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Dense Periodic Packings of Regular Polygons

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Abstract. — We show theoretically that it is possible to build dense periodic packings, with quasi 6- fold symmetry, from any kind of identical regular convex polygons. In all cases, each polygon is in contact with $z = 6$ other ones. For an odd number of sides of the polygons, 4 contacts are side to side contacts and the 2 others are side to vertex contacts. For an even number of sides, the 6 contacts are side to side contacts. The packing fraction of the assemblies is of the order of 90%. The predicted patterns have also been obtained by numerical simulations of annealing of packings of convex polygons.

1. Introduction

Many physical properties of granular media are related to their porosity or, alternately, to their packing fraction. For example, some properties of the grain space such as electrical (for conducting grains) or mechanical behaviours are improved by compaction.
Generally, realizations of dense packings do not allow to go much beyond packing fractions of the order of 80% in 2d or 60% in 3d. However, it is well known that in the case of identical grains (same shape, same size), provided they are not too exotic, higher packing fractions may be reached. In 2d, regular triangles, squares and hexagons may fill the plane and the densest configuration for identical discs ($C \approx 91\%$) is realized when their centers are the sites of a regular triangular array, while it is lower than 82% in the disordered case [1,2]; a similar behaviour is found for ellipses [3]. The situation is a little less clear in 3d: the densest known arrangement for identical spheres ($C = 74\%$) is the hexagonal close-packed structure, but this is not the only solution and it has not yet been proved that it has the highest possible packing fraction.

In all these cases, the densest solution is periodic. Surprisingly, a similar result was obtained in recent 2d compaction experiments on regular identical pentagons, although no long range order should be *a priori* expected here. We reached a packing fraction of 92% with the following characteristics: the arrangement is periodic, with a mirror symmetry and a quasi 6-fold

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symmetry [4]. Though it is not yet proved, it seems that this is the densest possible packing for regular pentagons. Actually, this configuration was predicted some years ago in the context of quasicrystal theory [5].

The aim of the present paper is to show that similar patterns hold for any kind of (identical) convex regular polygon assembly, i.e. that there exists a dense disposition of the grains which is periodic and quasi 6-fold. For obvious reasons, we have not considered triangles, squares and hexagons. For all other polygonal grains, the packing fraction is high and always close to 90%. In Section 2, we recall the pentagonal case and sketch briefly the experimental method of compaction — close to an annealing process [4]. In Section 3, we derive the possible 6-fold periodic arrangement for any kind of polygonal assemblies, by generalizing the theoretical calculation of reference [4]. Section 4 is devoted to numerical calculations for pentagons, heptagons and octagons which provide the predicted disposition. A short discussion is given in the conclusion.

2. Pentagonal Assemblies

It is known from some time that compaction of polygonal grains when friction forces are important provides disordered packings with a maximum packing fraction which increases with the number of sides of the grains from approximately 78% for pentagons up to C = 80% for ennagons and C = 84% for discs [6]. A better compaction is obtained when friction forces are suppressed, and this was realized for example on an air cushion table built in Rennes University for that purpose. We recall here briefly the experiment performed with regular pentagons [4].

The experimental device was described in detail in reference [7]: a wind machinery generates a vertical air flux through an horizontal porous table (50×50 cm^2). The strength of the flux can be controlled and the table is adjusted to be perfectly horizontal when the voltage at the ends of the ventilation system is 150 V. Small polygonal grains (6 mm sidelength and 1 mm thickness) made of polystyrene move above the table and rearrange permanently because of the small heterogeneities of the air flux, and after a short thermalization time the assembly reaches a stationary state. When the air flux is strong, a short range repulsion due to the air expulsion is present and the effective size of the grains may be 10% larger than the real one so that the collective behaviour of pentagonal grains is not very different from that of discs. When one decreases the voltage, the grains slow down, the effective radius decreases and the table bends down a little so that the grains concentrate in a smaller zone near the center of the table; compaction is thus the combination of the reduction of the air flux and the diminution of the active region.

This technique, similar to an annealing process, was performed progressively. At each step, we waited long enough so that the system reached again the equilibrium. Snapshots were taken at different times and we determined the corresponding diffusion patterns for the centers of the grains. For voltages less than 90 V, these patterns show the progressive setting of a quasi 6-fold symmetry; when the voltage is definitely turned off, the grains themselves are rearranged densely, in a periodic way, with a mirror symmetry. The theoretical lattice is shown in Figure 1, the 3 translational directions $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ ($\mathbf{a} + \mathbf{c} = \mathbf{b}$) are indicated. The 3 angles are respectively 59°3, 64°7, 56° and the 3 lengths a, b, c differ by less than 10% (Tab. I, first line). The unit cell is made of 2 pentagons plus 4 triangles in the void space. This configuration is quite remarkable as no *a priori* long range order could be expected with pentagonal grains. Actually, such a lattice was predicted using arguments related to quasi crystal theory [5]; some previous experimental evidence is referred to in [8].

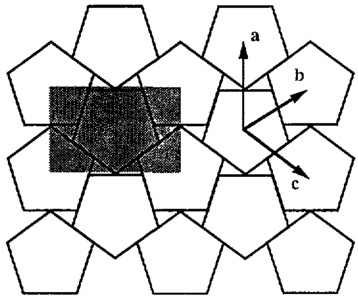


Fig. 1. — Theoretical crystal with pentagons. The 3 translational axes **a**, **b**, **c** are shown. Angles in the triangles of the void space are $2\pi/5$, $2\pi/5$ and $\pi/5$; the side to vertex contacts take place at the middle of the pentagon side and the same is true for the side to side contacts. The grey rectangle is the unit cell of the lattice.

Table I. — *Characteristics of the lattice when k is odd. The lengths are given in terms of the radius R of the circumscribed circle.*

k odd : $z_{ss} = 4$

k	n	C	a	b in terms of R	c	(**a**, **b**)	(**b**, **c**)	(**c**, **a**)
5	3	0.92131	1.8090	1.6583	1.7215	59°3	64°7	56°0 [4], [5]
7	4	0.89269	1.9010	1.9609	2.0393	63°7	56°7	59°6
9	5	0.89745	1.9397	1.9705	1.8806	57°5	60°4	62°1

The average number of contacts per grain is 6 and 6 is also the maximum possible number of contacts locally: two of them are vertex to side contacts, the other 4 are side to side contacts and we proved that 4 is the maximum average possible value for pentagons [4]. The packing fraction C is high ($C = 0.921$), slightly higher than for discs ($C = 0.907$), but we were not able to prove that it is the highest possible packing fraction: large scale reorganizations may occur which may yield a densest–less ordered–packing (R. Mosseri, private comm.).

3. Theoretical Predictions

We recovered this structure theoretically, counting the lines and vertices in the graph drawn by grains and the polygonal holes in the void space [4]. These arguments can be generalized to any kind of regular convex polygon assembly. We show below that we can get a dense periodic pattern with a quasi 6-fold symmetry. The packing fraction is high again and close to 90%.

3.1. Basic Equations. — The granular medium is made of regular convex polygons with k sides. The polygons cannot overlap (steric exclusion) but may be in contact. These contacts are generically of 2 kinds: side to side and side to vertex, other possibilities may be considered as limiting cases (Fig. 2). Let z_{ss} and z_{sv} be the average number of side to side and side to vertex contacts per polygon and let $z = z_{ss} + z_{sv}$ the total average coordination number.

The packing fraction may be estimated through the holes in the void (pore) space. The void space is made of non convex polygons with an unknown number n of sides (Fig. 3). Topological

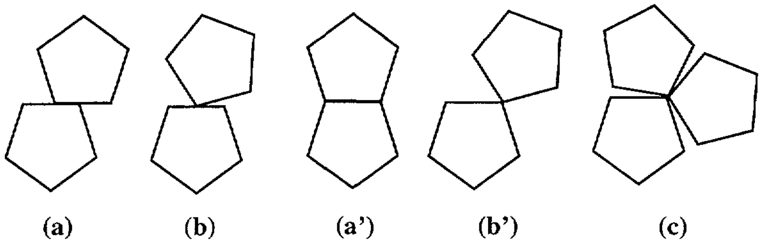


Fig. 2. — Definition of side to side (a) and vertex to side contacts (b) and corresponding limit cases (a$'$ and b$'$). For pentagons only (actually when $k \leq 6$), 3 grains may occur exceptionally at the same point but again, this case may be considered as a limit one (c).

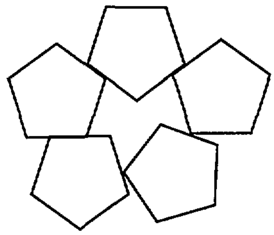


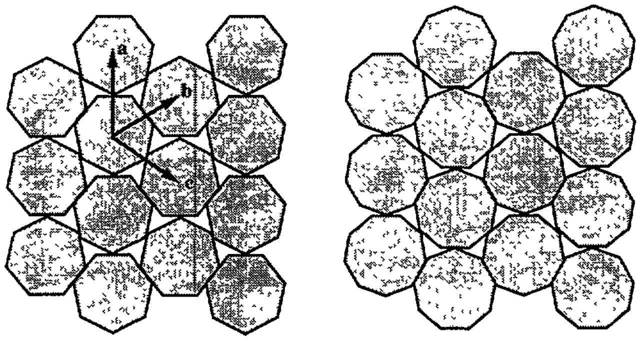
Fig. 3. — A polygonal hole in the void space (for $k = 5$). Here, $n = 8$, $\phi(n) = 3$ and $\alpha(n) = 3$. (See Appendix for notations).

and metric relations connect the distribution number P_n and angle repartition of the n-sided holes to the partial coordination numbers of the grains. They are derived in the Appendix (Eqs. (A.1)-(A.3)). For example, the number of holes per grain depends only on the total coordination number (Eq. (A.1a)) and the average coordination number z is less than 6 (Eq. (A.1d)). Actually, it may be shown that 6 is also the local maximum number of contacts.

3.2. Maximum Coordination Numbers. — The underlying assumption is that 6-fold compact packings are realized when $z = 6$ and z_{ss} is maximal.

i) $z = 6$. Then, equations (A.1b) and (A.1c) are identical. The number $\phi(n)$ of angles corresponding to the corners of the polygonal grains is equal to $n-3$. This means that in each hole only 3 grains are involved. Because of the metric relations (A.2), only 3 values of n are allowed, which depend on the parity of k, with a condition on the sum of the measures of the 3 acute angles.
k even: $k = 2p$ and $n = p, p+1, p+2$
k odd: $k = 2p+1$ and $n = p+1, p+2, p+3$.

ii) The further requirement that z_{ss} is maximum implies that the number of side to side contacts (≤ 3) in a hole polygon is maximum.
When k is even, 3 side to side contacts are possible if $n = p$.
When k is odd, the largest side to side contact number in a hole polygon is 2 when $n = p+1$. The remaining angle has a measure $\dfrac{\pi}{k}$.



(a) (b)

Fig. 4. — Periodic dense patterns with odd k. a) $k = 7$; b) $k = 9$. For $k = 9$, a few percent are lacking for having 2 sides in contact on their whole length. The packing fraction is $C = 0.8927$ for $k = 7$ and $C = 0.8975$ for $k = 9$.

3.3. Periodic Patterns. — Putting the above results all together, we focus on the case where only one species of hole is present in the void space i.e.:

$$k = 2p, \quad n = p \quad z_{ss} = z = 6. \tag{1a}$$

$$k = 2p + 1, \quad n = p + 1 \quad z_{ss} = 4, z = 6 \tag{1b}$$

Notice that all angles are then determined, but the lengths are not. We shall thus assume further that, in the void space

- all polygons are equal (same side lengths)
- some symmetry must hold

so that periodicity may exist. These configurations are actually possible and explicit realizations for $k = 7$, 9 and $k = 8$, 10 are shown in Figures 4 and 5 respectively.

In the odd case (Fig. 4), the side to vertex contacts take place at the middle of the side and the polygons are alternatively up and down with a minimum pattern involving 2 grains and 4 holes (mirror symmetry). The 3 directions **a**, **b**, **c** ($\mathbf{b} = \mathbf{a} + \mathbf{c}$) are shown for $k = 7$; the angles and lengths (reported to the radius R of the circumscribed circle) are given in Table I, last columns. There is a small distortion, less accentuated when the number of sides increases, as compared to the pure hexagonal case.

In the even case, one first notes two opposite limit cases: either 2 contacting grains have a common side or one of the contacts is restricted to a vertex to vertex contact. Both of them yield periodic patterns, with 2 orthogonal mirror symmetries and a minimum pattern involving 1 grain only. Two lengths and two angles are equal ($b = c$ and $(\mathbf{a}, \mathbf{b}) = (\mathbf{a}, \mathbf{c})$ in our notations, see Tab. II; for $k = 12$, the 6-fold symmetry is exact, as expected). The first possibility, shown in Figure 5a for $k = 8$ and $k = 10$, gives a packing fraction larger than the second one. Between the two limit cases, there is a set of configurations which can be obtained by continuous gliding of the grains but they have no longer the mirror symmetry. One of these intermediate situations is shown in Figure 5b.

As there are 2 holes for one grain (Eq. (A.1a)) , the packing fraction C is

$$C = \left[1 + 2\frac{\text{area of one hole}}{\text{area of the grain}}\right]^{-1} \tag{2}$$

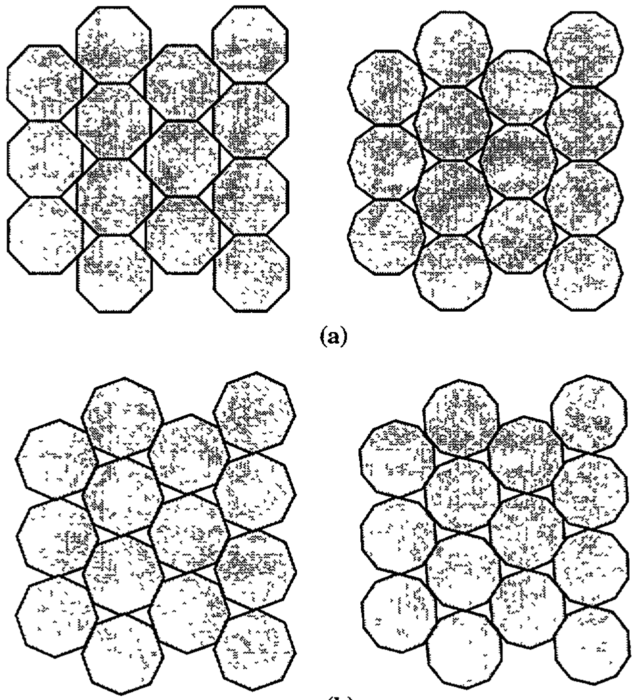


Fig. 5. — Periodic dense patterns with even k. a) limit case with 2 full side to side contacts; b) intermediate situation between the two possible limit cases. Left: $k = 8$; right: $k = 10$. In configurations (a), the packing fraction is $C = 0.9062$ for $k = 8$ and $C = 0.9137$ for $k = 10$; it is smaller in configurations (b).

Table II. — *The same as Table I when k is even. The 2 possible limit patterns are given. In the first case, the polygons of the void space are degenerated. Discs are indicated for comparison.*

k even : first case $z_{ss} = 6$
second case $z_{ss} = 4$ (+ 2 vertex to vertex contacts)

k	n	C	a	b (= c)	**(a, b) = (a, c) ≠ (b, c)**	
			in terms of R			
8	4 (---> triangles)	0.90616	1.8478	1.9254	61°3	57°4
	4	0.89180	2.	1.8748	57°75	64°5
10	5 (--> quadrilateral)	0.91371	1.9021	1.9667	61°1	57°8
	5	0.90450	2.	1.9077	58°4	63°2
12			$a = b = c$		**(a, b) = (b, c) = (a, c)**	
	6 (--> triangles)	0.92820	1.9318		60° [11]	
	6	0.86602	2		60° [11]	
[discs	∞	0.90689	2		60°]	

They are indicated in Tables I and II, column 3. In all cases, they are close to 90%. As z and z_{ss} are both maximum, the question arises whether this is or not the densest possible packing. This problem will be tackled in the last section.

4. Numerical Simulations

The above configurations may probably be recovered from densification on the air table as explained in Section 2; this will be done in a later work. At the present time, we began numerical simulations, first with the pentagonal case, then with hexagons, heptagons and octagons. We use a program performed by Tillemans and Herrmann in Jülich [9], which handles the evolution of an assembly of convex polygons (the polygons must have more than 3 sides) using molecular dynamics. Two forces are applied on each polygon of the system, a central force oriented towards the center of the packing and a viscous friction between the polygons and the floor. The trajectories are computed using a fifth order predictor corrector method [10]. The polygons which collide during their motion are allowed to have a small overlap but the elastic modulus and the central force are adjusted in order that the overlapping area remains very small compared to the area of a polygon. When two polygons overlap, two forces act on them at the point of contact (the point of contact is defined as the middle of the contact line built by taking the two points of intersection of the sides of the overlapping polygons), a restoration force proportional to the overlapping area and normal to the contact line and a normal dissipation proportional to the normal component of the relative velocity of the two polygons. A shear friction may also have been used but, as explained below, we set it to zero in the simulations.

We start with a random packing of regular n-sided polygons with an initial packing fraction $C = 0.15$. The central force is applied on the packing and we let the system evolve towards a steady configuration. Our aim is to find the configuration with the highest packing fraction. So we adjust the parameters of the simulations as follows. First, it is necessary to have energy dissipation to reach a steady state. But the energy dissipated during collision has to be as low as possible, otherwise there will be some sticking of the particles which will oppose the densification. In particular, the shear friction has to be zero in order to prevent arching. Thus we only keep a small normal dissipation and a small friction with the floor. We set those parameters in order to reach the steady state after about 80 000 time iterations. With those conditions, a lot of local rearrangements occurs before the stabilization (the final packing has a kinetic energy close to 0). Another point is that the central force introduces a singularity at the center of the attraction. If the force center is not exactly situated at the center of inertia of the packing, small oscillations of the packing around the force center appear, leading to long range shearing in the packing. These oscillations contribute to increase the final packing fraction.

In order to check the theoretical predictions of Section 3, we have made simulations with pentagons, hexagons, heptagons and octagons. Each packing was made of 500 polygons. All the simulations lead to wide well crystallized areas as predicted by the theory. An example of the resulting packing is shown in Figure 6 for octagons. One can see that the agreement with the theoretical packing of Figure 5a is very good. With hexagons, we get a perfect tiling of the plane. For an odd number of sides, the crystallized zones are smaller; this was also the case with pentagons in experiments on the air table, probably because the 2 side to vertex contacts are not very stable.

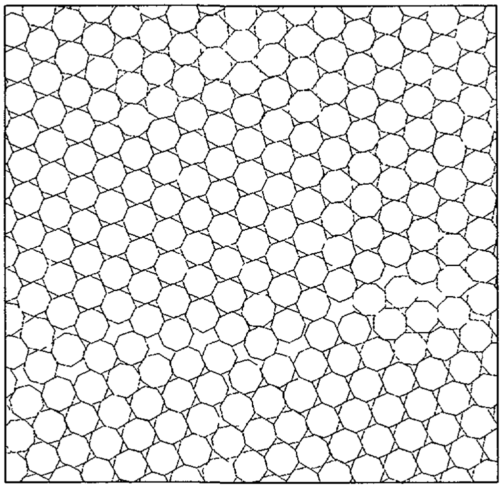


Fig. 6. — Packing of octagons obtained by numerical simulation.

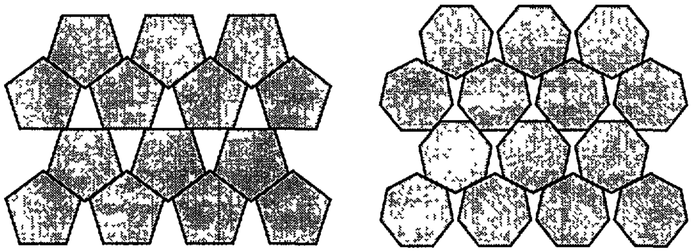
5. Discussion

We have extended to any kind of regular identical convex polygons the method initiated for pentagons. We found theoretically, then recovered numerically dense periodic configurations which

- optimize the average number of side to side and of all contacts
- are periodic with 2 orthogonal symmetries (even case) or a mirror symmetry (odd case)
- are quasi 6-fold with a small distortion which decreases when the order of the polygon increases
- have a high packing fraction, close to 90%.

Most of these patterns are new, and are not to be found in the reference book by Grünbaum and Shephard [11]. The odd case ($k = 7, 9, 11$) is specially interesting as no long range order from any kind seems to be *a priori* expected from such grains. The theoretical derivation is quite simple and relies mainly on the topological equations (A.1) but we were not able to find a close formula for the packing fraction at any k. Other periodic patterns may be obtained from theses relations, by imposing that all angles are $2\pi/k$ or π/k and/or only a finite (small) number of kind of holes are present. For example, we recover the periodic structures for pentagons shown in Figure 8 of reference [5]. Periodic patterns with 4 side to side contacts (and no side to vertex contacts) per grain exist for any k; some examples with odd k ($k = 5, 7$ - even k is straightforward) are shown in the Figure 7. To end off with these theoretical considerations, let us note that equations (A.1) hold with little change for any mixture of irregular different convex polygonal grains; then, $z = 6$ is a maximum average for any polydisperse assembly of convex grains.

The main difficulty left is deciding whether or not the patterns in Figures 4 and 5 are the densest ones for regular grains. It is a difficult mathematical problem as we are not sure that the simplest periodic arrangement yields the best packing fraction. It is probably true when k is even as the number z_{ss} ($= 6$) of side to side contacts is also the absolute local



(a) (b)

Fig. 7. — Periodic patterns when k is odd with a unique kind of hole and 4 contacts: a) $k = 5$; b) $k = 7$; this possibility may be extended to all odd k.

maximum number of contacts. It is less clear in the odd case, as the existence of side to vertex contacts is not a necessary ingredient for getting a higher packing fraction; nevertheless, analogical and numerical simulations support this assumption for $k = 5$ and 7. However, things become different for $k = 9$, 11: we have checked that some theoretical periodic patterns with $z = z_{ss} = 4$, which are generalizations of Figure 7 provide a higher packing fraction than those of Section 3. We are presently investigating in more detail these latter configurations and trying to recover them from the minimal energy requirement of our numerical program.

Finally, let us emphasize that only angles and orthogonal symmetries play a role in our theoretical derivation. Then, lengths may be modified in order to get other periodic patterns. A first possibility is provided by Apollonian fillings; in that case, $z = 6$ holds on the average only, the holes all have the same number of sides and same angle measures at the different stages of the building procedure, but they may be different in size and shape.

Another possibility consists in modifying differently the lengths of the edges of the grains, all angles unchanged. Pentagons excepted, at least 2 independent relative lengths are available. As true 6-fold symmetry implies no more than one (k even) or two (k odd) further condition(s), it may be realized for $k \geq 7$ with identical but slightly irregular grains; actually, in most cases, a continuous set of solutions exists and large packing fractions may be reached. For example, octagons with 2 different side lengths s_1 and s_2 ($s_2 = \sqrt{3/2}s_1 = 1.224\ldots s_1$) rearrange more densely ($C = 0.922\ldots$) than regular grains ($C = 0.906\ldots$) A crushing or stretching of the polygons along the vertical symmetry axis — angles modified but side lengths unchanged — should lead for some k to a similar result.

Acknowledgments

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Appendix A

We consider the figure made of P ($P \gg 1$) regular convex polygons (the grains) with k sides with steric exclusion. In a dense configuration, they may be in contact — but they cannot overlap. The contacts delimitate closed non convex polygons in the void (pore) space with an arbitrary number n of sides (Fig. 3). Their n angles have 3 origins:

- angles corresponding to the corners of the polygonal grains, with measure $\frac{k+2}{k}\pi$, let $\phi(n)(0 \leq \phi(n) \leq n-3)$ be their average number per polygon;
- angles arising from side to side contacts, with measure $2\pi/k$, average number $\alpha(n)$;
- angles $\beta_{i,n}(i = 1, \ldots n - \phi(n) - \alpha(n))$, corresponding to side to vertex contacts.

Actually, some other kinds of contacts may occur but they may be considered as limit cases of the preceding ones: vertex to vertex, or side to side with the 2 sides in contact on their whole length (Fig. 2). When $k \leq 6$, another kind of configuration can take place as 3 grains may occur at the same place but this is exceptional. All those limit cases will not be considered here.

A1. General Identities

By counting the number of sides and vertices in the whole graph and using Euler relation, we get topological relations between the number P_n of concave polygons with n sides and the average number z_{ss} and z_{sv} of side to side and side to vertex contacts per grain

$$\sum_{n\geq 3} P_n = \left(\frac{z}{2} - 1\right) P \tag{A.1a}$$

$$\sum_{n\geq 4} (n-3)P_n = \left(k + 3 - z - \frac{z_{ss}}{2}\right) P \tag{A.1b}$$

$$\sum_{n\geq 4} \phi(n)P_n = \left(k - \frac{z}{2} - \frac{z_{ss}}{2}\right) P \tag{A.1c}$$

where $z = z_{ss} + z_{sv}$ is the total coordination number; from $\phi(n) \leq n - 3$, we get

$$z \leq 6 \tag{A.1d}$$

which is both the average and local maximum value for the coordination number. Note that the relations above are average ones i.e. it means that these identities hold "almost always". Actually, these topological relations are true for any assembly of polygonal grains (any size, form and mixture...); then $z_{max} = 6$ appears as a generic property.

Equations (A.1) are completed by metric properties for the angles of the concave polygons in the porous space. For any polygon with n sides,

$$(n-2)\pi = \frac{k+2}{k}\pi\phi(n) + \frac{2}{k}\pi\alpha(n) + \sum_i \beta_{i,n} \tag{A.2a}$$

with

$$\beta_{i,n} < \frac{2}{k}\pi, \quad i = 1, \ldots n - \phi(n) - \alpha(n) \tag{A.2b}$$

Here, the numbers $\phi(n)$ and $\alpha(n)$ are integers and depend both on n and on the peculiar polygon which is considered. For example, when $k = 7$, $\phi(4) = 1$ is fixed but $\alpha(4) = 0, 1$ or 2. However, several values of $\phi(n)$ exist for large n; for instance, $\phi(14) = 8$ or 9. As a further consequence, note that

- no triangle exists in the pore space if $k \geq 7$, no quadrilateral if $k \geq 9, \dots$
- the triangles excepted, all the void polygons are not convex (i.e. $\phi(n) \geq 1$, when $n \geq 4$).
- setting all acute angles equal to $2\pi/k$, we get for $\phi(n)$ a lower bound

$$\phi(n) \geq \frac{k-2}{k} n - 2.$$

When taking the average over all configurations and all n, we get obviously

$$\langle \beta_{i,n} \rangle_{i,n} = \frac{\pi}{k} \tag{A.3a}$$

and

$$z_{\rm ss} P = \sum_n \alpha(n) P_n, \quad z_{\rm sv} P = \sum_n [n - \phi(n) - \alpha(n)] P_n \tag{A.3b}$$

A2. Maximum Coordination Number Hypothesis

We go now to the maximum coordination number $z = 6$. From (A.1b) - (A.1c), we get $\phi(n) = n - 3$, i.e. 3 grains and 3 contacts only are involved in each hole. As the sum of the 3 remaining angles is at most $\frac{6\pi}{k}$, the 3 possible values for n are $n = p, p+1, p+2$ (k even, $k = 2p$) and $n = p+1, p+2$ or $p+3$ (k odd, $k = 2p+1$).

If we assume that the number of side to side contacts must be maximum too, then

i) If $k = 2p$, the realization with maximum $z_{\rm ss}$ consists in choosing $n = p$ and all 3 acute angles equal to $\frac{\pi}{p}$ All contacts are side to side and $z_{\rm ss} = z = 6$.

ii) If $k = 2p+1$, the maximum possibility consists in 2 side to side contacts (angle $\frac{2\pi}{2p+1}$) and one side to vertex contact with an angle $\frac{\pi}{2p+1}$ Then $\alpha(p+1) = 2$ and $z_{\rm ss} = 4$. This is precisely what happened in the pentagonal case.

Actually, these requirements are necessary conditions; it remains to prove that such configurations are possible. The configurations are shown in Figures 4 and 5. For the even case, 2 possibilities are given, one of them — the most compact — corresponds to total side to side contacts; then, the polygons of the void space are degenerated (their degree is lowered, with an angle which is $\frac{2\pi}{p}$ instead of 2 angles $\frac{\pi}{p}$) quadrilaterals become triangles, pentagons become quadrilateral.. The less compact possibility is a limiting case where the side to side contact is replaced by a vertex to vertex symmetric contact.

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