From Eigenvalues To Fractals

A brief introduction to spectral theory and quantum mechanics

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Undergraduate Research Project, Fall 2018-Spring 2019

Eigenvalues of a finite dimensional matrix.

Eigenvalues of the matrix $H = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$$= \{E \mid H - E \cdot \mathrm{Id} = \begin{pmatrix} -E & 1 & 0 \\ 1 & -E & 1 \\ 0 & 1 & -E \end{pmatrix} \text{ is not invertible}\}$$
$$= \{E \mid \det(H - E)| = 0\}$$
$$= \{-\sqrt{2}, 0, \sqrt{2}\}$$

$\Longleftrightarrow$ Collection of E such that the linear system $Hx = Ex$ has a non-trivial solution $x \in \mathbb{R}^3$:

$$\begin{cases} 0 \cdot x_1 + 1 \cdot x_2 + 0 \cdot x_3 = Ex_1 \\ 1 \cdot x_1 + 0 \cdot x_2 + 1 \cdot x_3 = Ex_2 \\ 0 \cdot x_1 + 1 \cdot x_2 + 0 \cdot x_3 = Ex_3 \end{cases} , \quad x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in \mathbb{R}^3$$

Infinite dimensional matrix and Spectrum

$$3 \times 3 \Longrightarrow \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}_{4\times 4} \Longrightarrow \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix}_{5\times 5} \quad \cdots$$

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What are the "eigenvalues" for the following "$\infty \times \infty$ matrix"?

$$\begin{pmatrix} \cdots & \cdots & \cdots & & & & & & \cdots \\ \cdots & 1 & 0 & 1 & & & & 0 & \\ & & 1 & 0 & 1 & & \cdots & & \\ & & & 1 & 0 & 1 & & & \\ & & \cdots & & 1 & 0 & 1 & & \\ & 0 & & & & 1 & 0 & 1 & \cdots \\ \cdots & & & & & & \cdots & \cdots & \cdots \end{pmatrix}$$

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Matrix $\Longrightarrow$ Operator; Eigenvalue $\Longrightarrow$ Spectrum.

'Spectrum' in real life

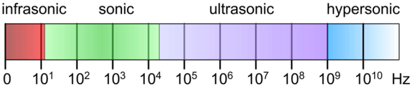


Figure 1: Sound spectrum

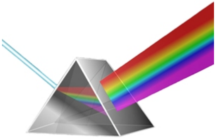
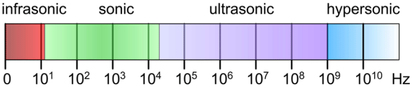


Figure 2: Light spectrum

‘Spectrum’ in real life



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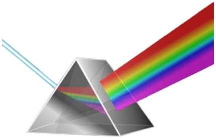


Figure 2: Light spectrum

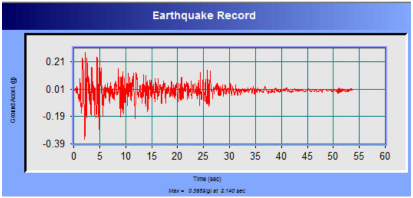


Figure 3: Earthquake Spectrum

‘Spectrum’ in real life

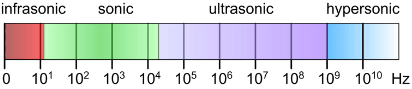
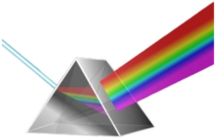


Figure 1: Sound spectrum



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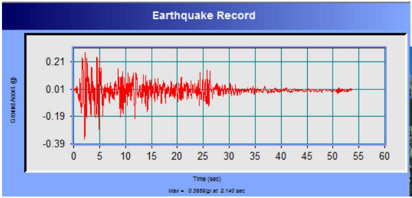

Figure 3: Earthquake Spectrum

Figure 4: Irvine Spectrum Center

Spectrum: The 'observable' quantity.

- Etymology: In Latin spectrum means "image" or "apparition".
- Mathematics-Physics:

$$\text{Eigenstate } x \xrightarrow{\text{input}} \boxed{\text{Operatored by } \mathsf{Hx}} \xrightarrow{\text{output}} \text{State } Ex$$

  The action (operation) behaves as multiplication: $Hx = Ex$, where E is the 'observable' energy.
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Definition

The spectrum of an operator H on a Hilbert space $\mathcal{H}$ is the subset of $\mathbb{C}$ given by

$$\sigma(H) := \{E \in \mathbb{C} | H - E \text{ is not invertible}\}$$

Quantum mechanics and Tight-binding model

- Vector/State $x = \{x_j\}$, $j \in \mathbb{Z}$ (or $j \in [1, 2, \cdots, n]$).
  Classical mechanics: position,momentum;
  Quantum mechanics: probability distribution/superposition of wave functions.
- In solid-state physics, the tight-binding model is an approach to the calculation of electronic band structure using an approximate set of wave functions for isolated atoms located at each atomic site.
- The name "tight binding" of the model suggests that the quantum mechanical model describes the properties of tightly bound electrons in solids.

Free Schrödinger operator H_0

- Kinetic energy/Momentum operator/Hopping operator

$$H_0 = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ \ddots & 1 & 0 & 1 & 0 & \ddots & \\ & 0 & 1 & 0 & 1 & 0 & \\ & \ddots & 0 & 1 & 0 & 1 & \ddots \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}$$

- H_0 acts on x as usual matrix multiplication:

$$H_0 x = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ \ddots & 1 & 0 & 1 & 0 & \ddots & \\ & 0 & 1 & 0 & 1 & 0 & \\ & \ddots & 0 & 1 & 0 & 1 & \ddots \\ & & & & \ddots & \ddots & \ddots \end{pmatrix} \begin{pmatrix} \vdots \\ x_0 \\ x_1 \\ x_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ x_{-1} + x_1 \\ x_0 + x_2 \\ x_1 + x_3 \\ \vdots \end{pmatrix}$$

More general hopping operators

- The j-th position of $H_0 x$ is $x_{j-1} + x_{j+1}$, which describes the interaction between jth position and its nearest neighborhoods ($j \pm 1$th position).
- In general, we can consider interactions given by the matrix

$$H_0 = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ \ddots & a_{0,-1} & 0 & a_{0,1} & a_{0,2} & \ddots & \\ & a_{1,-1} & a_{10} & 0 & a_{1,2} & a_{1,3} & \\ & \ddots & a_{2,0} & a_{2,1} & 0 & a_{2,3} & \ddots \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}$$

- Appropriate assumptions on $a_{i,j}$ are needed so that the model makes sense in physics. For example, the electrons in the T.B. model should have limited interaction with states on surrounding atoms of the solid.

Schrödinger operator with potential potential $\{v_n\}_{n\in\mathbb{Z}}$

- Potential energy/Multiplicative operator V:

$$V = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ \ddots & 0 & v_0 & 0 & 0 & \ddots & \\ & 0 & 0 & v_1 & 0 & 0 & \\ & \ddots & 0 & 0 & v_2 & 0 & \ddots \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}$$

- Total energy=Kinetic energy+Potential energy:

$$H = H_0 + V = \begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ \ddots & 1 & v_0 & 1 & 0 & \ddots & \\ & 0 & 1 & v_1 & 1 & 0 & \\ & \ddots & 0 & 1 & v_2 & 1 & \ddots \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}$$

Schrödinger equation

- Hx is defined in the same way as H_0x:

$$\begin{pmatrix} \ddots & \ddots & \ddots & & & & & \\ \ddots & 1 & v_0 & 1 & 0 & \ddots & & \\ & 0 & 1 & v_1 & 1 & 0 & & \\ & \ddots & 0 & 1 & v_2 & 1 & \ddots & \\ & & & & \ddots & \ddots & \ddots & \end{pmatrix} \begin{pmatrix} \vdots \\ x_0 \\ x_1 \\ x_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \vdots \\ x_{-1} + x_0 v_0 + x_1 \\ x_0 + x_1 v_1 + x_2 \\ x_1 + x_2 v_2 + x_3 \\ \vdots \end{pmatrix}$$

- The eigenvalue equation $Hx = Ex$ is called Schrödinger equation, which describes stationary quantum states of a quantum system.
- The the jth equation (j-th row of the sysytem):

$$x_{j-1} + v_j x_j + x_{j+1} = Ex_j$$

Eigenvalue problem on a finite lattice: Landscape theory

Theorem (M. L. Lyra, S. Mayboroda and M. Filoche)

If $H = \begin{pmatrix} v_1 & -1 & 0 & \cdots & 0 \\ -1 & v_2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & v_{n-1} & -1 \\ 0 & \cdots & 0 & -1 & v_n \end{pmatrix}$, $v_j \geq 2, j = 1, \cdots, n$, *and* $Hx = Ex$, *then for all* $j = 1, \cdots, n$,

$$\frac{|x_j|}{\max\limits_{1 \leq k \leq n} |x_k|} \leq E u_j, \quad \text{where} \quad H \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}.$$

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Remark

A finite lattice(linear algebra) problem can be highly non-trivial!

Eigenvalue equation for the free Schrödinger operator

- Let $x = (\cdots, x_0, x_1, \cdots)^T$. Eigenvalue equation of H_0:

$$H_0 x = E x \iff x_{n-1} + x_{n+1} = E\, x_n, n \in \mathbb{Z}$$

- Explicitly solvable for any $E \in \mathbb{C}$:

$$x_n = c_1\ \lambda^n + c_2\ \lambda^{-n}, \quad \lambda = \frac{E + \sqrt{E^2 - 4}}{2}$$

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- There is no eigenvalue since $\sum_{n \in \mathbb{Z}} |x_n|^2 = \infty$ for any E.
- For $E \notin [-2, 2]$, $|\lambda| > 1$ and $|x_n| \sim |\lambda|^{|n|}$, exponentially large.
- For $E \in [-2, 2]$, $|\lambda| = 1$ and $|x_n| < |c_1| + |c_2|$ for any n.
- Theorem of Schnol-Simon $\Longrightarrow \sigma(H_0) = [-2, 2]$

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- Theorem of Schnol-Simon $\Longrightarrow \sigma(H_0) = [-2, 2]$
- The spectrum of an infinite dimensional matrix is not the union of COUNTABLY many eigenvalues. It might be a whole INTERVAL.

Crystal and Schrödinger equation with periodic potential

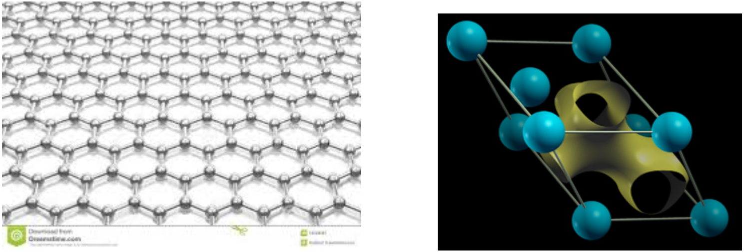

Figure 5: Periodically-repeating environment: Crystal.

Let $H = H_0 + V$. If v_n is a periodic sequence, then $\sigma(H)$ consists of finitely many intervals (spectrum bands).
e.g., $v_n = 2\cos(\pi n) = 2(-1)^n$ is a periodic sequence with period 2:

$$\cdots, 2, -2, 2, -2, 2, -2, \cdots$$

Harper's Equation.

- In general, we can consider $v_n = 2\cos(2\pi n\alpha)$, where $\alpha \in [0, 1]$ is some parameter. The Schrödinger equation (nth row) is:

$$x_{n+1} + x_{n-1} + 2\cos(2\pi n\alpha)\, x_n = E\, x_n$$

- The above equation is called Harper's Equation.

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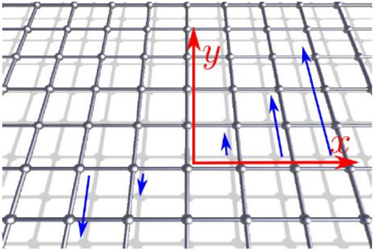
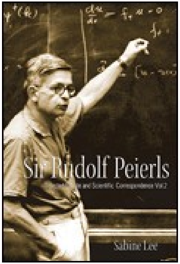
- The above equation is called Harper's Equation.
- If $\alpha = \frac{p}{q}$ is a rational number, the potential $v_n = 2\cos(2\pi n\frac{p}{q})$ is periodic.
- If α is irrational, v_n is no longer periodic but still has some recurrence properties, which is called quasi-periodic.
  e.g. $\alpha = \frac{\sqrt{5}-1}{2}$, v_n are: 2, -1.4747, 0.17485, 1.2169, -1.9694, 1.6875, -0.51921, -0.92181, 1.8786, -1.8487, 0.84769, 0.59857, -1.7304, 1.9534, -1.1503, -0.25702, 1.5293, -1.9983, 1.4177, -0.092383, -1.2814, 1.9821, $\cdots$

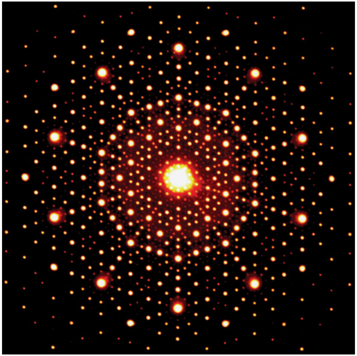
Energy levels of Bloch electrons in magnetic fields

- The Harper's equation (model) is used to study the theorised behaviour of Block electrons in a magnetic field.
- First introduced by R. Peierls in 1933 .
- Further studied by a Ph.D. student of Peierls, P.G. Harper (1955).
- α is a parameter equal to the ratio of flux through a lattice cell to one flux quantum.
- It is also called the almost Mathieu operator in math.





- The general quasi-periodic potential v_n and the associated Schrödinger equation are also close related to the study of quasicrystal.
- Quasicrystal, is a structure that is ordered but not periodic.
- D. Shechtman was awarded the 2011 Nobel Prize in Chemistry for the discovery of quasicrystals (in 1982).



The spectrum of Harper's Model at rational frequency

- In 1975 Douglas Hofstadter studied Harper's model numerically in his PhD thesis.

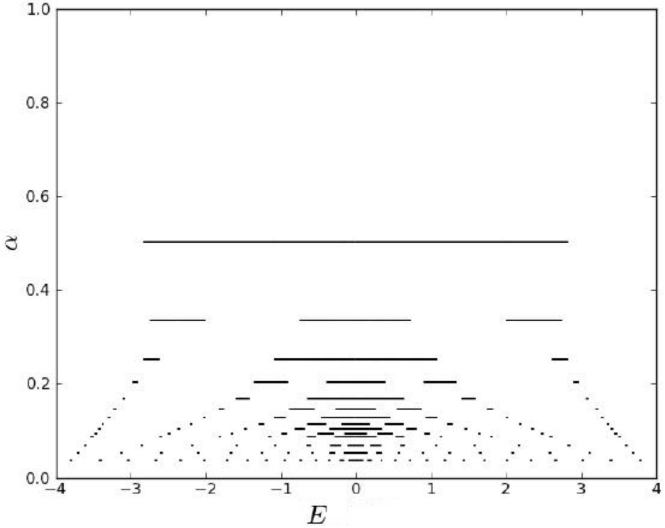
PHYSICAL REVIEW B VOLUME 14, NUMBER 6 15 SEPTEMBER 1976

Energy levels and wave functions of Bloch electrons in rational and irrational magnetic fields*

Douglas R. Hofstadter†
Physics Department, University of Oregon, Eugene, Oregon 97403
(Received 9 February 1976)

- He plotted the spectra for different rational values of the flux $\alpha = \frac{p}{q}$. Let q varies from 1 to 50.

Spectrum band for rational flux



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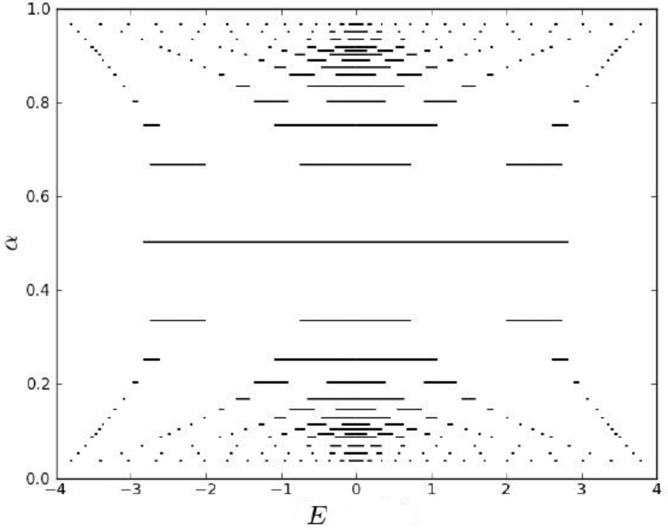
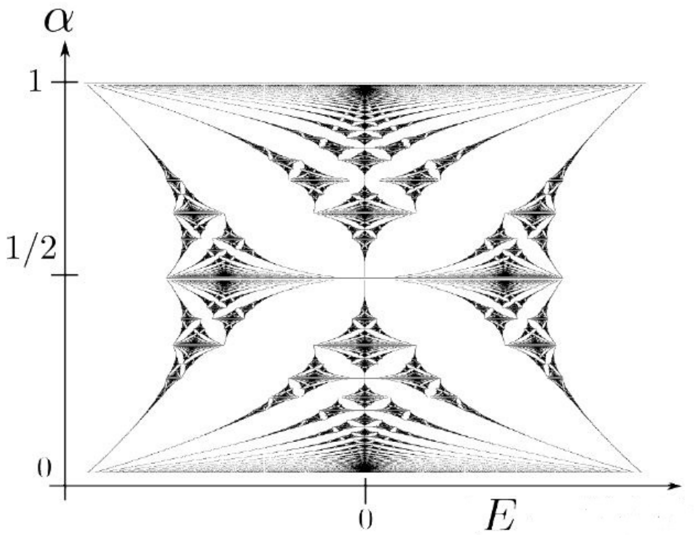
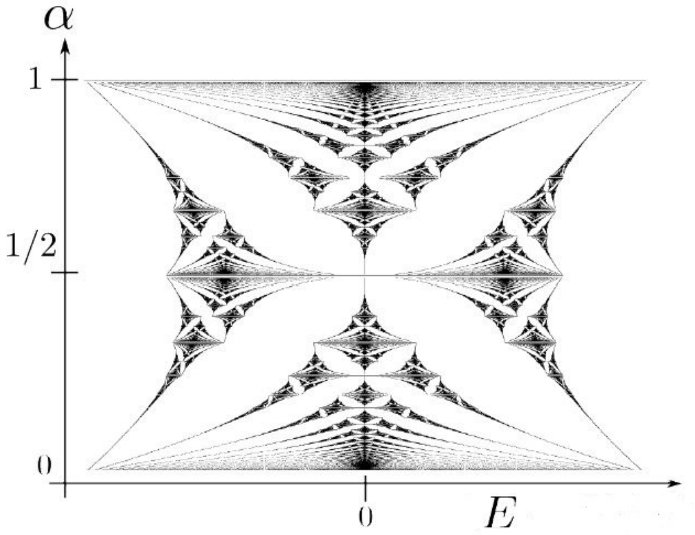
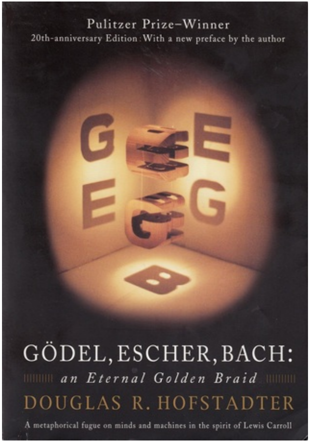



α
1
1/2
0
0
E

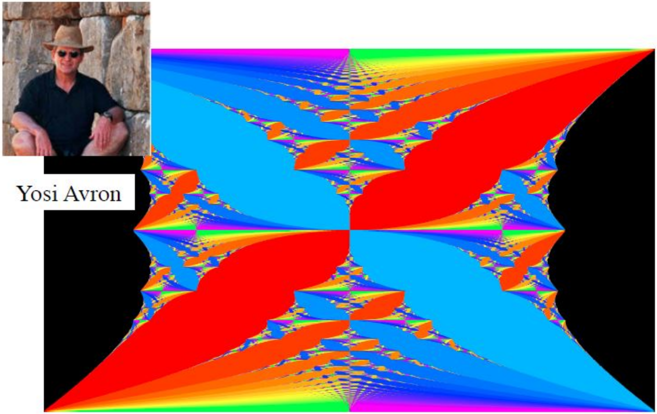
Hofstadter's butterfly



As Douglas Hofstadter mentioned in his PhD thesis, his friend David Jennings, on seeing the spectrum, described it as “a picture of God.”



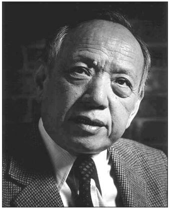
Colored Hofstadter's butterfly



The gaps in the spectrum correspond to integer values of the Hall conductance.
The figure shows the gaps, color coded according to the Hall conductance.
The warm colors represent positive values of Hall conductance, and the cold colors represent negative values.

Theory and experiment

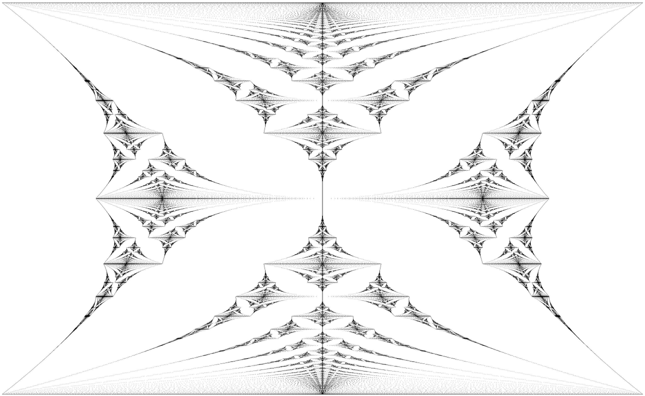
- Integer Quantum Hall Effect (von Klitzing, 1980)
- Theory of Thouless et all (1982) explains the quantization of charge transport in this effect as connected with certain topological invariants (Chern numbers). Central to their theory is the use of the Harpers model.
- Predictions of Thouless et al. verified experimentally by C. Albrecht, von Klitzing, et al. in a 2D electron gas in a superlattice potential (2001)
- In mathematics, Hofstadter's butterfly is one of the rare fractal structures discovered in physics.

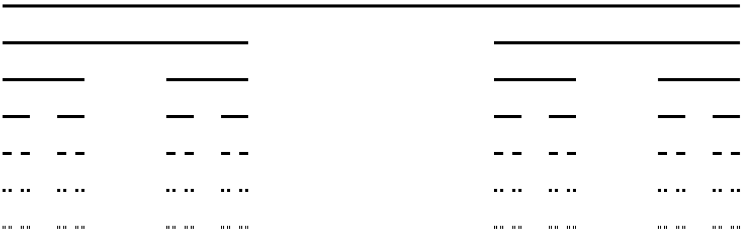
From rational to irrational: $\frac{p_n}{q_n} \to \alpha \in \mathbb{R} \backslash \mathbb{Q}$

If $v_n = 2\cos(2\pi n \frac{p}{q})$, then the spectrum $\sigma(H_{p/q})$ consists of up to q bands. What happens to $\sigma(H_\alpha)$ if $\frac{p_n}{q_n} \to \alpha \in \mathbb{R} \backslash \mathbb{Q}$?

e.g. $\alpha = \frac{\sqrt{5}-1}{2} \approx 0.61803398875\cdots$, $\frac{3}{5}, \frac{5}{8}, \frac{8}{13}, \frac{13}{21}, \frac{21}{34}, \frac{34}{55}, \cdots$



Cantor structure: Middle third Cantor Set



Nowhere dense: a set whose closure has empty interior.

Ten Martini Problem

Almost Mathieu Operator:

$$(H_{\lambda,\theta,\alpha}x)_n = x_{n+1} + x_{n-1} + 2\lambda\cos 2\pi(n\alpha+\theta)x_n$$

Ten Martini Problem: For all $\lambda \neq 0$, all irrational α and all θ, the spectrum of $H_{\lambda,\theta,\alpha}$ is a Cantor set.

- 1960s, conjectured by M. Azbel.
- Mark Kac in 1982 offered ten martinis for the proof of Azbel's Cantor set conjecture.
- It was dubbed the Ten Martini problem by Barry Simon who advertised it in his lists of 15 mathematical physics problems (1984) and later, mathematical physics problems for the XXI century (2001).

Ten Martini Problem

- Most substantial partial solutions were made in the work by J. Bellissard, B. Simon, Ya. Sinai, B.Hellfer, J. Sjostrand, G. Elliott, M.-D.Choi, S. Yui, Y. Last (between 1983-1994) and J. Puig (2003)
- Final solution in a joint work of Artur Avila (2014 Fields Medalist) and Svetlana Jitomirskaya in 2005.

Unfortunately Mark Kac is not there for offering the ten Martini.

Thank you!