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

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1 Notations

1.1 General

- 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.

1.2 Multifractal analysis

- $\alpha(x)$ 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 .

1.3 Renormalization parameters

$$z = \rho/2 \tag{1}$$

$$\overline{z} = \rho^2 \tag{2}$$

$$\lambda = 1/(2 + \rho^2) \tag{3}$$

$$\overline{\lambda} = 1/(1+2\rho^2) \tag{4}$$

$$c = 1 + \rho^2 \tag{5}$$

$$s = 1 - \rho^2 \tag{6}$$

We also introduce the notation $f_q(\rho) = f(\rho^q)$, where f can be any of the above renormalization parameters.

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

$$\rho \stackrel{\text{def}}{=} \frac{t_w}{t_s} \tag{7}$$

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

2.2.2 Molecular chains

2.3 Renormalization of the wavefunctions

2.3.1 Atomic chain

$$\begin{array}{c|cccc} & t_0 & t_1 & t_0 \\ \hline |0\rangle & |1\rangle & |2\rangle & |3\rangle \end{array}$$

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

$$\psi_i(E) = \beta_i \left(\{ \psi_{i'}(E/\bar{z}) \}_{i'} \right) \tag{8}$$

We assume that the transformation β is linear:

$$\psi_i(E) = \beta_{ii'}\psi_{i'}(E/\bar{z}) \tag{9}$$

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

$$\psi_i(E) = \sqrt{\lambda} \psi_{d_a(i)}(E/\bar{z}) \tag{10}$$

 λ is constrained by the unitarity of the wavefunction:

$$\Sigma^n \stackrel{\text{def}}{=} \sum_{i=1}^{F_n} |\psi_i|^2 = 1 \tag{11}$$

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

$$\sum_{i=1}^{F_n} |\psi_i|^2 = \sum_{i \in S_{a'}} \left(|\psi_i|^2 + |\psi_{i+2}|^2 + |\psi_{i-2}|^2 + |\psi_{i+4}|^2 + |\psi_{i-4}|^2 \right) + \sum_{i \in S_{m'}} \left(|\psi_i|^2 + |\psi_{i+2}|^2 + |\psi_{i+2}|^2 + |\psi_{i+4}|^2 \right)$$
(12)

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

$$\begin{cases} \Sigma_{a}^{n} &= \sum_{i \in S_{a'}} |\psi_{i}|^{2} + \sum_{i \in S_{m'}} |\psi_{i}|^{2} \\ \Sigma_{m}^{n} &= \sum_{i \in S_{a'}} \left(|\psi_{i+2}|^{2} + |\psi_{i-2}|^{2} + |\psi_{i+4}|^{2} + |\psi_{i-4}|^{2} \right) + \sum_{i \in S_{m'}} \left(|\psi_{i+2}|^{2} + |\psi_{i-2}|^{2} + |\psi_{i\pm 4}|^{2} \right) \end{cases}$$
(13)

Now, because of the way we assumed the wavefunction on atomic sites is renormalized (eq. (10)), we have

$$\Sigma_a^n = \bar{\lambda} \left(\sum_{i \in S_{a'}} |\psi_{d_a(i)}|^2 + \sum_{i \in S_{m'}} |\psi_{d_a(i)}|^2 \right)$$
(14)

$$= \bar{\lambda} \sum_{i=1}^{F_{n-3}} |\psi_i|^2 \tag{15}$$

$$=\bar{\lambda}\Sigma^{n-3} \tag{16}$$

and thus

$$\boxed{\Sigma_a^n = \bar{\lambda}} \tag{17}$$

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 ¹!

$$\begin{cases} \psi_{i\pm 2} &= -\rho\psi_i + \mathcal{O}(\rho E\psi_i) \\ \psi_{i\pm 4} &= \rho^2\psi_i + \mathcal{O}(\rho^4\psi_i) \end{cases}$$
(18)

Using this together with (10) we get 2 ,

$$\Sigma_m^n = \bar{\lambda} \left(2(\rho^2 + \rho^4) \Sigma_a^{n-3} + (2\rho^2 + \rho^4) \Sigma_m^{n-3} \right)$$
 (19)

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

$$\Sigma_m^n = \bar{\lambda} \left(2\rho^2 + \rho^4 + \bar{\lambda}\rho^4 \right)$$
 (20)

Finally,

$$\bar{\lambda}(\rho) = \frac{1}{1 + 2\rho^2} + \mathcal{O}(\rho^2)$$
(21)

2.3.2 Molecular chains

3 The fractal dimensions

3.1 Definitions

We distinguish between *spectral dimensions* depending on the spectral index a, and *local dimensions* depending on the spatial index i.

Dimension of the spectrum D_q , is given by the partition function

$$\Gamma(\tau) = \lim_{n \to \infty} \sum_{a=1}^{F_n} \frac{(\mu^n(I_a))^q}{(\Delta_a^n)^{\tau}}$$
(22)

where

$$d\mu^{n}(E) = \frac{1}{F_{n}} \sum_{a} \delta(E - E_{a}) dE$$
(23)

^{1.} 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.

^{2.} 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!!

or rather

$$\mathrm{d}\mu^n(E) = \frac{1}{F_n} \sum_a \mathrm{d}m_a^n(E) \tag{24}$$

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 ,

$$\tau(q) = (q-1)D_q \tag{25}$$

Spectral dimension of the wavefunctions $D_q^x(a)$ is given by

$$D_q^x(a) = \lim_{n \to \infty} \frac{1}{q-1} \frac{\log \chi_q^n(a)}{\log F_n}$$
 (26)

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

$$\chi_q^n(a) = \sum_{i=1}^{F_n} |\psi^n(i, a)|^{2q}$$
(27)

Averaged dimension of the wavefunctions $\overline{\overline{D_q^x}}$:

$$\overline{\chi_q^n} = \frac{1}{F_n} \sum_{a} \sum_{i} |\psi^n(i, a)|^{2q} \tag{28}$$

Local dimension of the local spectral measure $D_q^{\mu}(i)$

$$\Gamma^{\mu}(\tau(i)) = \lim_{n} \sum_{q} \frac{(\mu^{n}(i, \Delta_{a}^{n}))^{q}}{(\Delta_{a}^{n})^{\tau}}$$
(29)

where

$$d\mu^{n}(i,E) = \sum_{a} |\psi^{n}(i,a)|^{2} \delta(E - E_{a}) dE$$
(30)

or rather

$$d\mu^n(i,E) = \sum_a |\psi^n(i,a)|^2 dm_a(E)$$
(31)

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

Local dimension of the wavefunctions $\left| ilde{D}_q(i) \right|$

$$\tilde{\chi}_q^n(i) = \sum_a |\psi^n(i,a)|^{2q} \tag{32}$$

3.2 Conjectures

$$\tilde{D}_q(i) \underset{q \to 0}{\sim} D_q^x(a) \tag{33}$$

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

$$D_q^{\mu}(i) = \alpha(i)\tilde{D}_q(i) \tag{34}$$

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 independent! 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

$$3n_a + 2n_m = n \tag{35}$$

where n is the total number of renormalization steps³. So, in practice we only have to independent variables.

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

$$\begin{cases}
 x = n_m/n \\
 y = n_{ma}/n
\end{cases}$$
(36)

while for *spectral* dimensions we let

$$\begin{cases}
 x = n_l/n \\
 y = n_{lc}/n
\end{cases}$$
(37)

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

$$D_q^{\mu}(x,y) = \alpha(x)\tilde{D}_q(x,y)$$
(38)

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

This result can be understood qualitatively. Starting from

$$\Gamma^{\mu}(\tau, q; i) = \sum_{\alpha} \frac{|\psi_{i, \alpha}|^{2q}}{(\Delta_{\alpha})^{\tau}}$$
(39)

We use the local Hölder exponent of the spectrum to relate the bandwidth to the system size: $(\Delta_a)^{\alpha_a} \sim 1/F_n$. Thus,

$$\Gamma^{\mu}(\tau, q; i) = \sum_{a} |\psi_{i,a}|^{2q} (F_n)^{\tau/\alpha_a}$$
 (40)

But now, for q > 0 and in the strong quasiperioidicity limit, $|\psi_{i,a}|^{2q}$ is large only if the energy label, a, and the site label, i, have similar renormalization paths, in the sense that $x_a = x_i \stackrel{\text{def}}{=} x$. For these energy labels, $\alpha_a = \alpha(x)$. Thus,

$$\Gamma^{\mu}(\tau, q > 0; i) \underset{\rho \to 0}{\sim} (F_n)^{\tau/\alpha(x)} \tilde{\chi}(q; i) \tag{41}$$

We conclude that indeed,

$$\tau_q^{\mu,x} = \alpha(x)\tilde{\tau}_q^x \tag{42}$$

We also have that

$$\boxed{\overline{\tau_q^{\mu}} = D_{1 + \overline{\tilde{\tau}_q}} \times \overline{\tilde{\tau}_q}} \tag{43}$$

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

To test this relation, let us derive some inequalities:

$$\overline{\Gamma^{\mu}} \le \frac{1}{(\Delta_{\min})^{\tau}} \overline{\tilde{\chi}} \tag{44}$$

$$\geq \frac{1}{(\Delta_{\text{max}})^{\tau}} \overline{\tilde{\chi}} \tag{45}$$

and thus,

$$\overline{\tau^{\mu}} \ge \alpha_{\min} \overline{\tilde{\tau}} \tag{46}$$

$$\overline{\tau^{\mu}} \le \alpha_{\max} \overline{\tilde{\tau}} \tag{47}$$

Since $q \to D_q$ is non-increasing,

$$D_{+\infty} = \alpha_{\min} \le D_q \le D_{-\infty} = \alpha_{\max} \tag{48}$$

So, our relation seems plausible!

4 Asymptotic results

Averaged dimension of the wavefunctions $\overline{\overline{D_q^x}}$:

$$\tilde{D}_q(x,y)\log\omega = \frac{q}{q-1}\left(x\log\lambda + \frac{1-2x}{3}\log\overline{\lambda}\right) - \frac{1}{q-1}\left((x-y)\log\left(\frac{1}{2c_q}\right) + y\log\left(\frac{1}{2s_q}\right)\right) \tag{49}$$

since $\lambda, \overline{\lambda}, c_q, s_q$ are only known up to second order in ρ , we also have

$$\tilde{D}_q(x,y)\log\omega = x\log\left(\frac{1}{2}\right) - \frac{q}{q-1}\frac{4-5x}{6}\rho^2 - \frac{1}{q-1}(-x+2y)\rho^{2q}$$
(50)

4

References

^{4.} In particular, we have $\tilde{D}_q(x,y) \underset{\rho \to 0}{\sim} x \frac{\log 2}{\log \tau}$. This makes perfect sense: in that limit only isolated molecules remain, and on each molecular site we have presence probability $1/(2F_n)$.