Applications of Liouville Discrepancy to Quantum Dynamics

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REU in Semi-Algebraic Geometry in Schrödinger Equations.

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The Schrödinger Equation

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$$i\frac{\partial \psi}{\partial t} = \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi(x)$$

- This can be spatially discretized (eg. for a crystal lattice, numerical simulation), to obtain

$$i\frac{\partial \psi_n}{\partial t} = (\psi_{n+1} - 2\psi_n + \psi_{n-1}) + V_n\psi_n$$

where now ψ, V are sequences

Quantum Dynamics - Schrödinger Operators

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Definition 1.1: Schrödinger operator

A **Schrödinger operator** $H : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ acts on a *wavefunction* $\psi : \mathbb{Z} \to \mathbb{C}$ according to

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

where $V : \mathbb{Z} \to \mathbb{R}$ is the *potential*

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- Given $\psi(0) = \phi$, this has the exact solution $\psi(t) = e^{-itH}\phi$.
- $|\psi_n|^2$ represents the probability of measurement at site n.

Quantum Dynamics - Schrödinger Operators

A Schrödinger operator can be expressed as an infinte matrix

$$H = \begin{pmatrix} \ddots & & & & & & \\ & V_{-2} & 1 & 0 & 0 & 0 & \\ & 1 & V_{-1} & 1 & 0 & 0 & \\ & 0 & 1 & V_0 & 1 & 0 & \\ & 0 & 0 & 1 & V_1 & 1 & \\ & 0 & 0 & 0 & 1 & V_2 & \\ & & & & & & \ddots \end{pmatrix}$$

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We can consider its restriction to a finite interval, eg. [0,3]:

$$H_{[0,3]} = \begin{pmatrix} V_0 & 1 & 0 & 0 \\ 1 & V_1 & 1 & 0 \\ 0 & 1 & V_2 & 1 \\ 0 & 0 & 1 & V_3 \end{pmatrix}$$

Quantum Dynamics - Example 1

$$\phi_n = e^{-n^2/2} \qquad V_n = 0$$

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Insert diffusion example

Quantum Dynamics - Example 2

$$\phi_n = e^{ni-(n+\mu)^2/2} + e^{-ni-(n-\mu)^2/2} \qquad V_n = 0$$

Quantum Dynamics - Example 2

$$\phi_n = e^{ni-(n+\mu)^2/2} + e^{-ni-(n-\mu)^2/2} \qquad V_n = 0$$

Insert interference example

Quantum Dynamics - Example 3

$$\phi_n = e^{ni-(n+\mu)^2/2} \qquad V_n = \begin{cases} 1, & 140 \leq n \leq 150 \\ 0, & \text{otherwise} \end{cases}$$

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Insert reflection example

Definition 1.2: p^{th} moment

For an initial state ϕ, we define the p[th] **moment** as:

$$\langle |X_H|^p_\phi \rangle(t) = \sum_{n \in \mathbb{Z}} |n|^p |\psi_n(\tau)|^2$$

Then, we define the average p[th] **moment** as:

$$\langle |\tilde{X}_H|^p_\phi \rangle(t) = \frac{2}{t} \int_0^\infty e^{2\tau/t} \sum_{n \in \mathbb{Z}} |n|^p |\psi_n(\tau)|^2 \, d\tau$$

- Captures how $\psi(t) = e^{-itH}\phi$ spreads out over time

Transport - Example 1

If V is periodic, the p^{th} moment grows like

$$\langle X_H|_\phi^p\rangle \sim t^p$$

This is known as *ballistic transport* [Fil20].

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Insert periodic transport example

Transport - Example 2

If V is random, the p^{th} moment is bounded:

$$\langle X_H|_{\phi}^{p}\rangle \leq C \quad \text{for some } C > 0$$

This is known as *dynamic localization* [Klein].

Insert random transport example

Penrose Tilings

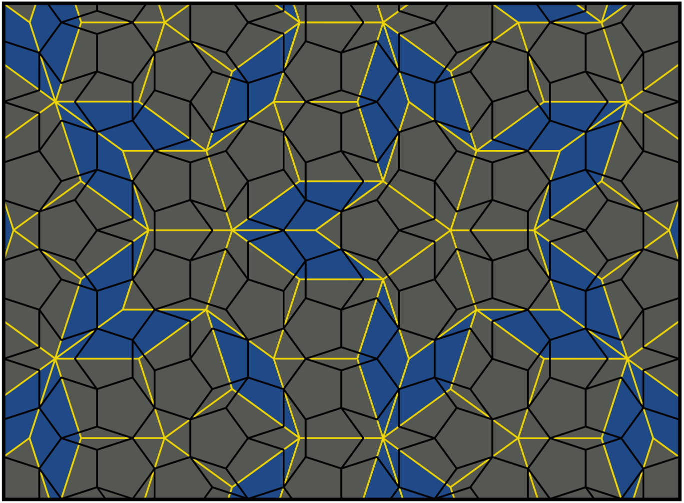


Figure: Image By Inductiveload - Own work, Public Domain, Link

The Fibonacci Hamiltonian

Consider a sequence S_N of words where $S_0 = 0$ and S_N is defined as the N-th application of the substitution rule

$$0 \mapsto 01 \quad \text{and} \quad 1 \mapsto 0$$

Taking the limit as $N \to \infty$, one obtains the Fibonacci Word (Hamiltonian) Eg.

$$0100101001001\cdots$$

Well studied model of Quasi-Crystals.

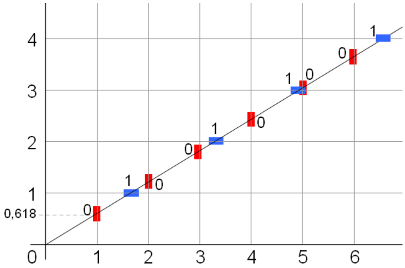


Figure: Line of Slope $\frac{1}{\phi}$. By Prokofiev - Own work, CC BY-SA 3.0, Link

Quasi-Periodic Potentials

Definition 1.3: Quasi-periodic

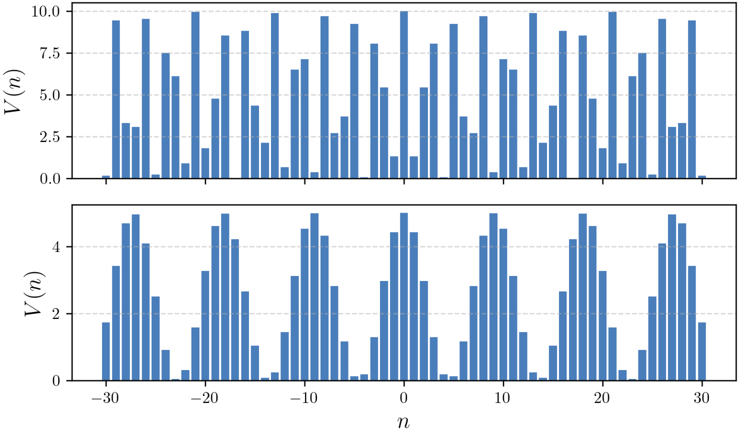
If $f : \mathbb{R} \to \mathbb{R}$ is a periodic, analytic function, and if α is an irrational number, we call

$$V(n) = f(n\alpha)$$

a **quasi-periodic** potential.

Quasi-Periodic Potentials

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



$$\alpha = \frac{\sqrt{5}-1}{2}$$

$$\alpha = \sum_{k=1}^{\infty} \frac{1}{10^{k!}}$$

Continued Fractions

Continued Fractions

Fact 1.5: Contined fraction expansion

Every positive real number can be expressed as a continued fraction of the form

$$\alpha = a_0 + \frac{1}{a_1 + \frac{1}{a_2 + \cdots}}$$

for $a_i \in \mathbb{N}$, and we write $\alpha = [a_0; a_1, a_2, \ldots]$.

Continued Fractions

Fact 1.6: Contined fraction expansion

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- Rational α have finite expansions

Fact 1.7: Contined fraction expansion

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Continued Fractions

Fact 1.9: Contined fraction expansion

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  - Growth rate of a_i determines how closely approximated by rationals α is.

Fact 1.10: Contined fraction expansion

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- Rational α have finite expansions
- Irrational α have infinite expansions
  - Terminating expansion gives the best rational approximation
  - Growth rate of a_i determines how closely approximated by rationals α is.

$$\frac{\sqrt{5}+1}{2} = [1; 1, 1, 1, \dots] \qquad \sum_{k=1}^{\infty} \frac{1}{10^{k!}} = [0; 9, 11, 99, 1, 10, 9, 999999999999, 1, \dots]$$

Diophantine Conditions

Consider what happens when we plot the sequence $e^{2\pi i n\alpha}$ for rational α:

Diophantine Conditions

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Rational animation

$$\alpha = \frac{3}{11}$$

Diophantine Conditions

$$x_n = e^{2\pi i n\alpha}$$

ϕ animation

Liouville animation

$$\alpha = \frac{\sqrt{5}+1}{2}$$

$$\alpha = \sum_{n=1}^{\infty} \frac{1}{10^{k!}}$$

Diophantine Conditions

Diophantine Conditions

Definition 1.7: Diophantine

We call $\alpha \in \mathbb{R}$ **diophantine** if there is some $\gamma > 0, \tau \geq 1$ such that for all $m \in \mathbb{Z}$,

$$\|m\alpha\| := \mathrm{dist}(m\alpha, \mathbb{Z}) \geq \frac{\gamma}{|m|^\tau}$$

We call these *poorly approximable by rationals*, or colloquially, “more irrational”

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Definition 1.8: Liouville

We call $m \in \mathbb{R}$ **Liouville** if, for all $\gamma > 0, \tau > 1$, there are infintely many $m \in \mathbb{Z}$ for which

$$\|m\alpha\| < \frac{\gamma}{|m|^\tau}$$

We call these *too well approximable by rationals*, or colloquially, "less irrational"

Transport - Example 3

If α is diophantine, the transport is similar to the random case [BG00]

Insert diophantine transport example

If α is Liouville, the transport is similar to the periodic case

Insert Liouville transport example

Main Results

We determine bounds on transport for a number of Diophantine-like conditions

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$$\|m\alpha\| \geq e^{-\kappa(\log|n|)^\gamma} \quad \Longrightarrow \quad \langle X_H|_\phi^p\rangle \leq e^{p(\log\log t)^c}$$

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Definitions

Definition 2.1: Discrepancy

Let $\{\mathbf{x}_n\}_{n\in\mathbb{N}}$ be a sequence in $[0,1)^d$. Define $P_N = \{\mathbf{x}_1, \mathbf{x}_2, ..., \mathbf{x}_N\}$ then define the **Discrepancy** of P_N as

$$D_N(P_N) = \sup_{I\subset[0,1)^d} \left| \frac{1}{N} \sum_{n=1}^{N} \chi_I(x_n) - \mathrm{Vol}(I) \right| \tag{3}$$

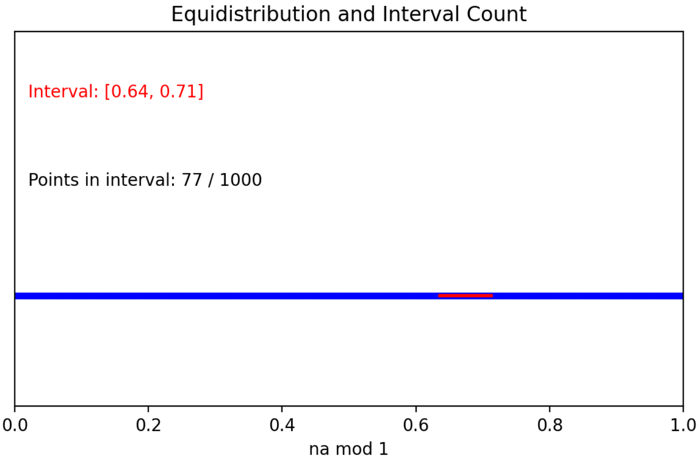
Where I is an axis-aligned rectangle.

Definition 2.2: Kronecker Sequence

Let $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_d) \in \mathbb{R}^d$. The **Kronecker Sequence** $\{\mathbf{x}_n\}_{n\in\mathbb{N}}$ of $\boldsymbol{\alpha}$ is defined via the relation:

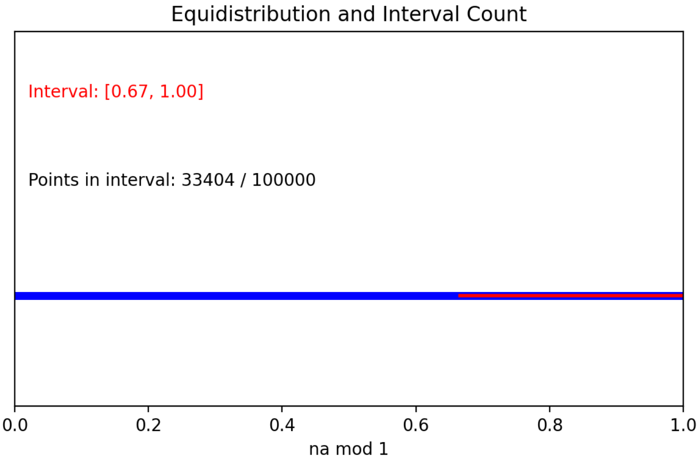
$$\mathbf{x}_n := n\boldsymbol{\alpha} \pmod{\mathbb{Z}^d} \tag{4}$$

Example 1 in $\mathbb{R}$



a $= \sqrt{2}$
Expected: $(0.71 - 0.64) \cdot 1000 = 70$
Discrepancy: $\frac{77-70}{1000} = 0.007$

Example 2 in $\mathbb{R}$

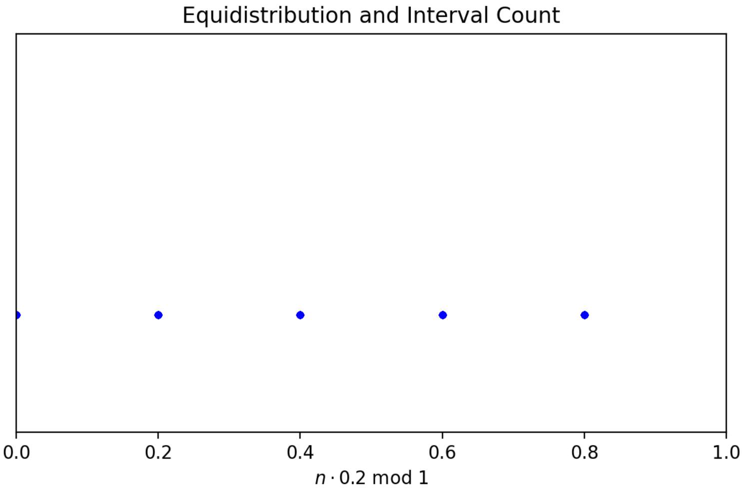


a $= \sqrt{2}$

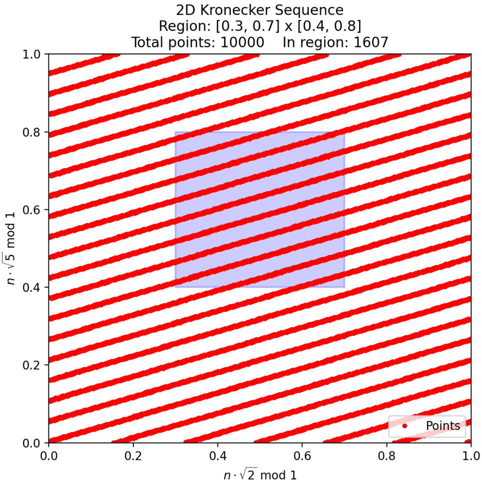
Expected: $(1 - 0.67) \cdot 100000 = 33000$

Discrepancy: $\frac{33404-33000}{100000} = 0.00404$

Example 3 in $\mathbb{R}$



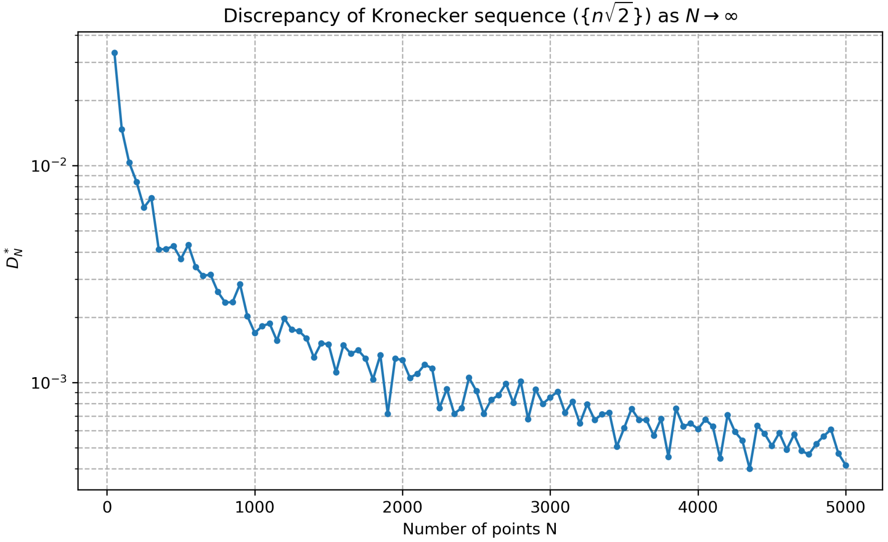
Example 4 in $\mathbb{R}^2$



Expected: $((0.7 - 0.3) \cdot (0.8 - 0.4)) \cdot 10000 = 1600$

Discrepancy: $\frac{1607-1600}{10000} = 0.0007$

Discrepancy as $N \to \infty$



Theorem 2.3: Denseness of Kronecker Sequences

Let $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, ..., \alpha_d) \in \mathbb{R}^d$ Then the Kronecker sequence $\{n\boldsymbol{\alpha}\}_{n\in\mathbb{N}}$ is dense in the unit torus $[0,1)^d$ iff $\{1, \alpha_1, ..., \alpha_d\}$ is linearly independent over the integers. We henceforth call this condition **rationally independent**.

- Hence, $D_N(\{n\boldsymbol{\alpha}\}) \to 0$ as $N \to \infty$ if and only if α is rationally independent.
- Interested in leading order approximation of D_N (logarithmic, exponential, polynomial?)
- Heavily depends on whether α is Diophantine or Liouville.

Previous Results

Theorem ([DT97])

Suppose $\boldsymbol{\alpha} \in \mathbb{R}^d$ *satisfies*

$$\|\boldsymbol{m\alpha}\| = \operatorname{dist}(\boldsymbol{m} \cdot \boldsymbol{\alpha}, \mathbb{Z}) \gtrsim \frac{\gamma}{|\mathbf{m}|^a} \tag{5}$$

for all $\mathbf{m} \in \mathbb{Z}^d$ *for some* $a \geq 1, \gamma > 0$*. Then for some* $\delta, C > 0$

$$D_N(\{\mathbf{x}_n\}) \leq CN^{-\delta} \tag{6}$$

Our Results

Theorem

Suppose $\boldsymbol{\alpha} \in \mathbb{R}^d$ *is such that for some* $\gamma, C > 0$

$$\|\boldsymbol{m\alpha}\| \gtrsim e^{-C|\mathbf{m}|^\gamma} \tag{7}$$

for all $\mathbf{m} \in \mathbb{Z}^d$ *and for some* $\gamma, C > 0$. *Then for some* $C_1 > 0$

$$D_N(\{\mathbf{x}_n\}) \leq C_1(\log N)^{-1/\gamma} \tag{8}$$

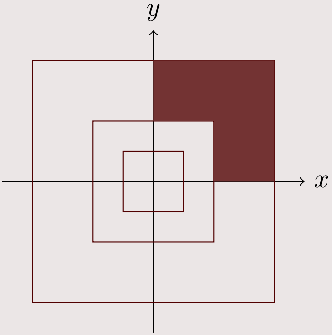
Proof.

1. Partition $\mathbb{Z}^d$ as in figure.
2. Bound each partition, and count the number within each partition.
3. Apply to Erdős-Turan inequality
4. Summing values together yields:

$$D_N \lesssim \frac{1}{M} + \frac{1}{N} + \frac{e^{(C(M-1)^{d\gamma})}(M-1)^d}{2N}$$

5. Choose $M = e^{.5CN^\gamma}$. Yields

$$D_N \le C_1(\log N)^{-1/\gamma}$$



□

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Theorem

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$$\|\boldsymbol{m\alpha}\| \gtrsim e^{-C(\log|\mathbf{m}|)^\gamma} \tag{9}$$

for all $\mathbf{m} \in \mathbb{Z}^d$. *Then for some* $\delta, C > 0$

$$D_N(\{\mathbf{x}_n\}) \leq \begin{cases} Ce^{-(\log N)^{1/\gamma}} & \gamma \geq 1 \\ CN^{-\delta} & \gamma < 1 \end{cases} \tag{10}$$

Counting using Discrepancy

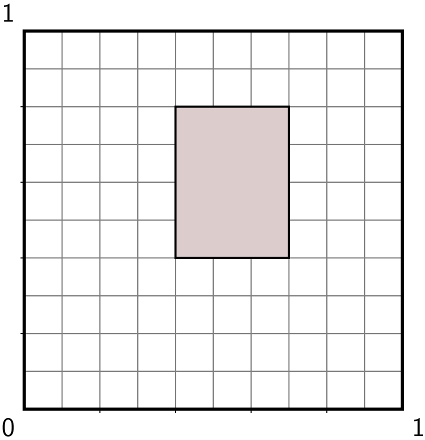
Recall

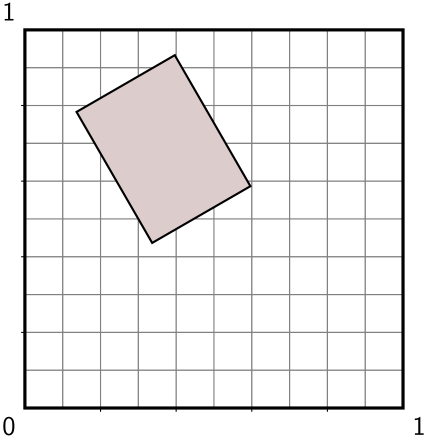
$$D_N(P_N) = \sup_{I \subset [0,1)^d} \left| \frac{1}{N} \sum_{n=1}^{N} \chi_I(n\boldsymbol{\alpha}) - \mathrm{Vol}(I) \right| \tag{11}$$

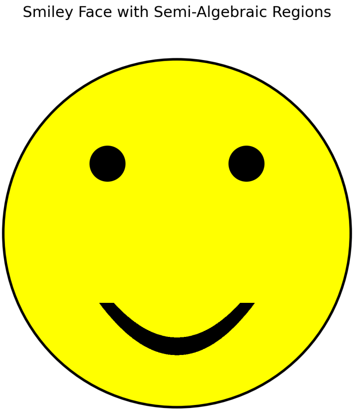
Hence, for a given rectangle

$$\sum_{n=1}^{N} \chi_I(n\boldsymbol{\alpha}) \leq N(D_N - \mathrm{Vol}(I)) \tag{12}$$

Expansion to Semi-Algebraic Sets







Definition 3.1: Semi-Algebraic Sets

A set $\mathcal{S}$ is **semi-algebraic** if it is a finite union of polynomial inequalities and equalities.

Head: $x^2 + y^2 \leq 1$

Left eye: $(x + 0.4)^2 + (y - 0.4)^2 \leq 0.01$

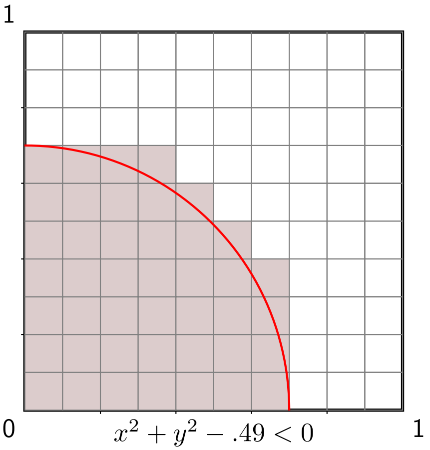
Right eye: $(x - 0.4)^2 + (y - 0.4)^2 \leq 0.01$

Smile: $1.5x^2 - 0.7 < y < 1.5x^2 - 0.6, \quad |x| < 0.5$

Expansion to Semi-Algebraic Sets

Theorem 3.2: [Bou05]

Let $\mathcal{S} \subseteq [0,1)^n$ be a semi-algebraic set of degree B. Let $\mathrm{Vol}(S) < \epsilon^n$ for some $\epsilon > 0$. $\mathcal{S}$ can be covered by $B^C(\epsilon)^{1-n}$ ϵ-balls.



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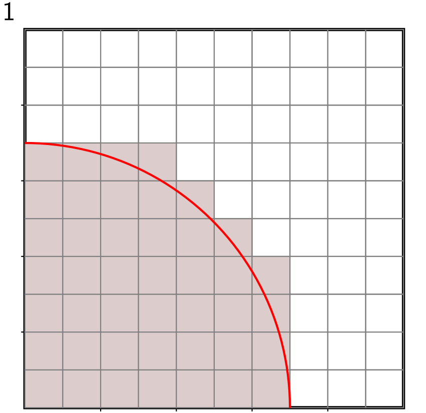
- Recall: V is analytic, hence V is well approximated by polynomials



Connection to Quantum Dynamics

Definition 4.1: Eigenvalues

Let $A \in M_{n\times n}(\mathbb{R})$. An eigenvalue- eigenvector pair are $\lambda \in \mathbb{C}$, $x \in \mathbb{R}^n$ which satisfy:

$$Ax = \lambda x$$

Alternatively, $\lambda \in \mathbb{C}$ is an eigenvalue iff

$$(A - \lambda I_n)^{-1} \text{ does not exist}$$

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- $H\psi = E\psi$
- Approximate H with finite dimensional H_N.

Connection to Quantum Dynamics

- Define $G_N(z;\theta) := (H_N(\theta) - zI_N)^{-1}$. Called the **Green's Function** of H.
- Since V is analytic, approximate with high-degree polynomial.
- Points where G_N doesn't exist are contained in Semi-Algebraic Set (Denote Θ_N).

Theorem 4.3: [HZ22] Large Deviation Estimates

$$\mathrm{Leb}\left\{\theta \in [0,1)^d : \det(H_N(\theta) - zI) < e^{-N^{1/2}}\right\} \leq e^{-N^{1/4}}$$

Theorem 4.4: Counting Estimates

$$\#\{|n| \leq N : \theta + n\alpha \in \Theta_N\} \text{ is } o(N^{-1})$$

Main Theorems

Theorem 4.5

If $\boldsymbol{\alpha}$ satisfies

$$\|\boldsymbol{m\alpha}\| > e^{-(\log|\mathbf{m}|)^{\gamma}} \tag{13}$$

Then,

$$\langle |X|_{\phi}^{p} \rangle(t) \lesssim e^{p(\log\log t)^{c}} \tag{14}$$

Theorem 4.6

If $\boldsymbol{\alpha}$ satisfies

$$\|\boldsymbol{m\alpha}\| > e^{-|\mathbf{m}|^{\gamma}} \tag{15}$$

Then,

$$\langle |X|_{\phi}^{p} \rangle(t) \lesssim e^{p(\log t)^{c}} \tag{16}$$

Proof.

Lemma 4.7

Let $z = E + \frac{i}{t}$. Assume that α is Liouvillian. Then for any j with $|j| \le M$,

$$|G(j,n)| \lesssim t^4 e^{-\frac{c}{20}|I|}$$

- Define

$$a(j,n,t) = \frac{2}{t}\int_0^\infty e^{2\tau/t} |(e^{-i\tau H}\delta_j, \delta_n)|^2 \, d\tau$$

- Hence,

$$\langle |X|_\phi^p \rangle = \sum_{n\in\mathbb{Z}} \sum_{|j|\le M} |n|^p a(j,n,t)$$

□

Proof of Theorem

Proof.

- By Parseval's Identity,

$$a(j,n,t) = \frac{1}{\pi t} \int_{\mathbb{R}} |G(z)(j,n)|^2 dz.$$

- Combes-Thomas Estimate, and the previous Lemma, we may estimate

$$a(j,n,t) \leq t^7 e^{-2c(\log(N))^C}$$

- By definition

$$\langle |X_H|^p_\phi \rangle(t) = \left(\sum_{|n| \leqslant R} + \sum_{|n|>R} \right) \sum_{|j| \leqslant M} |n|^p a(j,n,t)$$

- By construction

$$\langle |X_H|^p_\phi \rangle(t) \lesssim R^p + \sum_{|n|>R} \sum_{|j| \leq M} |n|^p a(j,n,t)$$

□

Proof of Theorem

Proof.

- Choose $R = e^{(\log T)^c}$
- Hence,

$$\langle |X_H|_\phi^p \rangle(t) \lesssim e^{p(\log T)^c}$$

$\square$

- Using this methodology, we may extend to general case (up to choice of R).

Conclusion

1. Quasi-Periodic Schrödinger Operators are fundamentally unique.
2. Summary of Tools used to find upper bounds.
    1. Discrepancy
    2. Semi-Algebraic Geometry
    3. Spectral Theory
3. Derived upper bounds show range of growth rates.

Open Problems

1. Lower Bounds
2. Does there exist an α such that $\langle |X|_{\phi}^{p} \rangle \sim T^{p/2}$?

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Thank You!