.

Numerical entropy and phason elastic constants of plane random tilings with any $2D$-fold symmetry

N. Destainville[1]

[1] *Laboratoire de Physique Théorique, IRSAMC - UMR CNRS/UPS 5152*
Université Paul Sabatier, 31062 Toulouse Cedex, France.

Abstract. – We perform Transition matrix Monte Carlo simulations to evaluate the entropy of rhombus tilings with fixed polygonal boundaries and $2D$-fold rotational symmetry. We estimate the large-size limit of this entropy for $D = 4$ to 10. We confirm analytic predictions of N. Destainville *et al.*, *J. Stat. Phys.* **120**, 799 (2005) and M. Widom *et al.*, *J. Stat. Phys.* **120**, 837 (2005), in particular that the large size and large D limits commute, and that entropy becomes insensible to size, phason strain and boundary conditions at large D. We are able to infer finite D and finite size scalings of entropy. We also show that phason elastic constants can be estimated for any D by measuring the relevant perpendicular space fluctuations.

Random tiling models [1,2] have been intensively studied since the discovery of quasicrystals in 1984, because they are good paradigmatic models of quasicrystals. These metallic compounds exhibit exotic symmetries (*e.g.* icosahedral) which are classically forbidden by crystallographic rules. This is accounted for by the existence of underlying quasiperiodic or random tilings. When tiles are decorated in some manner by atoms, these tilings become excellent candidates for modeling real quasycristalline compounds [3]. As compared to perfectly quasiperiodic tilings, some specific degrees of freedom, the so-called *phason flips*, are activated in random tilings, giving access to a large number of microscopic configurations. The number of configurations grows exponentially with the system size in contrast to perfectly quasiperiodic tilings where it only grows polynomially. The resulting configurational entropy lowers the free energy as compared to competing crystalline phases. Despite their random character, random tilings still display the required macroscopic point symmetries in their Fourier spectra. They are as good candidates as perfectly quasiperiodic tilings for modeling quasicrystals [1,2]. The statistical mechanics of random tilings is of central interest for quasi-crystallography. But the calculation of the thermodynamical observables of interest in random tiling models has turned out to be a formidable task. Even the calculation of configurational entropy in the case of *maximally* random tilings where all tilings have the same energy is a notoriously difficult problem. Very few models are exactly solvable [4–9], and a large majority of calculations rely on numerical simulations. In Refs. [10,11], an original analytic mean-field theory for plane rhombus tilings with $2D$-fold symmetry, in the large D limit, was proposed. Its ultimate goal is to derive valuable results on finite D tilings by estimating finite D corrections to the

infinite D limit. The present study intends to support numerically the analytic findings of this promising approach. We propose a calculation of the entropy per tile of rhombus tilings based on a Transition matrix Monte Carlo (TMMC) technique [12]. We get estimates of the large size limit of the entropy for $D \leq 10$ (Table I). Furthermore, we calculate the same entropy for large D tilings filling $2D$-gons of finite side length p. We confirm the theoretical predictions of Refs. [10, 11]: large D and large p limits commute. We also explore the large D behavior of a phason elastic constant by measuring the relevant perpendicular space fluctuations. We show that it decays like $1/D$.

We study tilings that fill centro-symmetric $2D$-gons (Fig. 1). Such fixed boundaries have a strong influence on tilings at finite D (see [11, 12] and references therein). Their most spectacular consequence is that the entropy per tile of fixed-boundary tilings is strictly smaller than its free- or periodic-boundary counterpart. It was also one of the goals of Ref. [11], where these questions are thoroughly discussed, to explore what this difference between fixed and free boundary conditions becomes in the large D limit. It was demonstrated there that, in this limit, all boundary conditions become equivalent. More generally, it was proved that under very weak conditions, the entropy per tile of large D tilings is independent of their size, shape, tile fractions and boundary conditions. The "universal" entropy per tile was estimated by a mean-field approach and numerically calculated : $\sigma_\infty \simeq 0.5676 \pm 0.0001$. It was also argued that some phason elastic constants associated with given strain modes vanish at large D. Our goal here is to explore numerically these predictions in a larger variety of situations.

The tiles considered in this paper are lozenges of unitary side length and of angles multiple of π/D. Their edges are collinear to the D vectors $\boldsymbol{e}_\alpha^\parallel$, $\alpha = 0, \ldots, D-1$ which make angles $\alpha\pi/D$ with an arbitrary direction. In the celebrated *cut-and-project* framework (see [1]), rhombic tiles are considered as the projections onto the 2-dimensional space of the 2-dimensional faces of a hypercube in a space of dimension D denoted by H. Conversely, any tiling in the bidimensional space can be "lifted" to a bidimensional continuous membrane embedded in the $\boldsymbol{Z}^D$ lattice. When this membrane is projected back into the 2-dimensional space, the facets of the D-dimensional lattice project precisely onto the rhombic tiles. The normalized basis vectors of H are denoted by $\boldsymbol{e}_\alpha$. The $\boldsymbol{e}_\alpha^\parallel$ are the normalized projections of the $\boldsymbol{e}_\alpha$ [10]. The physical 2-dimensional space is usually called the *parallel space* and it is denoted here by $\mathcal{E}^\parallel$. The $(D-2)$-dimensional space in H perpendicular to $\mathcal{E}^\parallel$ is called the *perpendicular space*. It is denoted by $\mathcal{E}^\perp$. The normalized projections of the $\boldsymbol{e}_\alpha$ in $\mathcal{E}^\perp$ are the $\boldsymbol{e}_\alpha^\perp$. The $2D$-gons filled by such tiles in the present publication have edges parallel to the $\boldsymbol{e}_\alpha^\parallel$. Their integral side lengths are denoted by p_α. When all p_α are equal to the same p, the tilings are said here to be *diagonal, of side p*. Local moves called single flips are usually used to explore configuration spaces of rhombus tilings. In dimension 2, they consist of the exchange of three tiles that locally fill a small elementary hexagon (see Fig. 1, left). Such flips connect configuration spaces in dimension 2.

Transition matrix Monte Carlo technique. – The previous estimates of the large D entropy [11] relied on an efficient numerical approach in the $p = 1$ case. It cannot, however, be applied to values of $p > 1$ of interest in the present paper, without inextricable technical complications. We chose to apply here a Transition matrix Monte Carlo technique [12]. It is a variant of the transition matrix method [13]. It uses a standard Metropolis Monte Carlo sampling to construct a numerical approximation to the transition matrix. The density of states is calculated from this transition matrix and provides the total number of configurations. The energy E used here in order to implement the Monte Carlo algorithm has no particular physical meaning as far as quasicrystals are concerned. It is related to the structure of the configuration space in terms of partial ordered sets (posets) theory [14]. It involves the description of

rhombus tilings with polygonal boundaries by means of *generalized partitions*, itself related to the cut-and-project technique. Its complete construction is detailed in Refs. [12] and [14] (where it is equal to the so-called "rank function"). There is a unique tiling t_{min} (resp. t_{max}) with minimal energy E_{min} (resp. maximal energy E_{max}) (see Fig. 1, bottom). The energy measures the distance from a given tiling t to t_{min}. A single flip as described above increases or decreases the energy by a single unit, according to whether it increases or decreases the distance from t_{min}. The structure of graded poset [14] ensures that the energy variation between any two tilings does not depend on the choice of the path of flips between these tilings. We find bellow that the energy of most tilings is close to $E_{mid} = (E_{min} + E_{max})/2$. The density of states is symmetric with respect to E_{mid}, because of the geometric centro-symmetry of the problem.
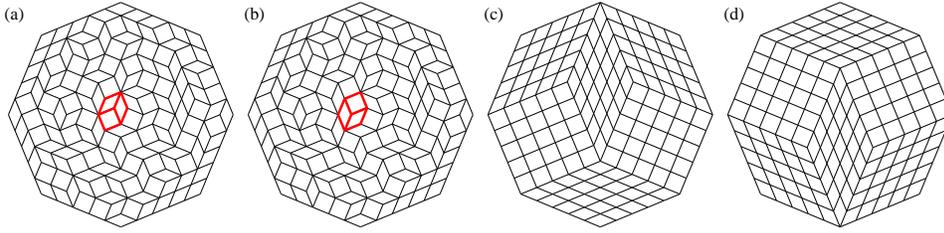

Fig. 1 – Several examples of tilings of side $p = 5$ with $D = 4$. (a,b): two typical random tilings differing by a single flip in the emphasized hexagon. (c,d): Tilings with minimal energy E_{min} (c) and maximal energy E_{max} (d). Tilings (a) and (b) have energies close to $E_{mid} = (E_{min} + E_{max})/2$.

In the Metropolis Monte Carlo algorithm, at temperature $T \geq 0$, a randomly chosen vertex is tried to be flipped if it is flippable. This change is accepted if it lowers the energy. If by contrast the change raises the energy, it is accepted with probability $\exp(-\Delta E/T)$, where ΔE is the energy variation *if the change was accepted*. At low T, tilings are close to t_{min}. At large T, they are in the maximum entropy region, close to E_{mid}. It will also be useful to take negative values of T after adapting suitably the previous transition probabilities. Now we use the fact that the energy variation associated with a single flip cannot be larger than ± 1. As in Ref. [12], we denote by $n_\pm(t)$ the number of tilings that can be reached from a given tiling t by single upwards or downwards flips. For any given tiling t, the numerical calculation of $n_\pm(t)$ is easy and exact. If N_V is the number of tiling vertices, then $n_+(t) + n_-(t) \leq N_V$. Remind that N_V is tiling-independent. In particular, it is unchanged through a single flip.

Now we can define the *transition matrix* $\omega(E, E')$ of dimension $E_{max} - E_{min} + 1$. It is equal to 0 everywhere except on its diagonal and two off-diagonals:

$$\omega(E, E \pm 1) = \frac{1}{W(E)} \sum_{t \in P(E)} \frac{n_\pm(t)}{N_V}, \tag{1}$$

where $P(E)$ is the set of tilings of energy E and $W(E)$ is their number. In addition $\omega(E, E) = 1 - \omega(E, E-1) - \omega(E, E+1)$. The matrix ω is not known and it is the goal of our Monte Carlo algorithm to estimate it by sampling the energy levels E and estimating the exact mean (1) by an approximate average on sampled configurations. The density of states can then be extracted as follows: $\omega_+(E)W(E) = \omega_-(E+1)W(E+1)$ because the total number of forward flips from energy E to energy $E+1$ is exactly equal to the total number of backward flips from energy $E+1$ to energy E. This equation reads $W(E+1) = \omega_+(E)W(E)/\omega_-(E+1)$. It allows

us to iteratively extract the $W(E)$ using uniqueness of the ground state t_{min}, $W(E_{min}) = 1$. Finally, the total number of tilings is $Z = \sum_E W(E)$, the configurational entropy is $S = \ln Z$, and the entropy per tile is $\overline{\sigma}_D(p) = S/N_T$, N_T the number of tiles. To ensure that all energy levels are (almost) uniformly visited, we perform sweeps over temperature, for both positive and negative temperatures. The minimum and maximum temperatures T_{min} and T_{max} must be suitably adjusted to ensure that this distribution is as uniform as possible in order to sample correctly all energy levels. We find that the density of states $W(E)$ is nearly Gaussian, at least near its maximum at E_{mid} [12].

Numerical results. – We first focus on the *diagonal* case where $p_\alpha = p$. Tilings are initialized at minimum energy E_{min} which is chosen to be equal to 0. The maximum energy can be calculated *a priori* [12,14]: $E_{max} = \binom{D}{3} p^3$. We accumulate statistics $n_\pm(t)$ to estimate the transition matrix. The degree to which symmetry of $S(E)$ with respect to E_{mid} is broken serves as an indicator of errors accumulated during the iterative calculation. The residual $R = \ln W(E_{max})$, that should ideally be equal to 0, reflects the cumulative errors in $W(E)$. It can be demonstrated [12] that R is a good indicator of the uncertainty on S at the end of the calculation. It will provide error bars on $\sigma_D(p)$ below. In all cases, error bars will be smaller than 10^{-4} (except for $D \geq 50$ where they will be smaller than 5.10^{-4}).

We begin with the infinite p limit of finite D entropies of diagonal tilings with fixed polygonal boundaries: $\overline{\sigma}_D = \lim_{p \to \infty} \overline{\sigma}_D(p)$. For $D = 4 - 10$, we extrapolate the large p limit by fitting the numerical data obtained *via* the previous algorithm. We choose a second order fit in $1/p$. Contrary to the three-dimensional case [12], we did not observe that logarithmic corrections improved the quality of the fit. Fig. 2 (left) displays $\overline{\sigma}_D(p)$ in function of $1/p$ and the second order fits. The extracted large p limits are listed in Tab. I. We applied the same procedure to the exactly solvable $D = 3$ case (see [1]) and we found that the method provides the exact expected value with a relative precision smaller than 1%. Therefore we anticipate that the relative errors for larger values of D are also smaller than 1%.
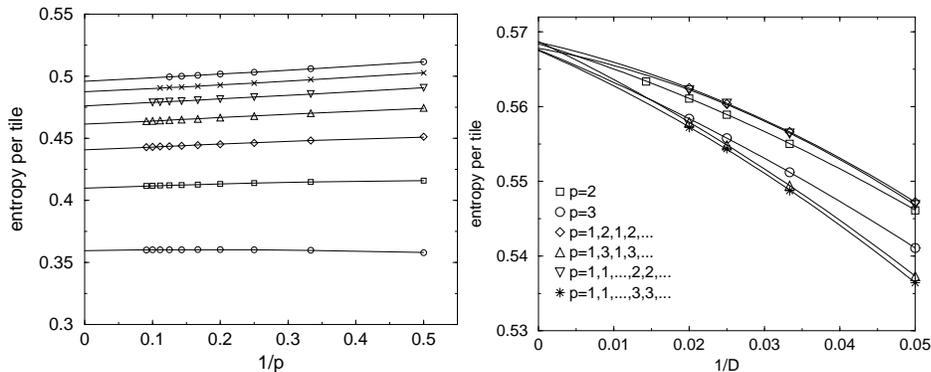

Fig. 2 – Left: Entropies per tile $\overline{\sigma}_D(p)$ *vs* $1/p$ for $D = 4, 5, 6, 7, 8, 9$ and 10 from bottom to top (symbols) and second order fits (lines). Error bars are much smaller than symbol sizes because all errors are smaller than $5 \ 10^{-4}$. Right: Entropies per tile *vs* $1/D$ in various situations (symbols; see text) and their fits at order 2 in $1/D$ (lines). All plots converge towards the "universal" value $\sigma_\infty \simeq 0.5676$ within our uncertainties.

To test the predictions stated above, we also extrapolate the limit $\overline{\sigma}_\infty = \lim_{D \to \infty} \overline{\sigma}_D = 0.563 \pm 0.006$ by fitting the finite D values at order 2 in $1/D$ [11]. The error bar also corresponds to a relative error of 1%. We get $\overline{\sigma}_\infty = \sigma_\infty$ within error bars. This is a first confirmation of

Table I – *Large size limits of the entropy per tile. Relative errors are smaller than 1% (see text).*

D	4	5	6	7	8	9	10
$\overline{\sigma}(D)$	0.360	0.410	0.441	0.461	0.476	0.487	0.496

the predictions under interest. To verify them further, we also calculate the large D limit for finite p. The case $p = 1$ was solely considered in Ref. [11]. We were able to perform more intensive numerical calculations here. The entropy is extrapolated from finite D entropies for $D = 20$ to 70 for $p = 2$, and $D = 20$ to 50 for $p = 3$. We find consistently $\overline{\sigma}_\infty(p = 2) = \overline{\sigma}_\infty(p = 3) = 0.568 \pm 0.006$. Then we consider boundary strains [11], with high frequency, $(p_\alpha) = (1, p, \ldots, 1, p)$, with $p = 2, 3$, as well as low frequency, $(p_\alpha) = (1, \ldots, 1, p, \ldots, p)$, with $D/2$ sides of length 1 (resp. of length $p = 2, 3$). Extrapolating data for $20 \leq D \leq 50$, we also find $\overline{\sigma}_\infty(1, 2, 1, 2, \ldots) = \overline{\sigma}_\infty(1, 3, 1, 3, \ldots) = 0.569 \pm 0.006$ at high frequency strain and $\overline{\sigma}_\infty(1, \ldots, 2, \ldots) = \overline{\sigma}_\infty(1, \ldots, 3 \ldots) = 0.568 \pm 0.006$ at low frequency. These calculations, summarized in Fig. 2 (right), also support the predictions of the "universality" of the large D limit [10, 11]. They also confirm the commutation of the large p and large D limits.

Now we examine finite p and finite D scalings. *A priori*, if there are not logarithmic corrections, the Taylor expansion of $\overline{\sigma}(D, p)$ at order 2 in powers of $1/p$ and $1/D$ reads

$$\overline{\sigma}(D, p) \simeq \overline{\sigma}_\infty + \frac{a}{p} + \frac{b}{D} + \frac{c}{p^2} + \frac{d}{p\,D} + \frac{e}{D^2}. \tag{2}$$

Since $\overline{\sigma}(\infty, p) = \overline{\sigma}_\infty$, $a = c = 0$. Moreover, at fixed $D = D_0$ and at first order in p, $\overline{\sigma}(D_0, p) \simeq \left(\overline{\sigma}_\infty + \frac{b}{D_0} + \frac{e}{D_0^2}\right) + \frac{d}{D_0}\frac{1}{p}$. From the fit of the data displayed in Tab. I, we get $b \simeq -0.57$ and $e \approx -1$. It is not possible to get a reliable estimate of d by fitting the available small D_0 data. Indeed, it appears that the slopes d/D_0 do not have reached their asymptotic regime at $D = 10$ because they are still increasing with D_0. However, fitting these available slopes at the second order in $1/D_0$ provides the rough estimate $d \approx 0.2$. In addition, at fixed $p = p_0$ and at first order in $1/D$, Eq. (2) becomes $\overline{\sigma}(D, p_0) \simeq \overline{\sigma}_\infty + (b + d/p_0)/D$. Fitting the data for $p_0 = 2$ and $p_0 = 3$ gives respectively $b + d/2 \simeq -0.31$ and $b + d/3 \simeq -0.41$, from which we get $b \simeq -0.61$ and $d \simeq 0.60$. These values are compatible with the previous ones. In particular, both values of b match very well, whereas they are extracted from the numerical data in a different way: in the first case, we take the infinite p limit first, and in the second case, the infinite D limit first. This confirms *a posteriori* the general expression (2). In particular the two limits commute; There are probably no logarithmic corrections in (2).

Phason elastic constants. – Now we use the previous algorithm to estimate phason elastic constants. Even though we are working on fixed-boundary tilings, our goal is to measure elastic constants associated with *free*-boundary ones. We use the notations and the conventions of Ref. [10]. In particular, the normalizations must be precisely prescribed: we define 3 scalar products in H, $\mathcal{E}^\parallel$ and $\mathcal{E}^\perp$ denoted by $\langle .|.\rangle_V$ where V is the space under consideration. If $\boldsymbol{x}, \boldsymbol{y} \in \mathcal{E}^\perp$, $\langle \boldsymbol{x}|\boldsymbol{y}\rangle_{\mathcal{E}^\perp} = s_\perp^2 \langle \boldsymbol{x}|\boldsymbol{y}\rangle_H$ with $s_\perp^2 = D/(D-2)$ [10]. In a similar way, $s_\parallel^2 = D/2$. With these conventions, we get $\|\boldsymbol{e}_\alpha\|_H = \|\boldsymbol{e}_\alpha^\perp\|_{\mathcal{E}^\perp} = \|\boldsymbol{e}_\alpha^\parallel\|_{\mathcal{E}^\parallel} = 1$, as desired.

We also employ here a useful variational principle (see [12] and references therein) to write the entropy in a practical field-theoretic manner. After coarse-graining [1], large size tilings are represented by regular height functions $\phi : \boldsymbol{R}^2 \to \boldsymbol{R}^{D-2}$. Such a "macroscopic" variable represents a large number $N(\phi)$ of tilings, whose membrane representation in $\boldsymbol{Z}^D$ is equal, after coarse-graining, to the graph of ϕ. Their micro-canonical entropy $\log(N(\phi))$ is equal to

a functional $S[\phi]$, which is the integral over the tiled domain Σ of a function $\sigma(\nabla\phi)$ of the gradients of ϕ [1]. The maximization of $S[\phi]$ gives a (unique) function $\phi^{(0)}$ which represents the dominant tilings in the statistical ensemble under consideration. The random tiling model states that $\sigma(\nabla\phi)$ has a unique maximum, corresponding to tile fractions maximizing (in the present case) the $2D$-fold rotational symmetry. The orientation of the real space $\mathcal{E}^{\parallel}$ is chosen so that the gradients are zero at this maximum, and the model states that the entropy density has a quadratic behavior near this maximum: $\sigma(\nabla\phi) = \sigma_{\max} - \frac{1}{2} \nabla\phi \cdot \mathbf{K} \cdot \nabla\phi + o(|\nabla\phi|^2)$. By analogy with an usual elastic theory, the tensor $\mathbf{K}$ is called the tensor of *phason elastic constants*. In the basis of the perpendicular space $\mathcal{E}^{\perp}$ where $\mathbf{K}$ is diagonal, the previous quadratic form becomes $\sigma(\nabla\phi) = \sigma_{\max} - \frac{1}{2} \sum_{i=0}^{D-3} \kappa_i (\nabla\phi_i)^2 + o(|\nabla\phi|^2)$. We denote by $\boldsymbol{\theta}_i$ the normalized (in $\mathcal{E}^{\perp}$) eigenvector of $\mathbf{K}$ corresponding to the eigenvalue κ_i. We set

$$O_i[\phi] = \int_{\Sigma} \phi(r) \cdot \boldsymbol{\theta}_i \, d^2 r. \tag{3}$$

$O_i[\phi]$ is the mean height of ϕ in the direction $\boldsymbol{\theta}_i$. As written above, the total entropy of a function ϕ is $S[\phi] = \int_{\Sigma} \sigma(\nabla\phi(r)) \, d^2 r$. To calculate the entropy $S(O_i)$ of the tilings of Σ whose mean height is O_i, we introduce the Lagrange multiplier λ_i and we now maximize $G_i[\phi] = S[\phi] + \lambda_i O_i[\phi]$. Without loss of generality we focus on G_0. Then differentiating G_0 with respect to ϕ, we get, at first order in ϕ and its gradients, the equations $\frac{\delta G_0}{\delta\phi_0} = \kappa_0 \Delta\phi_0 + \lambda_0 = 0$ and $\frac{\delta G_0}{\delta\phi_i} = \kappa_0 \Delta\phi_i = 0$ for $i > 0$, together with the condition that ϕ matches the boundary conditions induced by the tiling ones. Let $\phi^{(0)}$ be the function maximizing $S[\phi]$, which also satisfies $O_0[\phi^{(0)}] = 0$, and $\phi^{(1)} \equiv \phi - \phi^{(0)}$. By construction, $\phi^{(1)} \equiv 0$ at the boundary of Σ. The only non-zero coordinate of $\phi^{(1)}$ is $\phi_0^{(1)}$. It satisfies $\Delta\phi_0^{(1)} = -\lambda_0/\kappa_0$. At the large D limit, Σ tends towards a disk of radius $R = pD/\pi$ [10,11]. Taking into account the condition $\phi_0^{(1)} = 0$ on this circle, we get $\phi_0^{(1)}(r) = -\frac{\lambda_0}{4\kappa_0}(r^2 - R^2)$. Thus $O_0[\phi^{(1)}] = -\frac{\pi}{8}\frac{\lambda_0}{\kappa_0}R^4$ and $\lambda_0 = -\frac{8\kappa_0 O_0}{\pi R^4}$. One finally gets the relation (generalized to any i):

$$S(O_i) = S[\phi^{(0)} + \phi^{(1)}] = S(0) - \frac{1}{2} 8\pi^3 \kappa_i \left(\frac{O_i}{p^2 D^2}\right)^2 \tag{4}$$

for a diagonal tiling of side p with (large) $2D$-fold symmetry. Therefore at $T = \infty$, the equilibrium fluctuations of O_i satisfy $\langle O_i^2 \rangle = \frac{p^4 D^4}{8\pi^3 \kappa_i}$ because of the Gaussian character of the number $\exp(S(O_i))$ of tilings with mean height O_i. The measure of $\langle O_i^2 \rangle$ gives access to κ_i.

Before giving our numerical results, we discuss the validity of this calculation. It relies on the quadratic approximation above, which is itself valid if $\nabla\phi^{(0)} \cdot \mathbf{K} \cdot \nabla\phi^{(0)} \ll \sigma_{max} = O(1)$. Now $|\nabla\phi^{(0)}|^2 = O(1/D)$ in finite D tilings and phason elastic constants are bounded [10,11]. Thus the quadratic approximation is valid at large D and we get asymptotically exact estimates of the κ_i. But at finite D, this approach cannot be expected to provide accurate results. For example, if $D = 3$ one calculates that $|\nabla\phi^{(0)}|^2$ can be as large as 4 in large macroscopic regions near the boundary, and the previous argument collapses. We exemplify this procedure on $\boldsymbol{\theta}_z = \frac{\sqrt{D-2}}{D} \sum_{\alpha=0}^{D-1} (-1)^\alpha \boldsymbol{e}_\alpha$ [1]. One checks that $\|\boldsymbol{\theta}_z\|_{\mathcal{E}^{\perp}} = 1$. It is an eigenvector of $\mathbf{K}$ if and only if D is even because it belongs to a one-dimensional irreducible representation (irrep) in H of the symmetry group of the $2D$-gon, C_{2Dv}. This irrep exists only if D is even. $\boldsymbol{\theta}_z$ is a discrete component of $\mathcal{E}^{\perp}$ since for any α, $\langle \boldsymbol{\theta}_z | \boldsymbol{e}_\alpha^{\perp} \rangle_{\mathcal{E}^{\perp}} = \pm 1/\sqrt{D-2}$ and any tiling vertex is represented in $\mathcal{E}^{\perp}$ by a point of coordinate multiple of $1/\sqrt{D-2}$ along $\boldsymbol{\theta}_z$.

Table II – *Large p estimates of the phason elastic constant κ_z.*

D	5	7	9	11
κ_z	0.76	0.59	0.45	0.38

Tab. II gives the so-obtained values of κ_z in the large p limit for $D = 5, 7, 9, 11$. The limits are estimated by a fit of κ_z at order 2 in $1/p$. They clearly indicate that $\kappa_z \propto 1/D$ for the values considered here. Thus our conclusion is that κ_z vanishes at large D, proportionally to $1/D$, as predicted in Ref. [10]. However the elastic constants studied there were different from κ_z since they were associated with fluctuations of the de Bruijn lines separations, and existed whatever the parity of D. This result is in agreement with the universality of the large D entropy per tile: since $|\nabla\boldsymbol{\phi}^{(0)}|^2 = O(1/D)$, the corrections to σ_∞ vanish at large D like $1/D^2$.

We have mentioned that this method cannot be expected to give reliable results at finite D and it is indeed what we observed for $D = 3$. However, for $D = 5$, we already find, with the conventions of normalization of [1], $\kappa_z \simeq 0.26$. This value is close to the expected one $\kappa_z = 0.29$ [1]. In principle it is possible to apply the same procedure to other phason elastic constants κ_i. But determining the corresponding $\boldsymbol{\theta}_i$ is a tedious task, requiring a complete description of $\mathcal{E}^\perp$ in terms of irreps of C_{2Dv}. This goes beyond the scope of the present paper.

Conclusion. – The computational power provided by the Transition matrix Monte Carlo technique allowed us to investigate random tilings with $2D$-fold rotational symmetry in their large size, large D limit. The numerical entropies obtained strongly support the analytic predictions of previous publications [10, 11] and go into the direction of a large D "universal" entropy independent of size, shape, tile fractions and boundary conditions. This work shows that the knowledge of a few adjustable parameters that can be estimated by finite D and finite p fits is sufficient to get a good estimate of finite D entropies of physical interest (see Eq. (2)). For example, the fact that the numerical value of $|e|$ is of the order of 1 shows that the expansion of the finite D, infinite p, fixed-boundary entropies at the first order in $1/D$ is accurate within few percents as soon as $D \geq 4$. By contrast, the direct transposition of the present results to the more physically relevant, finite D free-boundary tilings, is less immediate since it requires the numerical knowledge of phason elastic constants.

We have demonstrated that the estimation of these phason elastic constants for free-boundary, finite D tilings is feasible with a good accuracy. However, we did not tackle this task in the general case but we have demonstrated its feasibility in a general framework. In the case studied here, the phason elastic constant κ_z falls off like $1/D$, in agreement with earlier predictions [10].

This work also illustrates that even though polygonal boundaries are not physical [12], fixed-boundary tilings are adapted to get valuable information on their free- or periodic-boundary counterpart. They present the great advantage of being conveniently coded and manipulated in a computer memory, in particular in relation with the *partition techniques* used in several publications (see [11, 12, 14] and references therein).

$$* * *$$

8

REFERENCES

[1] C.L. Henley, *Quasicrystals, the State of the Art*, edited by D.P. Di Vincenzo and P.J. Stein-
     hart (World Scientific, Singapour) 1991, p. 429.
[2] V. Elser, Phys. Rev. Lett., **54** (1985) 1730.
[3] M. Mihalkovic, *et al.*, Phys. Rev. B, **65** (2002) 104205.
[4] H.W.J. Blöte and H.J. Hilhorst, J. Phys. A: Math. Gen., **15** (1982) L631.
[5] M. Widom, Phys. Rev. Lett., **70** (1993) 2094.
[6] P. Kalugin, J. Phys. A: Math. Gen., **27** (1994) 3599.
[7] J. de Gier and B. Nienhuis, Phys. Rev. Lett., **76** (1996) 2918.
[8] J. de Gier and B. Nienhuis, J. Phys. A: Math. Gen., **31** (1998) 2141.
[9] B. Nienhuis, Phys. Rep., **301** (1998) 271.
[10] N. Destainville, M. Widom, R. Mosseri and F. Bailly, J. Stat. Phys., **120** (2005) 799.
[11] M. Widom, N. Destainville, R. Mosseri and F. Bailly, J. Stat. Phys., **120** (2005) 837.
[12] M. Widom, R. Mosseri, N. Destainville and F. Bailly, J. Stat. Phys., **109** (2002) 945.
[13] J.S. Wang, T.K. Tay and R.H. Swendsen, Phys. Rev. Lett., **82** (1999) 476.
[14] V. Desoutter and N. Destainville, J. Phys. A: Math. Gen., **38** (2005) 17.