Generalities on the Fibonacci Hamiltonian.

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9 décembre 2014

1 Constructing the Fibonacci Hamiltonian: the alphabet of couplings.

1.1 The Fibonacci sequence and its statistical properties

We consider the following inflation rule on the 2 letters alphabet $\mathcal{A} = \{t_s, t_w\}$:

$$r \stackrel{\text{def}}{=} \begin{cases} t_w & \to t_w t_s \\ t_s & \to t_w \end{cases} \tag{1.1}$$

Starting from the seed t_s, we define the nth *Fibonacci word* (aka *rabbit word*):

$$S_n \stackrel{\text{def}}{=} r^n(t_s) \tag{1.2}$$

One can show the S_n converges[1]. We call $S_\infty = \lim_{n\to\infty} S_n$ the *Fibonacci sequence*.

Statistical properties of the Fibonacci sequence

The inflation rule r has the substitution matrix

$$\mathrm{Sub}(r) = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \tag{1.3}$$

The eigenvalues of the substitution matrix are τ and $\omega \stackrel{\text{def}}{=} -1/\tau$, where $\tau = (1+\sqrt{5})/2$ is the golden ratio. More precisely, we have

$$\mathrm{Sub}(r) = \mathcal{R}(\theta) \begin{bmatrix} \tau & 0 \\ 0 & \omega \end{bmatrix} \mathcal{R}(\theta)^{-1} \tag{1.4}$$

1. For the product topology on $\mathcal{A}^{\mathbb{N}}$ induced by the discrete topology on $\mathcal{A}$.

where $\mathcal{R}(\theta)$ is the rotation by the angle θ such that

$$\begin{cases} \cos\theta = 1/\sqrt{2+\tau} \\ \sin\theta = 1/\sqrt{2+\omega} \end{cases} \tag{1.5}$$

Knowing this we can easily compute $\mathrm{Sub}(r^n) = \mathrm{Sub}(r)^n$. We immediately deduce the frequency of letters in S_n:

$$\begin{cases} \#\{t_s \in S_n\} & = F_{n-2} \\ \#\{t_w \in S_n\} & = F_{n-1} \end{cases} \tag{1.6}$$

where F_n is the nth *Fibonacci number* ($F_0 = 1$, $F_1 = 1$, $F_2 = 2$, ...). In particular, there are τ times more t_w than t_s in S_∞.

1.2 Deflation rules; atoms and molecules.

Consider the slightly different inflation rule

$$\tilde{r} = \begin{cases} t_w & \to t_s t_w \\ t_s & \to t_w \end{cases} \tag{1.7}$$

It has the same substitution matrix as r, and therefore the words produced by this rule have the same frequency of letters as the Fibonacci words. Furthermore they are locally undistinguishable from the Fibonacci words [2]. Any combination of these two substitution rules (eg $r\tilde{r}rr\tilde{r}$...) has again the same properties. We will also call words produced by such sequences Fibonacci words.

Molecules

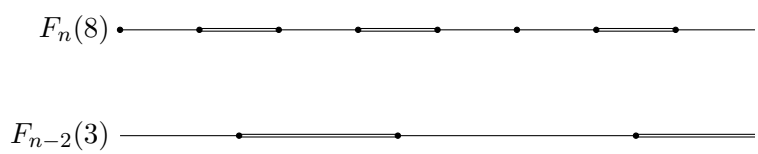

Figure 1.1 – The molecular deflation rule d_m illustrated on a length 8 Fibonacci word.

We have

$$\tilde{r}r = \begin{cases} t_w & \to t_s t_w t_w \\ t_s & \to t_s t_w \end{cases} \tag{1.8}$$

2. Both word sequences admit the same 3 local environments: $t_w t_s$, $t_s t_w$ and $t_w t_w$.

Which admits as an inverse the *deflation rule*

$$d_m = \begin{cases} t_w & \leftarrow t_s t_w t_w \\ t_s & \leftarrow t_s t_w \end{cases} \tag{1.9}$$

This deflation rule reduces a word of length F_n to word of length F_{n-2} (fig. (1.1)).

Atoms

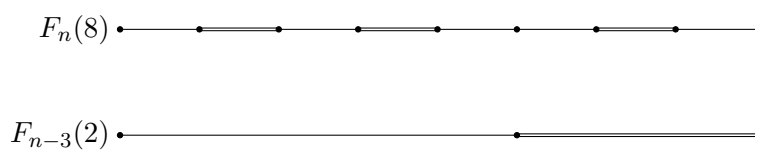

Figure 1.2 – The atomic deflation rule d_a illustrated on a length 8 Fibonacci word.

1.3 The Fibonacci Hamiltonian and its approximants

There is a natural quantum system associated to S_n. It is described by the tight-binding Hamiltonian H_n, whose sequence of couplings is given by S_n.

Boundary conditions: as there are F_n words in S_n, H_n has F_n couplings. These F_n couplings are jump amplitudes between two neighbouring atomic sites. There are thus *a priori* $F_n + 1$ atomic sites, but we are going identify the first and the last atomic sites, ie use *periodic boundary conditions*. See eq. (1.10) for the example of the sixth Hamiltonian, with $F_6 = 8$ atomis sites.

$$H_6 = \begin{bmatrix} 0 & t_w & & & & & & t_w \\ t_w & 0 & t_s & & & & & \\ & t_s & 0 & t_w & & & & \\ & & t_w & 0 & t_s & & & \\ & & & t_s & 0 & t_w & & \\ & & & & t_w & 0 & t_w & \\ & & & & & t_w & 0 & t_s \\ t_w & & & & & & t_s & 0 \end{bmatrix} \tag{1.10}$$

Tha Hamiltonian H_n is called the nth *approximant*. $H_\infty = \lim_{n\to\infty} H_n$ is called the *Fibonacci Hamiltonian*.

2 Some results on the Fibonacci Hamiltonian

The transformation $\lambda \to \lambda H$ leaves the spectrum and the wavefunctions unchanged. Therefore, the properties of the Fibonacci Hamiltonian relevant for the physics only depend on the parameter

$$\rho = \frac{t_w}{t_s} \tag{2.1}$$

2.1 The $\rho = 1$ case.

In that case the Hamiltonian is periodic. As we are going to see, this case is very special, and differs from the case $\rho < 1$ in almost every respect.

However, we start by analyzing this well known case to gain some insight on the physics of the model.

Spectrum of the nth approximant It is a tedious but easy exercice of linear algebra to diagonalize the $H_n(k)$ matrix. One finds that the F_n energy states are indexed by an integer $a \in [0, F_n)$, and write

$$E_a(k) = 2\cos\left(\frac{2a\pi + k}{F_n}\right) \tag{2.2}$$

Then, finding the wavefunction $|\psi_a\rangle$ associated to E_a is easy enought. Calling $\psi(i, a)$ the coefficient of this wavefunction at site i, we have the recurrence relation

$$\psi(i-1, a) + \psi(i+1, a) = E_a \psi(i, a) \tag{2.3}$$

for a site i that is not at the edges of the chain: $i > 0$ and $i < F_n - 1$. Thus $\psi(i, a)$ is a linear combination of $\exp(2I\pi ia/F_n)$ and $\exp(-2I\pi ia/F_n)$. If $k = 0, \pi$, the coefficients must be real ($H_n(0, \pi)$ being a *real* symmetric matrix, it can be diagonalized by real vectors), we have, for i integer, $i \in [0, F_n)$,

$$\psi(i, a) = \mathcal{N}_a \cos\left(\frac{2ai\pi}{F_n}\right) \tag{2.4}$$

where $\mathcal{N}_a$ is a normalization coefficient. Note that in the limit $n \to \infty$ it is no longer possible to normalize these extended eigenstates.

I find

$$\mathcal{N}_a \underset{n\to\infty}{\sim} \frac{1}{\sqrt{F_n}} \frac{1}{\sqrt{\frac{1}{2}\left(1 + \frac{\sin(4a\pi)}{4a\pi}\right)}} \tag{2.5}$$

Fractal dimensions In the case $\rho = 1$ the fractal dimensions of the spectrum can be computed analytically without much effort – cf. appendix B. We find

$$\tau(q \leq 2) = q - 1 \tag{2.6}$$

$$\tau(q \geq 2) = \frac{q}{2} \tag{2.7}$$

In particular, as expected, the Hausdorff dimension is 1. Performing a Legendre transform, we realize that the pointwise Hölder exponent can only take 2 values:

$$\alpha(q \leq 2) = 1 \text{ and } f(1) = 1 \tag{2.8}$$

$$\alpha(q \geq 2) = \frac{1}{2} \text{ and } f(1/2) = 0 \tag{2.9}$$

$f(1/2) = 0$ indicates that the set of points having Hölder exponent $1/2$ forms at most a countable subset of the spectrum. It is actually constituted of the 2 points at the edges of the spectral band $[-2, 2]$. At these points – known as Van Hove singularities – the local density of state is non-smooth (and here even diverges). This is reflected by a smaller than 1 value of the Hölder exponent.

2.2 The $\rho \to 1$ limit

In this limit the Hamiltonian is periodic. Interestingly, physical quantities does not have a smooth limit when $\rho \to 1$. For example if $\rho = 1$ the spectrum is absolutely continuous, but as soon as $\rho < 1$, the spectrum becomes singular continuous. Physically that means that gaps open almost everywhere in the – previously – continuous spectral band $[-2, 2]$.

The fractal dimensions of the spectrum become smaller than one, indicative of its factal nature. It was found [RS96] that, at first order in $(1 - \rho)$,

$$q(\tau \leq 1) = 1 + \tau + (1 - \rho)4\pi^{-2}\tau \tag{2.10}$$

$$q(\tau \geq 1) = 2\tau \tag{2.11}$$

which is easily inverted to deduce that

$$D(q \leq 2) = 1 - (1 - \rho)4\pi^{-2} \tag{2.12}$$

Note that the $q \geq 2$ dimensions remain unaffected at first order, indicating that the Van Hove singularities are unperturbed.

2.3 The $\rho \to 0$ limit

In this limit, the t_s is much stronger than t_w. As t_s becomes stronger and stronger, the gap width becomes larger and larger.

To begin with, we investigate the $\rho = 0$ case. In that – rather trival – case, because $t_w = 0$ the chain decouples into isolated atoms (the ones linked to their neighbours by weak bounds), and isolated molecules (two atoms linked by a strong bound). We will in the following refer to them respectively as "atoms" and "molecules".

The Hamiltonian is then a direct sum of Hamiltonians decribing an atom or a molecule. Atomic Hamiltonians give rise to a 0 energy level, while molecular Hamiltonians give rise to two levels: $\pm t_s$. The spectrum has thus a boring zero Hausdorff dimension. As for the wavefunctions, their fractal dimensions are not even properly defined since the energy levels are degenerate [3].

In the $\rho \to 0$ limit, the atoms and the molecules weakly couple to each other, thus rising the degeneracy of the energy levels. To our delight, the Fibonacci hierarchy of gaps – indexed according to the gap labelling theorem – appears. The Hausdorff dimension of the spectrum satisfyingly becomes non trivial. It is given by

$$D(q=0) \underset{\rho\to 0}{\sim} \frac{\log(\sqrt{2}-1)}{\log \rho} \tag{2.13}$$

What about the dimensions of the wavefunctions? We have

$$D(q;a) = x_a \frac{\log 2}{\log \tau} \tag{2.14}$$

where x_a is the fraction of renormalization time the energy labelled by a spends in molecular clusters.

Let us prove it! Call $\psi_n(i,a)$ the wavefunction associated to the energy E_a, at site i. Call $I_n(i,a) = |\psi_n(i,a)|^2$ the associated intensity (or presence probability). We are interested in computing

$$\chi_n(q;a) = \sum_{i=0}^{F_n-1} (I_n(i,a))^q \tag{2.15}$$

3. The fractal dimension of a linear combination is not the linear combination of the fractal dimensions. But a linear combination of eigenfunctions of a degenerate energy level is again an eigenfunction. Hence the fractal dimensions of the eigenfunctions of a degenerate level are ill-defined.

In the $\rho \to 0$ limit the intensity at site i, at energy E_a, only depends on x_a. So, given a, the intensity does not depend on the site! In other words the intensity is uniform, which means that the fractal dimensions are independant of q.

Normalization gives us $I_n(i,a) = 2^{-nx_a}$, so that

$$\chi_n(q;a) = \left(\frac{1}{2^{nx_a}}\right)^{q-1} \tag{2.16}$$

and

$$D_n(q;a) = x_a \frac{\log 2}{\log(F_n^{1/n})} \tag{2.17}$$

hence the result (2.14).

A The thermodynamical formalism: a reminder.

We make an extensive use of the thermodynamical formalism to compute the fractal dimensions of the spectrum and of the wavefunctions. We simply wish here to set up some definitions and recall some useful results.

A.1 General formalism

To compute the fractal dimensions of a fractal set $\mathcal{S}$, the thermodynamical formalism defines at each point $a \in \mathcal{S}$ a sequence of open sets $\Delta_a^n \supset \Delta_a^{n+1} \supset ... \supset \{a\}$. To each of these open sets is associated the propability to draw a point from $\mathcal{S}$ belonging to it. We call it p_a^n. We define the partition function

$$\Gamma^n(q,\tau) = \sum_a \frac{(p_a^n)^q}{(\Delta_a^n)^\tau} \tag{A.1}$$

Then, one can show [HJK86] that the fractal dimensions are given by $\tau(q) = (q-1)D_q$ with $\tau(q)$ defined by

$$\Gamma^n(q,\tau > \tau(q)) \to +\infty \tag{A.2}$$

$$\Gamma^n(a,\tau < \tau(q)) \to 0 \tag{A.3}$$

A.2 Application to the spectrum and to the wavefunctions

We consider the nth approximant of the infinite chain. We will say that is has L_n sites ($L_n = F_n$ in the case of the Fibonacci chain).

In the case of the spectrum, we take Δ_a^n to be the width of the ath energy band. If each energy band has the same degeneracy, we can take $p_a^n = 1/L_n$.

In the case of the wavefunctions, we let $p_i^n = |\psi_i^n|^2$.

B Fractal dimensions in the periodic limit.

The periodic case is interesting, because the partition function (cf appendix A) can be computed exactly. We have

$$\Gamma^n = \left(\frac{1}{L_n}\right)^q \sum_{a=0}^{L_n-1} \frac{1}{(\Delta_a^n)^\tau} \tag{B.1}$$

$$= 2\left(\frac{1}{L_n}\right)^q \sum_{a=0}^{L_n/2-1} \frac{1}{(\Delta_a^n)^\tau} \tag{B.2}$$

because of the symmetry of the band structure. Also,

$$\Delta_a^n \underset{n\to\infty}{\sim} \frac{\pi}{L_n}\left|\sin\left(\frac{2a\pi}{L_n}+\frac{\pi}{2L_n}\right)\right| \tag{B.3}$$

We see that in the large n limit, the bandwidths tend to be continuous functions of the band index. We will exploit this fact to transform the sum appearing in the partition function in an integral. To this end we define $u = 2(a+1/4)/L_n$. Then,

$$\Gamma^n \underset{n\to\infty}{\sim} \frac{(L_n)^{\tau+1}}{(L_n)^q}\frac{1}{\pi^\tau}\underbrace{\int_{1/(2L_n)}^{1-3/(2L_n)} \frac{\mathrm{d}u}{|\sin(\pi u)|^\tau}}_{=I_n(\tau)} \tag{B.4}$$

At the edges, the integrand behaves as $1/u^\tau$. Thus if $\tau < 1$, $I_n(\tau)$ converges. We call $I_\infty(\tau)$ its limit. Thus,

$$\Gamma^n(\tau<1) \underset{n\to\infty}{\sim} \frac{(L_n)^{\tau+1}}{(L_n)^q}\frac{I_\infty(\tau)}{\pi^\tau} \tag{B.5}$$

We deduce that

$$\boxed{q(\tau<1) = 1+\tau} \tag{B.6}$$

This is the "trivial" case, where all the fractal dimensions are equal to 1.

On the other hand, if $\tau > 1$, the integral diverges. We have to evaluate how fast $I_n(\tau)$ diverges. The divergencies come from the 2 egdes. At these points, the integrand behaves as $1/u^\tau$, and thus

$$I_n(\tau>1) \underset{n\to\infty}{\sim} \mathrm{cst}(\tau)\times(L_n)^{\tau-1} \tag{B.7}$$

We conclude that

$$\boxed{q(\tau>1) = 2\tau} \tag{B.8}$$

C Fractal dimensions in the strong quasiperiodicity limit.

We use again the thermodynamic formalism to compute the fractal dimensions. We introduce the thermodynamic function on the nth approximant:

$$\Gamma_n(q,\tau;\rho) = \sum_{a=0}^{F_n-1} \frac{(1/F_n)^q}{(\Delta_a^n(\rho))^\tau} \tag{C.1}$$

At first order in ρ, atomic and molecular chains are decoupled. Each of the 2 molecular chains involves a fraction F_{n-2}/F_n of the sites, while the atomic chain involves the remaining F_{n-3}/F_n fraction of the sites. So,

$$\Gamma_n(q,\tau;\rho) = 2\left(\frac{F_{n-2}}{F_n}\right)^q \Gamma_{n-2}(q,\tau;d_m(\rho)) + \left(\frac{F_{n-3}}{F_n}\right)^q \Gamma_{n-3}(q,\tau;d_a(\rho)) \tag{C.2}$$

After a molecular deflation, the coupling ρ is renormalized: $d_m(\rho) = z\rho$ with $z = \rho/2$. Similarly, $d_a(\rho) = \bar{z}\rho$ with $\bar{z} = \rho^2$. See [NN90], [PBJ95]. Because the bandwidths are proportional to the coupling, we obtain,

$$\Gamma_n(q,\tau;\rho) = 2\left(\frac{F_{n-2}}{F_n}\right)^q z^{-\tau}\Gamma_{n-2}(q,\tau;\rho) + \left(\frac{F_{n-3}}{F_n}\right)^q \bar{z}^{-\tau}\Gamma_{n-3}(q,\tau;\rho) \tag{C.3}$$

Thus, $\tau(q) = (q-1)D(q)$ is given by

$$\boxed{1 = 2\omega^{2q} z^{-(q-1)D(q)} + \omega^{3q}\bar{z}^{-(q-1)D(q)}} \tag{C.4}$$

Now, we look for the Hausdorff dimension, so we take $q = 0$. We search a $D(0)$ of the form

$$D(0) = \frac{\log x}{\log \rho} \tag{C.5}$$

then we have an almost-second order equation for x:

$$x^2 = 1 + 2x2^{\frac{\log x}{\log \rho}} \tag{C.6}$$

Assuming that x oblidgingly converges to a non-zero constant as $\rho \to 0$, we have in this limit

$$x^2 = 1 + 2x \tag{C.7}$$

hence the result (2.13).

References

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