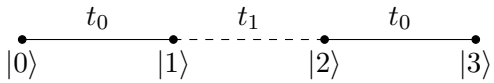
The hierarchical chain (tight binding model)

October 9, 2014

1 The model



We consider the tight-binding Hamiltonian:

$$H = \sum_i t(i) \left|i-1\right\rangle \left\langle i\right| + \text{h. c.} \tag{1}$$

where

$$t(i) \stackrel{\text{def}}{=} t_k, \text{ with } k \text{ the number of times 2 divides } i. \tag{2}$$

Such a Hamiltonian has a the structure of a binary tree. This binary hierarchy must somehow show up in its spectrum, at least given a reasonable set of t_ks.

2 Strong hierarchy: $t_0 \gg t_1 \gg ... \gg t_1^2 \gg t_2^2 \gg ... \gg t_1^3 \gg t_2^3 \gg ...$

In that case, we can treat the problem perturbatively ; first integrate out the diatomic molecules (two atoms liked by a t_0 bond), then the the diatomic molecules of diatomic molecules (two diatomic molecules linked by a t_1 bond), etc.

At the first order in perturbation theory the spectrum is

$$E_{\epsilon_1\epsilon_2...} = (-1)^{\epsilon_1} t_0 + (-1)^{\epsilon_2} \frac{t_1}{2} + (-1)^{\epsilon_3} \frac{t_2}{4} + ... \tag{3}$$

At zeroth order in perturbation theory, the eigenstate assiated to $E_{\epsilon_1\epsilon_2...}$ can be constructed using the following procedure:

— If $\epsilon_1 = 0/1$ construct the symmetric/antisymmetric linear combination of atomic states linked by a t_0 bond. That is to say, construct the vector

$$\left|\psi^0_{\epsilon_1}\right\rangle = \frac{1}{\sqrt{2}}(\left|0\right\rangle + (-1)^{\epsilon_1} \left|1\right\rangle) + \frac{1}{\sqrt{2}}(\left|2\right\rangle + (-1)^{\epsilon_1} \left|3\right\rangle) + ... \tag{4}$$

We shall define $\left|i, \epsilon_1\right\rangle \stackrel{\text{def}}{=} (\left|2i\right\rangle + (-1)^{\epsilon_1} \left|2i+1\right\rangle)/\sqrt{2}$. We shall call the $\left|i, \epsilon_1\right\rangle$ the *diatomic states*. If $\epsilon_1 = 0/1$ we say that the diatomic state i is *antibonding/bonding*.

— If $\epsilon_2 = 0/1$ construct the symmetric/antisymmetric linear combination of diatomic states linked by a t_1 bond. That is to say, construct the vector

$$\left|\psi^1_{\epsilon_1\epsilon_2}\right\rangle = \frac{1}{\sqrt{2}}(\left|0, \epsilon_1\right\rangle + (-1)^{\epsilon_2} \left|1, \epsilon_1\right\rangle) + \frac{1}{\sqrt{2}}(\left|2, \epsilon_1\right\rangle + (-1)^{\epsilon_2} \left|3, \epsilon_1\right\rangle) + ... \tag{5}$$

We shall define the *quadriatomic states* $\left|i, \epsilon_1\epsilon_2\right\rangle \stackrel{\text{def}}{=} (\left|2i, \epsilon_1\right\rangle + (-1)^{\epsilon_2} \left|2i+1, \epsilon_1\right\rangle)/\sqrt{2}$

— If $\epsilon_n = 0/1$ construct the symmetric/antisymmetric linear combination of 2^{n-1}-atomic states linked by a t_{n-1} bond.

At the n^{th} step of this procedure, we obtain $|\psi^{n-1}_{\epsilon_1 \dots \epsilon_n}\rangle$, the zeroth order eigenvector of a 2^n size hierarchical chain associated with the energy $E_{\epsilon_1 \dots \epsilon_n}$.

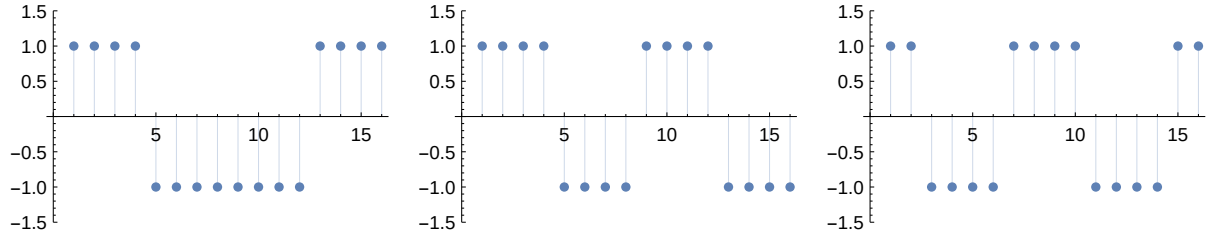


Figure 1 – From left to right: 2^4-atomic states associated with the energies $\epsilon_1\epsilon_2\epsilon_3\epsilon_4 = 0010, 0011, 0100$, in the atomic states basis.

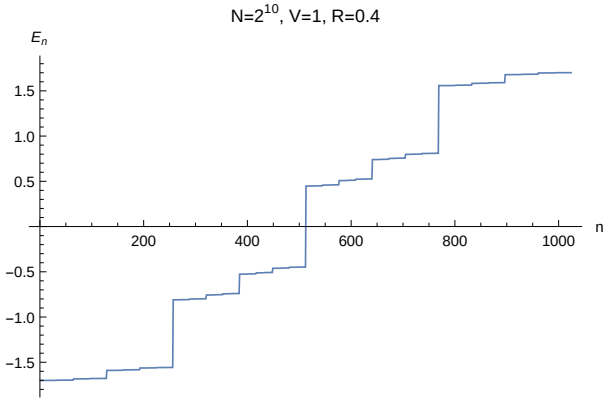
3 Geometric hierarchy: $t_{k\geq 2} = Rt_{k-1}$

In that case, we may no longer be able to organize the perturbation theory hierarchically (for example second order perturbation theory applied to the 2^2 chain will involve corrections of order $t_2^2 = R^2 t_1^2$, but since $t_3 = R^2 t_1 = t_2^2/t_1$, depending on the value of t_1, these second order corrections may be involved when dealing with the 2^3 chain at first order.).

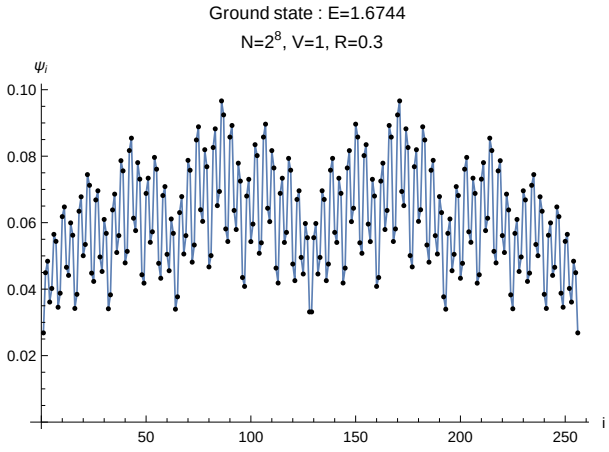
Following [1], we chose

$$t_k = \begin{cases} 1 & \text{if } k = 0 \\ V & \text{if } k = 1 \\ R^{k-2}V & \text{if } k > 1 \end{cases} \tag{6}$$

3.1 Spectrum and wavefunctions



(a) Spectrum of the isolated chain of N atomic sites.



(b) Ground state of the chain of N atomic sites.

Figure 2 – Numerical results for the isolated chain with geometric hierarchy.

As before, we consider an isolated chain of $N = 2^n$ atoms.

Numerically, we can easily compute its spectrum (fig. (2a)) and the corresponding wavefunctions (fig. (2b)). It looks like both spectrum and wavefunctions have a hierarchical structure.

To further analize the hierarchical character of the spectrum, we wish to compute its fractal dimensions (aka Rényi dimensions or Rényi entropy or generalized dimensions)

3.2 Fractal dimensions

We consider our spectrum as a subset of some set (say the unit interval $I = [0, 1]$), that we partition into boxes of length ϵ. Following [2] we then define p_i as the fraction of points of our spectrum lying inside the i^{th} box. The q^{th} generalized/fractal/Rényi dimension is then

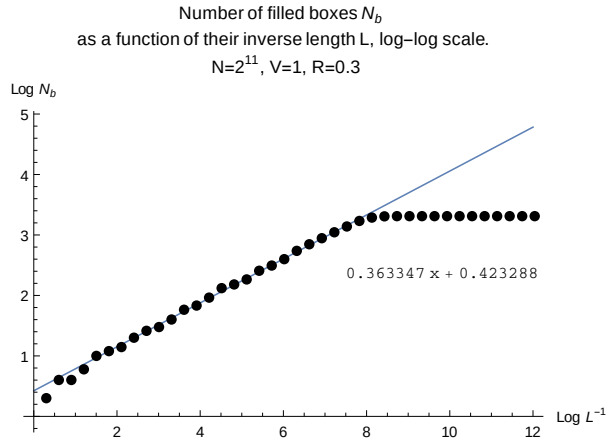
$$D_q = \frac{1}{q-1} \lim_{\epsilon \to 0} \frac{\log \sum_i p_i^q}{\log \epsilon^{-1}} \tag{7}$$

3.2.1 Box-counted Hausdorff dimension

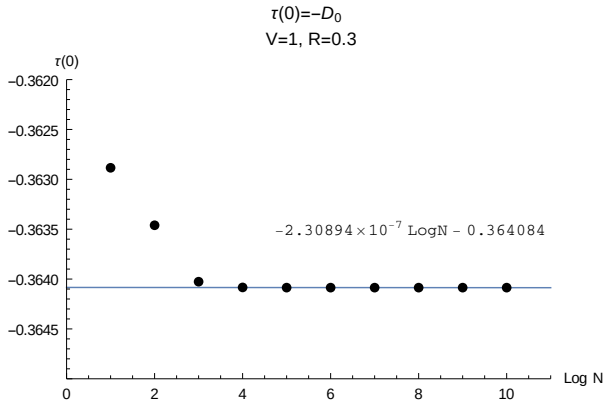
We have

$$D_0 = -\lim_{\epsilon \to 0} \frac{\log N_b}{\log \epsilon^{-1}} \tag{8}$$

where N_b is the number of boxes containing at least one point of the spectrum. This is the reason why D_0 is called the *box-counting* dimension. In most cases the Hausdorff dimension coincides with the box-counting dimension [1].



(a) D_0 obtained by direct box-counting.



(b) D_0 obtained with the partition function.

Figure 3 – Box-counting.

Figure (3a) shows how $\log N_b$ evolve as $\epsilon \to 0$, in $\log - \log$ scale. For an infinite size system (that is, for the spectrum of the infinite chain) we expect this function to have a linear asymptotic behaviour, the slope of the asymptote being $-D_0$. For our numerical, finite size spectrum however, we expect finite size effects to come into play when ϵ is too small. This is indeed what happens (fig. (3a)). For this computation we took a sequence of boxes of length $\epsilon_i = \delta^{-i}$. We noted that when δ is taken to be a power of 2, $\log N_b$ becomes constant when ϵ is sufficiently small (in fig. (3a) δ was set to 2). Whereas when δ is not a power of 2, $\log N_b$ seems to be taking random values when ϵ is sufficiently small. This probably means that the energy states are indexed by a binary integer, at least for finite size chains.

1. In fact D_0 is always greater or equal to the Hausdorff dimension. Indeed, countable sets increase the dimension D_0 – obtained by box-counting – when they have accumulation points, while they do not contribute to the Hausdorff dimension.

3.2.2 Partition function

The *partition function* Γ is another tool one can use to compute the fractal dimensions.

Let us consider a partition $\mathcal{P} = \{S_i\}_i$ of the set S whose fractal dimensions we are interested in. Each subset S_i is contained in a ball of radius l_i. This ball contains a fraction p_i of the points of S. We assume that the balls radii are smaller than a control radius ϵ. Then we define the *partition function*:

$$\Gamma(q, \tau; \mathcal{P}, \{l_i\}) \stackrel{\text{def}}{=} \sum_i \frac{p_i^q}{l_i^\tau} \tag{9}$$

Next, we chose the partition such as to minimize/maximize Γ depending on whether q is positive/negative:

$$\Gamma(q, \tau) \stackrel{\text{def}}{=} \begin{cases} \inf\limits_{\mathcal{P}} \Gamma(q, \tau; \mathcal{P}, \{l_i\}) & \text{if } q > 0 \\ \max\limits_{\mathcal{P}} \Gamma(q, \tau; \mathcal{P}, \{l_i\}) & \text{if } q < 0 \end{cases} \tag{10}$$

It is not clear for me at the moment how we chose the radii l_i. In the limit $\epsilon \to 0$, the above partition function is finite only when $\tau \stackrel{\text{def}}{=} \tau(q)$. We have the important property

$$\tau(q) = (q-1)D_q \tag{11}$$

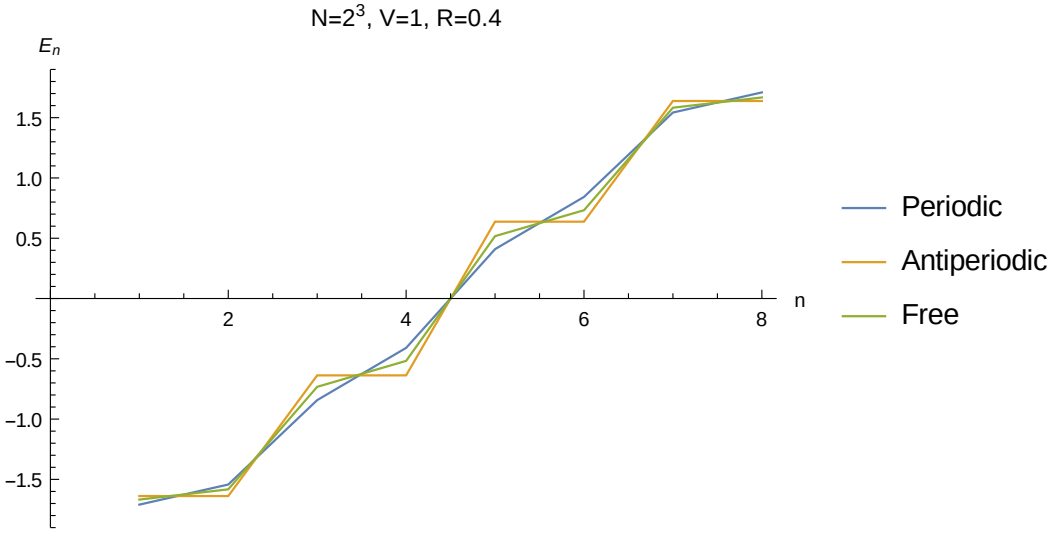


Figure 4 – Spectrum of the chain with 2^3 sites for different boundary conditions.

In our case, the set S is the spectrum of the infinite chain. We can compute a sequence of spectra $\{S_n^p\}_n, \{S_n^a\}_n$, S_n^p and S_n^a being the spectrum of the chain of length 2^n with periodic/antiperiodic boundary conditions. In the limit $n \to \infty$ both spectra become equal to S. If we wish to compute $\Gamma_n(q, \tau)$, the n^{th} approximant of the partition function, we must find a suitable partition $\mathcal{P}_n$ and a suitable associated set of radii l_i. As the spectra S_n^p, S_n^a are finite sets, it seems natural to partition them into insolated points. To each point we must now associate a ball of radius l_i. What should we take as a radius ? I don't know why, but it turns out to be a great idea to chose l_i to be the distance betweeen a point S_n^p and the corresponding point of S_n^a. The chain of length 2^n with any boundary condition has energies sandwiched between the associated energy for the periodic boundary conditions and the associated energy for antiperiodic boundary conditions (fig (4)). Thus, we understand that $\Gamma_n(q, \tau; \mathcal{P}, \{l_i\})$ is a good candidate for the partition function of the spectrum of the chain of length 2^n with any boundary condition Of course $p_i = 2^{-n}$ as the 2^n sites chain has 2^n (nondegenerate) energies.

To evaluate numerically $\tau(q)$ we can either find τ such that $\Gamma_{n\to\infty}$ is finite, or find τ such that

$$\lim_{n\to\infty} \frac{\Gamma_{n+1}}{\Gamma_n} = 1 \tag{12}$$

The latter method seems more accurate. We solved $\Gamma_{n+1}/\Gamma_n = 1$ for increasing values of n. The result is fig (3b). The convergence seems to be quite quick. The Hausdorff dimension obtained with this method agrees with the one obtained by direct box-counting up to the third decimal place.

3.3 Transition matrices

3.3.1 Definition

For a nearest-neighbours tight-binding system, the Schrödinger equation writes

$$E\psi_n = t_{n,n-1}\psi_{n-1} + t_{n,n+1}\psi_{n+1} \tag{13}$$

where $\psi_n = \langle n|\psi\rangle$. In the hierarchical chain case, the hopping amplitudes are real-valued: $t_{n,n+1} = t^*_{n+1,n} = t_{n+1,n} \stackrel{\text{def}}{=} t(n)$.

In general, we can define a *transition matrix*:

$$T(t_r, t_l; E) \stackrel{\text{def}}{=} \begin{bmatrix} \frac{E}{t_r} & -\frac{t_l}{t_r} \\ 1 & 0 \end{bmatrix} \tag{14}$$

and we have the important property that

$$\underbrace{T(t_{n,n+1}, t_{n,n-1}; E)}_{\stackrel{\text{def}}{=} T_{n,n-1}} \begin{pmatrix} \psi_n \\ \psi_{n-1} \end{pmatrix} = \begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} \tag{15}$$

3.3.2 Application to the (periodic) hierarchical chain

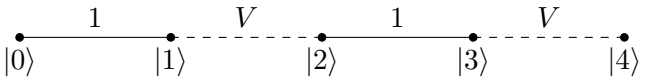


Figure 5 – First periodic approximant of the hierarchical chain. Two periods are shown.

We now consider the n^{th} periodic approximant of the infinite hierarchical chain. It is defined as the infinite chain obtained by the replacement

$$t_{k>n} \to t_n \tag{16}$$

The n^{th} periodic approximant has period 2^n.

First periodic approximant: because the first periodic approximant has period 2, we have

$$T(1, V; E)T(V, 1; E) \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = T_{2,1}T_{1,0} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} = \begin{pmatrix} \psi_3 \\ \psi_2 \end{pmatrix} = e^{2ik} \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix} \tag{17}$$

We see that the vector (ψ_1, ψ_0) is an eigenvector of $T_{2,1}T_{1,0}$, associated to the eigenvalue $\lambda_1 = \exp(2ik)$. Moreover, because of the periodicity,

$$\det T_{2,1}T_{1,0} = 1 \tag{18}$$

So that $\lambda_1\lambda_2 = 1$. Thus $\lambda_2 = \lambda_1^* = \exp(-2ik)$, and

$$\operatorname{tr} T_{2,1}T_{1,0} = \frac{E^2 - V^2 - 1}{V} = 2\cos(2k) \tag{19}$$

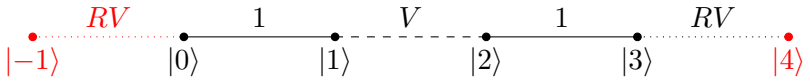


Figure 6 – Second periodic approximant. One period is shown (in black), as well as the surrounding environment (in red).

Solving this second-order polynomial in E gives us the two energy bands of this first periodic approximant.

Second periodic approximant and decimation: For this second periodic approximant, the period is $2^2 = 4$. We do not wish to compute directly the 4 bands, but rather to decimate half the sites of this period 4 system in order to recover a system equivalent to the previously studied period 2 system.

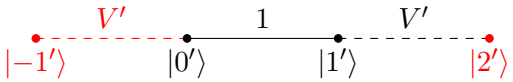


Figure 7 – First periodic approximant with renormalized couplings.

We chose to decimate the two sites surrounding the V coupling (sites $|1\rangle$ and $|2\rangle$ in fig (6)). We will thus obtain a first periodic approximant with renormalized couplings (fig (7)).

Using transition matrices, this means that we wish to make the identification

$$T(RV,1;E)T(1,V;E)T(V,1;E)T(1,RV;E) = T(V',1;E')T(1,V';E') \tag{20}$$

$$\Leftrightarrow \quad T_{3,2}T_{2,1}T_{1,0}T_{0,-1} = T'_{1',0'}T'_{0',-1'} \tag{21}$$

$$\Leftrightarrow \quad \begin{bmatrix} \frac{(E^2-1)^2-E^2V^2}{RV^2} & -\frac{E}{V}(E^2-V^2-1) \\ \frac{E}{V}(E^2-V^2-1) & -R(E^2-V^2) \end{bmatrix} = \begin{bmatrix} \frac{E'^2-1}{V'} & -E' \\ E' & -V' \end{bmatrix} \tag{22}$$

And thus, we conclude that the second approximant reduces to the first with the renormalized couplings

$$\begin{cases} V' &= R(E^2-V^2) \\ E' &= \frac{E}{V}(E^2-V^2-1) \end{cases} \tag{23}$$

n^{th} periodic approximant and decimation: We now wish to extend this decimation procedure to an arbitrary long approximant. This is easily done, because

$$T(R^2V,1;E)T(1,V;E)T(V,1;E)T(1,RV;E) = T(RV',1;E')T(1,V';E') \tag{24}$$

and

$$T(RV,1;E)T(1,V;E)T(V,1;E)T(1,R^2V;E) = T(V',1;E')T(1,RV';E') \tag{25}$$

with the same renormalized couplings E' and V'. The n^{th} periodic approximant with couplings E_n and V_n thus reduces to the $(n-1)^{\text{th}}$ one with the renormalized couplings

$$\begin{cases} V_{n-1} &= R(E_n^2-V_n^2) \\ E_{n-1} &= \frac{E_n}{V_n}(E_n^2-V_n^2-1) \end{cases} \tag{26}$$

References

[1] HA Ceccatto, WP Keirstead, and BA Huberman. Quantum states of hierarchical systems. *Physical Review A*, 36(11):5509–5512, 1987.

[2] TC Halsey, MH Jensen, and LP Kadanoff. Fractal measures and their singularities: the characterization of strange sets. *Physical Review A*, 33(2), 1986.