2D quasiperiodic stuff

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Disclaimer: the purpose of these notes is to nicely sum up what is known about 2D models of quasicrystals.

1 Geometry and tiling theory

This section lists (in no precise order) the useful tools for building or understanding 2D tilings.

1.1 Lift

Ammann-Beenker tiling (AB for short) involves 4 edges, which can be mapped onto the 4 base vectors of the $\mathbb{Z}^4$ lattice. Then, each lattice point lifts to a point in 4D, and the set of these points in exactly $\mathbb{Z}^4 \cap E + [0, 1)$ where E is the *physical space* (or parallel space). It is the plane of *Grassmann coordinates*:

$$G_{\mathrm{AB}} = (1, \sqrt{2}, 1, 1, \sqrt{2}, 1), \tag{1}$$

where the coefficients are ordered lexicographically (more on Grassmann coordinates later).

More generally, one can define an *octagonal* tiling as a 2D tiling using as tiles the 6 parallelograms generated by 4 noncolinear edges. Then this tiling can be lifted to $\mathbb{Z}^4$. It is said to be *planar* if the lift is contained into the slice $E + [0, t)$ with t finite. Then of course the tiling can be recovered by projecting points of $\mathbb{Z}^4 \cap E + [0, t)$ onto E (this is the cut and project method). t is called the *thickness* of the tiling. Note that if the points of an octagonal tiling are projected onto $E_\perp$, they fall on a compact space, the *window*, that has the shape of an (in general irregular) octagon. Hence the name "octagonal tiling".

Remark 1 (AB has maximal symmetry) *The AB tiling is the only octagonal tiling whose window is a regular octagnon. In this sense it is the one that is maximally symmetric. We are going to see that it has other "maximal symmetry" properties.*

1.2 Grassmann coordinates

Grassmann coordinatesare useful to describe planes in high dimensional spaces, in that the store all the information about the plane, in a compact way. Formally, let $E \in \mathbb{R}^4$ be the plane generated by $\mathbf{u}$ and $\mathbf{v}$. Then the Grassmann coordinates of E are the second minors of the matrix whose rows are $\mathbf{u}$ and $\mathbf{v}$. Explicitly, $G_{i,j} = u_i v_j - u_j v_j$.

Below we list some useful properties of Grassmann coordinates.

Theorem 1 *The Grassmann coordinates are base-independent, up to a global multiplicative factor.*

Theorem 2 (Plücker relation) *The 6 Grassmann coordinates are constrained by*

$$G_{12}G_{34} - G_{13}G_{24} + G_{14}G_{23} = 0 \tag{2}$$

Theorem 3 *The vectors*

$$\mathbf{u} = (0, G_{12}, G_{13}, G_{14}) \tag{3}$$
$$\mathbf{v} = (-G_{12}, 0, G_{23}, G_{24}) \tag{4}$$

direct E.

Theorem 4 (Frequencies of tiles) *Consider a planar octagonal tiling of physical plane E. Call $\pi_{\parallel}$ the orthogonal projection on E, and $(\mathbf{e}_i)_i$ the canonical base of $\mathbb{Z}^4$. Then $G_{i,j}$ is proportional to the frequency of the tile generated by $\pi_{\parallel}(\mathbf{e}_i)$ and $\pi_{\parallel}(\mathbf{e}_j)$.*

1.3 Shadows and subperiods

Consider an octagonal tiling whose physical plane contains no integer vector. Then this tiling cannot be periodic. Conversely, an aperiodic octagonal tiling has a physical plane which contains no integer vector. However, it may exist rational relations between vectors in the physical plane. Then, even if the tiling has no periods, it may have *subperiods*.

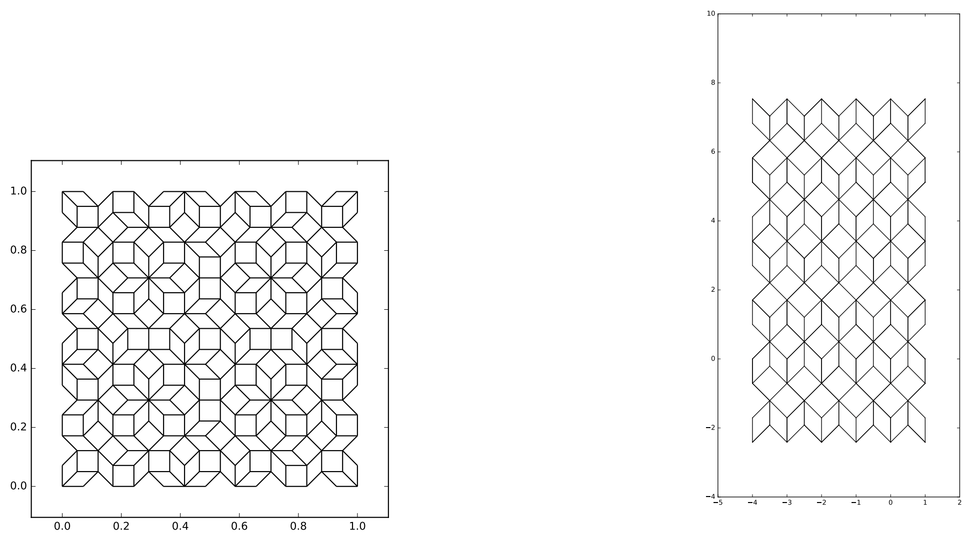

Figure 1 – A piece of the AB tiling, and a shadow of that piece (obtained by projecting the lift along $\mathbf{e}_2 - \mathbf{e}_4$). This amounts to removing the edges of the tiling along $\pi_{\parallel}(\mathbf{e}_1)$ (since $\pi_{\parallel}(\mathbf{e}_1) \propto \pi_{\parallel}(\mathbf{e}_2) - \pi_{\parallel}(\mathbf{e}_4)$). The shadow is quasiperiodic in one direction, and periodic in another one.

1.4 Local rules

Subperiods can be enforced by local rules. Hence, one can wonder is specifying subperiods is constraining enough to enforce a specific tiling. The answer is "sometimes, yes". For example, the *golden octagonal tiling* specified by the Grassmann coordinates $(1, \tau, 1, \tau, \tau, 1)$ has subperiods $\mathbf{e}_3 + \mathbf{e}_4$, $\mathbf{e}_1 + \mathbf{e}_3$, $\mathbf{e}_2 + \mathbf{e}_4$, $\mathbf{e}_1 + \mathbf{e}_2$. These subperiods respectively enforce $G_{23} = G_{24}$, $G_{14} = G_{34}$, $G_{12} = G_{14}$, $G_{13} = G_{23}$. Together with the Plücker relation, this is enough to specify to slope of the tiling.

The AB tiling provides us with a counterexample. The subperiods of the AB tiling are $\mathbf{e}_2 + \mathbf{e}_4$, $\mathbf{e}_1 + \mathbf{e}_3$, $\mathbf{e}_2 + \mathbf{e}_4$, $\mathbf{e}_1 - \mathbf{e}_3$. These subperiods respectively enforce $G_{23} = G_{34}$, $G_{14} = G_{34}$, $G_{12} = G_{14}$, $G_{12} = G_{23}$. Together with the Plücker relation, this enforces that the slope is

$$E_t = (1, t, 1, 1, 2/t, 1), \ t \in \mathbb{R} \tag{5}$$

Thus, the subperiods merely specify a one-parameter family of tilings (the AB tiling is $E_{\sqrt{2}}$). It is thus not enough to enforce the AB tiling to know its subperiods. This argument can be extended to show that no local rules can enforce the AB tiling. See [**?**] for more details.

Remark 2 (subperiods + extremization gives the AB tiling) *The square tiles of the E_t tiling are either spanned by the edges $\mathbf{e}_1$ and $\mathbf{e}_3$ or by $\mathbf{e}_2$ and $\mathbf{e}_4$. Therefore, the frequency of squares in the tiling E_t is proportional to $t + 2/t$. This frequency is extremal (in fact, minimal) for $t = \sqrt{2}$, which corresponds to the AB tiling. Thus the AB tiling can be recovered from its subperiod, together with an extremization argument. See [**?**] for details (well written ++).*

We can also remark the AB tiling is the most symmetric tiling among the family of tilings E_t that have the same subperiods, in the sense that it is the only one that has the same area covered by squares and by lozenges.

1.5 Coordination zones

We define the k^{th} *coordination zone of* r as $z_k(r)$, the set of k^{th} neighbors of site r (ie sites that are exactly k hops away from r). For the AB tiling $z_k(r)$ becomes a regular octagon as $k \to \infty$.

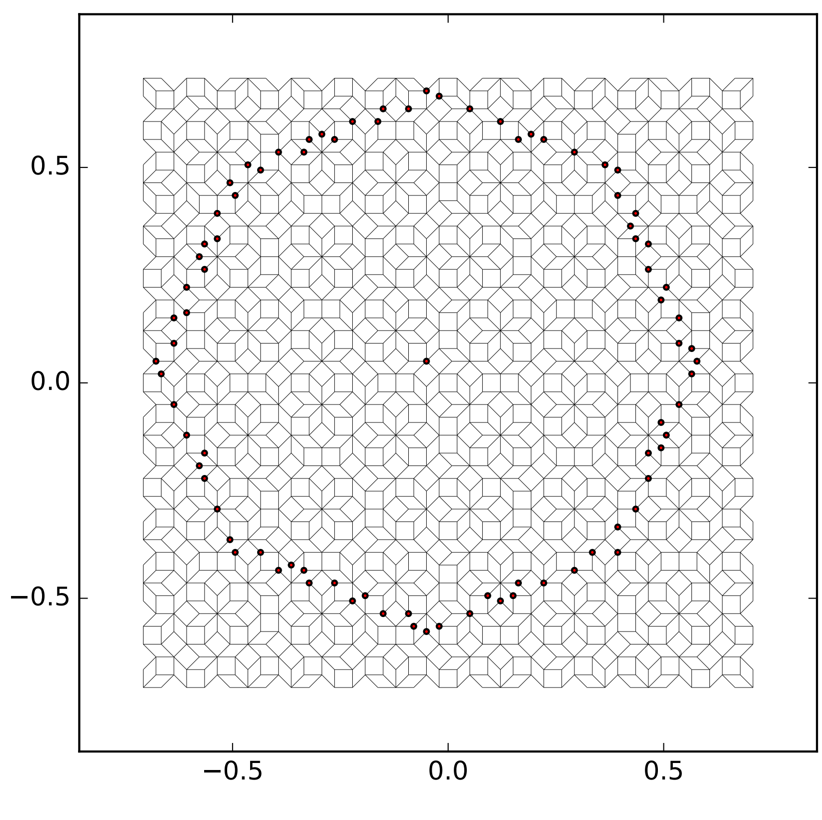

Figure 2 – A large coordination zone on a patch of the AB tiling.

1.6 Matching rules and a deterministic construction algorithm

1.7 The field of arrows, and the field of heights

There are several ways to introduce the field of arrows on the AB tiling:

1. **Inflation.** A given square can be inflated in four nonequivalent ways. For a given square on an AB tiling, one of them is compatible with the AB rules, while the others are not. A way to correctly decide how to inflate the squares is to draw arrows on the neighboring lozenges, pointing to their acute vertices (or leaving them, depending on the convention).

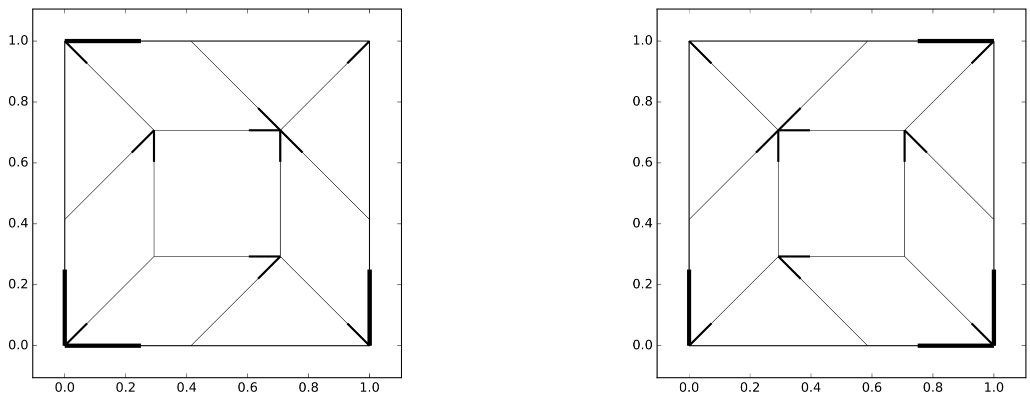

Figure 3 – Two of the four nonequivalent ways to inflate a square (note that they are linked to each other by a rotation). The initial square has thick edges and big arrows, the pieces resulting from inflation have thin edges and small arrows. Arrows are figured by a thick segment stuck to the vertex the arrow is pointing to (that's the default behavior of NetworkX).

2. **Local environments.** The arrow between two sites is always pointing to (or leaving, depending on the convention) the one the farther away from the center of the internal space (Rémy's remark).
3. **Cohomology classes of the Hull.** Let $[\omega]$ be a cohomology class of the first cohomology group of the *hull* (the notion of hull is unclear for me, as is the notion of cohomology groups (which cohomology are we talking about by the way?)). Then, according to Pavel [**?**] $\omega \in [\omega]$ can be pulled back on E. Its pullback is the differential of a scalar function, and this function is the integral of an arrow field (what I call a *height function*). The first cohomology group of the hull of AB has only one element, so a single field of arrows can be defined on AB tilings.
4. **Local rules.** Attaching arrows to the edges of the tiles is equivalent to forbidding certain configurations of tiles. This is enough to enforce the subperiods (cf [**?**]), and sometimes this is in turn enough to enforce a specific tiling (eg Penrose), and sometimes not (eg AB).

1.8 Height distribution

We want to compute $f_\mu(m)$, the probability that a type μ site has potential m. For that, we define $N_\mu^{(l)}(m)$, the number of type μ sites having potential m, on the tiling obtained from l inflations of an initial pattern. The goal is to obtain a recurrence relation for $N^{(l)}$, and to obtain the probabilities from it.

First, let us compute $N_\mu^{(l)}$, the number of type μ environments at step l. There are powerful techniques to evaluate these numbers, notably the dualization of the tiles, see [**?**, **?**]. However here we shall use a very basic approach.

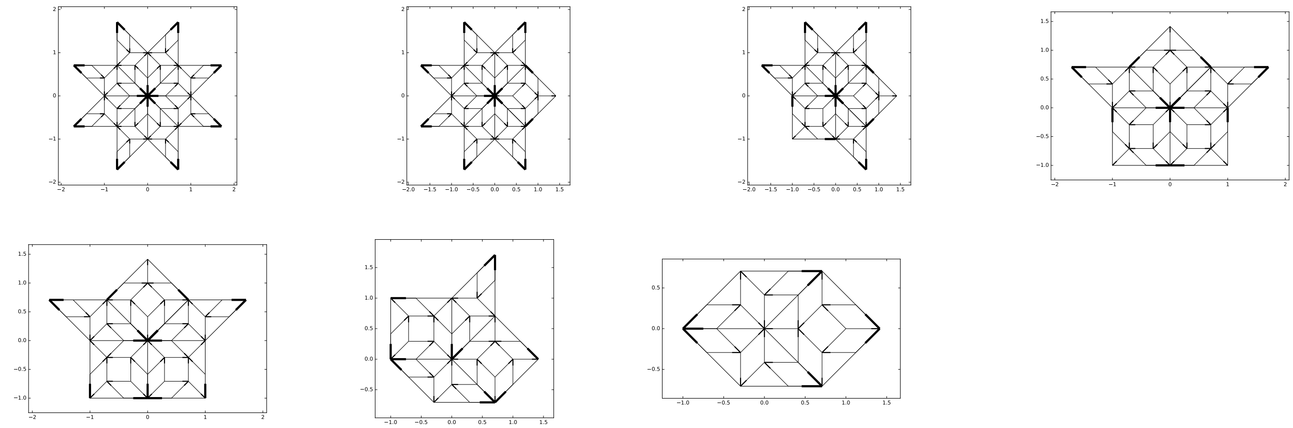

Figure 4 – The 7 local environments, and their first inflation.

We see that after one inflation (fig (3)) a given site becomes a site A, B, C or D_1. More precisely, their number becomes

$$\begin{pmatrix} N_A^{(l+1)} \\ N_B^{(l+1)} \\ N_C^{(l+1)} \\ N_{D1}^{(l+1)} \end{pmatrix} = \underbrace{\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}}_{=M_0} \begin{pmatrix} N_A^{(l)} \\ N_B^{(l)} \\ N_C^{(l)} \\ N_{D1}^{(l)} \\ N_{D2}^{(l)} \\ N_E^{(l)} \\ N_F^{(l)} \end{pmatrix} \tag{6}$$

After inflation, D_2, E and F sites must be new sites, and thus nearest neighbors of old sites. Thus it suffices to look at the nearest neighbors of old sites on fig (4) to count them. We get

$$\begin{pmatrix} N_{D_2}^{(l+1)} \\ N_E^{(l+1)} \\ N_F^{(l+1)} \end{pmatrix} = \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 2 & 3 & 2 \\ 8 & 8 & 8 & 8 & 5 & 2 & 0 \end{bmatrix}}_{=M_1} \begin{pmatrix} N_A^{(l)} \\ N_B^{(l)} \\ N_C^{(l)} \\ N_{D1}^{(l)} \\ N_{D2}^{(l)} \\ N_E^{(l)} \\ N_F^{(l)} \end{pmatrix} \tag{7}$$

$M = M_0 + M_1$ is the geometrical inflation (or *substitution*) matrix, describing the statistics of the 7 local environments of the AB tiling. As such, its highest eigenvalue is λ^2, the inflation factor of the AB tiling. The corresponding eigenvector, $\mathbf{f}$, has positive entries, proportional to the frequencies of the local environments:

$$\mathbf{f} = (\mu^4, \mu^5, 2\mu^2, \mu^3, \mu^3, 2\mu^2, \mu) \tag{8}$$

where $\mu = 1/\lambda = \sqrt{2} - 1$. It can be checked that these entries are indeed the frequencies of the local environments, for example compare to [?].

Now, we repeat our construction, but this time tracking the evolution of the height together with the evolution of the environment.

1. The effect of inflation on the old tiles is to change the direction of the arrows along their edges (this is also true for Penrose, is it true in general?). Hence the potential on old sites only changes

sign under inflation:

$$m_{\text{old}}^{(l+1)} = -m_{\text{old}}^{(l)} \tag{9}$$

2. New sites are connected to old ones by one bond, and the arrow on this bond is always directed from new to old (or old to new, depending on the convention we choose). Hence,

$$m_{\text{new}}^{(l+1)} = m_{\text{old}}^{(l+1)} - 1 \tag{10}$$

$$= -m_{\text{old}}^{(l)} - 1 \tag{11}$$

Looking at (9) and (10) we get

$$N_\mu^{(l)}(-m) = (M_0)_{\mu,\nu} N_\nu^{(l)}(m) + (M_1)_{\mu,\nu} N_\nu^{(l)}(m-1) \tag{12}$$

After two inflations, the potential has changed sign twice and we have

$$N_\mu^{(2l+2)}(m) = (M_0 M_1)_{\mu,\nu} N_\nu^{(l)}(m-1) + (M_0^2 + M_1^2)_{\mu,\nu} N_\nu^{(l)}(m) + (M_1 M_0)_{\mu,\nu} N_\nu^{(l)}(m+1) \tag{13}$$

Generating function of the height distribution

We consider the generating function of the height counting function:

$$\widetilde{N}_\mu^{(t)}(z) = \sum_m z^m N_\mu^{(t)}(m) \tag{14}$$

It obeys the simple recursion

$$\widetilde{N}_\mu^{(2l+2)}(z) = T_{\mu,\nu}(z) \widetilde{N}_\nu^{(2l)}(z) \tag{15}$$

with $T(z) = M_0^2 + M_1^2 + z M_0 M_1 + 1/z M_1 M_0$. Let $\omega(z)$ be the largest eigenvalue of $T(z)$. Let $\widetilde{\mathbf{f}}(z)$ be the associated eigenvector. Both can be computed analytically. Then,

$$\widetilde{N}_\mu^{(t)}(z) \sim \omega^t(z) \widetilde{f}_\mu(z) \tag{16}$$

Moments of the height distribution

Now, using the generating function, we can compute the moments of the height distribution. For example, the average height on environment μ is

$$\langle m_\mu \rangle = \lim_{t\to\infty} \frac{\sum_m m N_\mu^{(t)}(m)}{\sum_m N_\mu^{(t)}(m)} \tag{17}$$

And using (14) and (16),

$$\langle m_\mu \rangle = \lim_{t\to\infty} \frac{\partial \log \omega^t(z) \widetilde{f}_\mu(z)}{\partial \log z}|_{z=1} \tag{18}$$

This expression can be further simplified using that $\omega'(1) = 0$. We end up with

$$\boxed{\langle m_\mu \rangle = \frac{\partial \log \widetilde{f}_\mu(z)}{\partial \log z}|_{z=1}} \tag{19}$$

Remark: the averages are defined up to a constant since the origin of the heights is arbitrary. This is reflected by the fact that the eigenvector $\widetilde{f}_\mu$ is defined up to a normalization constant. For example, if we set the origin of the heights at a A site, then we find

$$\mathbf{m} = \frac{1}{12} \begin{pmatrix} 0 \\ 2+\sqrt{2} \\ 3(2+\sqrt{2}) \\ 14+5\sqrt{2} \\ 2+5\sqrt{2} \\ -2+3\sqrt{2} \\ -10+\sqrt{2} \end{pmatrix} \tag{20}$$

Similarly, we compute the variance:

$$\langle m_\mu^2 \rangle - \langle m_\mu \rangle^2 = \lim_{t\to\infty} \frac{\partial^2 \log \omega^t(z) \widetilde{f}_\mu(z)}{\partial \log^2 z}|_{z=1} \tag{21}$$

Now, since $\omega''(1) \neq 0$, the $\omega^t(z)$ term gives the dominant contribution and

$$\boxed{\langle m_\mu^2 \rangle - \langle m_\mu \rangle^2 \sim t \frac{\partial^2 \log \omega(z)}{\partial \log^2 z}|_{z=1}} \tag{22}$$

The linear dependence on the number of inflations t is reminiscent of a diffusion process. With that in mind, we introduce the diffusion constant D, defined by $\sigma^2 = 2Dt$. We have

$$D = \frac{1}{2} \frac{\partial^2 \log \omega(z)}{\partial \log^2 z}|_{z=1} = \frac{1}{6\sqrt{2}} \tag{23}$$

Height distribution

To compute the height distribution analytically, we rewrite eq (13) as

$$\mathbf{P}^{(t+2)}(m) = W_l \mathbf{P}^{(t)}(m-1) + W_0 \mathbf{P}^{(t)}(m) + W_r \mathbf{P}^{(t)}(m+1) \tag{24}$$

where $P_\mu^{(t)}(m)$ is the probability to find environment μ with height m after t inflations. The transition rates W are proportional to the matrices involved in (13), and the proportionality coefficient is here to ensure the probabilities are correctly normalized. For example, if the initial condition is

$$\mathbf{P}_0(m) = \begin{cases} \mathbf{f} & \text{if } m = 0 \\ 0 & \text{if } m \neq 0 \end{cases} \tag{25}$$

then the proportionality coefficient is the square of the inflation factor, λ^4.

Eq (24) looks like a Fokker-Planck, and numerically $\mathbf{P}^{(t)}(m)$ looks like a vector of Gaussians at large times. We are thus hinted to think of (24) as the multidimensional version of the Fokker-Planck equation

$$\partial_t p_t(x) = D \partial_x^2 p_t(x) \tag{26}$$

whose solution is known to be $p_t(x) = 1/\sqrt{4\pi Dt} \exp\big(-(x-x_0)^2/(4Dt)\big)$, if the initial condition is $\delta(x-x_0)$.

We therefore guess the form of the probability law for the heights:

$$\boxed{P_\mu^{(t)}(m) = \frac{f_\mu}{\sqrt{4\pi Dt}} \exp\left(-\frac{(m - \langle m_\mu \rangle)^2}{4Dt}\right)} \tag{27}$$

where D and $\langle m_\mu \rangle$ are given above. The agreement with numerics is perfect, which suggests this is the correct asymptotic form of the probability distribution.

Estimate of the generating function

If we admit that the distribution of heights is Gaussian (eq. (27)), then it is easy to estimate the distribution function:

$$\widetilde{N}_\mu^{(t)}(z) = \sum_{m=-t/2}^{t/2} z^m N_\mu^{(t)}(m) \tag{28}$$

We introduce the variable $u = m/t$ to keep the bounds of the sum fixed:

$$\widetilde{N}_\mu^{(t)}(z) = \sum_{u=-1/2}^{1/2} t z^{tu} N_\mu^{(t)}(tu) \tag{29}$$

In the long time limit, we can transform the sum into an integral:

$$\widetilde{N}_{\mu}^{(t)}(z) \sim \int_{-1/2}^{1/2} \mathrm{d}u t z^{tu} N_{\mu}^{(t)}(tu) \tag{30}$$

Now, if, according to (27), $N_{\mu}^{(t)}$ is a Gaussian peaked around $tu = \langle m_\mu \rangle$, and of vanishing spreading (in the variable u) $\sigma = \sqrt{2Dt}/t$, then wen can integrate on the whole real line in the large time limit. The integral is Gaussian, and therefore yields straightforwardly

$$\widetilde{N}_{\mu}^{(t)}(z) \sim z^{\langle m_\mu \rangle} \exp\bigl(Dt(\log z)^2\bigr) \tag{31}$$

Refining local environments.

Looking at numerical data for the local part of the groundstate [?], we see that it varies about as strongly inside of envs E and F as between envs A and B. This hints that we should refine our local environment subdivision. We propose here to divide envs E and F into two categories, labeled 1 and 2. Envs E_1 and F_1 have as nearest neighbors only inner sites (ie sites A to D_1), while envs E_2 and F_2 are connected to an outer site, namely a D_2 site. This distinction is perhaps physically relevant. Anyway, it seems so by looking at the numerics of [?]. The substitution matrix M is now 9×9. The inner part M_0 is only changed trivially (since $N_{C/D_1}^{(l+1)} = N_{E/F}^{(l)} = N_{E_1/F_1}^{(l)} + N_{E_2/F_2}^{(l)}$). The outer part is changed to:

$$M_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 2 & 2 \\ 0 & 0 & 0 & 0 & 2 & 2 & 2 & 0 & 0 \\ 8 & 8 & 8 & 8 & 3 & 0 & 0 & 0 & 0 \\ 8 & 8 & 8 & 8 & 2 & 2 & 2 & 0 & 0 \end{bmatrix} \tag{32}$$

2 Gap labelling

3 IPR and moments of the ground state

We assume Pavel's Ansatz holds true (ie the groundstate can be decomposed into a local part that depends only on the local configuration of the bonds, and a part that depends only on the arrow field). Then we write the groundstate as

$$|\psi\rangle = \sum_i C_{\mu(i)} \beta^{h(i)} |i\rangle \tag{33}$$

where μ depends only on the local environment, and h is the integral of the arrow field. Then we write the q moment of the ground state as:

$$\chi_q^{(t)} = \frac{\sum_\mu |C_\mu|^{2q} \sum_h \beta^{2qh} N_\mu^{(t)}(h)}{\left(\sum_\mu |C_\mu|^2 \sum_h \beta^{2h} N_\mu^{(t)}(h)\right)^q} \tag{34}$$

Now, we are seeking to evaluate the moments in the thermodynamic limit $t \to \infty$, and in particular their scaling

$$\tau_q = \lim_{t\to\infty} -\frac{\log \chi_q^{(t)}}{\log N^{(t)}} \tag{35}$$

We rewrite

$$\chi_q^{(t)} = \frac{\sum_\mu |C_\mu|^{2q} \widetilde{N}_\mu^{(t)}(\beta^{2q})}{\left(\sum_\mu |C_\mu|^2 \widetilde{N}_\mu^{(t)}(\beta^2)\right)^q} \tag{36}$$

where $\widetilde{N}_\mu^{(t)}$ is the generating function of the distribution of heights (14). Crucially, the generating functions have a universal scaling, ie it does not depend on the local environment:

$$\widetilde{N}_\mu^{(t)}(\beta^{2q}) \sim \omega^{t/2}(\beta^{2q})\widetilde{f}_\mu \tag{37}$$

And since the local environment part of the wavefunction no longer evolves with t in the thermodynamic limit, we conclude that τ_q *is insensitive to the local environment part of the wavefunction.* In particular, Sutherland's wavefunction [?] (which is obtained by setting $C_\mu = 1$ in (33)) has the same scaling as the more complicated Ansatz of Pavel.

We readily find

$$\boxed{\tau_q = \frac{1}{2}\frac{\log\bigl(\omega(\beta^2)^q/\omega(\beta^{2q})\bigr)}{\log\lambda^2}} \tag{38}$$

where the 1/2 factor comes from the fact that ω is the scaling factor after two consecutive inflations. We note that this quantity depends only on the geometry of the AB tiling, not on the particular details of the Hamiltonian. However, the moments χ_q do depend on these details.

4 Variational Ansätze

We consider the Hamiltonian

$$H(t) = -tH_{\mathrm{PH}} + (1-t)H_{\mathrm{OS}} \tag{39}$$

This is the Hamiltonian first introduced by Sire (see eg [?, ?]). Let us also define $H^{(l)}(t)$ as the Hamiltonian on the finite-size system obtained from l inflations of an initial set of tiles.

There are 3 notable values of t:

1. $t = 1$ gives the pure-hopping Hamiltonian
2. $t = 1/2$ gives the Laplacian model
3. $t = 0$ gives the purely onsite, local Hamiltonian.

The onsite limit is the easiest one. In this limit, the spectrum consists of 6 infinitely degenerate levels, each of which lives on a particular class of sites (sites are classified up to their first coordination zone here). Inspired by this remark, we write an Ansatz for the wavefunctions:

$$|\psi_0\rangle = \sum_i C_{\mu(i)}\,|i\rangle \tag{40}$$

where μ runs of over the different classes of the sites:

$$\mu \in \{A(8), B(7), C(6), D_1(5), D_2(5), E(4), F(3)\} \tag{41}$$

where the coordination of each class of site is put in parenthesis. We distinguish D_1 and D_2 although they have the same coordination, because we see numerically that they correspond to two distinct energy levels as soon as $t \neq 0$.

4.1 Choice of the Ansatz

As we are going to see later, the overlap $\langle \psi^{(l)} \mid \psi_0 \rangle$ (where $|\psi^{(l)}\rangle$ is the exact ground state wavefunction of $H_{\mathrm{PH}}^{(l)}$) worsen as l increases. This contrasts with the situation for the Rauzy tiling, where the overlap saturates at a finite value. We conclude that for the AB tiling, *nonlocal fluctuations* become more and more important as the size of the approximant grows. These fluctuations must be related to the only nonlocal geometrical quantity defined on the tiling: the field of arrows. Guided by the exact ground state described by Pavel [?], we chose as our Ansatz a wavefunction that incorporated a local part and a height-dependent part:

$$|\psi\rangle = \sum_i C_{\mu(i)} \beta^{m(i)} |i\rangle \tag{42}$$

where $m(i)$ is the height at site i, and β is a parameter of the model, constrained by the variational equations.

4.2 The variational energy

As the onsite Hamiltonian is trivial, let us focus on the pure-hopping part. We want to extremize $E(\{C\},\beta) = \langle\psi\,|\,H_{\rm PH}\,|\,\psi\rangle\,/\,\langle\psi\,|\,\psi\rangle$ wrt the 7 parameters $\{C_\mu\}_\mu$ and wrt β. This is going to give us 8 variational equations, the solution of which should be a reasonable approximation of the exact groundstate of our Hamiltonian.

Evaluation of the norm $\langle\psi\,|\,\psi\rangle$.

We have

$$\langle\psi\,|\,\psi\rangle = \sum_\mu C_\mu^2 \sum_m \beta^{2m} N_\mu^{(2l)}(m) \tag{43}$$

$$= \sum_\mu C_\mu^2 \widetilde{N}_\mu^{(2l)}(\beta^2) \tag{44}$$

Now, $\widetilde{N}_\mu^{(2l)}(\beta^2) = T(\beta^2)^l_{\mu,\nu} \widetilde{N}_\nu^{(0)}(\beta^2)$ (where $\widetilde{N}$ is the generating function of N, as defined in the Height distribution section). If the starting vector has a component along the eigenvector associated to the largest eigenvalue of T (which we will assume), then $\widetilde{N}_\mu^{(2l)}(\beta^2) = \omega(\beta^2)^{2l} f_\mu(\beta^2)$, where ω^2 is the largest eigenvalue of T, and f_μ the corresponding eigenvector. Hence

$$\langle\psi\,|\,\psi\rangle = \omega(\beta^2)^{2l} \sum_\mu C_\mu^2 f_\mu(\beta^2) \tag{45}$$

The factor $\omega(\beta^2)^{2l}$ can be incorporated in the normalization of the wavefunction. We will assume it is the case from now on. Hence our final expression is

$$\langle\psi\,|\,\psi\rangle = \sum_\mu C_\mu^2 f_\mu(\beta^2) \tag{46}$$

Evaluation of the average $\langle\psi\,|\,H_{\mathbf{PH}}\,|\,\psi\rangle$

Now, we evaluate

$$\langle\psi\,|\,H_{\rm PH}\,|\,\psi\rangle = \sum_{\mu,\nu} C_\mu C_\nu \sum_m \beta^{2m+\epsilon(\mu\to\nu)} N_\nu(\mu,m) \tag{47}$$

$N_\nu(\mu,m)$ is the number of bonds (μ,ν) with μ having potential m. $\epsilon(\mu\to\nu) = \pm 1$ resp if the arrow goes from μ to ν or the reverse. We can write $N_\nu(\mu,m) = z(\nu|\mu,m)N_\mu(m)$ with $z(\nu|\mu,m)$ the average number of type ν sites around type μ sites that have potential m. If the number of ν sites around μ is always the same, then $z(\nu|\mu,m) = z(\nu|\mu)$. This is the case for $\mu<\nu$ (lexicographic order: $1=A, 2=B, 3=C, 4=D_1, 5=D_2, 6=E, 7=F$). Assuming $\mu<\nu$, we have

$$\sum_m \beta^{2m} N_\nu(\mu,m) = z(\nu|\mu) \sum_m \beta^{2m} N_\mu(m) \tag{48}$$

$$= z(\nu|\mu) \widetilde{N}_\mu(\beta^2) \tag{49}$$

Because the Hamiltonian is real symmetric, $\beta^{\epsilon(\mu\to\nu)}N_\nu(\mu,m)$ is symmetric under the exchange of μ and ν. In particular, if $\mu > \nu$,

$$\beta^{\epsilon(\mu\to\nu)}\sum_m \beta^{2m}N_\nu(\mu,m) = \beta^{\epsilon(\nu\to\mu)}\sum_m \beta^{2m}N_\mu(\nu,m) \tag{50}$$

$$= \beta^{\epsilon(\nu\to\mu)}z(\mu|\nu)\widetilde{N}_\nu(\beta^2). \tag{51}$$

So, finally

$$\langle\psi\,|\,H_{\mathrm{PH}}\,|\,\psi\rangle = \sum_{\mu,\nu} C_\mu h_{\mu,\nu} C_\nu \tag{52}$$

where h is the symmetric 7×7 matrix

$$h_{\mu,\nu} = \beta^{\epsilon(\mu\to\nu)}z(\nu|\mu)f_\mu(\beta^2) \text{ if } \mu<\nu \tag{53}$$

$$= \beta^{\epsilon(\nu\to\mu)}z(\mu|\nu)f_\nu(\beta^2) \text{ if } \mu>\nu. \tag{54}$$

Evaluation of $\langle\psi\,|\,H(t)\,|\,\psi\rangle$

This straightforwardly amounts to replacing $h_{\mu,\nu}$ by

$$-\,th_{\mu,\nu} + (1-t)z_\mu f_\mu(\beta^2)\delta_{\mu,\nu} \tag{55}$$

with z_μ the coordination of type μ sites.

4.3 The variational equations

Extremizing the energy wrt a parameter p yields

$$\partial_p\,\langle\psi\,|\,H\,|\,\psi\rangle = E(p)\partial_p\,\langle\psi\,|\,\psi\rangle \tag{56}$$

Here we have two kinds of parameters: the C's and β. Let us consider each in turn.

Extremization wrt C

Let us first extremize for H_{PH}. Since h is symmetric, we have

$$\sum_\nu h_{\mu,\nu}C_\nu = Ef_\mu C_\mu \tag{57}$$

So, $\mathbf{C}(\beta)$ is an eigenvector of the matrix $Z_{\mu,\nu} = h_{\mu,\nu}(\beta)/f_\mu(\beta^2)$, with eigenvalue E. There are thus 7 independent solutions for $\mathbf{C}(\beta)$, for each value of β. The extension to $H(t)$ is simple: $Z_{\mu,\nu}$ becomes

$$Z_{\mu,\nu} = -th_{\mu,\nu}(\beta)/f_\mu(\beta^2) + (1-t)z_\mu\delta_{\mu,\nu} \tag{58}$$

Extremization wrt to β

Since h is symmetric, we can write

$$\langle\psi\,|\,H_{\mathrm{PH}}\,|\,\psi\rangle = 2\sum_{\mu<\nu} C_\nu z(\nu|\mu)f_\mu\beta^{\epsilon(\mu\to\nu)}C_\mu \tag{59}$$

Then, extremization yields

$$2\sum_{\mu<\nu} C_\nu z(\nu|\mu)\partial_\beta\left(f_\mu\beta^{\epsilon(\mu\to\nu)}\right)C_\mu = E\sum_\mu C_\mu^2\partial_\beta f_\mu \tag{60}$$

(There should be a way to simplify this expression, making use of (57).) The extension to $H(t)$ is, again, straightforward.

4.4 Results and comparison to numerics

We solve the minimization equations numerically: Solving the variational equation for $\mathbf{C}$ (57) at fixed β we obtain $\mathbf{C}(\beta)$. We then vary β until the variational equation for β (60) is satisfied. Remark: we have checked numerically that (60) is satisfied only at a single point $\{\beta, \mathbf{C}(\beta)\}$ (this is not trivial, as this equation is nonlinear). This holds true for any value of t.

Ground state

	Uniform	Var, no β	Var, β	Exact
$-E_{\mathrm{GS}}$	4	4.21936	4.22091	4.221697
β_{GS}			0.907397	0.858100

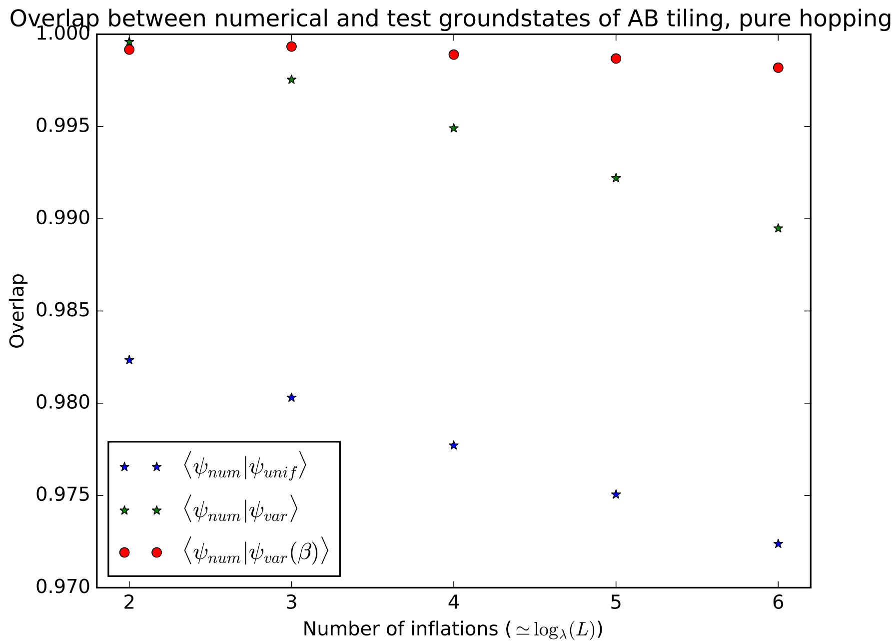

Figure 5 – Overlap between the numerical groundstate and test states, as a function of the log of the linear size of the numerical system.

For the pure-hopping Hamiltonian ($t = 1$), we compare our results to the known exact result [?] in the table (4.4). We can also compute the groundstate numerically on a large lattice, and look at the overlap between the numerical and the variational states as a function of the lattice size. If the overlap decreases as a function of the system size, but has a finite limit, then the variational state is a good approximation of the exact groundstate. If, on the other hand, the overlap goes to zero, then the variational state is does not describe well the exact groundstate.

Figure (5) shows the overlap for the different trial states. The overlap using the variational state without β has the same decay as the overlap using the uniform state. So clearly it is not enough to take into account the local environments. The field of heights (which is nonlocal) must play a role in the groundstate. Indeed, the overlap using the variational state including β has a slower decay. However it is unclear whether the overlap still decays to zero in this case or not (in the former case, this would mean that local environments at larger and larger scales become relevant as the system size is increased).

We can also look at how our Ansatz predicts β will behave as a function of t (fig (6)). We know that $\beta(1/2) = 1$ since the groundsate of the Laplacian model is uniform. This is indeed what we find. No surprise here, the Ansatz should give the exact result if the true groundstate is uniform. According to

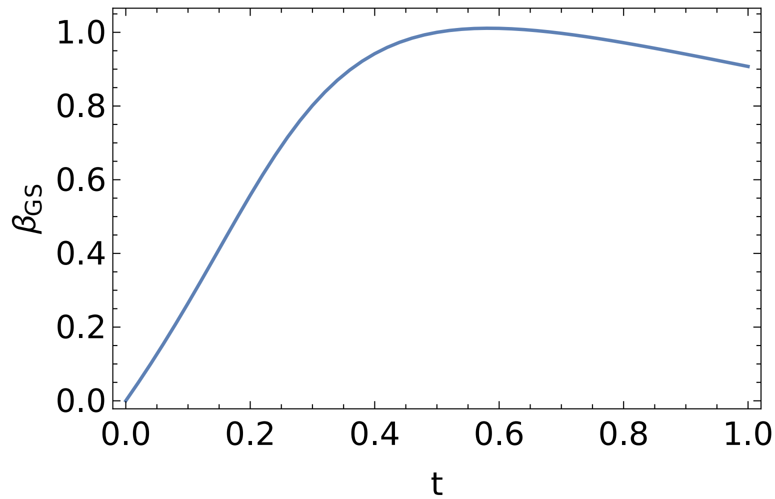

Figure 6 – The variational β for the grounstate of $H(t)$.

Rémy, numerically β is always smaller than 1. However, we find β slightly larger than 1 for t just above 1/2. We also find that $\beta \to 0$ as $t \to 0$, a result I still do not understand.

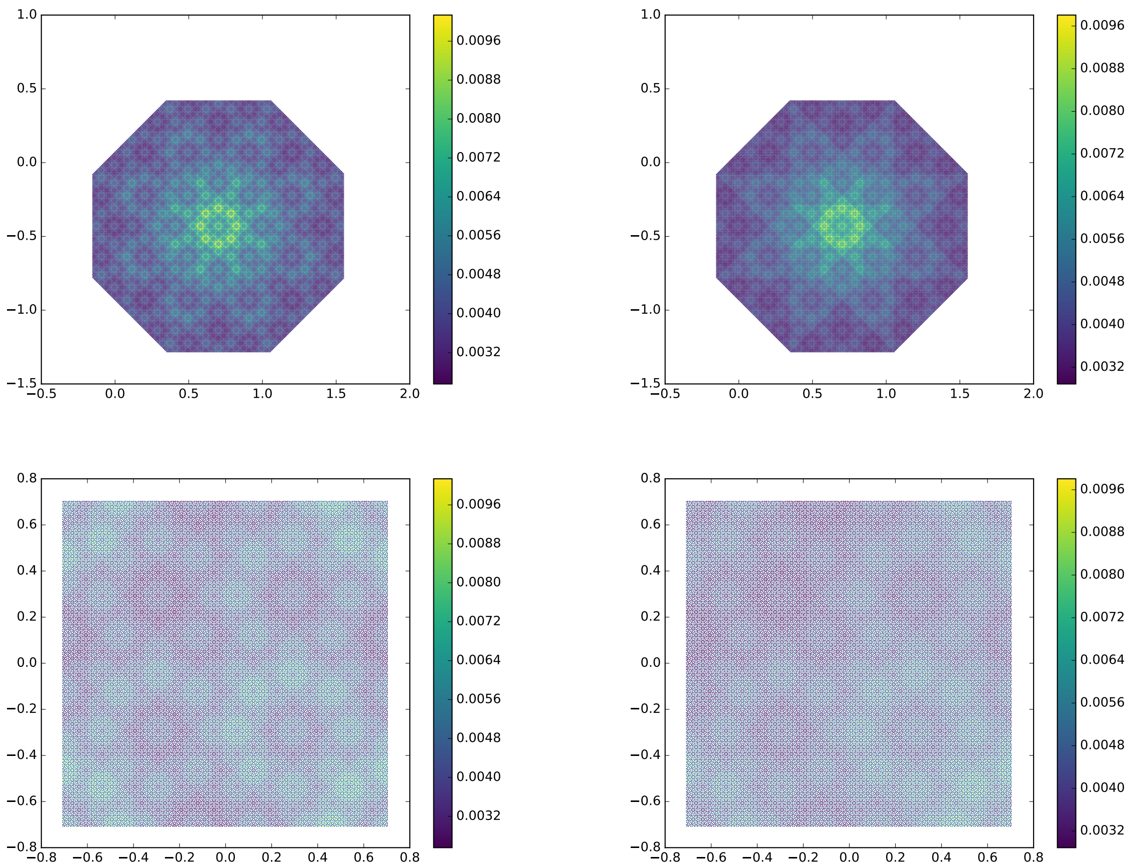

Figure 7 – The numerical and variational groundstates of the pure-hopping Hamiltonian. Top row: in internal space, bottom row: in real space. Numerical groundstate is computed on the sixth inflation of a square (47321 sites), with periodic boundary conditions. Variational state is put on the same lattice for comparison. Left column: numerical, right: variational.