2-1-2014

Asymptotic Spectral Properties of the Schrödinger Operator With Thue-Morse Potential

William Clark
Ohio University

Rachael Kline
St. John Fisher College, rmk09830@sjfc.edu

Michaela Stone
Louisiana State University

Asymptotic Spectral Properties of the Schrödinger Operator With Thue-Morse Potential

Abstract

The open problem

Study the Thue-Morse trace map; in particular, find the asymptotics of the Hausdorff dimension of the spectrum as the coupling constant tends to zero or infinity.

Our research

• We studied the dynamics of the Thue-Morse trace map.

• We developed MATLAB code to help approximate the box-counting dimension, thickness, and Hausdorff measure of the Schrödinger operator with Thue-Morse potential.

• We analysed the resulting data, which confirmed conjectures about the asymptotic behavior of the fractal dimensions of the operator. Asymptotic Spectral Properties of the Schr¨odinger Operator with Thue-

Disciplines

Mathematics

Comments

Presented at the Nebraska Conference for Undergraduate Women in Mathematics on February 1, 2014.

Asymptotic Spectral Properties of the Schrödinger Operator With Thue-Morse Potential

William Clark - Ohio University • Rachael Kline - St. John Fisher College • Michaela Stone - Louisiana State University
Advisors: May Mei and Andrew Zemke

The open problem

Study the Thue-Morse trace map; in particular, find the asymptotics of the Hausdorff dimension of the spectrum as the coupling constant tends to zero or infinity.

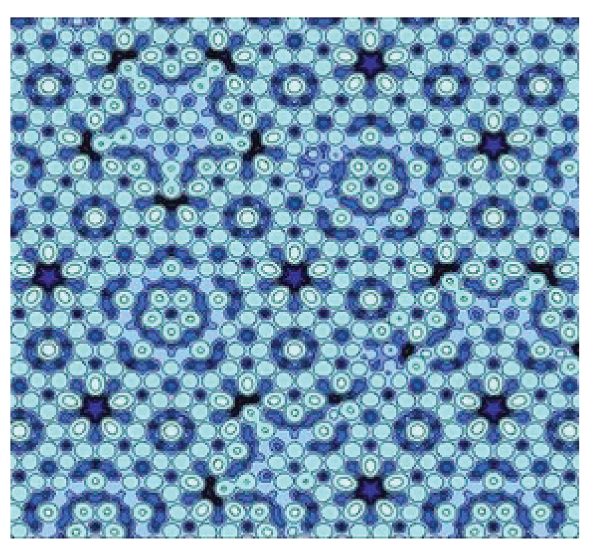
Our research

- We studied the dynamics of the Thue-Morse trace map.
- We developed MATLAB code to help approximate the box-counting dimension, thickness, and Hausdorff measure of the Schrödinger operator with Thue-Morse potential.
- We analysed the resulting data, which confirmed conjectures about the asymptotic behavior of the fractal dimensions of the operator.

Historical background

1984
Discovery of the icosahedral phase of the AlMn alloy was interpreted as a quasiperiodic crystal, giving rise to new questions about tilings.

Figure : Aperiodic quasicrystalline diffraction pattern.



Note that while several of the subpatterns are repeated, there is no regular lattice structure.

Why do we care?

Understanding the mathematics behind aperiodic tilings allows us to model the behavior of electrons traveling through quasicrystals.

Properties:

- Directionally varying electrical conductivity
- Poor heat conductivity

Uses:

- Surgical instruments
- LED lights
- Non-stick cookware

Modeling quasicrystals

A possible construction of these structures is generated using "inflation rules" that utilize a finite alphabet to represent the tiling. A substitution, σ, assigns a finite string of letters to each letter in the alphabet.

Definition
Letter - a single representative of the alphabet $(a, b, c, \ldots)$
Word - a collection of letters $(ab, ba, abc, \ldots)$

The Thue-Morse sequence

One specific sequence, the Thue-Morse sequence, uses two letters, a and b with the substitutions $\sigma(a) = ab, \sigma(b) = ba$. We denote the sequence as $\underline{u}$ where $\underline{u}_n$ is the n^{th} letter in the sequence. Suppose $u_0 = a$, using the substitution we obtain the sequence:

$$\underline{u} = abbabaabbaababba\ldots$$

where the sequence is the limit of the substitutions as the length of the sequence goes to infinity.

The 1D discrete Schrödinger operator with a Thue-Morse potential defined on the discrete 1-D lattice $\mathbb{Z}$ where V is the coupling constant, is

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

where $V(n) = V(-n-1)$ and $V(n) = V$ whenever the n^{th} letter of $\underline{u}$ is a and $V(n) = -V$ otherwise (by convention $u_0 = a$).

Understanding the trace map

The trace map is defined by

$$f(x, v) = (x^2 - 2 - v, v(v + 4 - x^2))$$

with the initial conditions $v_1 = 4V^2$, and $x_1 = E^2 - V^2 - 2$.

Definition
A point (x, v) is called *unstable* if there is a neighborhood $\mathscr{U}$ of (x, v) and an integer n_0 such that for all (x_1, v_1) in $\mathscr{U}$ and all $N \geq n_0$, the iterated $(x_N, v_N) = f^N(x_1, v_1)$ satisfies $|x_N| > 2$.

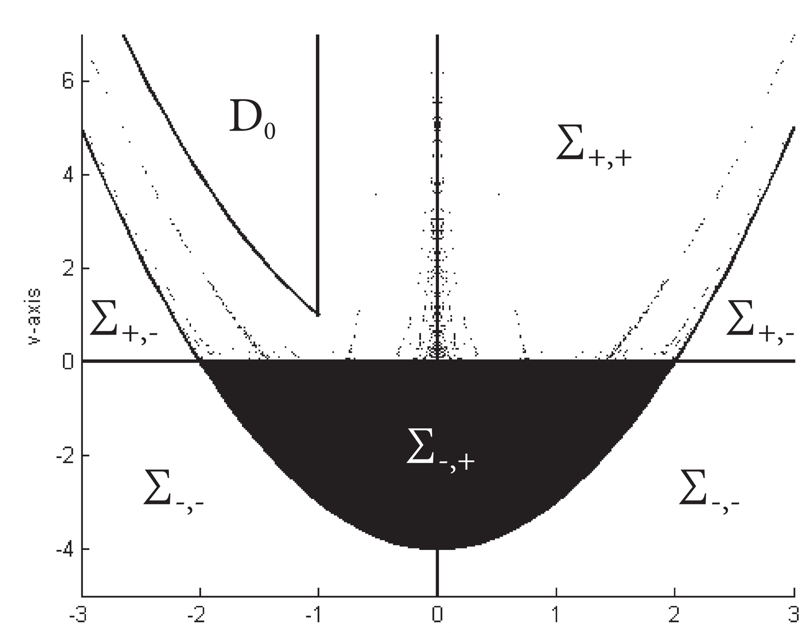


Figure : Stability domains in the (x, v)-plane for the trace map. $D_0, \Sigma_{+,-}$ and $\Sigma_{-,-}$ are unstable regions, $\Sigma_{-,+}$ is a not unstable region and $\Sigma_{+,+}$ contains both not unstable and unstable points. Not unstable points are represented by the black dots.

Proposition
E, energy, values corresponding to unstable points are out of the spectrum of the operator (Bellissard 1990).

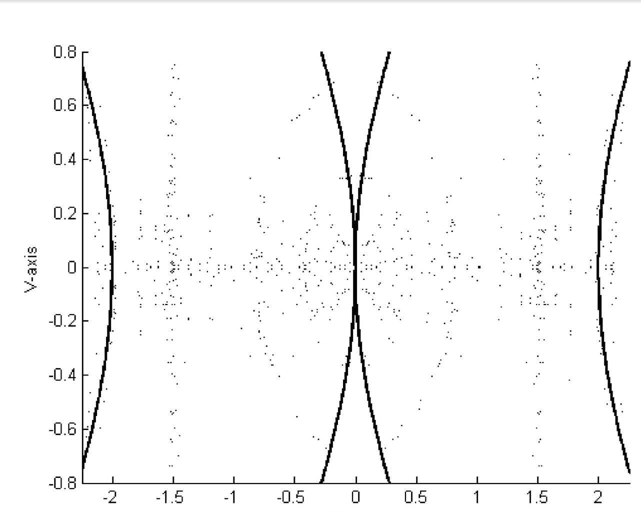


Figure : Plot of not unstable points in the (E, V)-plane instead of the (x, v)-plane in the previous figure.

Fractal Dimension

Since the spectrum is a Cantor set with measure zero, we wish to analyse the fractal dimension of the spectrum for different coupling constants, V. The notions of fractal dimension we will be using include:

- Box-counting dimension
- Thickness
- Hausdorff dimension

In an arbitrary set, F, we have the following relation:

$$\frac{\log 2}{\log\left(2 + \frac{1}{\tau}\right)} \leq \dim_H(F) \leq \dim_B(F):$$

where τ is the thickness, $\dim_H(F)$ is the Hausdorff dimension, $\dim_B(F)$ is box-counting dimension (Falconer 2005, Palis et al. 1993).

Box-counting Dimension

The Box-counting dimension of a set F is:

$$\dim_H F = \lim_{\delta \to 0} \frac{\log N_\delta(F)}{-\log \delta}$$

This equation is assuming that the measure of the set F obeys the power law:

$$N_\delta(F) \sim c\delta^{-s}$$
$$\log(N_\delta) \sim \log(c) - s\log(\delta)$$

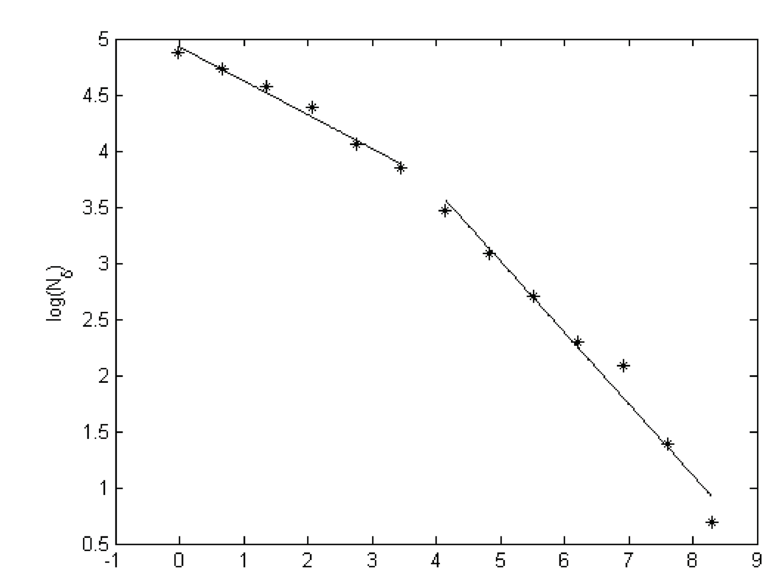


Figure : This is a log-log plot of δ versus N_δ with a coupling constant of 0.3 and with the resolution checking 2^{17} points under 10,000 iterations. The results are partitioned into two groups so the data is being fitted with two best-fit lines for the upper and lower estimates on the box-counting dimension.

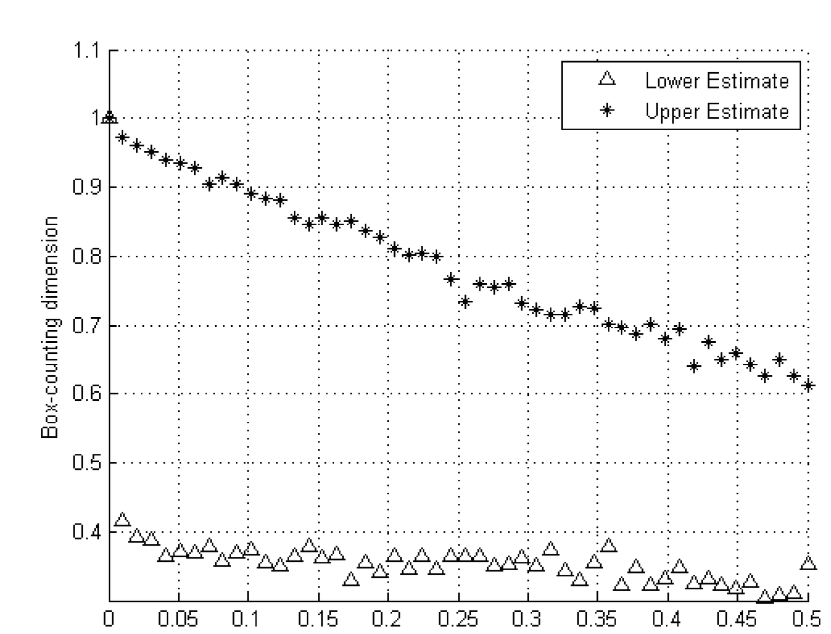


Figure : This graph is a V versus $\dim_B$ plot, where V is the coupling constant and $\dim_B$ is the box-counting dimension of the spectrum cross-section at that V. The graph includes both the upper and lower estimates for the box-counting dimension as described above.

Thickness

Another type of fractal dimension we will consider is the thickness of a Cantor set.

Definition
Let $K \subset \mathbb{R}$. A *gap* of K is a connected component $\mathbb{R}\backslash K$; a bounded gap is a bounded connected component of $\mathbb{R}\backslash K$. Let U be any bounded gap and u be a boundary point of U, so $u \in K$. Let C be the *bridge* of K at u, i.e. the maximal interval in $\mathbb{R}$ such that
- u is a boundary point of C,
- C contains no point of a gap U' whose length $\ell(U')$ is at least the length of U.

Definition
The thickness of K at u is defined as $\tau(K, u) = \ell(C)/\ell(U)$. The *thickness* of K, denoted by $\tau(K)$, is the infimum over these $\tau(K, u)$ for all boundary points u of bounded gaps.

We cannot compute this directly as a lower bound for the Hausdorff dimension. We plug the calculation of thickness into the function:

$$\frac{\log 2}{\log\left(2 + \frac{1}{\tau}\right)}$$

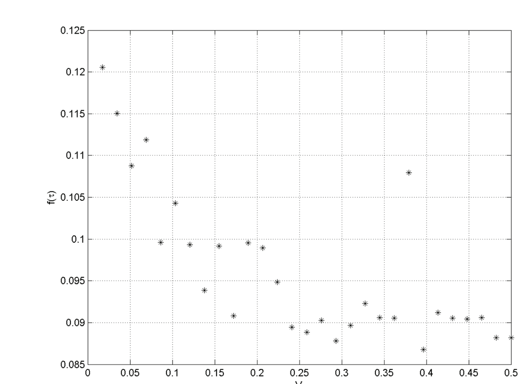


Figure : A plot of V versus $f(\tau)$ where $f(\tau) = \log 2/\log(2 + (1/\tau))$ which is a lower bound on the Hausdorff dimension.

Hausdorff Dimension

Before the Hausdorff dimension can be defined, the Hausdorff measure of a set must be defined:

Definition
The Hausdorff measure of a set F of dimension s, denoted by $\mathscr{H}^s(F)$, is:

$$\mathscr{H}^s(F) = \lim_{\delta \to 0}\left\{\inf\left\{\sum_{i=1}^{\infty}|U_i|^s : \{U_i\} \text{ is a } \delta - \text{cover of } F\right\}\right\}$$

With this in mind, we can define the Hausdorff dimension as follows:

Definition
The Hausdorff dimension of a set F, denoted by $\dim_H(F)$, is:

$$\dim_H(F) = \inf\{s \geq 0 : \mathscr{H}^s(F) = 0\} = \sup\{s : \mathscr{H}^s(F) = \infty\}$$

Specifically, $\dim_H(F)$ is the value of s where the Hausdorff measure 'jumps' from ∞ to 0.

We computed the Hausdorff measure of the spectrum, using both the trace map and also via Laplacian matrix truncation. In both cases the estimated dimension was between 0.4 and 0.8.

Research supported by

Cornell University
Department of Mathematics
Summer Math Institute

This work was supported by NSF grant DMS-0739338.