda > 0$,

$$\alpha^\pm \geq \dim_B(\Sigma_\lambda).$$

Wave packet spreading: illustration

Consider the following discrete simulation with the same periodic, random, and Fibonacci potentials whose spectra were illustrated earlier.



Simulation with $N = 1000$ and $\psi_n(0) = \delta_{500}$.

Sütő's periodic potentials

Sütő [1987] showed that if we replace ϕ in the Fibonacci potential with the ratio of successive Fibonacci numbers, $\phi_k = F_k/F_{k-1}$, we obtain

$$V_k(n) = \begin{cases} \lambda, & (n/\phi_k \bmod 1) \geq 1 - 1/\phi_k; \\ 0, & \text{otherwise.} \end{cases}$$

The potential V_k is *periodic*, as seen in the following table with $\lambda = 1$.

k	F_k	periodic potential values for level-k approximation
1	1	11111111111111111111111111111111111111111111111111111111111111111111
2	2	10101010101010101010101010101010101010101010101010101010101010101010
3	3	11011011011011011011011011011011011011011011011011011011011011011011
4	5	10110101101011010110101101011010110101101011010110101101011010110101
5	8	10110110101101101011011010110110101101101011011010110110101101101011
6	13	10110101101101011010110110101101011011010110101101101011010110110101
7	21	10110101101101011011010110101101101011011010110101101101011011010110
8	34	10110101101101011010110110101101101011010110110101101011011010110110
∞	∞	10110101101101011010110110101101101011010110110101101011010110110110...

Sütő's periodic potentials: polynomials

Furthermore, Sütő [1987] showed that the spectrum of the associated Hamiltonian

$$(H_k\psi)(n) = \psi(n+1) + \psi(n-1) + V_k(n)\psi(n)$$

can be determined from the polynomials

$$\begin{aligned} p_{-1}(E) &= 2 \\ p_0(E) &= E \\ p_1(E) &= E - \lambda \\ &\vdots \\ p_{k+1}(E) &= p_k(E)p_{k-1}(E) - p_{k-2}(E) \end{aligned}$$

The spectrum of H_k is given by

$$\sigma_k := \{E \in \mathbf{R} : |p_k(E)| \leq 2\}.$$

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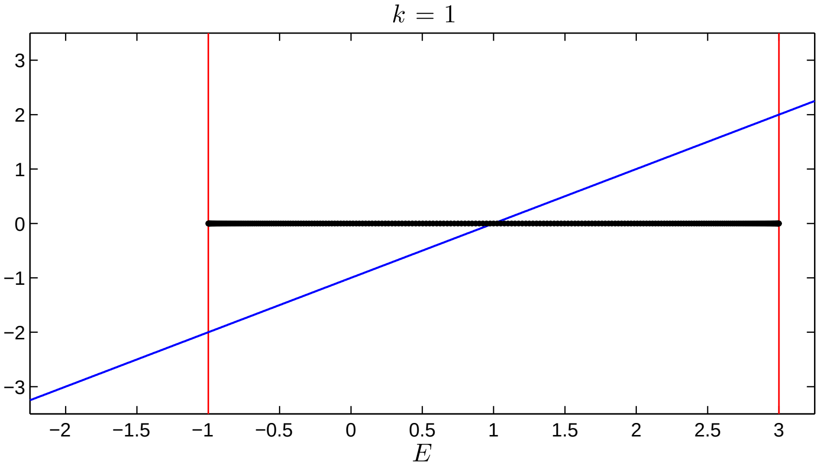
For $k \ge 0$, note that $\deg(p_k) = F_k$, the kth Fibonacci number.
For example, $\deg(p_{100}) > 5.73 \times 10^{20}$.

Sütő's approximate spectrum for $\lambda = 1$

The blue line shows $p_k(E)$.
The red lines show where $|p_k(E)| = 2$.
The black dots show eigenvalues for a 500×500 finite section.



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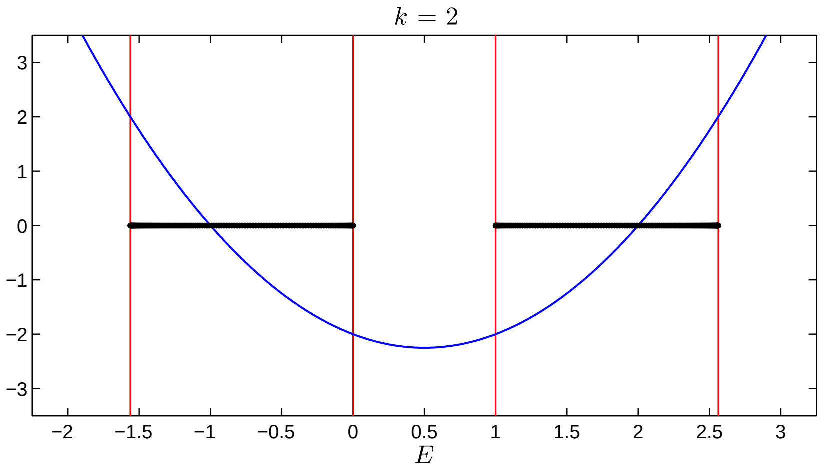

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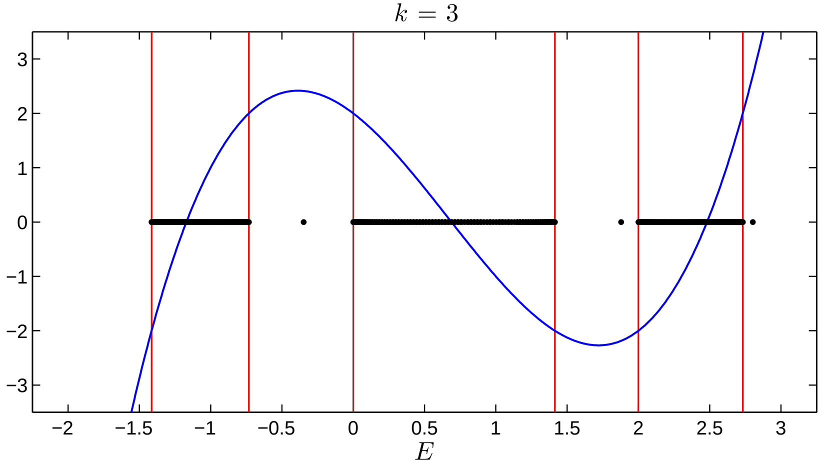

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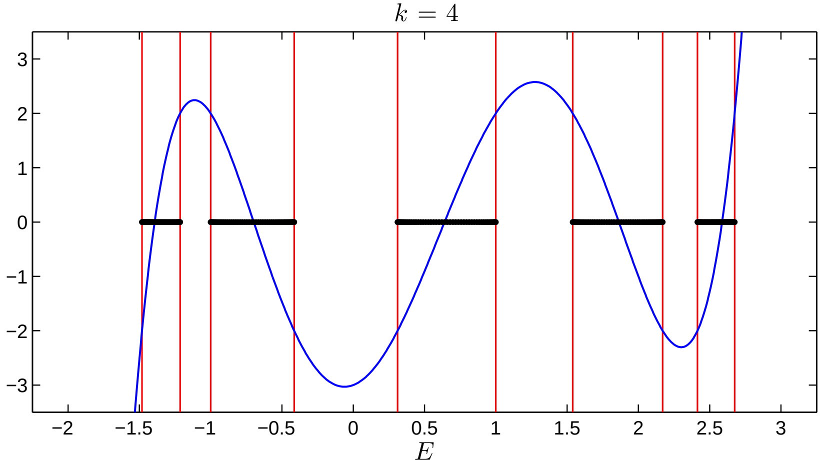
The blue line shows $p_k(E)$.
The red lines show where $|p_k(E)| = 2$.
The black dots show eigenvalues for a 500×500 finite section.



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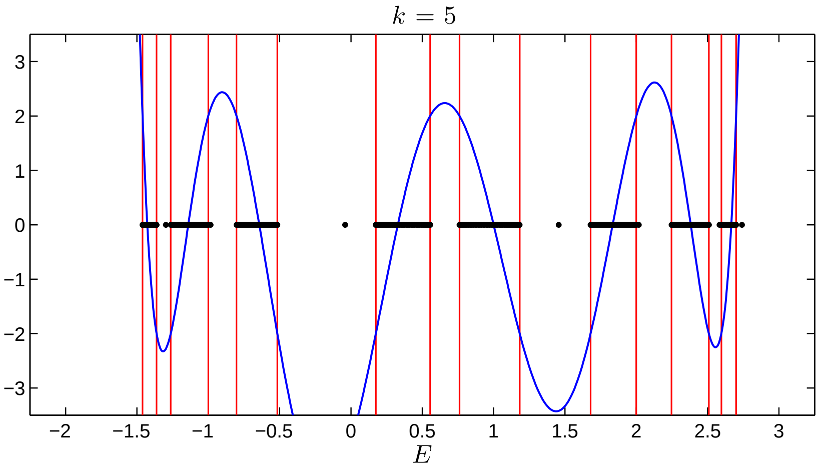
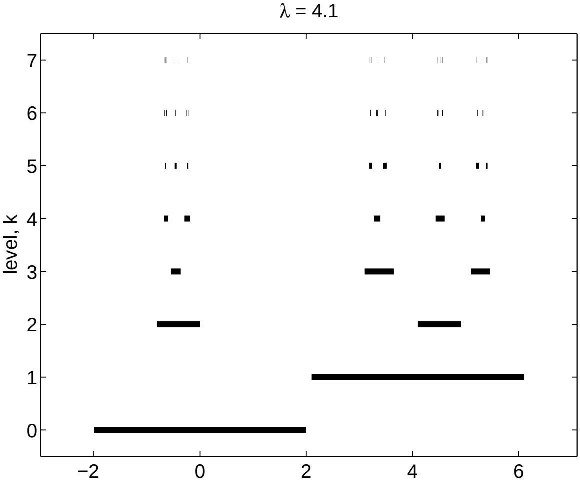


Spectral estimates based on Sütő's polynomials



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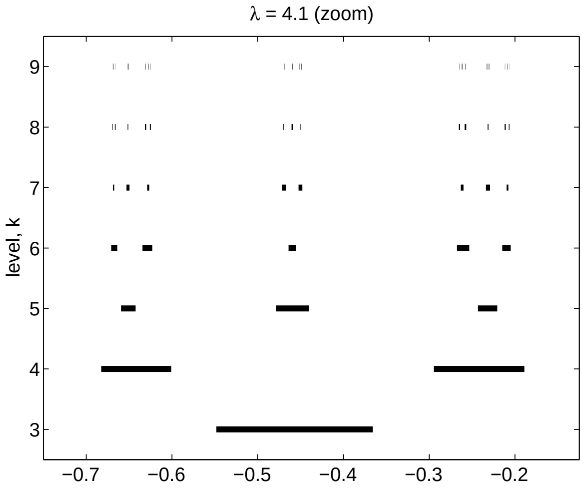

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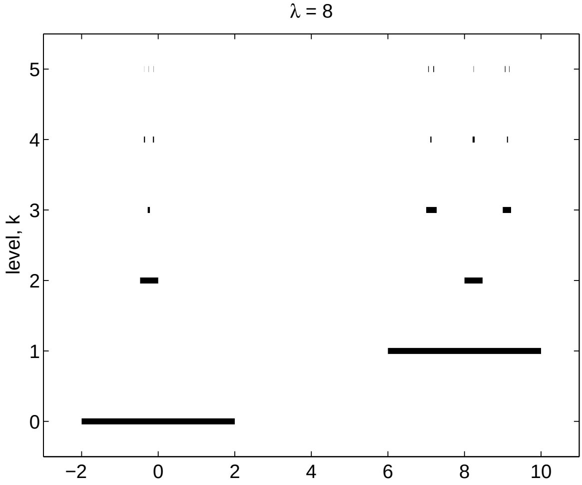

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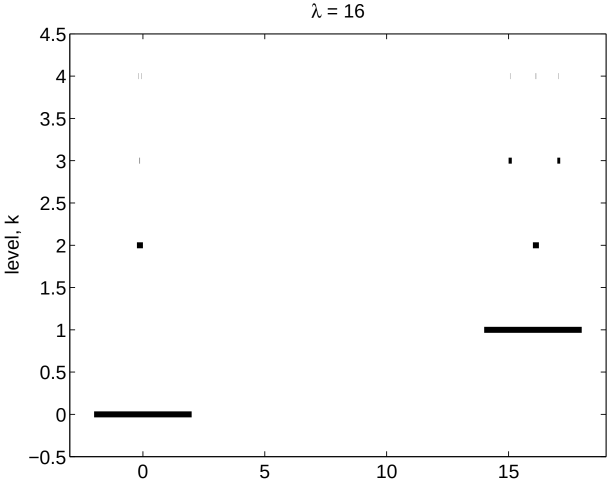
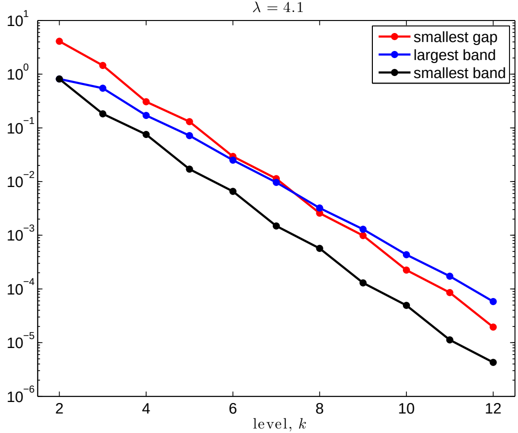


Spectral statistics for Sütő's approximation

At level k, the periodic approximation has F_k bands.
These bands are shrinking in width and getting closer as k increases.
These properties make computation of the bandwidths nontrivial.



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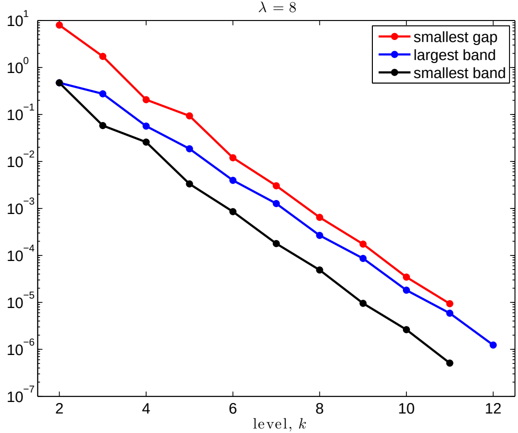

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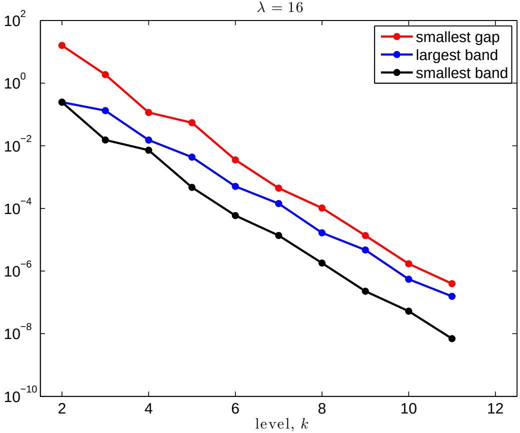


Classification of bands in σ_k

Sütő [1987] also showed that

$$(\sigma_k \cup \sigma_{k+1}) \subset (\sigma_{k-1} \cup \sigma_k)$$

and

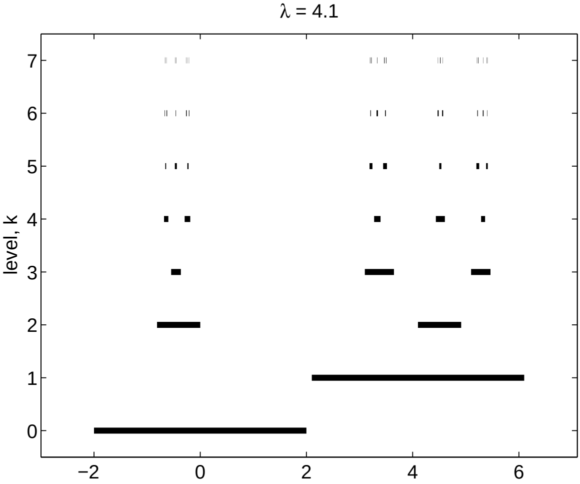
$$\sigma(H) = \bigcap_{k \geq 1} (\sigma_k \cup \sigma_{k+1}).$$

[Killip, Kiselev, Last 2003]: All bands I_k in σ_k can be classified in one of two ways:

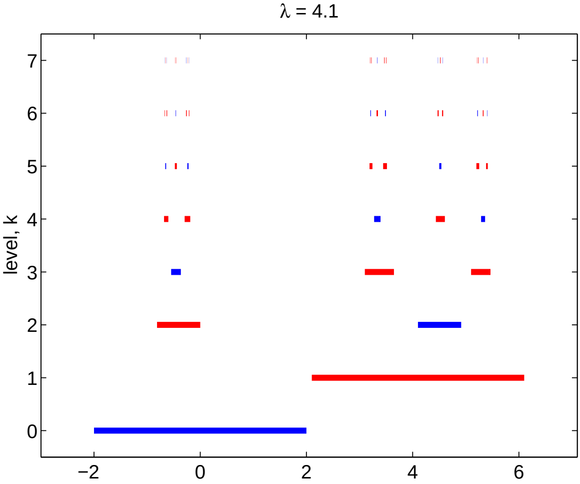
- If $I_k \subset \sigma_{k-1}$, it is called 'Type A';
- If $I_k \subset \sigma_{k-2}$, it is called 'Type B'.

We can write down a recurrence for the bands of each type at each level k, and asymptotically measure the width of these bands.

Spectral Estimates Based on Sütő's Polynomials



Spectral Estimates: A bands (blue) and B bands (red)



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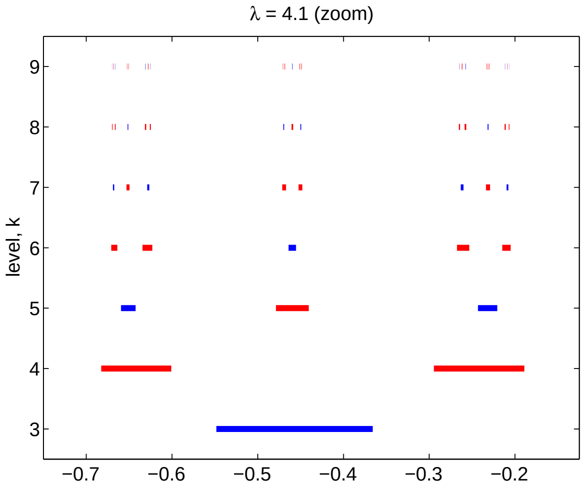

Classification of bands in σ_k

Moreover, we can describe how bands overlap at each level:

$$a_{k,m} = \text{number of type-A bands } I \text{ in } \sigma_k \text{ with } \#\{0 \le j < k : I \cap \sigma_j \ne \emptyset\} = m;$$

$$b_{k,m} = \text{number of type-B bands } I \text{ in } \sigma_k \text{ with } \#\{0 \le j < k : I \cap \sigma_j \ne \emptyset\} = m.$$

We have a recurrence for these values:

$$\begin{aligned} a_{k,m} &= b_{k-1,m-1} \\ b_{k,m} &= a_{k-2,m-1} + 2b_{k-2,m-1} \end{aligned}$$

with $a_{0,m} = a_{1,m} = b_{0,m} = b_{1,m} = 0$ except for

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Can we find explicit formulas for $a_{k,m}$?

Values of $a_{k,m}$ (k on vertical axis, m on horizontal axis)

	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
0	1																				
1																					
2		1																			
3			1																		
4			2																		
5				3																	
6				4	1																
7					8																
8					8	5															
9						20	1														
10						16	18														
11							48	7													
12							32	56	1												
13								112	32												
14								64	160	9											
15									256	120	1										
16									128	432	50										
17										576	400	11									
18										256	1120	220	1								
19											1280	1232	72								
20											512	2816	840	13							
21												2816	3584	364	1						
22												1024	6912	2912	98						
23													6144	9984	1568	15					
24													2048	16640	9408	560	1				
25														13312	26880	6048	128				
	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20

Closed form expressions for $a_{k,m}$ and $b_{k,m}$

We have $a_{k,m} = 0$ unless $\lceil k/2 \rceil \leq m \leq \lfloor 2k/3 \rfloor$, in which case:

$$a_{k,m} = 2^{2k-3m-1} \frac{m}{k-m} \binom{k-m}{2m-k}.$$

Then for all $k, m \geq 0$:

$$b_{k,m} = a_{k+1,m+1}.$$

Computing the fractal dimension as $\lambda \to \infty$

Using Stirling's approximation, we obtain $k/2 \leq m \leq 2k/3$,

$$\frac{1}{\sqrt{k}} \exp(m\, f(m/k)) \lesssim a_{k,m} \lesssim \sqrt{k} \exp(m\, f(m/k)),$$

where

$$f(x) = \frac{1}{x}\Big((2-3x)\log 2 + (1-x)\log(1-x) \\ - (2x-1)\log(2x-1) - (2-3x)\log(2-3x)\Big)$$

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From this we deduce that

$$\lim_{k\to\infty} \max_m \frac{\log a_{m,k}}{m} = f^*,$$

where f^* is the maximum of f over $x \in [1/2, 2/3]$.

Summary

Using properties of the band widths, we arrive at:

Theorem. If $\lambda > 16$, then

$$\frac{f^*}{\log S_u(\lambda)} \leq \dim_B(\Sigma_\lambda) \leq \frac{f^*}{\log S_l(\lambda)},$$

where

$$S_u(\lambda) = 2\lambda + 22, \qquad S_l(\lambda) = \frac{1}{2}\left((\lambda - 4) + \sqrt{(\lambda - 4)^2 - 12}\right)$$

and

$$f^* = \log(1 + \sqrt{2}).$$

Corollary.

$$\lim_{\lambda \to \infty} \dim(\Sigma_\lambda) \cdot \log \lambda = f^*.$$

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$$\lim_{\lambda \to \infty} \dim(\Sigma_\lambda) \cdot \log \lambda = f^*.$$

D. Damanik, M. Embree, A. Gorodetski, S. Tcheremchantsev.
The Fractal dimension of the spectrum of the Fibonacci Hamiltonian.
Comm. Math. Phys. 280 (2008) 499–516.

See also the subsequent article:
Q.-H. Liu, J. Peyrière, Z.-Y. Wen. Dimension of the spectrum of one-dimensional discrete Schrödinger operators with Sturmian potentials.
C. R. Acad. Sci. Paris, Ser. I 345 (2007) 667-672.