

Notes - RMS asymptotic behavior; Summary of the paper by Mosseri

Our numerical results for the triadic Cantor set spectrum in the tight-binding model indicate that $\langle \Delta x^2(t) \rangle \sim_{t \rightarrow \infty} t^\alpha$, with

$$\langle \Delta x^2(t) \rangle = \frac{1}{t} \int_0^t \sum_{k \geq 0} k^2 |\psi(k, t')|^2 dt'$$

and $\alpha = \frac{\ln 2}{\ln 3}$ the fractal dimension of the triadic Cantor set. Numerical results seem to indicate that the time-averaged RMS is, asymptotically, a scaling function. The value we found for the characteristic exponent α is not confirmed by the literature, and seems in contradiction with predictions from Mantica [1], namely : $\langle \Delta x^2(t) \rangle \sim_{t \rightarrow \infty} t^{2\alpha}$.

However, the quantum system described by Mantica is different from ours; we shall give some details later. Other papers deal with the question of the characteristic exponent : Piéchon [2], Mosseri [3] and Dunne, Teplyaev, Akkerman [4]; but the spectral measure and the definition of de spectral dimension varies from a paper to another, which makes the comparasion difficult.

This note is organized as follows :

- 1) Summary and comment of the paper by Mosseri
- 2) Comparison with papers by Piéchon and Akkerman
- 3) Comparison with the paper by Mantica
- 4) Conclusion and some ideas

The goal is to answer (or at least give ideas) to answer the questions :

- Are our results in contradiction with the literature ?
- Is the asymptotic exponent of $\langle \Delta x^2(t) \rangle$ the spectral dimension ?

Summary and comment of Mosseri's paper

In [3], Mosseri studies theoretically and numerically the Harper model and the Fibonacci model, in the tight-binding model, for dimensions 1D, 2D and 3D.

Consider an electron placed on a lattice of finite size (N sites). The system is described by the Hamiltonian $H = \sum_i u_i |i\rangle \langle i| + \sum_{i,j} v_{i,j} |i\rangle \langle j|$, and the wavefunction of the electron evolves according to : $i \frac{d}{dt} \Psi(t) = H \Psi(t)$. The wavepacket is initially localized at site $n = 0$. Thus, the amplitude of the wavefunction at time t , on the site n , is given by :

$$\psi_n(t) = \sum_j \phi_0(\epsilon_j)^* \phi_n(\epsilon_j) e^{-i\epsilon_j t}$$

with $\phi(\epsilon_j)$ the eigenfunction of H corresponding to the eigenvalue ϵ_j .

The spectral dimension D_2 is defined as follows : consider

$$R(l) = \iint_{|\epsilon - \epsilon'| < \frac{l}{2}} d\mu(\epsilon) d\mu(\epsilon')$$

where $\mu(\epsilon)$ is the spectral measure (not explicetly given here). If, for $l \rightarrow 0$, $R(l) \sim_{l \rightarrow 0} l^\delta$, then set $D_2 = \delta$.

Mosseri focuses on the time-averaged return probability :

$$C(t) = \frac{1}{t} \int_0^t P(t') dt'$$

with

$$P(t) = |\psi_0(t)|^2 = \left| \sum_j |\phi_0(\epsilon_j)|^2 e^{-i\epsilon_j t} \right|^2$$

Using standard calculation, the following equivalence is proven :

$$R(l) \sim_{l \rightarrow 0} l^\delta \Leftrightarrow C(t) \sim_{t \rightarrow \infty} t^{-\delta} \quad (1)$$

Note : This confirms our analytical results for the triadic Cantor set, with the uniform measure we defined : in this case, $\delta = \frac{\ln 2}{\ln 3}$. Furthermore, we showed that, for any measure with a scaling symmetry, $C(t)$ is asymptotically a scaling function (e.g. $C(t) \sim_{t \rightarrow \infty} t^{-\delta}$), and that δ is the spectral measure in the sense of Mosseri.

The Fibonacci and Harper model are then studied numerically in 1D, 2D and 3D. It is demonstrated that the (numerical) spectral dimension for the Fibonacci model depends on the choice of the model (diagonal or off-diagonal) and on the amplitude of the potential. It is therefore difficult to compare the numerical results with the other results in the literature.

However, it is worth noticing that Mosseri uses a local spectral measure : $\mu(\epsilon)$ is the measure at the site where the wavepacket is initially localized, e.g. $\mu(\epsilon) = |\phi_0(\epsilon)|^2 d\epsilon$.

The RMS $d(t) = \sqrt{\sum_n n^2 |\psi_n(t)|^2}$ is only briefly mentioned : Mosseri reminds that, according to the literature, $d(t) \sim_{t \rightarrow \infty} t^\beta$. However, the question of whether or not the exponent β is related to the spectral dimension of the measure is not discussed.

Conclusion and comments

To conclude on this paper, it confirms what we derived for the time-averaged return probability and its connection to the spectral measure, but does not give us many information about the exponent of the RMS.

However, one could use the duality (1), which gives the relation between the spectral dimension associated to the measure μ and the decay of the time-averaged probability, for the study of the RMS (further details are given in the last paragraph).

Comparison with papers [2], [4]

In [2], Piéchon studies the dynamics of a wave packet evolving in a Fibonacci potential in the tight-binding model. The time and space averaged RMS, is studied numerically and theoretically ; however, the spectral dimension is different from the one defined by Mosseri (which is the definition we also used). The approach here is to consider a space averaged measure, e.g. the average of all the local measures at sites n . Assuming that the time-averaged probability of having the wave packet at site k after a time t is a scaling function of both space and time :

$$\langle |\psi(k, t)|^2 \rangle = t^{-\sigma} f(kt - \sigma)$$

leads to the following asymptotic expression of the time-averaged RMS : $\langle d(t) \rangle \sim_{t \rightarrow \infty} t^{d_s}$, with d_s the spectral dimension associated to the measure.

However, it is not clear that such a scaling relation exists. In fact, our study of the tight-binding model showed that the eigenfunctions can be written as polynomials in the energy ; the detail of the calculation is not give here but it seems that the return probability, even after a space average, does not have a simple scaling symmetry in space.

The paper [4] is about diffusion on a fractal ; the problem is thus not exactly the same, but very similar. The time-averaged probability to diffuse over a distance n at time t , $P(r, t) = \sum_k \phi_k(\epsilon)^* \phi_{k+n}(\epsilon) e^{-i\epsilon t}$ (for Piéchon, the corresponding probability is the square module of this probability amplitude). It is of the form :

$$P(r, t) = t^{-d_s/2} f(kt^{-d_s/2})$$

d_s being the spectral dimension. The RMS is then defined as $\langle d^2(t) \rangle = \sum_n n^2 P(n, t)$, and has the asymptotic behavior : $\langle d^2(t) \rangle \sim_{t \rightarrow \infty} t^{d_s}$, which is consistent with the results by Piéchon.

Comparison with papers by Mantica

In [1], Mantica develops a different approach : starting from a spectral measure μ , with associated spectral dimension d_s , he derives a set of orthonormal polynomials $q_k(x)$ (in the sense of μ) :

$$\int_{\text{spectrum}} q_k(x) q_l(x) d\mu(x) = \delta_{k,l} \quad (2)$$

and builds the "tight-binding Hamiltonian" (a tridiagonal matrix) having the polynomials as eigenfunctions. Then, a numerical study gives the typical exponent of the time-averaged RMS :

$$\langle d^2(t) \rangle \sim_{t \rightarrow \infty} t^{2d_s}$$

However, it is difficult to compare this result to our numerical results, since the Hamiltonian studied by Mantica does not rigourosly have the form of a tight-binding Hamiltonian. Furthermore, in our case (see reminder in the following paragraph), even if the eigenfunctions are also gien by some polynomials $p_k(\epsilon)$, the orthogonality relation (2) does not hold a priori.

Conclusion - Some ideas

This section summarizes some ideas to go further in the study of the exponent of the time-averaged RMS :

$$\langle d^2(t) \rangle = \sum_n (n - n_0)^2 \langle |\psi_n(t)|^2 \rangle$$

We focus on the tight-binding model in the case of a triadic Cantor spectrum K . We wish to use the duality (1) from Mosseri's paper, to study the time-averaged RMS.

In fact, the time-averaged RMS $\langle d^2(t) \rangle$ is given by :

$$\begin{aligned} \langle d^2(t) \rangle &= \sum_n n^2 \langle |\psi_n(t)|^2 \rangle \\ &= \sum_n n^2 \iint \phi_0(\epsilon)^* \phi_n(\epsilon) \phi_0(\epsilon') \phi_n(\epsilon')^* \text{sinc}((\epsilon - \epsilon')t) d\mu(\epsilon) d\mu(\epsilon') \\ &= \iint \left(\sum_n n^2 \iint \phi_0(\epsilon)^* \phi_n(\epsilon) \phi_0(\epsilon') \phi_n(\epsilon')^* \right) \text{sinc}((\epsilon - \epsilon')t) d\mu(\epsilon) d\mu(\epsilon') \end{aligned}$$

which is, formally, the wavelet transform associated to the "measure"

$$\left(\sum_n n^2 \iint \phi_0(\epsilon)^* \phi_n(\epsilon) \phi_0(\epsilon') \phi_n(\epsilon')^* \right)$$

The dimension δ associated to this measure is, a priori, different from the local spectral measure $\mu(\epsilon) = |\phi_0(\epsilon)|^2 d\epsilon$.

To calculate δ , we need to study the asymptotic behavior, for $l \rightarrow 0$, of :

$$R_K(l) = \iint_{|\epsilon - \epsilon'| < \frac{l}{2}} \left(\sum_n n^2 \iint \phi_0(\epsilon)^* \phi_n(\epsilon) \phi_0(\epsilon') \phi_n(\epsilon')^* \right) d\mu(\epsilon) d\mu(\epsilon')$$

If $R(l) \sim_{l \rightarrow 0} l^{-\delta}$, then $\langle d^2(t) \rangle \sim_{t \rightarrow \infty} t^\delta$.

Remind that, in the tight-binding model, the eigenfunctions $\phi(\epsilon)$ are given by :

$$\phi_n(\epsilon) = \phi_0(\epsilon) p_n(\epsilon)$$

were $p_n(x)$ is a polynomial of degree $n - 1$, defined recursively by :

$$p_{k+1}(\epsilon) = (2 + V(k) - \epsilon) p_k(\epsilon) - p_{k-1}(\epsilon)$$

$$\text{with initial conditions : } \begin{cases} p_1(\epsilon) = 1 \\ p_2(\epsilon) = 2 + V(1) - \epsilon \end{cases}$$

The wave packet is initially localized at site $n = 1$. At time t , the amplitude of the wave function at site k is given by :

$$\begin{aligned} \psi(k, t) &= \int_K \phi_\epsilon(1)^* \phi_\epsilon(k) e^{-i\epsilon t} d\mu(\epsilon) \\ &= \int_K |\phi_\epsilon(1)|^2 p_k(\epsilon) e^{-i\epsilon t} d\mu(\epsilon) \end{aligned}$$

Let us define the local spectral measure $d\mu(\epsilon) \equiv |\phi_\epsilon(1)|^2 d\mu(\epsilon)$. We assume that this measure verifies the scaling property characteristic of the triadic Cantor set :

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

Thus, the wave function is given by :

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

Due to the orthonormality of the eigenfunction, the polynomials p_k verify :

$$\sum_k p_k(\epsilon)p_k(\epsilon') = \delta_{\epsilon,\epsilon'} \quad (4)$$

Furthermore, the initial condition translates into :

$$\iint_{K \times K} p_k(\epsilon)p_k(\epsilon')d\mu(\epsilon)d\mu(\epsilon') = \delta_{k,1} \quad (5)$$

Thus :

$$R_K(l) = \iint_{|\epsilon-\epsilon'| < \frac{l}{2}} \left(\sum_n (n-1)^2 p_n(\epsilon)p_n(\epsilon') \right) d\mu(\epsilon)d\mu(\epsilon')$$

I did not manage to do this calculation ; however, one can notice that, from (5), we get : $R_K(2) = 0$, and since $\int_K |p_k(\epsilon)|^2 d\mu(\epsilon) > 0$, we deduce that $R_K(0) > 0$. Thus, R_K seems to be a decreasing function.

References

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