Fractal dimensions of the Fibonacci chain *via* a perturbative renormalization group.

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1 Constructing the Fibonacci chain: the alphabet of couplings.

1.1 The Fibonacci sequence and its statistical properties

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

$$r \stackrel{\text{def}}{=} \begin{cases} t_w & \to t_w t_s \\ t_s & \to t_w \end{cases} \tag{1}$$

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

$$S_n \stackrel{\text{def}}{=} r^n(t_s) \tag{2}$$

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

$$\text{Sub}(r) = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \tag{3}$$

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. There are thus τ times more t_w than t_s in S_∞. More precisely, we have

$$\text{Sub}(r) = \mathcal{R}(\theta) \begin{bmatrix} \tau & 0 \\ 0 & \omega \end{bmatrix} \mathcal{R}(\theta)^{-1} \tag{4}$$

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

$$\begin{cases} \cos\theta = 1/\sqrt{2+\tau} \\ \sin\theta = 1/\sqrt{2+\omega} \end{cases} \tag{5}$$

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

$$\begin{cases} \#\{t_s \in S_n\} & = F_{n-2} \\ \#\{t_w \in S_n\} & = F_{n-1} \end{cases} \tag{6}$$

where F_n is the nth *Fibonacci number* ($F_0 = 1$, $F_1 = 1$, $F_2 = 2$, ...).

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

1.2 Deflation rules; atoms and molecules.

Consider the slightly different inflation rule

$$\tilde{r} = \begin{cases} t_w & \to t_s t_w \\ t_s & \to t_w \end{cases} \tag{7}$$

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.
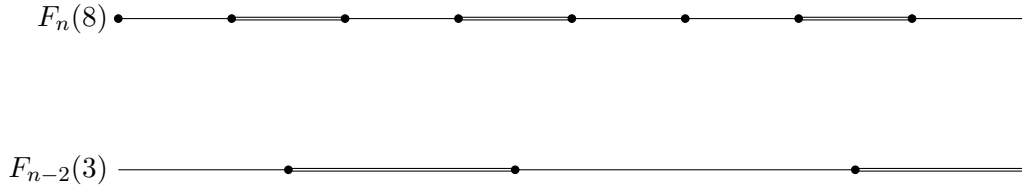
Molecules

Figure 1 – The molecular deflation rule d_m illustrated on a length 8 Fibonacci word.

We have

$$\tilde{r}r = \begin{cases} t_w & \to t_s t_w t_w \\ t_s & \to t_s t_w \end{cases} \tag{8}$$

Which admits as an inverse the *deflation rule*

$$d_m = \begin{cases} t_w & \leftarrow t_s t_w t_w \\ t_s & \leftarrow t_s t_w \end{cases} \tag{9}$$

This deflation rule reduces a word of length F_n to word of length F_{n-2} (fig. (1)).
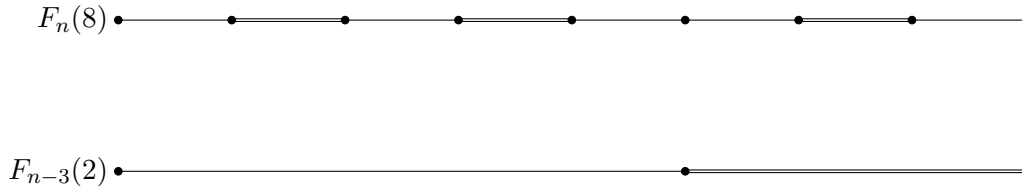
Atoms

Figure 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 contiditons: 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

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

we are going identify the first and the last atomic sites, ie use *periodic boundary conditions*. See eq. (10) for the example of the sixth Hamiltonian, with $F_6 = 8$ atomis sites.

$$H_6 = \begin{bmatrix} 0 & t_w & & & & & & t_w \\ t_w & 0 & t_s & & & & & \\ & t_s & 0 & t_w & & & & \\ & & t_w & 0 & t_s & & & \\ & & & t_s & 0 & t_w & & \\ & & & & t_w & 0 & t_w & \\ & & & & & t_w & 0 & t_s \\ t_w & & & & & & t_s & 0 \end{bmatrix} \tag{10}$$

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

2 The renormalization equations

2.1 Threefold decimation

We wish to consider the sequence of approximants in the *strong quasiperiodicity limit*: $t_s/t_w \ll 1$. In view of passing to this perturbative framework, we define the small parameter

$$\rho \stackrel{\text{def}}{=} \frac{t_w}{t_s} \tag{11}$$

At leading order in ρ weak bonds disappear: $t_w = 0$. Therefore we can diagonalize separately *molecules*, ie atomic sites linked by a strong coupling, and *atoms*, ie atomic sites surrounded by two weak couplings.

At next-to-leading order, two neighbouring molecules/atoms can interact, and the study of the chain S_n is naturally equivalent to the study of an atomic chain $d_a(S_n) = S_{n-3}$ and two molecular chains $d_m(S_n) = S_{n-2}$.

The *deflation* of the chain S_n translates into a *renormalization* of the Hamiltonian H_n: H_n is related to H_{n-2} by the decimation of atomic sites, and to H_{n-3} by the decimation of molecular sites. Though the action of the deflation rules d_a and d_m on S_n is simple, the action of the decimation rules on H_n is far from trivial. In particular, after a decimation, couplings and wavefunctions are renormalized. We are now interested in characterizing this renormalization.

2.2 Renormalization of the couplings

2.2.1 Atomic chain

In [?] one can find an exact renormalization group transformation linking a large chain (density of sites 1), to three smaller chains:
— a chain of atomic sites (density of sites $1/\tau^3$)
— two chains of molecular sites (density of sites $1/\tau^2$).
In view of passing to a perturbative framework, we define

$$\rho \stackrel{\text{def}}{=} \frac{t_w}{t_s} \tag{12}$$

A renormalization group operation generically translates the spectrum (because the one-sites energy are all renormalized by the same amount), and rescales it (because the hopping energies are all renormalized

by the samed amount). To take into account these effects, it is a good idea to look at the spectrum in the "co-moving frame":

$$x_\alpha(E) \overset{\text{def}}{=} \frac{E - V_\alpha}{t_\alpha} \tag{13}$$
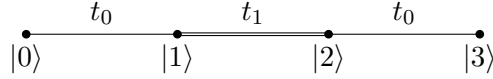
where $\alpha \in \{s, w\}$.

The renormalization equations given in [?] rewrite

$$\bar{x}_w = x_w + 2\rho^2 \frac{1}{x_s(1 - x_s^2)} \tag{14}$$

2.2.2 Molecular chains

2.3 Renormalization of the wavefunctions

2.3.1 Atomic chain

At leading order in ρ, an atomic wavefunction of energy E is sent by d_a to a *not necesarily atomic* wavefunction of energy $E/\bar{z}$. If i is the label of an atomic site of the chain S_n, we have

$$\psi_i(E) = \beta_i \left(\{ \psi_{i'}(E/\bar{z}) \}_{i'} \right) \tag{15}$$

We assume that the transformation β is linear:

$$\psi_i(E) = \beta_{ii'} \psi_{i'}(E/\bar{z}) \tag{16}$$

and even more than that, that it is a simple homothety: $\beta_{ii'} = \sqrt{\lambda} \delta_{d_a(i)i'}$. We therefore have

$$\psi_i(E) = \sqrt{\lambda} \psi_{d_a(i)}(E/\bar{z}) \tag{17}$$

λ is constrained by the unitarity of the wavefunction:

$$\Sigma^n \overset{\text{def}}{=} \sum_{i=1}^{F_n} |\psi_i|^2 = 1 \tag{18}$$

Let us note that we can partition the set of atomic sites of S_n into the set of atomic sites that remain atomic sites after deflation $S_{a'}$ and the set atomic sites that become molecular sites after deflation $S_{m'}$. Using this partition to transform the sum on all sites, we get

$$\sum_{i=1}^{F_n} |\psi_i|^2 = \sum_{i \in S_{a'}} \left(|\psi_i|^2 + |\psi_{i+2}|^2 + |\psi_{i-2}|^2 + |\psi_{i+4}|^2 + |\psi_{i-4}|^2 \right) + \sum_{i \in S_{m'}} \left(|\psi_i|^2 + |\psi_{i+2}|^2 + |\psi_{i-2}|^2 + |\psi_{i\pm4}|^2 \right) \tag{19}$$

We can also partition this sum into a sum over atomic sites Σ_a^n and over molecular sites Σ_m^n. We have

$$\begin{cases} \Sigma_a^n &= \sum_{i \in S_{a'}} |\psi_i|^2 + \sum_{i \in S_{m'}} |\psi_i|^2 \\ \Sigma_m^n &= \sum_{i \in S_{a'}} \left(|\psi_{i+2}|^2 + |\psi_{i-2}|^2 + |\psi_{i+4}|^2 + |\psi_{i-4}|^2 \right) + \sum_{i \in S_{m'}} \left(|\psi_{i+2}|^2 + |\psi_{i-2}|^2 + |\psi_{i\pm4}|^2 \right) \end{cases} \tag{20}$$

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Now, beacause of the way we assumed the wavefunction on atomic sites is renormalized (eq. (17)), we have

$$\Sigma_a^n = \bar{\lambda} \left(\sum_{i \in S_{a'}} |\psi_{d_a(i)}|^2 + \sum_{i \in S_{m'}} |\psi_{d_a(i)}|^2 \right) \tag{21}$$

$$= \bar{\lambda} \sum_{i=1}^{F_{n-3}} |\psi_i|^2 \tag{22}$$

$$= \bar{\lambda} \Sigma^{n-3} \tag{23}$$

and thus

$$\boxed{\Sigma_a^n = \bar{\lambda}} \tag{24}$$

Now, in the perturbative limit, the great thing is that the wafunction at molecular sites can be expressed in terms of the wavefunction at atomic sites [3]!

$$\begin{cases} \psi_{i \pm 2} & = -\rho \psi_i + \mathcal{O}(\rho E \psi_i) \\ \psi_{i \pm 4} & = \rho^2 \psi_i + \mathcal{O}(\rho^4 \psi_i) \end{cases} \tag{25}$$

Using this together with (17) we get [4],

$$\Sigma_m^n = \bar{\lambda} \left(2(\rho^2 + \rho^4)\Sigma_a^{n-3} + (2\rho^2 + \rho^4)\Sigma_m^{n-3} \right) \tag{26}$$

Since $\Sigma_m^{n-3} + \Sigma_a^{n-3} = 1$, and knowing that $\Sigma_a^{n-3} = \bar{\lambda}$, we have finally

$$\boxed{\Sigma_m^n = \bar{\lambda} \left(2\rho^2 + \rho^4 + \bar{\lambda}\rho^4 \right)} \tag{27}$$

Finally,

$$\boxed{\bar{\lambda}(\rho) = \frac{1}{1 + 2\rho^2} + \mathcal{O}(\rho^2)} \tag{28}$$

2.3.2 Molecular chains

3 The fractal dimensions

Conventions:
— Indices $a, b, c...$ will be used to label energy bands, while indices $i, j, k...$ will label sites.
— The superscript n is used to denote the nth approximant of the Fibonacci chain. This approximant is constituted of F_n sites, with periodic boundary conditions.
— $\alpha(x)$ is the pointwise Hölder exponent at point x, of some fractal set X that could be the spectrum, or the set of components of a wavefunction, etc. α is also the conjugate variable (by a Legendre transform) of q.
— $f(\alpha)$ is the Hausdorff dimension of the set $H_\alpha = \{x \in X | \alpha(x) = \alpha\}$. It is also the Legendre transform of τ.

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3. To derive these relations, we use the fact that E being an atomic energy, it is at most of order ρ. We also use the fact that at leading order the wavefunction is of the same order on all atomic sites.

4. If energy really is at most of order ρ, the formula below is correct only up to order ρ^2, and the terms of order ρ^4 should be dropped!!

3.1   Definitions

Spectral dimension $\boxed{D_q}$, is given by the partition function

$$\Gamma(\tau) = \lim_{n\to\infty} \sum_{a=1}^{F_n} \frac{(\mu^n(I_a))^q}{(\Delta_a^n)^\tau} \tag{29}$$

where

$$d\mu^n(E) = \frac{1}{F_n} \sum_a \delta(E - E_a)dE \tag{30}$$

or rather

$$d\mu^n(E) = \frac{1}{F_n} \sum_a dm_a^n(E) \tag{31}$$

where m_a^n is the spectral (Lebesgue) measure on the interval $I_a^n = [E_a, E_a + \Delta_a^n[$. Here, since the bands are non-degenerate, m_a^n is normalized to unity: $m_a^n(I_b^n) = \delta_{a,b}$.

$\Gamma(\tau)$ is finite and nonzero for a single value of τ,

$$\tau(q) = (q-1)D_q \tag{32}$$

Local wavefunction dimension $\boxed{D_q^x(a)}$ is given by

$$D_q^x(a) = \lim_{n\to\infty} \frac{1}{q-1} \frac{\log \chi_q^n(a)}{\log F_n} \tag{33}$$

where $\chi_q^n(a)$ is the weighted probability sum

$$\chi_q^n(a) = \sum_{i=1}^{F_n} |\psi^n(i,a)|^{2q} \tag{34}$$

Averaged wavefunction dimension $\boxed{\overline{D_q^x}}$:

$$\overline{\chi_q^n} = \frac{1}{F_n} \sum_a \sum_i |\psi^n(i,a)|^{2q} \tag{35}$$

Local spectral dimension $\boxed{D_q^\mu(i)}$

$$\Gamma^\mu(\tau(i)) = \lim_n \sum_a \frac{(\mu^n(i,\Delta_a^n))^q}{(\Delta_a^n)^\tau} \tag{36}$$

where

$$d\mu^n(i,E) = \sum_a |\psi^n(i,a)|^2 \delta(E - E_a)dE \tag{37}$$

or rather

$$d\mu^n(i,E) = \sum_a |\psi^n(i,a)|^2 dm_a(E) \tag{38}$$

Note that $d\mu^n(i,E) = d\mu^n(E)$ for plane waves.

Local spectral wavefunction dimension $\boxed{\tilde{D}_q(i)}$

$$\tilde{\chi}_q^n(i) = \sum_a |\psi^n(i,a)|^{2q} \tag{39}$$

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3.2 Conjectures

$$\tilde{D}_q(i) \underset{\rho \to 0}{\sim} D_q^x(a) \tag{40}$$

if $a = i$ (assuming we label energy bands by increasing energy, and that we label sites in the co-numerotation). Clearly this does no longer hold when ρ is finite. However there may exist a value of q for which the equality holds nonperturbatively.

$$\tilde{D}_q(i) = \alpha(i) D_q^\mu(i) \tag{41}$$

Actually, at least in the perturbative limit we find that *spatial* fractal dimensions only depend on the fraction of (renormalization group) time spent in molecular/atomic clusters, and on the fraction of time we switch from molecular to atomic clusters, and not on the order in which we visit atomic/molecular clusters.

Similarly, *spectral* fractal dimensions only depends on the fraction of time spent in lateral/central energy clusters, and on the fraction of time we switch from lateral to central clusters.

So, *a priori* the spatial fractal dimensions depend on n_m, time spent on molecular clusters, n_a, time spent on atomic clusters and on n_{ma}, time spent switching from molecular to atomic clusters. This makes 3 variables, but they are not independant! Because when we renormalize to an atomic cluster the number of sites is reduced by a factor F_{n-3}/F_n, while when we renormalize to a molecular cluster the reduction factor is F_{n-2}/F_n, we have

$$3n_a + 2n_m = n \tag{42}$$

where n is the total number of renormalization steps [5]. So, in practice we only have to independant variables.

To encode these informations, for *spatial* dimensions we let

$$\begin{cases} x = n_m/n \\ y = n_{ma}/n \end{cases} \tag{43}$$

while for *spectral* dimensions we let

$$\begin{cases} x = n_l/n \\ y = n_{lc}/n \end{cases} \tag{44}$$

In the perturbative limit, we thus have the slightly more general relation

$$\tilde{D}_q(x,y) = \alpha(x) D_q^\mu(x,y) \tag{45}$$

where x is a spatial label for spatial dimensions, and a spectral label for α.

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5. This is only valid in the limit $n \to \infty$. For n finite we actually have $3n_a + 2n_m = n \pm 1$.