Flip Dynamics in Octagonal Rhombus Tiling Sets

N. Destainville

Laboratoire de Physique Quantique–UMR CNRS-UPS 5626–IRSAMC, Université Paul Sabatier, 118, route de Narbonne, 31062 Toulouse Cedex 04, France

(Received 13 February 2001; published 3 January 2002)

We investigate the properties of classical single flip dynamics in sets of two-dimensional random rhombus tilings. Single flips are local moves involving three tiles which sample the tiling sets via Monte Carlo Markov chains. We determine the ergodic times of these dynamical systems (at infinite temperature): they grow with the system size N_T like const. $\times N_T^2 \ln N_T$; these dynamics are rapidly mixing. We use an inherent symmetry of tiling sets and a powerful tool from probability theory, the coupling technique. We also point out the interesting occurrence of Gumbel distributions.

DOI: 10.1103/PhysRevLett.88.030601 PACS numbers: 05.40.–a, 02.50.Ga, 61.44.Br

After the discovery of quasicrystals [1], quasiperiodic tilings [2] as well as their randomized counterpart, random rhombus tilings [3], rapidly appeared to be suitable paradigmatic models for quasicrystalline alloys [4]. Simultaneously, these systems also became an active topic in discrete mathematics (see [5] or [6] for examples). Figure 1 displays a random tiling, which belongs to the class of plane tilings with octagonal symmetry. Beyond this case, plane tilings with larger symmetries including Penrose tilings [2] and space tilings with icosahedral symmetries were proposed to model every kind of quasicrystal. The present Letter is devoted to dynamical properties of random rhombus tilings in terms of local dynamical rules, the so-called *phason flips,* which consist of local rearrangement of tiles (Fig. 1). These dynamics are of interest for several reasons. On the one hand, it is more and more clear that phason flips exist in real quasicrystals [7] and can be modeled in a first approximation by tile flips; they are a new source of atomic mobility, as compared to usual crystalline materials. In particular, they could carry their own contribution to self-diffusion [8], even if the efficiency of such processes remains controversial [9]. They are also involved in some specific mechanical properties of quasicrystals, such as plasticity via dislocation mobility [10]. Therefore a complete understanding of flip dynamics is essential in quasicrystal physics. The present work is a first step in this direction. On the other hand, a lot of numerical work has been carried out to characterize statistical properties of tiling sets, a part of which was based on Monte Carlo techniques which rely on a faithful sampling of tiling sets (see [11,12]). So far, no systematic study of the relaxation times between two independent numerical measures has been accomplished, whereas it is an essential ingredient for a suitable control of error bars. However, there exist exact results in the simplest case of random rhombus tilings with hexagonal symmetry [13–15] and several estimates of relaxation times in larger symmetries, either numerical or in the approximate frame of Langevin dynamics [11,16].

Random rhombus tilings are made of rhombi of unitary side length. They are classified according to their global symmetries [3]. The simplest class of hexagonal tilings—made of 60° rhombi with three possible orientations—has been widely explored [13–15]. Tilings with octagonal symmetry are made of six different tiles (characterized by their shape *and* orientation): two squares and four 45° rhombi (Fig. 1). Beyond these two cases, one can define tilings with higher symmetries (e.g., Penrose tilings [2]) or of higher dimensions [3]. For sake of technical simplicity, we focus on tilings filling a centrally symmetric polygon with integral side lengths (Fig. 1). We are interested in the large size limit where the polygon becomes large keeping a fixed shape. Such tilings can schematically be seen as frozen near their boundary, and strain-free in their central region [17]. Dynamics of fixed boundary tilings should be the manifestation of dynamics of their strain-free center, thus relating both boundary conditions. Here we suppose that all tilings have the same probability; we work at infinite temperature.

The set of all the tilings of such a region together with the flip dynamical rule define a discrete time Markov chain: at each step, a vertex of the tiling is uniformly chosen at random and if this vertex is surrounded by three tiles in flippable configuration, then we flip it. Since sets of plane rhombus tilings are connected via elementary flips [18], this process can reach any tiling. It converges toward the uniform equilibrium distribution, since it satisfies detailed balance. All the difficulty is to characterize how many flips

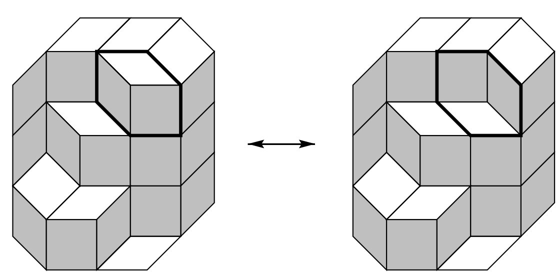

FIG. 1. Examples of octagonal fixed boundary tiling and of elementary flip. We have also displayed (in gray) the de Bruijn lines of a family, among four families. They are lines of adjacent tiles sharing an edge with a fixed orientation.

one needs to get close to equilibrium. Generally speaking, let us consider a Markov chain on a finite configuration space L, which converges toward a stationary distribution π. Let x_0 be any initial configuration and $P(x,t \mid x_0, 0)$ be the probability that the process has reached the configuration x after t steps. Then

$$\Delta(t,x_0) = 1/2 \sum_{x \in L} |P(x,t \mid x_0, 0) - \pi(x)| \qquad (1)$$

usually measures the distance between both distributions [19]. Given $\varepsilon > 0$ we define the *ergodic* or *mixing* time $\tau(\varepsilon)$ so that whatever x_0, after $\tau(\varepsilon)$ steps, one is sure to stay within distance ε of equilibrium:

$$\tau(\varepsilon) = \max_{x_0} \min_{t_0} \{t_0 / \forall\ t \geq t_0, \Delta(t,x_0) \leq \varepsilon\}. \qquad (2)$$

In this Letter, we prove that for a tiling of N_T tiles

$$\tau(\varepsilon) \leq \text{const} \times (N_T)^{\nu} \ln N_T \ln(1/\varepsilon). \qquad (3)$$

More precisely, we establish, with the help of reduced numerical work, that such a bound holds for $\nu = 3$, then we argue that $\nu = 2$ should be the correct exponent. Whatever this exponent, this proves that flip dynamics are rapidly mixing at infinite temperature. As for the $\ln(N_T)$ correction in (3), as discussed in [15], it is a feature of our choice of distance $\Delta(t,x_0)$: a Euclidean norm would not display this correction, but it is less natural in the context of measure of probability distributions convergence.

The coupling technique [19] has been successfully applied to estimate mixing times of several systems, such as hexagonal tilings [13–15]. It relies on the surprising idea that following the dynamics of *couples* of configurations instead of a single one might provide the properties of the original dynamics on single configurations. A *coupling* is a Markov chain on $L \times L$; couples of configurations are updated simultaneously and are strongly correlated, but each configuration, viewed in isolation, performs transitions of the original Markov chain. Moreover, the coupled process is designed so that when both configurations happen to be identical, then they follow the same evolution and remain identical forever. Then the central idea of the technique is that the average time the two configurations need to couple (or to *coalesce*) provides a good upper bound on the original mixing time $\tau(\varepsilon)$: given an initial couple (x_0, y_0) at time $t = 0$, define the *coalescence* time $T(x_0, y_0)$ as the minimum time that both configurations need to coalesce, and the *coupling* time as

$$T = \max_{(x_0,y_0) \in L \times L} \langle T(x_0, y_0) \rangle, \qquad (4)$$

where the last mean is taken over realizations of the coupled Markov chain. The following theorem, central in the coupling approach, provides an upper bound for the ergodic times of the original (*not coupled*) process [19]:

$$\tau(\varepsilon) \leq Te \ln(1/\varepsilon) + 1 \simeq Te \ln(1/\varepsilon), \qquad (5)$$

where $e = \exp(1)$. If the configuration set L can be endowed with a partial order relation $\succeq$ with unique minimum and maximum elements $\hat{0}$ and $\hat{1}$, the implementation of the technique is highly facilitated, provided the coupled dynamics is *monotonous*; i.e., if $x(t) \succeq y(t)$, then $x(t + 1) \succeq y(t + 1)$: let (x_0, y_0) be any initial couple such that $\hat{1} \succeq x_0 \succeq y_0 \succeq \hat{0}$. After any number of steps, the four configurations remain in this order. When the iterates of $\hat{0}$ and $\hat{1}$ have coalesced, the iterates of x_0 and y_0 also have. Thus $T(x_0, y_0) \leq T(\hat{0}, \hat{1})$ and $T = \langle T(\hat{0}, \hat{1}) \rangle$.

A convenient representation of random rhombus tilings was introduced by de Bruijn [20]. It consists of following in tiling lines made of adjacent tiles sharing an edge with a fixed orientation (Fig. 1). The set of lines associated with an orientation is called a de Bruijn family. In an octagonal tiling, there are four families. When removing a family from an octagonal tiling, one gets a hexagonal tiling. Conversely, this enables one to propose a convenient construction of tilings [12,18,21]: directed paths are chosen on a hexagonal tiling, called the *base* tiling. They are represented by dark lines in Fig. 2. They go from left to right without crossing (but they can have contacts). When they are "opened" following a new edge orientation, they generate de Bruijn lines of the fourth family. In this one-to-one representation, a tiling flip involving tiles of the fourth family becomes a path flip: the path jumps from one side of a tile to the opposite side.

Defining couplings on the whole octagonal tiling sets seems to be an infeasible task. We instead use the paths-on-tiling point of view to decompose the configuration space into smaller subsets where couplings can be defined: let J_a denote the set of tilings which have the same base hexagonal tiling a, called "fibers" [18]. L is a disjoint union of fibers. The only possible flips inside J_a are those which involve the fourth de Bruijn family. Note that we can construct four such fibrations, one for each family.

Now, let $\mathcal{M}$ denote the symmetric transition matrix associated with the Markov chain on the whole set L: given two configurations x and y, the matrix entry $\mathcal{M}(x,y)$ is equal to the transition probability $P(x, t + 1 \mid y, t)$. In the same way, we define the symmetric transition matrices

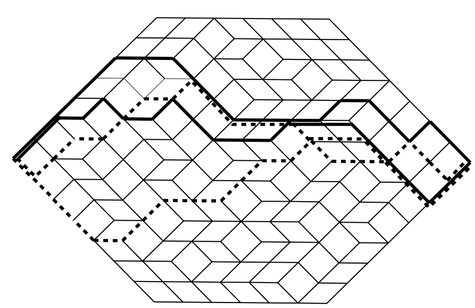

FIG. 2. Example of two-line coupling in the directed path representation. Dark lines represent a configuration and dotted lines the second one. Both configurations form a couple.

$\mathcal{M}_i$ associated with the Markov chains where only flips involving the ith de Bruijn family are allowed. Since fibers have been disconnected, $\mathcal{M}_i$ is block diagonal. The following result interconnects the four fibrations:

$$\mathcal{M} = (\mathcal{M}_1 + \mathcal{M}_2 + \mathcal{M}_3 + \mathcal{M}_4)/3 - \mathrm{Id}/3, \quad (6)$$

where Id is the identity. Indeed, each coefficient $\mathcal{M}(x, y)$ appears in all four matrices $\mathcal{M}_i$ but one, since the corresponding flip involves three de Bruijn lines.

Now we implement the above *coupling technique on each fiber*. To begin with, we suppose that there is only one line in the flipping family, denoted by ℓ. As in Ref. [13], in order to have a monotonous coupling, we slightly modify the Markov chain: at each step, we choose uniformly at random an internal vertex of ℓ, the nth one starting from the left, *and* a number $r \in \{0, 1\}$. If this vertex is flippable upward (downward) and $r = 0$ ($r = 1$), then we flip it. Note that this Markov chain has a time unit different from the original one.

We now define the order relation ($\succeq$): given two lines ℓ_1 and ℓ_2, $\ell_1 \succeq \ell_2$ if ℓ_1 is entirely above ℓ_2. The maximum (minimum) configuration clearly lies on the top (bottom) boundary of the hexagonal domain. If the two flips on ℓ_1 and ℓ_2 occur with the same n and r and if $\ell_1 \succeq \ell_2$, then their images satisfy the same relation. Indeed, as in Ref. [13], thanks to the introduction of r, if a flip could bring ℓ_1 below ℓ_2, then the same flip would also apply to ℓ_2, thus preserving the order between lines: the coupling is monotonous.

In the general case with p nonintersecting lines in each configuration (Fig. 2), let us denote by $\ell_i^{(j)}$, $j = 1, \dots, p$, the p lines of each configuration γ_i. Then $\gamma_1 \succeq \gamma_2$ if for any j, $\ell_1^{(j)} \succeq \ell_2^{(j)}$. The configuration γ is maximum (minimum) when each of its lines is maximum (minimum). At each step, the index j of the line to be flipped is chosen between 1 and p, the same j for both γ_i.

To begin with, we numerically study the diagonal case, where the four sides of the octagonal tilings are equal to k. For a given base tiling $\mathcal{T}_a$, we run a number m of couplings until they coalesce, and then estimate the coupling time $T(\mathcal{T}_a)$. We then make a second average on M different tilings, in order to get the time $\overline{T}$ averaged on tilings $\mathcal{T}_a$. We also keep track of the standard deviation ΔT. From our numerical data (see Fig. 3), we draw the following conclusions: $\Delta T/\overline{T}$ decreases toward a constant ($\simeq 0.07$) as $k \to \infty$, which means that the average coupling time $T(\mathcal{T}_a)$ goes on depending on the base tiling $\mathcal{T}_a$ at the large size limit. However, most $T(\mathcal{T}_a)$ are of order $\overline{T}$, and the mixing times $\tau(\varepsilon)$ on most fibers are controlled by $\overline{T}$. Nevertheless, the effect of few "slower" fibers will deserve a detailed discussion below. Moreover, the measures of $\overline{T}$ are compatible with a $k^4 \ln k$ behavior (Fig. 3, inset). In particular, this fit with logarithmic corrections is much better than a simple power-law fit. This result is consistent with known results in the case of hexagonal tilings [13,15], where T also grows like $k^4 \ln k$.

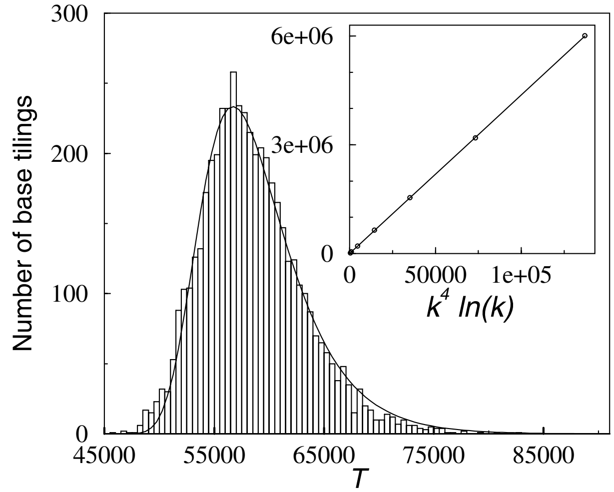

FIG. 3. A distribution of coupling times T in the case of a diagonal base tiling ($k = 10$) and $p = 1$, fitted by a Gumbel distribution [continuous curve; see Eq. (9)]. Inset: in the diagonal case ($k = p$), numerical estimates of $\overline{T}$ in a function of $k^4 \ln k$ (circles), up to $k = 15$, and linear fit. Error bars are smaller than the size of symbols. The slope is 25.51 ± 0.05.

We also have explored coupling times on fibers in nondiagonal cases and our conclusions remain identical. As a consequence, couplings in fibers behave like couplings in hexagonal tiling problems, up to different numerical prefactors: the dynamics on each fiber is rapidly mixing.

Now we return to the dynamics on the whole set of tilings. Examining Fig. 4, one remarks that two fibrations are to a certain extent "transverse": in octagonal tiling sets, one can connect any two tilings using flips of only two fibers [22]; if the dynamics is rapidly mixing in each fiber, the combination of dynamics on two (and even four) fibrations will certainly also be rapidly mixing. We now establish properly this point: it is common in the field of Markov processes to relate rates of convergence to spectra of transition matrices. Generally speaking, given a transition matrix M, 1 is always the largest eigenvalue in modulus, and the difference $g(M)$ between 1 and the second largest eigenvalue is called the first gap of M. Then

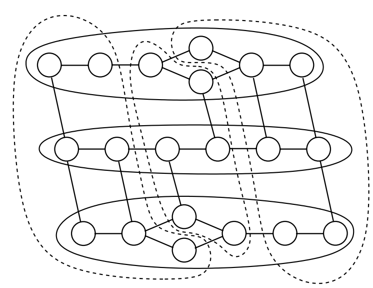

FIG. 4. The lattice of tilings filling an octagon of sides 1, 1, 1, and 2. The edges represent possible flips. Two fibrations among four are represented (continuous and dotted lines).

$\tau(\varepsilon) \simeq \ln(1/\varepsilon)/g(\mathcal{M})$ for small ε [14]. By simple arguments from linear algebra and Euclidean geometry (since matrices are symmetric), the following central gap relation can be established [22], based upon (6) and the smallness of the intersection of two fibers:

$$g(\mathcal{M}) \geq \inf_i\bigl(g(\mathcal{M}_i)\bigr). \tag{7}$$

This result restores the symmetry lost in the fibration process. It implies that the mixing time $\tau(\varepsilon)$ on L is smaller than the mixing time on the slowest fibration derived from (5). Hence $\tau(\varepsilon)$ is smaller than the mixing time on the slowest fiber. We have seen that the average coupling time $\overline{T}$ grows like $k^4 \ln k$ in diagonal cases. Since the number of tiles is $N_T = 6k^2$, $\overline{T} \simeq \kappa_4 N_T^2 \ln(N_T)$, where $\kappa_4 = 1.189 \pm 0.003$ in the original time unit. However, the coupling time T depends on the base tiling $\mathcal{T}_a$ and the distribution of times T in a given fibration have a certain width around $\overline{T}$ (Fig. 3). And even if the typical values of coupling times are of the order of magnitude of the previous average value, this does not exclude the existence of rare slow fibers in the upper tails of these distributions. However, we recall that coupling times T are maxima of coalescence time distributions (4). Therefore the expected shape of the distribution of $T(\mathcal{T}_a)$ ought to be sought in the specific class of extreme-value distributions, namely Gumbel distributions [23]: consider N independent identical random variables T_a, whose probability densities decay rapidly at large T:

$$p(T) \simeq \frac{C_1}{T^\alpha} \exp(-C_2 T^\beta), \tag{8}$$

where C_1, C_2, $\beta > 0$. If $T_{\max} = \max_a T_a$, then at large N, the probability density of $T_{\max}$ satisfies

$$p(u) = \exp[-u - \exp(-u)], \tag{9}$$

where $u = (T_{\max} - T_0)/\delta T$ is a suitably rescaled variable.

Now, even if coalescence times are not strictly speaking independent variables [22], our numerical distributions appear to be well fitted by this kind of distribution (Fig. 3). This result provides the large T behavior of coupling time distributions: $p(T_{\max}) \sim \exp(-u) \sim \exp(-T_{\max}/\delta T)$, and therefore an estimation of the largest coupling time. Let us focus on diagonal cases: T_0 as well as δT behave like $k^4 \ln k$. But for a fibration i, there are N_i base tilings $\mathcal{T}_a$. Therefore if T^* is the largest coupling time on all tilings $\mathcal{T}_a$, it is estimated by $N_i \exp(-T^*/\delta T) \approx 1$. Now N_i grows exponentially with the number of tiles [18]: $\ln N_i \approx C_1 k^2$. Thus

$$T^* \approx C_2 k^6 \ln k \approx C_3 N_T^3 \ln N_T \tag{10}$$

and $\tau(\varepsilon) \leq C_4 N_T^3 \ln N_T \ln(1/\varepsilon)$. However, these extreme values should not be relevant: because of the exponential decay of $p(u)$, slow fibers are rare and can be bypassed via rapid ones. More precisely, perturbation theory arguments suggest that rare slow fibers can be seen as a small perturbation of an otherwise rapid transition matrix and have a vanishing influence on its spectral gap [22]: they do not significantly slow rapid dynamics and the typical coupling time $\overline{T}$ drives the dynamics on fibers, leading to $\nu = 2$ in (3) and const $\approx e\kappa_4$.

What does this analysis become in the case of larger symmetry tilings or of higher dimensional tilings, such as icosahedral ones? Plane rhombus tilings with $2D$-fold symmetry could be addressed by our approach without significant technical complication, leading to laws similar to (3), up to different prefactors, const [22]. As for higher dimensional tilings, the fibration process remains valid, but the connectivity of fibers is not established [18], making impossible a naïve generalization of this approach.

I thank M. Latapy, K. Frahm, R. Mosseri, and D. S. Dean for fruitful discussions.

[1] D. Shechtman *et al.,* Phys. Rev. Lett. **53**, 1951 (1984).
[2] R. Penrose, Bull. Inst. Math. Appl. **10**, 226 (1974).
[3] C. L. Henley, in *Quasicrystals, The State of The Art,* edited by D. P. Di Vincenzo and P. J. Steinhardt (World Scientific, Singapore, 1991).
[4] D. Levine and P. J. Steinhardt, Phys. Rev. Lett. **53**, 2477 (1984); V. Elser, Phys. Rev. Lett. **54**, 1730 (1985).
[5] H. Cohn *et al.,* New York J. Math **4**, 137 (1998).
[6] M. Latapy, in Proceedings of the 12th International Conference on Formal Power Series and Algebraic Combinatorics (to be published).
[7] S. Lyonnard *et al.,* Phys. Rev. B **53**, 3150 (1996).
[8] P. A. Kalugin and A. Katz, Europhys. Lett. **21**, 921 (1993).
[9] R. Blüher *et al.,* Phys. Rev. Lett. **80**, 1014 (1998).
[10] D. Caillard, in *Quasicrystals, Current Topics* (World Scientific, Singapore, 2000).
[11] L. H. Tang, Phys. Rev. Lett. **64**, 2390 (1990); L. J. Shaw, V. Elser, and C. L. Henley, Phys. Rev. B **43**, 3423 (1991).
[12] M. Widom *et al.,* in *Proceedings of the 6th International Conference on Quasicrystals* (World Scientific, Singapore, 1998).
[13] M. Luby, D. Randall, and A. Sinclair, SIAM J. Comput. (to be published).
[14] D. Randall and P. Tetali, J. Math. Phys. (N.Y.) **41**, 1598 (2000).
[15] D. B. Wilson (to be published).
[16] C. L. Henley, J. Stat. Phys. **89**, 483 (1997).
[17] N. Destainville, J. Phys. A **31**, 6123 (1998).
[18] N. Destainville *et al.,* J. Stat. Phys. **102**, 147 (2001).
[19] D. Aldous, in *Séminaire de probabilités XVII,* Springer Lecture Notes in Mathematics Vol. 986 (Springer-Verlag, Berlin, 1983), p. 243.
[20] N. G. de Bruijn, J. Phys. (Paris) **47**, C3–9 (1986).
[21] R. Mosseri and F. Bailly, Int. J. Mod. Phys. B **6&7**, 1427 (1993).
[22] N. Destainville (to be published).
[23] E. J. Gumbel, *Statistics of Extreme* (Columbia University Press, Columbia, 1958).