

Notes du 1 juin 2015 - quantum dynamics for a Cantor spectrum, tight-binding model

Introduction

This is a summary of the discussion of June 1, on quantum dynamics for the tight-binding model, with some complementary results obtained since. After the discussion, we decided that the following questions should be examined :

- the dynamics of the wave packet depends on the functions : $h_k(t) = \int_K e^{-i\epsilon t} \epsilon^k d\mu(\epsilon)$, which are not scaling functions, but do have a certain structure ; can we approximate the $h_k(t)$ by scaling functions, thus implying that the RMS is, in first approximation, a scaling function ?
- if not, how does the characteristics of the $h_k(t)$ affect the dynamics ?

After further numerical study, I found that the $h_k(t)$ can not easily be approximated by scaling functions. However, a numerical study shows that there is clearly an almost-proportional relation between $h_k(t)$ and $h_{k-1}(t/3)$, which can be justified theoretically by the relations between the zeroes and maxima of the $h_k(t)$; I have no better theoretical explanation so far.

If the $h_k(t)$ were scaling functions, so would be the RMS. That is, if we assume that : $h_k(t) \propto h_{k-1}(t/3)$, we deduce that the RMS is of the form : $\Delta x(t) = t^{-\ln 2 / \ln 3} G(\frac{\ln t}{\ln 3})$. However, since the $h_k(t)$ are not scaling functions, we do not expect $\Delta x(t)$ to have this exact behaviour, and in fact a numerical study of $\Delta x(t)$ shows that this quantity is not of that form. Nevertheless, the structure of the $h_k(t)$ (scaling relations between zeroes and maxima) does translate to the RMS. In fact, I found numerically that the RMS is a power-law modulated by oscillations, which appear to have a log-periodic envelope.

I give first a reminder of the framework and of previous results, then I discuss and give a partial answer to the questions above. I also did a complementary study of the Fibonacci potential, to compare the behaviour of the $h_k(t)$ in the case of a triadic Cantor spectrum and in the case of a Fibonacci potential.

Reminder of previous results

We consider an infinite 1D lattice, with sites k labelled from 0 to ∞ . We define a potential V on this system such that the discrete Schrodinger operator : $H = -\Delta + V$, which acts on $l_2(\mathbb{Z})$, has a triadic Cantor set spectrum. The eigenfunctions of H verify :

$$H\phi_\epsilon = \epsilon\phi_\epsilon$$

Using transfer matrices, the above equation becomes :

$$\begin{pmatrix} \phi_\epsilon(k) \\ \phi_\epsilon(k-1) \end{pmatrix} = \begin{pmatrix} 2 + V_k - \epsilon & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \phi_\epsilon(k) \\ \phi_\epsilon(k-1) \end{pmatrix}$$

Imposing $\phi_\epsilon(0) = 0$, we find that the eigenfunctions $\{\phi_\epsilon\}_{\epsilon \in K}$, evaluated on the sites k , can be seen as polynomials in ϵ :

$$\phi_\epsilon(k) = \phi_\epsilon(1)p_k(\epsilon) \tag{1}$$

with

$$\begin{pmatrix} p_k(E) & q_k(E) \\ p_{k-1}(E) & q_{k-1}(E) \end{pmatrix} = \prod_{j=k}^1 \begin{pmatrix} 2 + V_j - E & -1 \\ 1 & 0 \end{pmatrix}$$

We are interested of the evolution of a wave packet, described by the normalized wave function $\psi(t)$, evolving according to Schrodinger's equation :

$$i \frac{d\psi(t)}{dt} = H\psi(t)$$

The wave function is initially localized at the site 1 : $\langle k|\psi(t=0)\rangle = \delta(k-1)$. At time t , the system is in the state : $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$, and the value of the wave function at site k is given by :

$$|\psi(k, t)| = \int_K \phi_\epsilon(1)^* \phi_\epsilon(k) e^{-i\epsilon t} d\mu$$

Using (1), we obtain :

$$\begin{aligned} \psi(k, t) &= \int_K \phi_\epsilon(1)^* \phi_\epsilon(k) e^{-i\epsilon t} d\mu \\ &= \int_K p_1(\epsilon) p_k(\epsilon) e^{-i\epsilon t} d\mu \\ &= \sum_{j_k \leq k} c_{j_k} \int_K \epsilon^{j_k} e^{-i\epsilon t} d\mu \end{aligned}$$

with $p_k(x) = \sum_{0 \leq j_k \leq k} c_{j_k} x^{j_k}$. Thus, the dynamical behaviour of the system depends essentially on the functions :

$$h_k(t) = \int_K e^{-i\epsilon t} \epsilon^k d\mu(\epsilon)$$

aka the Fourier transforms on K of the moments x^k .

Expanding the exponential in $h_k(t)$, we obtain :

$$h_k(t) = \sum_{n \leq 0} \frac{(-it)^n}{n!} \mu_{n+k}$$

with $\mu_n = \int_K x^n d\mu$.

The fingerprint of the scaling symmetry of the spectrum is carried by the $\mu_n = \int_K x^n d\mu$. It can be shown that, for $n \rightarrow \infty$ (see [1])

$$\mu_n = n^{-\ln 2 / \ln 3} F(\ln n / \ln 3) (1 + O(\frac{1}{n}))$$

where F is a log-periodic function of period 1.

The $h_k(t)$ do not verify a scaling property (of the form $f(x) = bf(ax)$); however, there is a structure and there are some scaling invariance.

First, there is a recurrence relation verified by the $h_k(t)$:

$$\begin{aligned} h_k(t) &= \int_K e^{-i\epsilon t} \epsilon^k d\mu \\ &= \frac{3^{-k}}{2} \int_K e^{-i\epsilon t/3} \epsilon^k d\mu + \frac{3^{-k} e^{-i2t/3}}{2} \int_K e^{-i\epsilon t/3} (\epsilon + 2)^k d\mu \\ &= \frac{3^{-k}}{2} h_k(t/3) + \frac{3^{-k}}{2} e^{-i2t/3} \sum_{j=0}^k \binom{k}{j} h_j(t/3) 2^{k-j} \end{aligned}$$

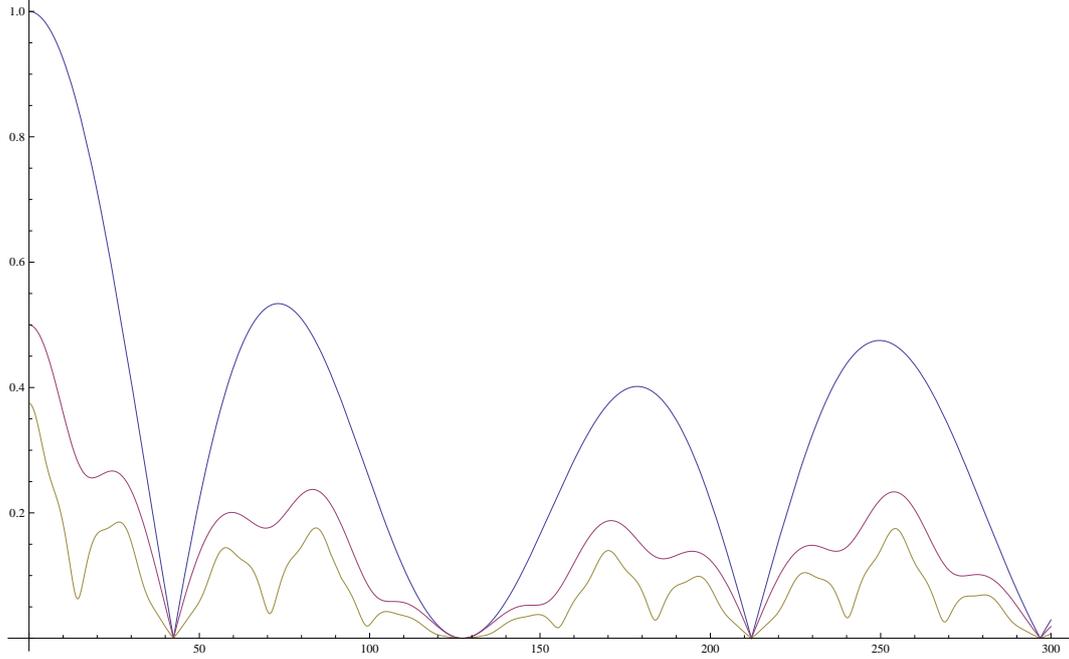


FIGURE 1 – Numerical curves of $|h_0(t/9)|$ (blue), $|h_1(t/3)|$ (red) and $|h_2(t)|$ (yellow).

From this relation, we can show by recurrence that the zeroes of $h_k(t)$ is the set :

$$Z_k = \{t_{m,k} = \frac{\pi}{2}(2m + 1)3^{k+1}, m \in \mathbb{Z}\}$$

Thus, the zeroes of $h_k(t)$ are those of $h_{k-1}(t/3)$, as illustrated in fig. 1.

Moreover, the $h_k(t)$ all have local maxima at points of the form $m_{n,l} = n\pi 3^l$. I did not manage to prove this rigorously for $k > 0$ (the case $k = 0$ is straightforward, the detail is given in annexe), but the numerics support this assumption and one can intuitively understand why it is so from the definition of $h_k(t)$:

$$h_k(t) = \int_K x^k e^{-ixt} d\mu = \lim_{n \rightarrow \infty} \frac{3^n}{2^n} \sum_{a_{jn} \in K_n} \int_{a_{jn}}^{a_{jn} + 3^{-n}} x^k e^{-ixt} dx$$

$|h_k(t)|$ is maximal at points t such that the phase e^{-ixt} varies as little as possible as x goes through K . K is composed of real numbers which have only 0 and 2 in their decomposition in base 3, e.g. $x = \sum_{k \leq 1} \frac{\beta_k}{3^k}$ with $\beta_k \in \{0, 2\}$. Now, for $t = n\pi 3^l$, we see that for any $x \in K$ whose decomposition in base 3 has only 0 after the l first terms, we have $e^{-ixt} = 1$: the phase does not change.

At these local maxima, the amplitude of the functions $h_k(t)$ decreases with k (as a consequence of Riemann-Lebesgue theorem).

We wish now to examine how this structure translates in terms of physical dynamical quantities.

Numerical study

The relation between the zeroes of the $h_k(t)$ is very well verified numerically (fig. 1).

We observe that the amplitude of h_k decreases with k (see fig. 2), thus we wish to make the assumption : $h_k(t) \propto h_{k-1}(t/3)$.

Approximation of $h_k(t)$ by a scaling function

Using

$$\begin{aligned} h_k(t) &= \int_K e^{-i\epsilon t} \epsilon^k d\mu \\ &= \frac{3^{-k}}{2} \int_K e^{-i\epsilon t/3} \epsilon^k d\mu + \frac{3^{-k} e^{-i2t/3}}{2} \int_K e^{-i\epsilon t/3} (\epsilon + 2)^k d\mu \\ &= \frac{3^{-k}}{2} h_k(t/3) + \frac{3^{-k}}{2} e^{-i2t/3} \sum_{j=0}^k \binom{k}{j} h_j(t/3) 2^{k-j} \end{aligned}$$

we wish to keep only the dominant terms of the sum on the right side to approximate $h_k(t)$.

Let us test the validity of the approximation : $h_k(t) = \frac{3^{-k} e^{-2it/3}}{2} 2^k h_0(t/3)$. We find (see fig. 3) that this is quite accurate for small k , but falls for $k \leq 4$.

I have tried a few other approximation by scaling functions, which did not work well. So far, it seems that the relations between the zeroes of h_k and the behaviour at the local maxima alone can justify the numerical observation that "from afar" $h_k(t) \propto h_{k-1}(t/3)$.

This almost re-scaling relation translates to the RMS. The details of how the wave packet is constructed is given in the annexe. The wave packet is initially localized on the first site $k = 1$. Figure 4 shows the graphs of $\Delta x(t)$ and $\Delta x(t/3)$. We find that $\Delta x(t)$ displays a log-periodic structure. $\Delta x(t)$ is a power-law modulated by oscillations, which have a log-periodic envelope of period $\log 3$; inside the envelope, the period of the oscillations increases with time, which is consistent with the behaviour of $h_k(t)$ under the transformation $t \rightarrow t/3$. I also find that : $\Delta x(t) \approx \frac{3}{2} \Delta x(t/3)$ (see fig. 5), but I have no explanation for the value of this coefficient so far.

Application to the Fibonacci potential

We study numerically the case of a Fibonacci potential. The potential is defined with the Fibonacci algorithm. For the numerics we choose $V(k) = \pm 0.6$ (note : for $|V(k)| > 2$, the spectrum is continuous and not singular continuous). The fig. 6 is the spectrum associated to this potential.

The spectrum in this case is not a pure Cantor set, but a superposition of Cantor sets; however, we can use the following approximate scaling symmetry : $N(\epsilon) = 3N(\epsilon/5)$ where $N(\epsilon)$ is the IDOS (see fig. 7).

We find, in this case, that, as for the triadic Cantor set, the functions $h_k(t)$ seem almost proportional to one another for $k \geq 1$. The function $h_0(t)$ has a very different behaviour. We find that $h_1(t) \approx h_0(t/5)$ (see fig. 8).

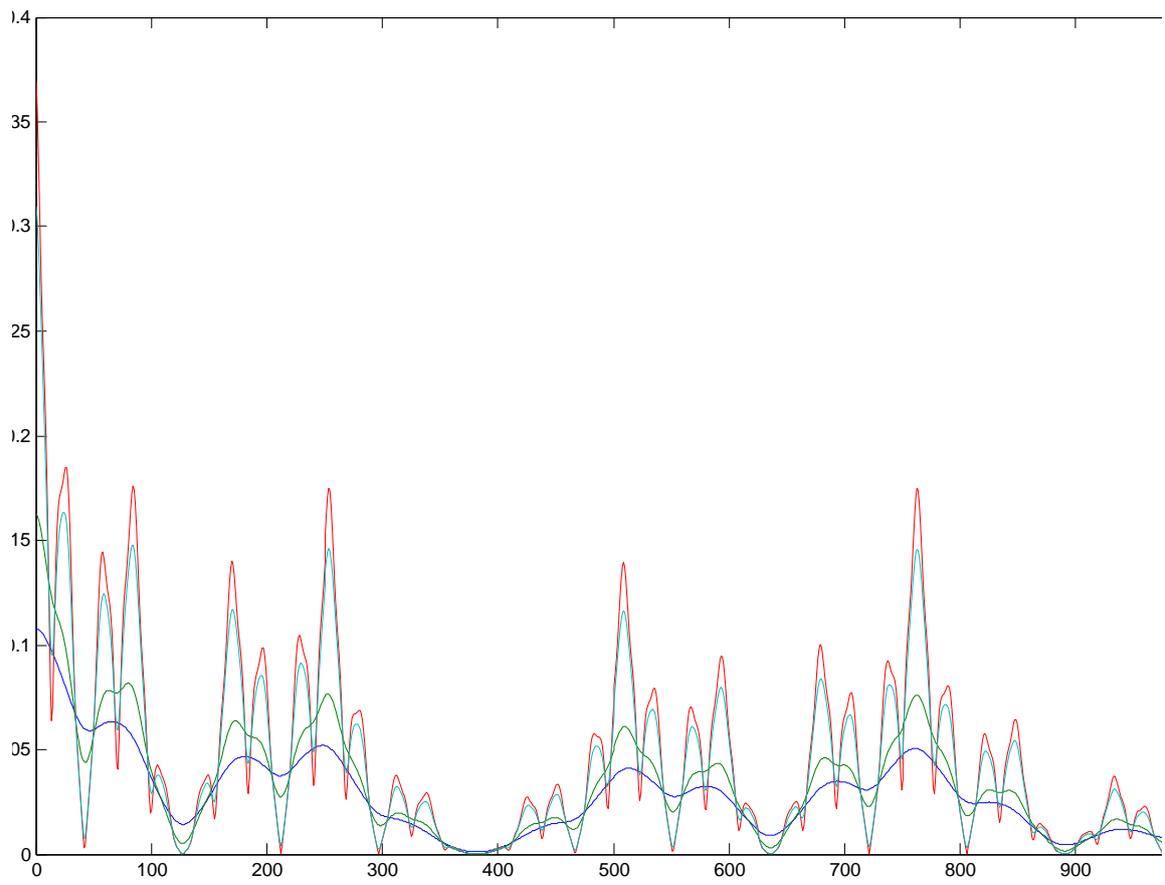


FIGURE 2 – $h_1(t), h_2(t), h_{10}(t), h_{20}(t)$ for a triadic Cantor set spectrum.

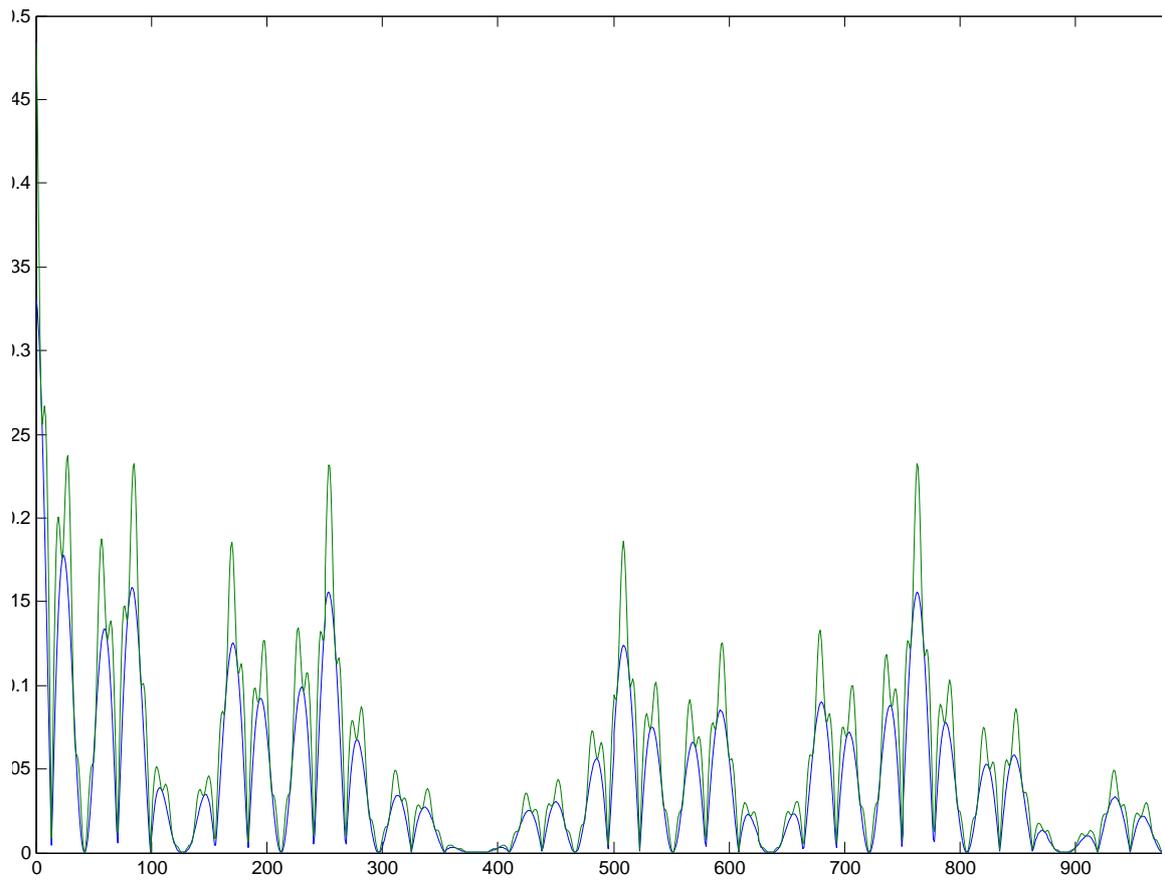


FIGURE 3 – $h_1(t)$ and $\frac{1}{3}h_0(t/3)$ for a Cantor spectrum.

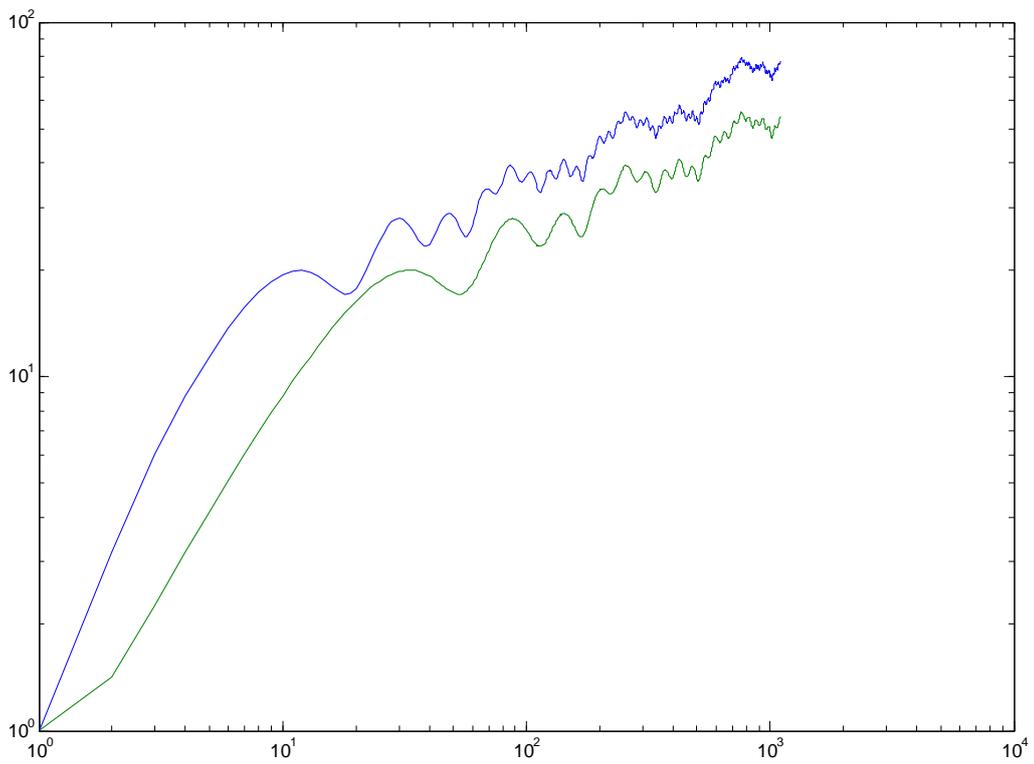


FIGURE 4 – RMS for a triadic Cantor spectrum ; blue : $\Delta x(t)$, green : $\Delta x(t/3)$.

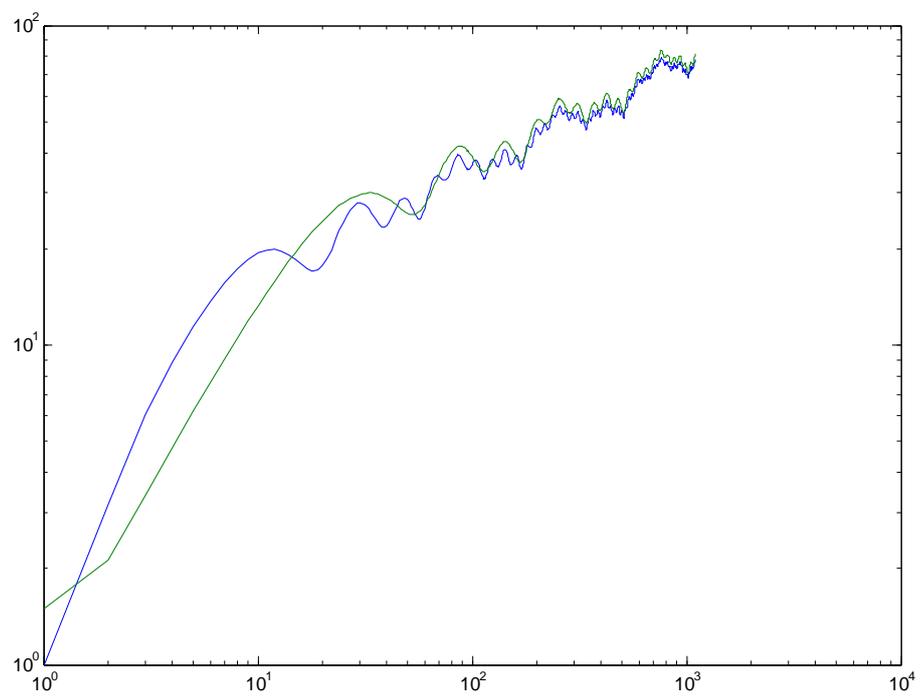


FIGURE 5 – RMS for a triadic Cantor spectrum as a function of time, in loglog scale; blue : $\Delta x(t)$, green : $\frac{3}{2}\Delta x(t/3)$.

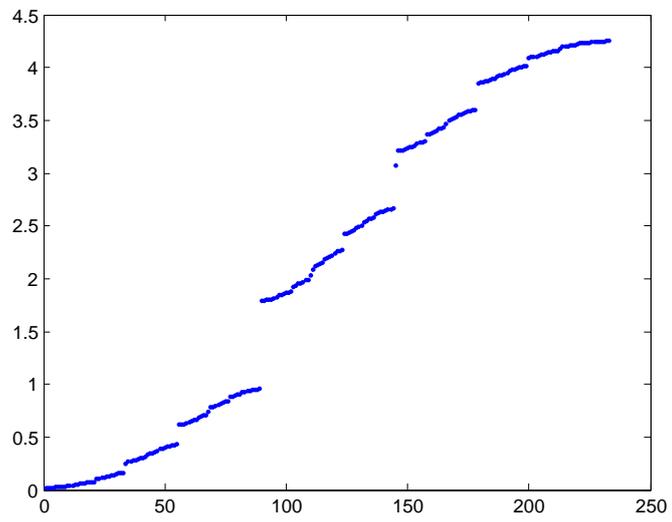


FIGURE 6 – Spectrum for a Fibonacci potential, $V(k) = \pm 0.6$.

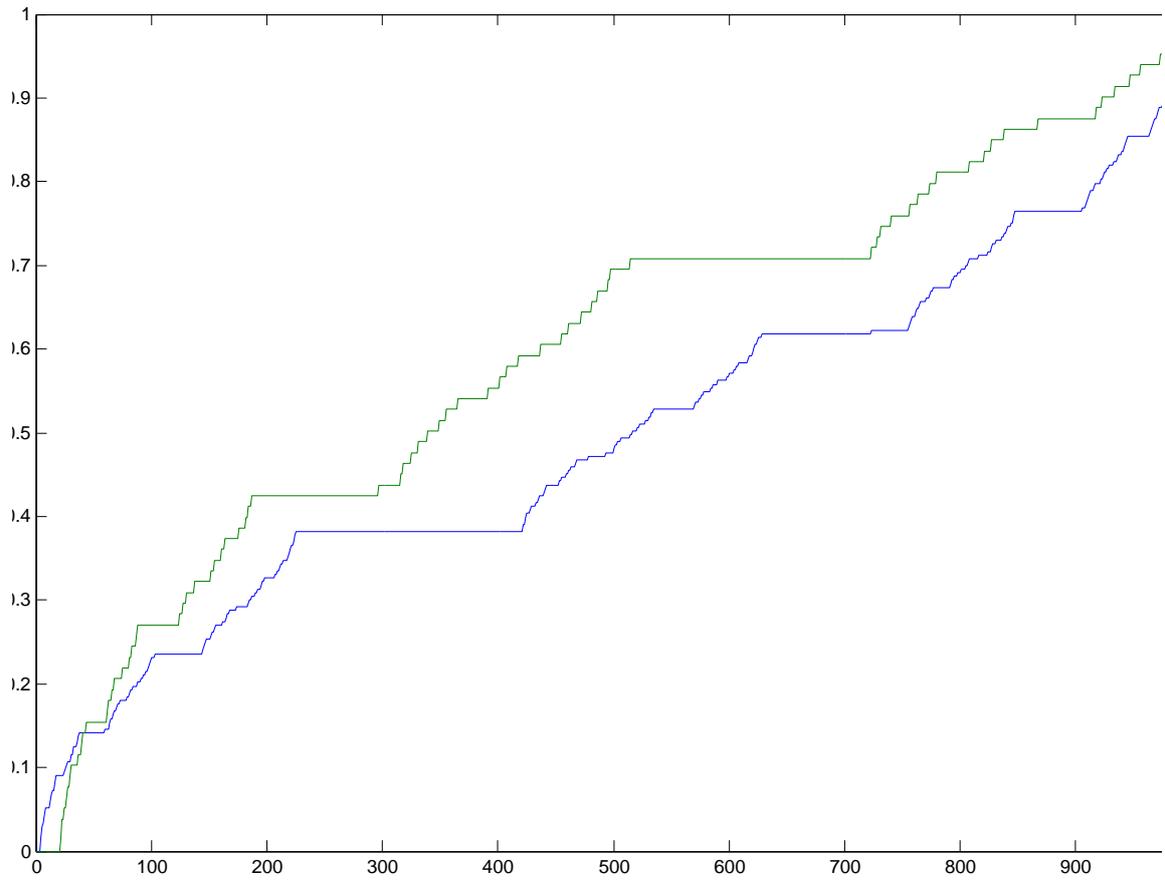


FIGURE 7 –

Assuming the pure scaling symmetry for this spectrum ($N(\epsilon) = 3N(\epsilon/5)$), we find the following theoretical expression for $h_0(t)$:

$$h_0^{th}(t) = \prod_{k=1}^{\infty} \frac{1 + e^{-2it/5^k} + e^{-4it/5^k}}{3}$$

However, this expression does not fit well with the numerical graph; this is due to the fact that the spectrum does not have such a simple scaling relation (see fig. 7). Nevertheless, we observe, as for the Cantor set case, that for $t < 100$, the zeroes of h_0 do seem to be stable under the transform $t \rightarrow t/5$ (see fig. 9). We thus expect the RMS to be stable under the transform $t \rightarrow t/5$. We find numerically that $\Delta x(t)$ is a power-law modulated by log-periodic oscillations of very small amplitude for $0 < t < 300$. For larger t , the function starts to decay and has a very wild behaviour, probably due to numerical approximations.

Annexe

Maxima of $h_0(t)$ for the triadic Cantor set

Using the scaling symmetry of the spectrum :

$$\int_K f(x) d\mu(x) = \frac{1}{2} \int_K f\left(\frac{x}{3}\right) d\mu(x) + \frac{1}{2} \int_K f\left(\frac{x+2}{3}\right) d\mu(x) \quad (2)$$

we find that :

$$\begin{aligned} h_0(t) &= \int_K e^{-iet} d\mu \\ &= \frac{1}{2} \int_K e^{-iet/3} d\mu + \frac{e^{-i2t/3}}{2} \int_K e^{-iet/3} d\mu \\ &= \frac{1 + e^{-i2t/3}}{2} h_0(t/3) \end{aligned}$$

By repeating this process, and using $h_0(0) = \int_K 1 d\mu = 1$, we find the exact expression of $h_0(t)$:

$$h_0(t) = \prod_{k \geq 1} \frac{1 + e^{-i2t/3^k}}{2} \quad (3)$$

thus :

$$|h_0(t)| = \prod_{k \geq 1} \cos t/3^k \quad (4)$$

The derivative :

$$|h_0(t)|' = - \sum_{k \geq 1} 3^{-k} \sin t/3^k \prod_{j \neq k} \cos t/3^j \quad (5)$$

is null for t of the form : $t = m_{n,l} = \pi n 3^l$, with $n \in \mathbb{Z}$ and $l \in \mathbb{N}^*$.

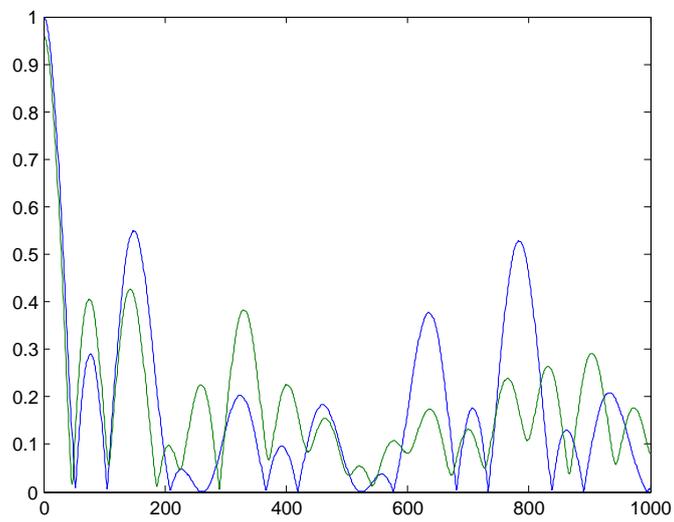


FIGURE 8 –

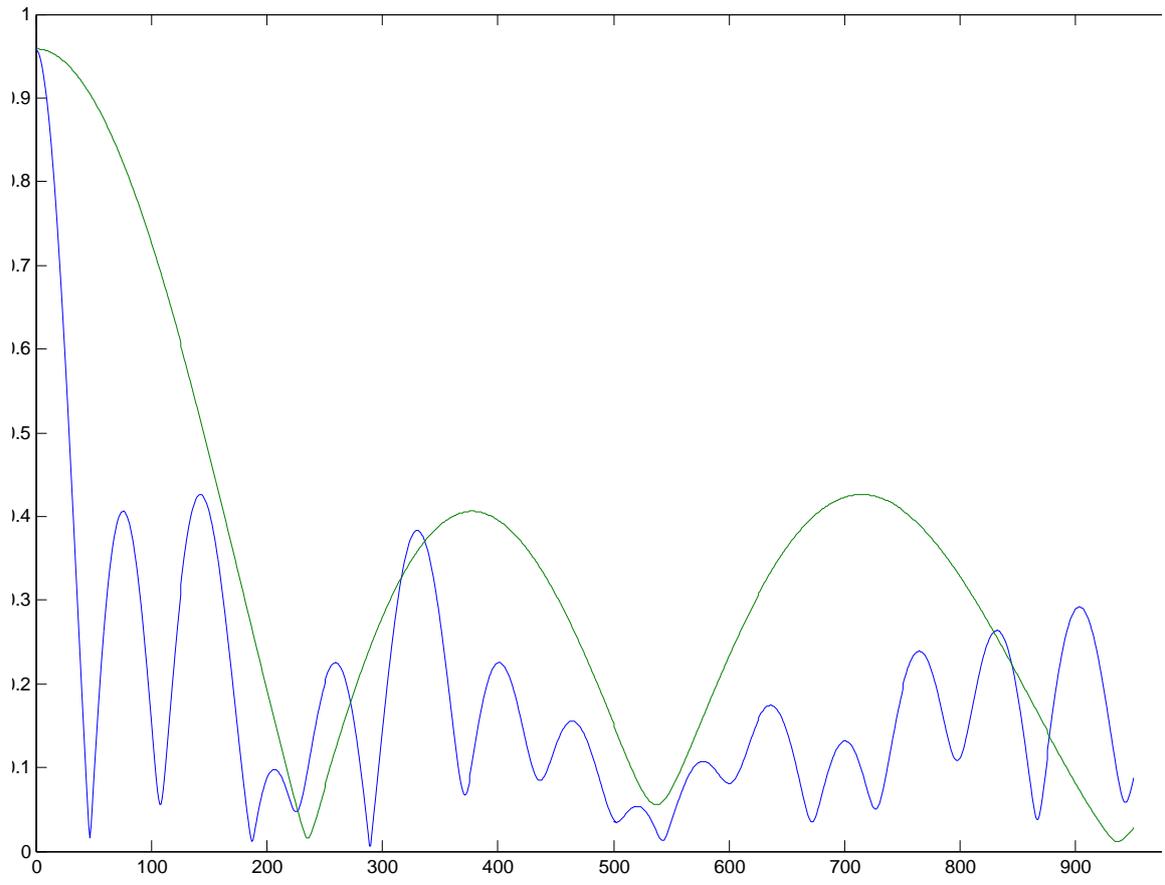


FIGURE 9 –

Construction of the wave packet for the triadic Cantor set spectrum

I first tried to build a potential V whose associated spectrum would be a triadic Cantor set, but it was difficult to obtain something close enough so that the properties of the $h_k(t)$ would still be verified. Therefore, I considered the case of $V = 0$, with an associated continuous spectrum, and I built a wave packet using only eigenfunctions associated to energies belonging to the triadic Cantor set embedded in the spectrum.

I used a finite lattice of size $2^8 = 256$, and an associated finite Cantor set of size 256. The Hamiltonian is a 256×256 matrix H of diagonal elements equal to 2, off-diagonal elements $H_{i,i+1} = H_{i+1,i} = -1$ and the other elements equal to zero. The theoretical eigenfunctions are constructed using :

$$\phi_\epsilon(k) = \phi_\epsilon(1)p_k(\epsilon)$$

with $p_k(x)$ constructed as explained earlier. The boundary values $\phi_\epsilon(1)$ are obtained numerically from the eigenvectors of the matrix H .

The wave packet is constructed so as to be initially located on the site $k = 1$ (see fig. 10 for the evolution in time).

References

- [1] P.J. Grabner , H. Prodinger, Statistics & Probability Letters 26 (1996) 243-248

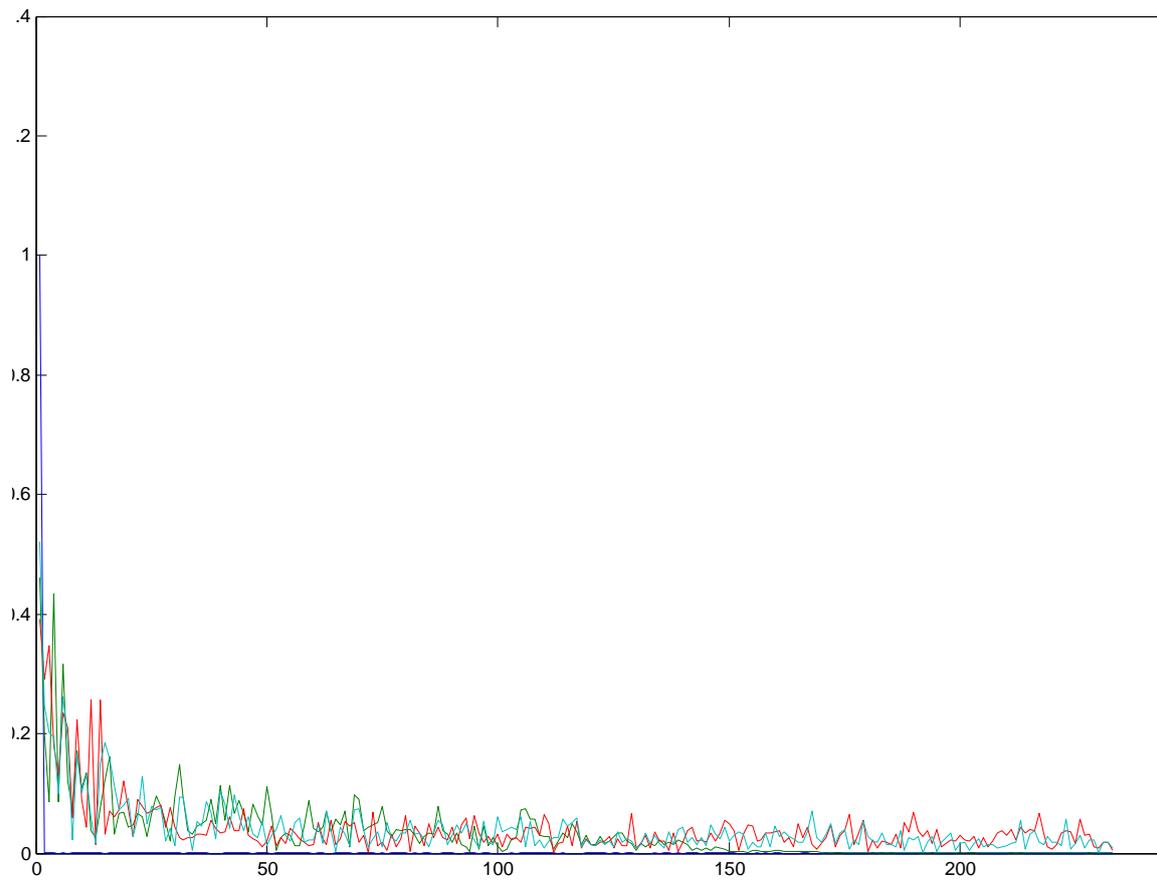


FIGURE 10 –