Aperiodic Order: Schrödinger Operators

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The Schrödinger Equation

The fundamental equation of quantum mechanics is the Schrödinger equation

$$i\partial_t \psi = H\psi.$$

Here, ψ is a time-dependent element of a Hilbert space $\mathcal{H}$ and H is a self-adjoint operator in $\mathcal{H}$.

Typically, $\mathcal{H}$ is given by $L^2(\mathbb{R}^d)$ or $\ell^2(\mathbb{Z}^d)$, but in the context of aperiodic order, it is also useful to consider $\ell^2(\Lambda)$ with a suitable countable $\Lambda \subset \mathbb{R}^d$. In these cases, there is a natural notion of a space variable.

The state ψ is normalized (a property which is preserved by the time evolution), so that its modulus squared serves as a probability distribution on $\mathbb{R}^d$ or Λ. That is,

$$\mathrm{Prob}(\text{state is in } A) = \int_A |\psi|^2.$$

The Schrödinger Operator

Just as $\mathcal{H}$ is in practice a concrete space such as $L^2(\mathbb{R}^d)$ or $\ell^2(\Lambda)$, the self-adjoint operator H appearing in

$$i\partial_t\psi = H\psi$$

is in practice a concrete operator of the form

$$H = -\Delta + V.$$

Here, Δ is the Laplace operator and V is a multiplication operator. Schrödinger operators H studied in the context of aperiodic order often come in two standard forms:

- The space is $\mathbb{R}^d$ or $\mathbb{Z}^d$ and the aperiodic order is encoded in the potential V.
- The space is an aperiodically ordered point set Λ and the potential is for simplicity set equal to zero.

Transport Exponents

If we wish to study the solutions of the Schrödinger equation

$$i\partial_t \psi = H\psi$$

with initial state $\psi(0) = \psi_0$, the spectral theorem says that we need to consider $e^{-itH}\psi_0$. We ask whether $\psi(t)$ spreads out in space over time. For example, if the Hilbert space in question is $\ell^2(\Lambda)$, then $n \in \Lambda$ is the natural space variable.

Spreading is then studied via the growth of

$$\langle |X|^p_{\psi_0} \rangle(t) = \sum_n |n|^p |\langle e^{-itH}\psi_0, \delta_n \rangle|^2.$$

Transport Exponents

If the spectral measure of (H, ψ_0) is singular continuous, Wiener's theorem suggests that we average in time. We do this as follows. If $f(t)$ is a function of $t > 0$ and $T > 0$ is given, we denote the time-averaged function at T by $\langle f \rangle(T)$:

$$\langle f \rangle(T) = \frac{2}{T} \int_0^\infty e^{-2t/T} f(t)\, dt.$$

Then, the corresponding upper and lower transport exponents $\tilde{\beta}^+_{\psi_0}(p)$ and $\tilde{\beta}^-_{\psi_0}(p)$ are given, respectively, by

$$\tilde{\beta}^+_{\psi_0}(p) = \limsup_{T \to \infty} \frac{\log \langle \langle |X|^p_{\psi_0} \rangle \rangle(T)}{p \log T},$$

$$\tilde{\beta}^-_{\psi_0}(p) = \liminf_{T \to \infty} \frac{\log \langle \langle |X|^p_{\psi_0} \rangle \rangle(T)}{p \log T}.$$

Transport Exponents

The transport exponents $\tilde{\beta}^{\pm}_{\psi_0}(p)$ belong to $[0,1]$ and are non-decreasing in p, and hence the following limits exist:

$$\tilde{\alpha}_l^{\pm} = \lim_{p \to 0} \tilde{\beta}^{\pm}_{\psi_0}(p),$$
$$\tilde{\alpha}_u^{\pm} = \lim_{p \to \infty} \tilde{\beta}^{\pm}_{\psi_0}(p).$$

Theorem (Last 96, Guarneri-Schulz-Baldes 99)

If $\mathcal{H} = \ell^2(\mathbb{Z}^d)$, then

$$\tilde{\alpha}_l^{-} \geq d^{-1} \dim_H \mu_{H,\psi_0} \quad \textit{and} \quad \tilde{\alpha}_l^{+} \geq d^{-1} \dim_P \mu_{H,\psi_0}.$$

Existence of the IDS

The integrated density of states (IDS) arises in a variety of ways. For example:

- One can restrict H to a finite box B and count the number of eigenvalues of $H|_B$ that are less than $E \in \mathbb{R}$, normalized by the volume of the box. As B exhausts space, the limit is called $N(E)$.
- One can embed the operator H in an ergodic family of operators and average suitable spectral measures with respect to the ergodic measure. The distribution function of the resulting (density of states) measure $d\nu$ is $N : \mathbb{R} \to \mathbb{R}$.

This works out particularly nicely if there is a unique ergodic probability measure. Corresponding uniform convergence statements have been studied by Hof, Lenz, Stollmann, and others.

Zero-Measure Spectrum in 1D

Consider a finite alphabet $\mathcal{A}$ and the full shift $\mathcal{A}^{\mathbb{Z}}$, equipped with discrete/product topology, together with the shift transformation $(T\omega)_n = \omega_{n+1}$. A closed T-invariant subset Ω of $\mathcal{A}^{\mathbb{Z}}$ is called a subshift.

Given a subshift Ω, choose some continuous $f : \Omega \to \mathbb{R}$ and define potentials $\{V_\omega\}_{\omega \in \Omega}$ via

$$V_\omega(n) = f(T^n \omega).$$

This gives rise to Schrödinger operators $\{H_\omega\}_{\omega \in \Omega}$ in $\ell^2(\mathbb{Z})$.

For any ergodic probability measure μ, there is an associated spectrum Σ (so that $\sigma(H_\omega) = \Sigma$ for μ-a.e. $\omega \in \Omega$).

Zero-Measure Spectrum in 1D

Let $\Omega \subset \mathcal{A}^{\mathbb{Z}}$ be a strictly ergodic subshift with unique T-invariant Borel probability measure μ. It satisfies the *Boshernitzan condition* (B) if

$$\limsup_{n\to\infty}\left(\min_{w\in\mathcal{W}_\Omega(n)} n\cdot\mu([w])\right) > 0.$$

Here, $\mathcal{W}_\Omega(n)$ denotes the set of words of length n that occur in elements of Ω, and $[w]$ denotes the cylinder set associated with a finite word w, that is, $[w] = \{\omega \in \Omega : \omega_1 \ldots \omega_{|w|} = w\}$.

Theorem (D.-Lenz 06)

Suppose the subshift Ω is strictly ergodic and satisfies (B), the sampling function $f : \Omega \to \mathbb{R}$ is locally constant, and the resulting potentials V_ω are aperiodic. Then, Σ is a Cantor set of zero Lebesgue measure.

A Case Study: The Fibonacci Hamiltonian

The Fibonacci Hamiltonian is the following family of discrete one-dimensional Schrödinger operators,

$$[H_{\lambda,\omega} u](n) = u(n+1) + u(n-1) + \lambda \chi_{[1-\alpha,1)}(n\alpha + \omega \text{ mod } 1) u(n),$$

acting in $\ell^2(\mathbb{Z})$, where $\lambda > 0$ is the coupling constant, $\alpha = \frac{\sqrt{5}-1}{2}$ is the frequency, and $\omega \in \mathbb{T} = \mathbb{R}/\mathbb{Z}$ is the phase. Alternatively, the potential of this operator can be generated by the Fibonacci substitution $a \mapsto ab$, $b \mapsto a$.

The Spectrum of the Fibonacci Hamiltonian

The spectrum of $H_{\lambda,\omega}$ does not depend on ω, let us denote it by Σ_λ.

Theorem (Sütő 89)

For every $\lambda > 0$, Σ_λ is a Cantor set of zero Lebesgue measure.

Theorem (Casdagli 86, D.-Gorodetski 09, D.-G.-Yessen 16+)

For every $\lambda > 0$, Σ_λ is a dynamically defined Cantor set. In particular, its box counting dimension exists, coincides with its Hausdorff dimension, and belongs to $(0, 1)$.

The Spectrum of the Fibonacci Hamiltonian

Here is a plot of a numerical approximation of the spectrum:

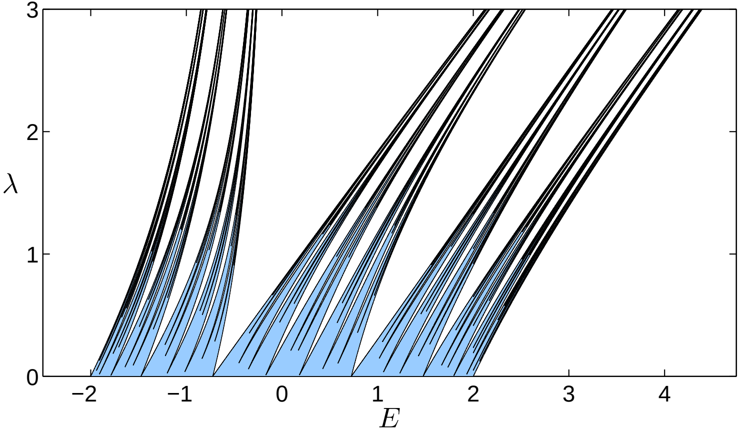

Figure: The set $\{(E, \lambda) : E \in \Sigma_\lambda,\ 0 \leq \lambda \leq 3\}$.

The Spectrum of the Fibonacci Hamiltonian

Theorem (D.-Embree-Gorodetski-Tcheremchantsev 08, D.-Gorodetski 11)

We have $\lim_{\lambda \to 0} \dim_H \Sigma_\lambda = 1$ *and*

$$\lim_{\lambda \to \infty} \dim_H \Sigma_\lambda \cdot \log \lambda = \log(1 + \sqrt{2}) \approx 1.83156 \log \varphi$$

Moreover, as the coupling is turned on, all gaps open linearly. That is, given any one-parameter continuous family $\{U_\lambda\}_{\lambda > 0}$ *of gaps of* Σ_λ*, we have that*

$$\lim_{\lambda \to 0} \frac{|U_\lambda|}{|\lambda|}$$

exists and belongs to $(0, \infty)$*.*

The Density of States of the Fibonacci Hamiltonian

By the spectral theorem, there are Borel probability measures $\mu_{\lambda,\omega}$ on $\mathbb{R}$ such that

$$\langle \delta_0, g(H_{\lambda,\omega})\delta_0 \rangle = \int g(E)\, d\mu_{\lambda,\omega}(E)$$

for all bounded measurable functions g. The *density of states measure* ν_λ is given by the ω-average of these measures with respect to Lebesgue measure, that is,

$$\int_{\mathbb{T}} \langle \delta_0, g(H_{\lambda,\omega})\delta_0 \rangle \, d\omega = \int g(E)\, d\nu_\lambda(E)$$

for all bounded measurable functions g.

The Density of States of the Fibonacci Hamiltonian

By general principles, the density of states measure is non-atomic and its topological support is Σ_λ. The fact that Σ_λ has zero Lebesgue measure therefore implies that ν_λ is singular continuous for every $\lambda > 0$.

Moreover, by an 07 result of Simon, ν_λ is the equilibrium measure in the sense of logarithmic potential theory associated with the set Σ_λ. Motivated by results of Makarov and Volberg for the standard Cantor set, Simon conjectured the following: $\dim_H \nu_\lambda < \dim_H \Sigma_\lambda$.

Theorem (D.-Gorodetski 12, D.-Gorodetski-Yessen 16+)

For every $\lambda > 0$, $\dim_H \nu_\lambda < \dim_H \Sigma_\lambda$.

The Density of States of the Fibonacci Hamiltonian

The asymptotics of the dimension of the density of states measure are given in the following theorem.

Theorem (D.-Gorodetski 12, D.-Gorodetski-Yessen 16+)

For every $\lambda > 0$, the density of states measure ν_λ is exact-dimensional. Namely, for every $\lambda > 0$, the limit (called the scaling exponent of ν_λ at E)

$$\lim_{\varepsilon \downarrow 0} \frac{\log \nu_\lambda(E - \varepsilon, E + \varepsilon)}{\log \varepsilon}$$

ν_λ-almost everywhere exists and is constant. Moreover, denoting this almost everywhere limit by d_λ, we have $\lim_{\lambda \to 0} d_\lambda = 1$ and

$$\lim_{\lambda \to \infty} d_\lambda \cdot \log \lambda = \frac{5 + \sqrt{5}}{4} \log \varphi$$

Transport Exponents of the Fibonacci Hamiltonian

It had been conjectured since the mid-1980's that the transport associated with the Fibonacci Hamiltonian is anomalous, which means that the transport exponents are different from $1, 1/2, 0$. That is, transport is neither ballistic, nor diffusive, nor absent.

Here is a p-dependent lower bound that improves on the general Guarneri-Last estimate:

Theorem (D.-Tcheremchantsev 05)

Suppose $\lambda > 0$ and set $\gamma = D\log(2+\sqrt{8+\lambda^2})$ (where D is some universal constant) and $\kappa = \log\left[\frac{\sqrt{17}}{20\log\varphi}\right]$. Then,

$$\tilde{\beta}^{\pm}_{\delta_0}(p) \geq \begin{cases} \frac{p+2\kappa}{(p+1)(\gamma+\kappa+1/2)}, & p \leq 2\gamma+1; \\ \frac{1}{\gamma+1}, & p > 2\gamma+1. \end{cases}$$

Transport Exponents of the Fibonacci Hamiltonian

Here is a result that concerns the regime of large λ and p:

Theorem (D.-Tcheremchantsev 07/08)

For $\lambda > \sqrt{24}$, we have

$$\tilde{\alpha}_u^{\pm} \geq \frac{2 \log \varphi}{\log(2\lambda + 22)}$$

and for $\lambda \geq 8$, we have

$$\tilde{\alpha}_u^{\pm} \leq \frac{2 \log \varphi}{\log \left(\frac{1}{2} \left[(\lambda - 4) + \sqrt{(\lambda - 4)^2 - 12} \right] \right)}$$

In particular,

$$\lim_{\lambda \to \infty} \tilde{\alpha}_u^{\pm} \cdot \log \lambda = 2 \log \varphi$$

Transport Exponents of the Fibonacci Hamiltonian

The transport exponents are expected to approach the value 1 as $\lambda \to 0$. Notice that the lower bound from the '05 result does not imply this. Using different methods an improved lower bound can be shown, which does give the desired consequence.

Theorem (Damanik-Gorodetski 15)

There is a constant $c > 0$ such that for $\lambda > 0$ sufficiently small, we have

$$1 - c\lambda^2 \leq \tilde{\alpha}_u^{\pm} \leq 1$$

The Square Fibonacci Hamiltonian

The square Fibonacci Hamiltonian is the bounded self-adjoint operator

$$
\begin{aligned}
[H_{\lambda_1,\lambda_2,\omega_1,\omega_2}\psi](m,n) &= \psi(m+1,n) + \psi(m-1,n) + \\
&\quad + \psi(m,n+1) + \psi(m,n-1) + \\
&+ \Big(\lambda_1 \chi_{[1-\alpha,1)}(m\alpha + \omega_1 \bmod 1) + \lambda_2 \chi_{[1-\alpha,1)}(n\alpha + \omega_2 \bmod 1)\Big)\psi(m,n)
\end{aligned}
$$

in $\ell^2(\mathbb{Z}^2)$, with $\alpha = \frac{\sqrt{5}-1}{2}$, coupling constants $\lambda_1, \lambda_2 > 0$ and phases $\omega_1, \omega_2 \in \mathbb{T} = \mathbb{R}/\mathbb{Z}$.

The spectrum is again independent of the phases and may be denoted by $\Sigma_{\lambda_1,\lambda_2}$. The associated density of states measure will be denoted by $\nu_{\lambda_1,\lambda_2}$.

The Square Fibonacci Hamiltonian

The theory of separable operators implies that

$$\Sigma_{\lambda_1,\lambda_2} = \Sigma_{\lambda_1} + \Sigma_{\lambda_2} \quad \text{and} \quad \nu_{\lambda_1,\lambda_2} = \nu_{\lambda_1} * \nu_{\lambda_2},$$

where the sum of sets is defined by

$$S + T = \{s + t : s \in S, \ t \in T\}$$

and the convolution of measures is defined by

$$\int_{\mathbb{R}} g(E)\, d(\mu * \nu)(E) = \int_{\mathbb{R}} \int_{\mathbb{R}} g(E_1 + E_2)\, d\mu(E_1)\, d\nu(E_2).$$

The Spectrum of the Square Fibonacci Hamiltonian

Recall the plot of a numerical approximation of Σ_λ:

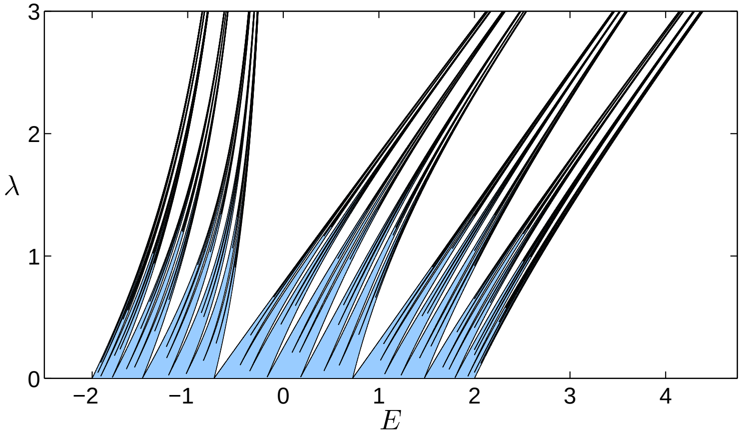

Figure: The set $\{(E, \lambda) : E \in \Sigma_\lambda,\ 0 \leq \lambda \leq 3\}$.

The Spectrum of the Square Fibonacci Hamiltonian

This gives rise to a numerical approximation of $\Sigma_{\lambda,\lambda} = \Sigma_\lambda + \Sigma_\lambda$:

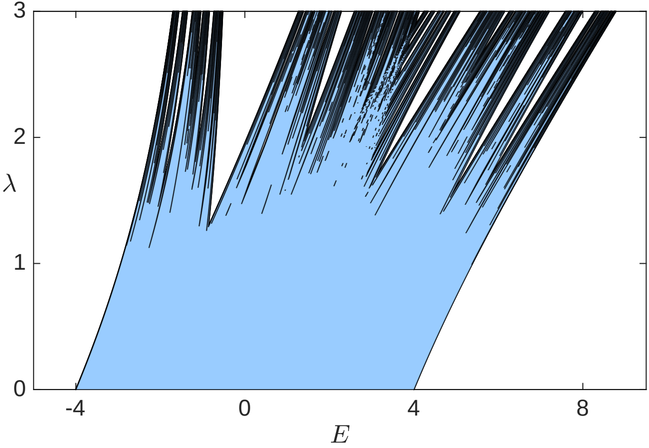

Figure: The set $\{(E,\lambda) : E \in \Sigma_{\lambda,\lambda},\ 0 \le \lambda \le 3\}$.

The Spectrum of the Square Fibonacci Hamiltonian

Theorem (D.-Embree-Gorodetski-Tcheremchantsev 08)

If λ_1, λ_2 are large enough, then $\Sigma_{\lambda_1,\lambda_2}$ is a Cantor set of zero Lebesgue measure.

Theorem (D.-Gorodetski 11)

If λ_1, λ_2 are small enough, then $\Sigma_{\lambda_1,\lambda_2}$ is an interval.

Theorem (D.-Gorodetski-Solomyak 15)

For Lebesgue almost all sufficiently small λ_1, λ_2, $\nu_{\lambda_1,\lambda_2}$ is absolutely continuous.

The Spectrum of the Square Fibonacci Hamiltonian

Theorem (D.-Gorodetski 16+)

Suppose that for all pairs (λ_1, λ_2) *in some open set* $U \subset \mathbb{R}^2_+$, *we have* $\dim_{\mathrm{H}} \Sigma_{\lambda_1} + \dim_{\mathrm{H}} \Sigma_{\lambda_2} > 1$. *Then, for Lebesgue almost all pairs* $(\lambda_1, \lambda_2) \in U$, $\Sigma_{\lambda_1,\lambda_2}$ *has positive Lebesgue measure.*

Theorem (D.-Gorodetski 16+)

Suppose that $\dim_{\mathrm{H}} \nu_{\lambda_1} + \dim_{\mathrm{H}} \nu_{\lambda_2} < 1$. *Then,* $\nu_{\lambda_1,\lambda_2}$ *is singular, that is, it is supported by a set of zero Lebesgue measure.*

The Spectrum of the Square Fibonacci Hamiltonian

Recall that for every $\lambda > 0$, we have

$$0 < \dim_{\mathrm{H}} \nu_\lambda < \dim_{\mathrm{H}} \Sigma_\lambda < 1.$$

Thus the curves

$$\{(\lambda_1, \lambda_2) \in \mathbb{R}_+^2 : \dim_{\mathrm{H}} \nu_{\lambda_1} + \dim_{\mathrm{H}} \nu_{\lambda_2} = 1\}$$

$$\{(\lambda_1, \lambda_2) \in \mathbb{R}_+^2 : \dim_{\mathrm{H}} \Sigma_{\lambda_1} + \dim_{\mathrm{H}} \Sigma_{\lambda_2} = 1\}$$

are disjoint. Consider the following three regions in $\mathbb{R}_+^2$:

$$\begin{aligned}
U_{\mathrm{acds}} &= \{(\lambda_1, \lambda_2) \in \mathbb{R}_+^2 : \dim_{\mathrm{H}} \nu_{\lambda_1} + \dim_{\mathrm{H}} \nu_{\lambda_2} > 1\}, \\
U_{\mathrm{pmsd}} &= \{(\lambda_1, \lambda_2) \in \mathbb{R}_+^2 : \dim_{\mathrm{H}} \Sigma_{\lambda_1} + \dim_{\mathrm{H}} \Sigma_{\lambda_2} > 1 \text{ and} \\
&\qquad \dim_{\mathrm{H}} \nu_{\lambda_1} + \dim_{\mathrm{H}} \nu_{\lambda_2} < 1\}, \\
U_{\mathrm{zmsp}} &= \{(\lambda_1, \lambda_2) \in \mathbb{R}_+^2 : \dim_{\mathrm{H}} \Sigma_{\lambda_1} + \dim_{\mathrm{H}} \Sigma_{\lambda_2} < 1\}.
\end{aligned}$$

The Spectrum of the Square Fibonacci Hamiltonian

Theorem (D.-Gorodetski 16+)

(a) *Each of the regions* U_{acds}, U_{pmsd}, U_{zmsp} *is open and non-empty.*

(b) *The regions* U_{acds}, U_{pmsd}, U_{zmsp} *are disjoint and the union of their closures covers the parameter space* $\mathbb{R}_+^2$.

(c) *For Lebesgue almost every* $(\lambda_1, \lambda_2) \in U_{\mathrm{acds}}$, $\nu_{\lambda_1,\lambda_2}$ *is absolutely continuous, and hence* $\Sigma_{\lambda_1,\lambda_2}$ *has positive Lebesgue measure.*

(d) *For every* $(\lambda_1, \lambda_2) \in U_{\mathrm{pmsd}}$, $\nu_{\lambda_1,\lambda_2}$ *is singular, but for Lebesgue almost every* $(\lambda_1, \lambda_2) \in U_{\mathrm{pmsd}}$, $\Sigma_{\lambda_1,\lambda_2}$ *has positive Lebesgue measure.*

(e) *For every* $(\lambda_1, \lambda_2) \in U_{\mathrm{zmsp}}$, $\Sigma_{\lambda_1,\lambda_2}$ *has zero Lebesgue measure, and hence* $\nu_{\lambda_1,\lambda_2}$ *is singular.*