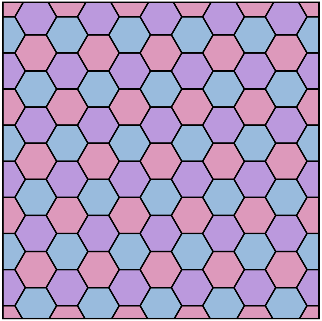
Improved Spectral Calculations for Discrete Schrödinger Operators

Charles Puelz

Rice University

April 3, 2013

Types of crystals



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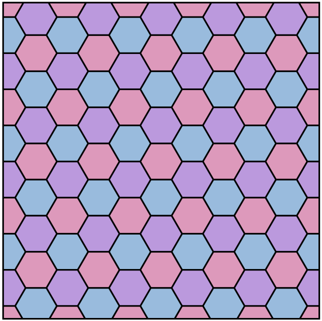

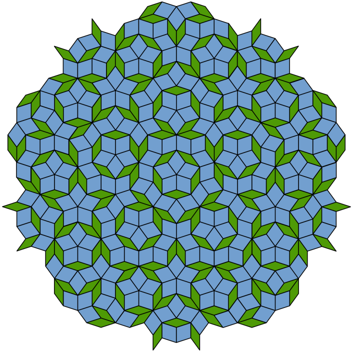

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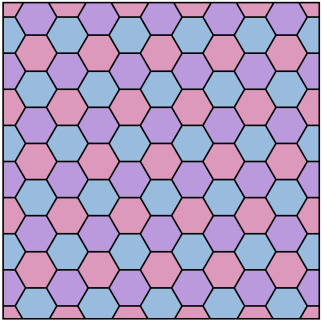
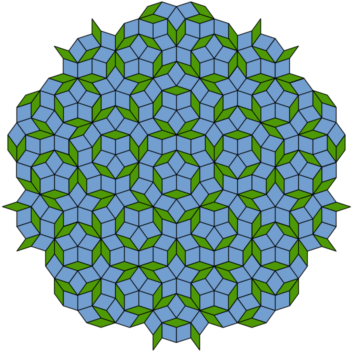


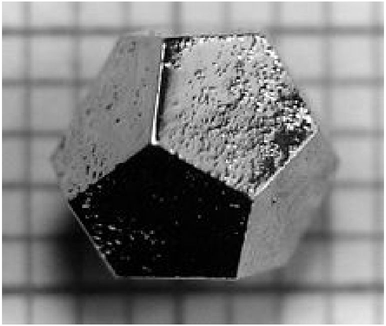


Drake, N., "Prospecting for Quasicrystals," *Science News*, Nov. 3, 2012.

`http://en.wikipedia.org/wiki/File:Tiling_Regular_6-3_Hexagonal.svg`

`http://en.wikipedia.org/wiki/File:Penrose_Tiling_(Rhombi).svg`

Synthetic Quasicrystal



http://en.wikipedia.org/wiki/File:Ho-Mg-ZnQuasicrystal.jpg

PDE model: Schrödinger Equation

To investigate electronic properties of quantum systems,
we seek solutions of:

$$\imath \partial_t \Psi(x,t) = \mathcal{H}\Psi(x,t)$$

$$\mathcal{H} = \Delta + V(x) \text{ and } \Psi(\cdot,t) \in L^2(-\infty,\infty).$$

$|\Psi(\cdot,t)|^2$ is the probability density of the quantum particle in space.

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Separations of variables with $\Psi(x,t) = \psi(x)\phi(t)$ yields

$$\mathcal{H}\psi = E\psi.$$

We analyze a finite difference approximation of $\mathcal{H}$.

Schrödinger Operators

Instead of working directly with $\mathcal{H}$, consider $\mathbf{H} : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$.

$$(\mathbf{H}\psi)_n = \psi_{n-1} + v_n \psi_n + \psi_{n+1},$$

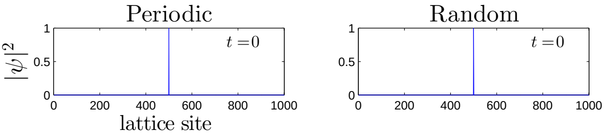
where $\{v_n\} \in \ell^\infty(\mathbb{Z})$ determined by physical system.

Examples:

- Periodic: $1, 0, 1, 0, 1, 0, 1, 0, \ldots$
- Random: v_n uniform random in $[0, 1]$.
- Somewhere "in between" (quasicrystal models)

Periodic versus Random

$$\psi(t) = e^{-\imath \mathbf{H} t}\psi(0).$$



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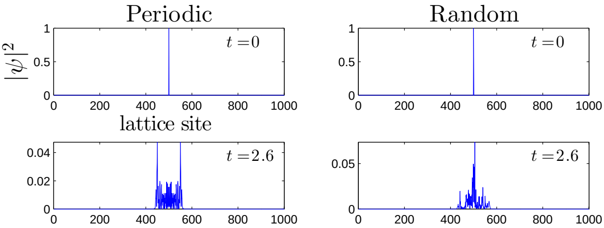

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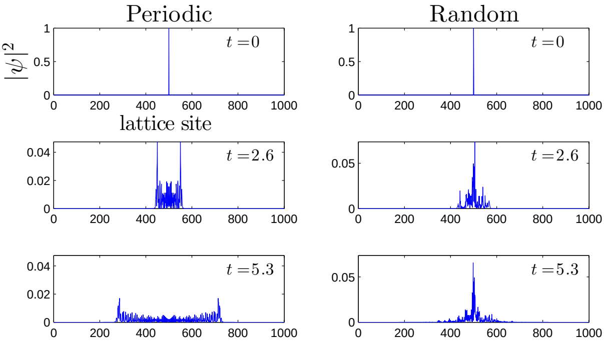

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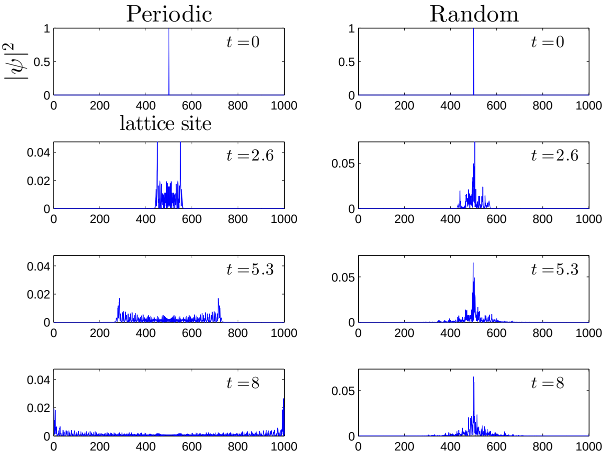

Quasiperiodic

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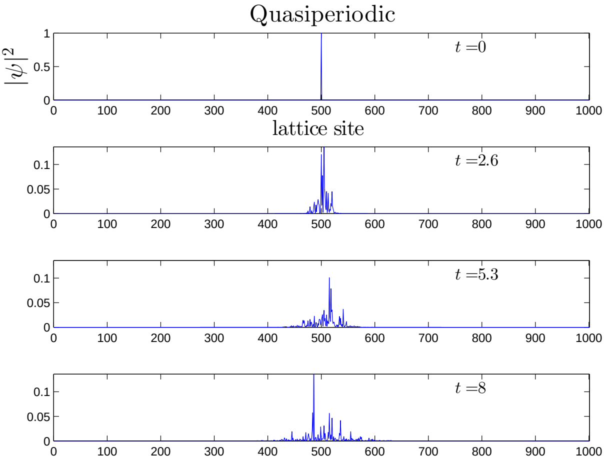

Aperiodic model: The Fibonacci Hamiltonian

Potential: $v_n = \lambda\chi_{[1-\phi^{-1},1)}(n\phi^{-1} \text{mod } 1)$, $\phi = \frac{1+\sqrt{5}}{2}$, $\lambda > 0$.
i.e. with $\lambda = 1$, the main diagonal starting with $n = 1$ is

$$\ldots 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, 1, 0, 1, 0, 1, 1, 0, 1, 0 \ldots$$

- $\sigma(\mathbf{H})$ is a Cantor set (Sütő 1989), dynamically defined for λ sufficiently large and small.

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- Approximate $\sigma(\mathbf{H})$ with σ_k = spectrum of periodic operator with potential $v_n^{(k)}$ given by replacing ϕ with F_k/F_{k-1}.

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- $\sigma(\mathbf{H}) = \bigcap_{k\geq 1} \sigma_k \cup \sigma_{k+1}$
- $\sigma_k \cup \sigma_{k+1} \subset \sigma_{k-1} \cup \sigma_k$ (Sütő 1987).

"Good approximation" for larger k

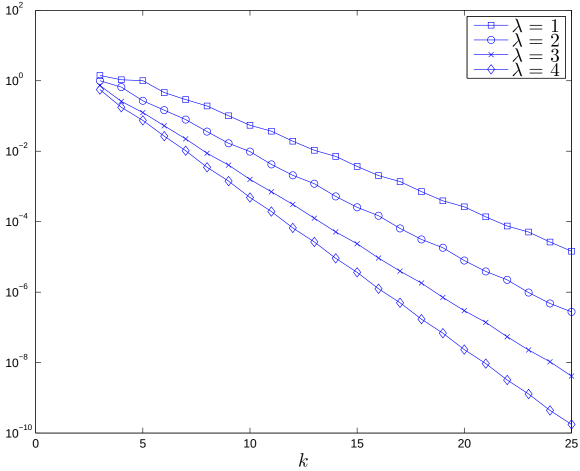

Figure: Maximum interval length in $\sigma_k \cup \sigma_{k+1}$

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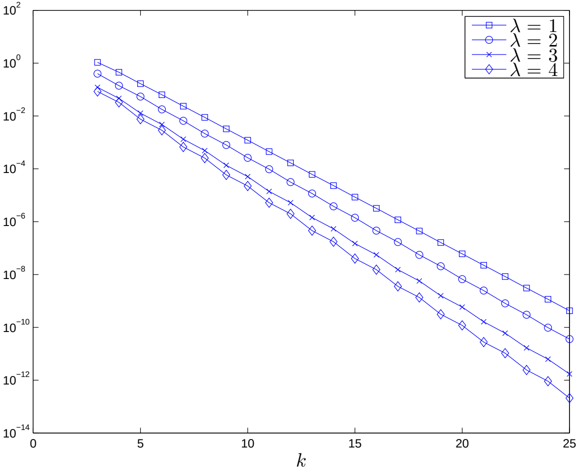

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How to compute σ_k?

Two ways:

- From a particular dynamical map: not robust.
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- From a particular dynamical map: not robust.
  - Kohmoto, Sutherland, and Tang (1987).
  - Naka, Ino, and Kohmoto (2005).
- Eigenvalues of matrices: great! but a large-scale eigenvalue problem...
  - Lamoureux, for Almost Mathieu (1997).
  - Mandel and Lifshitz (2006, 2008). $\mathbf{k = 15}$, $\mathbf{N = 987}$.
  - Damanik, Embree, and Gorodetski (2012). $\mathbf{k = 21}$, $\mathbf{N = 17711}$.

The sets σ_k for $k = 1, \ldots, 5$

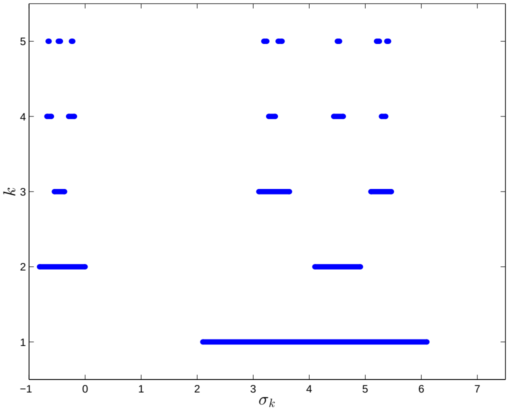

Figure: Plot of σ_k for $\lambda = 4.1$.

I compute to $k = 26$, so σ_k has $F_k = 196418$ intervals.

Dynamical Map to compute σ_k

Lemma (Sütő 1987)

Given the following initial conditions $x_{-1} = 2$, $x_0 = E$, $x_1 = E - \lambda$ *and the map* $x_{k+2} = x_{k+1}x_k - x_{k-1}$,

$$\sigma_k = \{E : |x_k(E)| \leq 2\}.$$

Idea: Root-finding algorithm for $x_k(E) \pm 2$.

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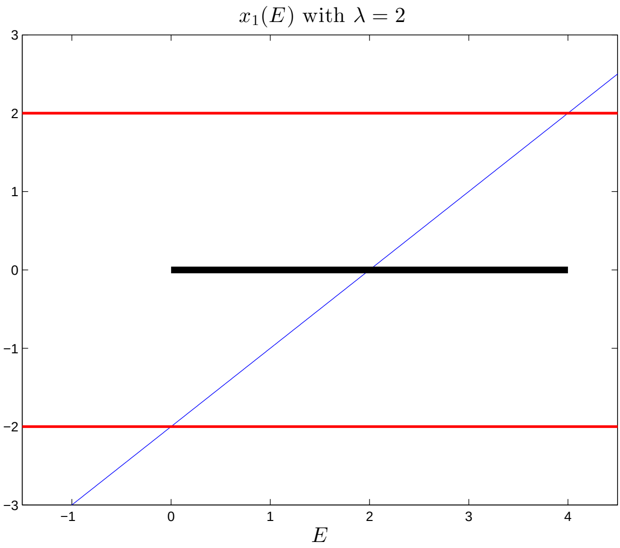
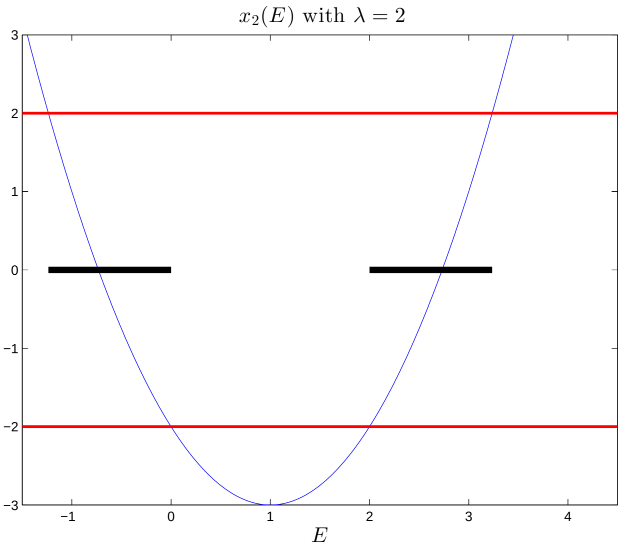
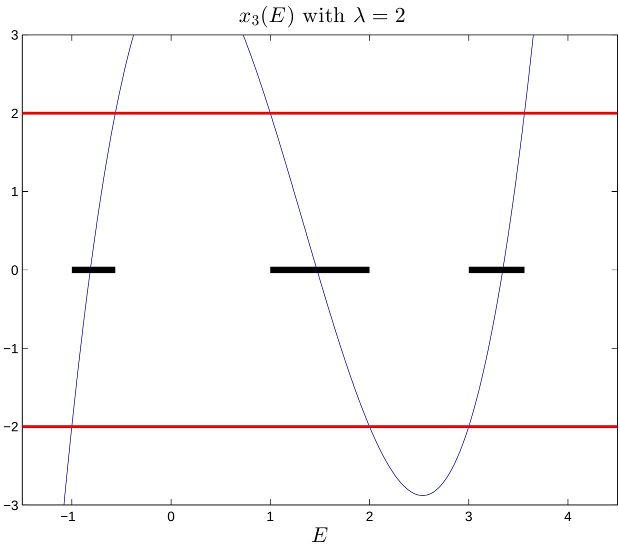
For example, with $\lambda = 5$:

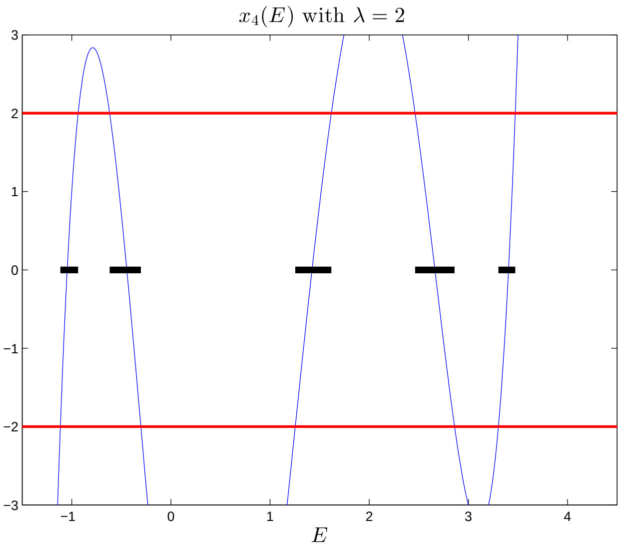
$$x_6(E) = x^{13} - 40x^{12} + 687x^{11} - 6560x^{10} + 37440x^9 - 125550x^8$$
$$+211169x^7 + \ldots + 2210.$$

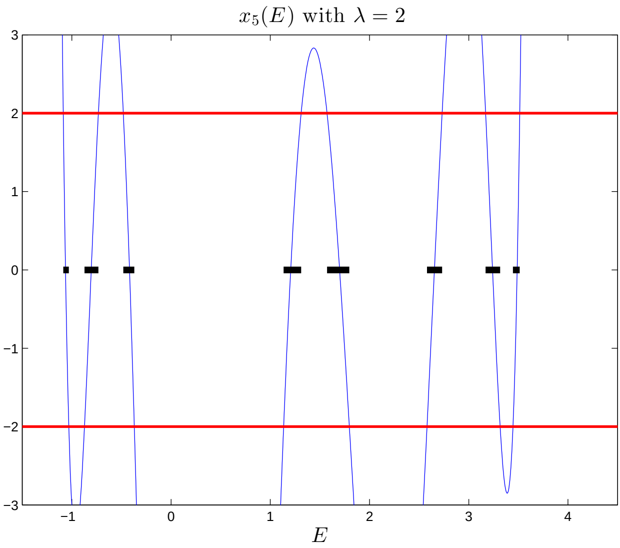

$x_1(E)$ with $\lambda = 2$
3
2
1
0
−1
−2
−3
−1
0
1
2
3
4
E


$x_2(E)$ with $\lambda = 2$
3
2
1
0
−1
−2
−3
−1
0
1
2
3
4
E



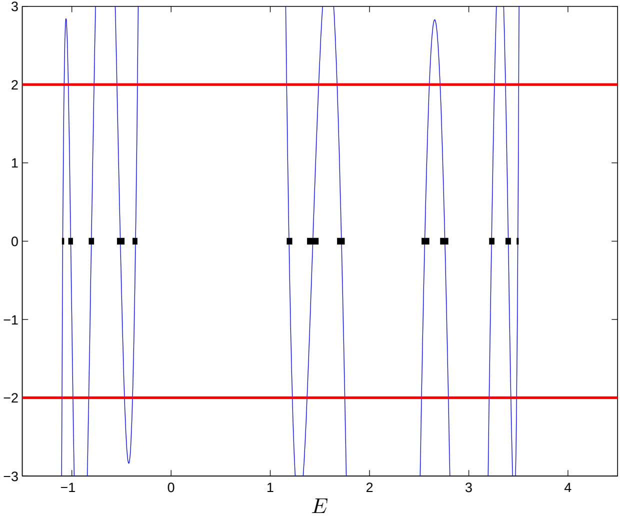
$x_3(E)$ with $\lambda = 2$
3
2
1
0
−1
−2
−3
−1
0
1
2
3
4
E


$x_4(E)$ with $\lambda = 2$
3
2
1
0
−1
−2
−3
−1
0
1
2
3
4
E

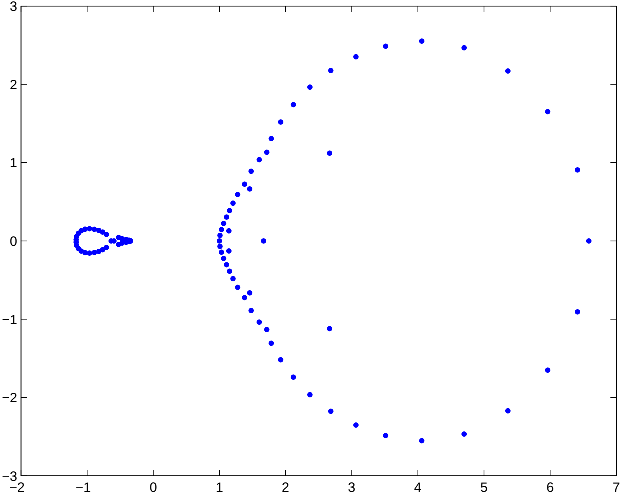


$x_5(E)$ with $\lambda = 2$
3
2
1
0
−1
−2
−3
−1
0
1
2
3
4
E

$x_6(E)$ with $\lambda = 2$



roots of $x_{10}(E) - 2$ for $\lambda = 2$



Eigenvalue Problem for σ_k

$\sigma_k = \cup_{j=1}^{F_k} [E_{2j-1}, E_{2j}]$, where E_i's are the sorted eigenvalues of the finite dimensional matrices (see e.g. Teschl 2000):

$$\mathbf{J}_\pm = \begin{bmatrix} v_1^{(k)} & 1 & & & \pm 1 \\ 1 & v_2^{(k)} & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & v_{F_{k-1}}^{(k)} & 1 \\ \pm 1 & & & 1 & v_{F_k}^{(k)} \end{bmatrix}.$$

Goal: An efficient algorithm for computing the spectrum of $\mathbf{J}_\pm$.

Proposed algorithm (for $\mathbf{J}_+$)

Split $\mathbf{J}_+ = \mathbf{T} + \mathbf{w}\mathbf{w}^*$ with $\mathbf{w} = \mathbf{e}_1 + \mathbf{e}_{F_k}$. If the spectral decomposition is $\mathbf{T} = \mathbf{Q}\mathbf{D}\mathbf{Q}^*$, equivalently compute the eigenvalues of

$$\mathbf{D} + (\mathbf{Q}^*\mathbf{w})(\mathbf{Q}^*\mathbf{w})^*. \tag{1}$$

1. Compute the eigenvalues of $\mathbf{T}$ (with the QR iteration).
2. Sequentially compute the eigenvectors of $\mathbf{T}$ with inverse iteration and store the first and last components.
3. Compute roots of the secular equation corresponding to (1).

J.R. Bunch, C.P. Nielsen, and D.C. Sorensen. "Rank-one modification to the symmetric eigenproblem." *Numer. Math.*, 31:31-38, 1978

Secular Equation

If all the components of $\mathbf{z}$ are nonzero, then E is an eigenvalue of $\mathbf{D} + \mathbf{z}\mathbf{z}^*$ $\iff$ E is a root of the *secular equation*

$$g(x) := 1 + \sum_{j=1}^{N} \frac{|z_j|^2}{d_j - x}.$$

Bunch, Nielsen, and Sorensen devised a Newton-type method to compute the roots efficiently.

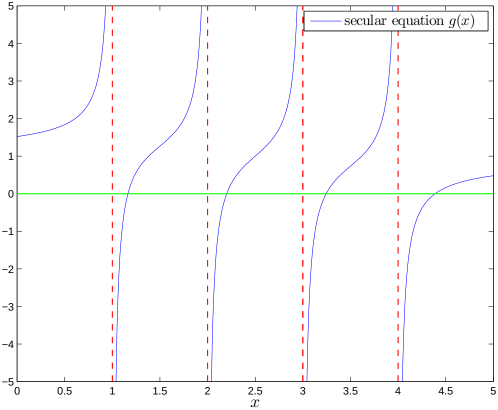


Figure: $\mathbf{D} = \mathbf{diag}([1;2;3;4])$ and $\mathbf{z} = 0.5^*[1;1;1;1]$.

Implementation

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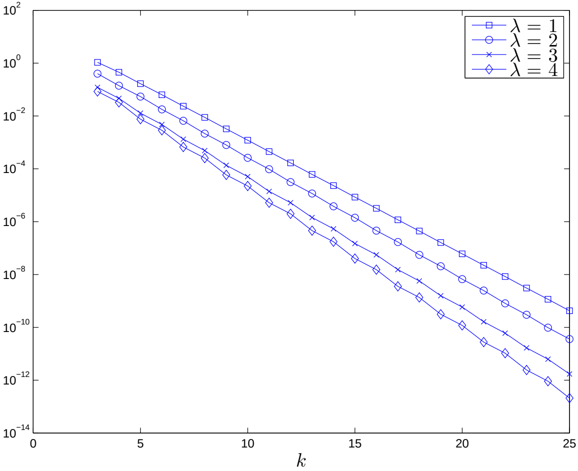

Figure: Minimum interval length in $\sigma_k \cup \sigma_{k+1}$

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  - Larger λ requires finer resolution in exponentially close eigenvalues.

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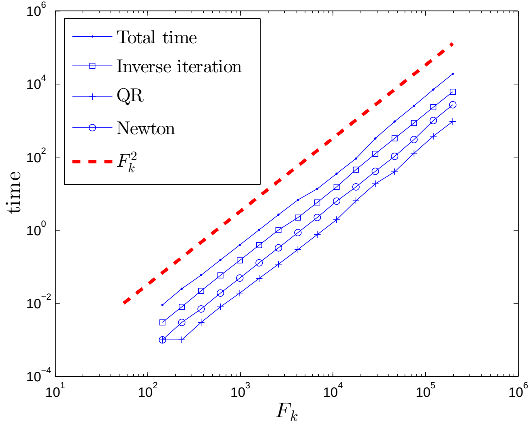
  - Larger λ requires finer resolution in exponentially close eigenvalues.
- Benchmarked on matrices with 1's on super- and sub- diagonal, zero on the diagonal, and corner entries (Gear 1969).

Timing results (Intel core i3, 3.3 GHz with 4 GB RAM)



Approximating fractal dimensions of $\sigma(\mathbf{H})$

Definition

Let $S \subset \mathbb{R}$. Let $\{C_l\}$ be a Δ-cover of S and consider the function

$$h^\alpha(S) = \lim_{\Delta \to 0} \inf_{\Delta\text{-covers}} \sum_{l \geq 1} |C_l|^\alpha,$$

with $\alpha \in [0, 1]$. The *Hausdorff dimension* of S is

$$\dim_H S = \inf\{\alpha : h^\alpha(S) < \infty\}.$$

Approximating fractal dimension

Let $\sigma_k \cup \sigma_{k+1} = \cup_{j=1}^{N_k} B_j^{(k)}$. The approximate dimension $\tilde{\alpha}_k$ is the root of

$$d_k(\alpha) = \sum_{j=1}^{N_k} |B_j^{(k)}|^\alpha - \sum_{j=1}^{N_{k+1}} |B_j^{(k+1)}|^\alpha.$$

We want to investigate the convergence of $\tilde{\alpha}_k$ as $k \to \infty$.

Thomas C. Halsey, Mogens H. Jensen, Leo P. Kadanoff, Itamar Procaccia, and Boris I. Shraiman. "Fractal measures and their singularities: The characterization of strange sets." *Phys. Rev. A*, 33:11411151, Feb 1986.

Table: Approximate Hausdorff dimension $\tilde{\alpha}$ computed with the covers $\sigma_k \cup \sigma_{k+1}$ and $\sigma_{k+1} \cup \sigma_{k+2}$.

k	$\lambda = 1$	$\lambda = 2$	$\lambda = 3$	$\lambda = 4$
3	0.629184721644038	0.546264141212987	0.550922327994936	0.488025115075937
8	0.780389915333086	0.612894523364685	0.513532576522766	0.452726564745786
13	0.772999910983101	0.611241269469838	0.515071697768937	0.454572409187434
18	0.772856924165551	0.611296934295102	0.514997379296334	0.454460072332500
19	0.772860487019160	0.611294102304395	0.515002805673527	0.454470411042160
20	0.772858831782941	0.611295550849554	0.514999829522381	0.454464482921194
21	0.772859571887832	0.611294809816774	0.515001463458351	0.454467874686662
22	0.772859243100286	0.611295188819406	0.515000573873506	0.454465912748311
23	0.772859393255526	0.611294994922469	0.515001056835674	0.454467035392032
24	0.77285 9324719459	0.61129 5094167910	0.51500 0778375714	0.45446 5398123737

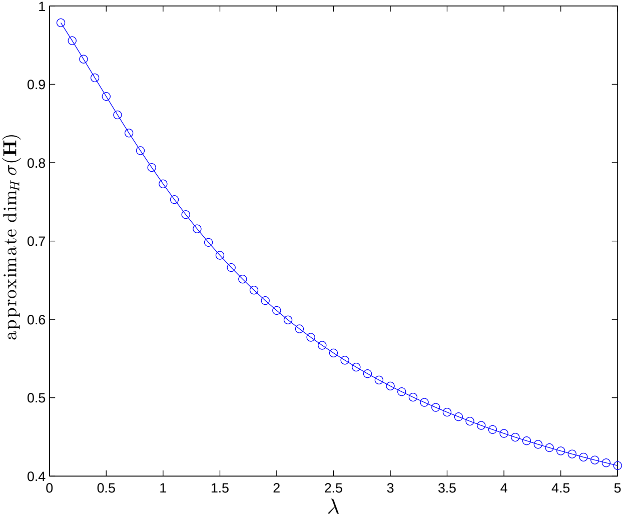


Figure: Approximate Hausdorff dimension computed with covers $\sigma_k \cup \sigma_{k+1}$ with k =23, 24.

Table: Estimation of λ such that $\dim \Sigma_\lambda = 1/2$ by determining root of $\dim_H \Sigma_\lambda - 1/2$ in the interval $[3, 4]$.

k	root of $\dim_H \Sigma_\lambda - 1/2$
5	3.358132165787465
6	3.136023908556593
7	3.252443323604985
8	3.188369245375197
9	3.223061231166874
10	3.203897752346325
11	3.214420790092100
12	3.208597301692052
13	3.211813603439293
14	3.210032038473626
15	3.211018258537230
16	3.210471722049607
17	3.210774542902178
18	3.210606689833002
19	3.210699725856641
20	3.210648145088315
21	3.210676725662388
22	3.2106 61023369781

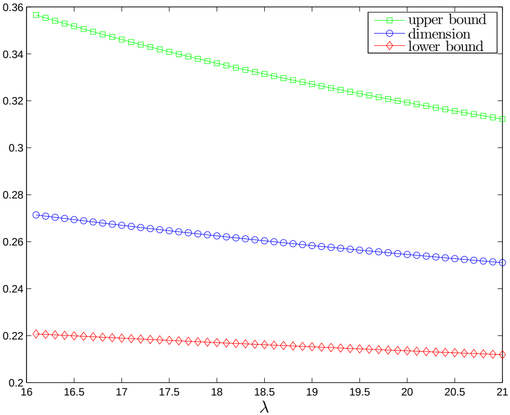


Figure: Approximate dimension computed with covers $\sigma_k \cup \sigma_{k+1}$ with k =13, 14.

D. Damanik, M. Embree, A. Gorodetski, and S. Tcheremchantsev. "The Fractal Dimension of the Spectrum of the Fibonacci Hamiltonian." *Commun. Math. Phys.*, 280:499516, 2008.

Band Combinatorics of σ_k

Lemma (Killip, Kiselev, and Last 2003)

Take $\lambda > 4$ and $k \geq 1$.

- *Every type A band $I \subset \sigma_k$ contains only one type B band in σ_{k+2} and no bands in σ_{k+1}.*
- *Every type B band $I \subset \sigma_k$ contains only one type A band in σ_{k+1} and two type B bands in σ_{k+2} sitting on either side of I.*

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- Investigate combinatorics for $\lambda \in (0, 4]$.
- Apply results to refine approximations to fractal dimensions from the covers $\sigma_k \cup \sigma_{k+1}$ (see e.g. Damanik et al. 2008).

Combinatorics of bands in σ_k

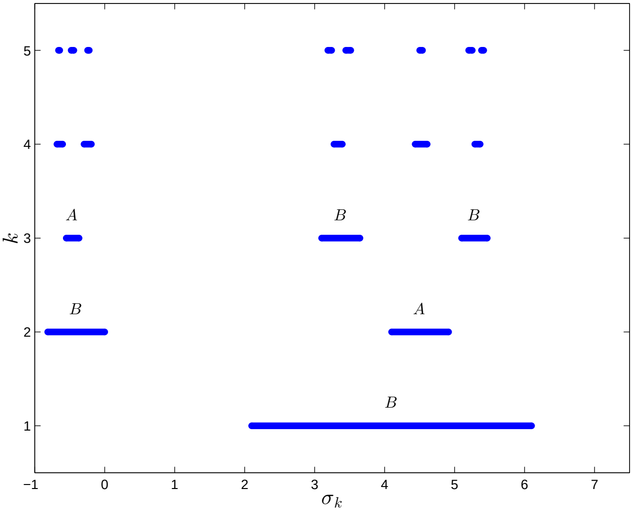
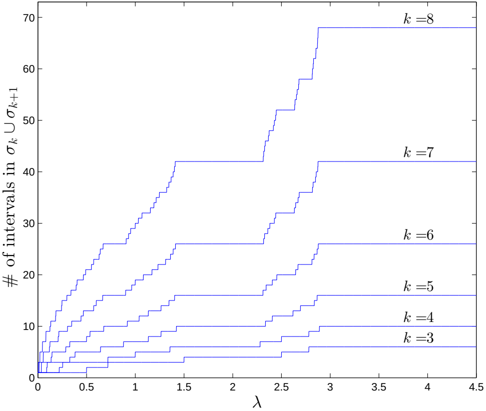


Figure: Plot of σ_k for $\lambda = 4.1$.

Combinatorics for $\lambda \in (0, 4]$

Calculations suggest that for k sufficiently large, the number of intervals in $\sigma_k \cup \sigma_{k+1}$ obeys the Fibonacci recurrence.



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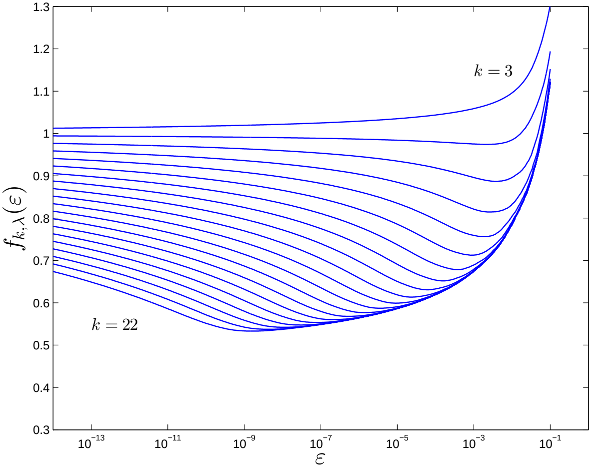
Future work

Numerical

- Develop robust extrapolation of box-counting dimension.

Future work



1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
$f_{k,\lambda}(\varepsilon)$
$k = 3$
$k = 22$
10^{-13}
10^{-11}
10^{-9}
10^{-7}
10^{-5}
10^{-3}
10^{-1}
ε

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- Develop robust extrapolation of box-counting dimension.
- Refine techniques for approximating fractal dimensions (with knowledge of intervals combinatorics).
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Theoretical (Joint with Paul Munger)

- Study combinatorics of bands in σ_k in intermediate coupling regime (extend ideas from Killip et al. 2003).
- Investigate λ where fractal dimension is $1/2$.
- Understand the spectra of two and three dimensional Fibonacci Hamiltonians.