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Compaction and arching in tapped pentagon deposits

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Abstract We simulate the process of compaction under vertical tapping for a two-dimensional system of particles deposited in a rectangular box. The particles consist in regular pentagons and our main objective is to analyze the novel behavior recently found for the packing fraction as a function of the tapping strength applied to the system (Vidales et al. in Phys Rev E 77:051305, 2008). We will relate the behavior of the number and type of arches, mean coordination number and number and type of contacts to the peculiar packing density increase found for increasing tapping strength. Finally, we present results of an annealed tapping on our packings to compare the results to the constant tapping protocol. All our results are compared with the analogous simulations carried out on disks.

Keywords Granular matter · Arching · Pentagons · Compaction

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1 Introduction

Compaction of granular matter under vertical tapping is still a subject with many open questions. The densification of granular beds subjected to vertical tapping is generally studied both as a function of the number of taps and as a function of the tapping intensity.

Most works in the literature deal with simulations or experiments performed on rounded particles, specially spheres and disks, but studies on pointed objects are less common and harder to carry out. In this sense, a first experimental investigation [1] used assemblies of spheres to build up more complex objects which however retain the smooth edges of the constituents.

In a pioneering work, Duparcmeur et al. [2], studied the densification of a 2D horizontal assembly made of regular pentagons. Pentagons resting on a concave blowing air table were allowed to pack as the air pressure under the particles was slowly decreased. Particles rearrange their positions and orientations continuously due to the aerodynamic interactions with the air flux which introduce a background vibration. Thus, the structure of the assembly evolves increasing its packing fraction. They found that the final configurations attained by pentagons show crystal like structures and tend to maximize the average number of contacts and the average number of side-to-side contacts. This large numbers of side-to-side contacts at high packing fractions are due to the continuous reorganization promoted by the background vibration on the table. In [3], the same authors studied the densification of regular polygon packings (pentagons and heptagons) generated by simulations reproducing the crystallization features seen in their experiments. Crystallization was also observed in Monte Carlo simulations of pentagons in the modeling of fluids with symmetry mismatch [4].

In a recent work [5], we have studied the compaction of pentagon deposits under tapping, showing that these objects unpack when gentle vibrations are applied to the system. These results show a novel behavior for pointed granular matter compared to rounded objects.

Arches are basic structural entities in granular deposits. The number and type of the arches found in the granular packing determine the overall packing fraction and coordination number [6,7] as well as the ability to jam an opening during flow [8–11].

In this paper, we present a detailed analysis on the particle–particle contacts and on the arches formed by the pentagons. Comparisons with disk packings obtained with an analogous method are drawn. Packings of pentagons present a response to vertical tapping which is significantly different from that observed in packings of rounded grains like disks or spheres.

2 Packing regular pentagons: simulation algorithm

We perform simulations of regular pentagons [5] that comprise three phases: (1) the generation of an irregular base of pentagons followed by a sequential deposition of particles that create the initial packing, (2) the tapping driven through a vertical homogeneous expansion of the particles followed by small random rearrangements, and (3) the simultaneous deposition of the pentagons using a pseudo molecular dynamics method (PMDM).

2.1 Preparation of the sample

For the present simulations we use a nearly monodisperse size distribution (5% dispersion). This small dispersion helps to avoid typical round-off errors in off-lattice simulations. One thousand regular pentagons are sampled from a uniform size distribution. A number of them are placed at the bottom of a rectangular box in a disorder way in order to create an irregular base. Arranged in this manner, the N base particles fix the wall-to-wall width of the box which is about 40 particle diameters. These pentagons remain still over the course of the tapping protocol. The remaining pentagons are poured one at a time from the top of the box and from random horizontal positions and random orientations avoiding overlaps with the walls of the container. Each grain falls following a steepest descendent algorithm. When a pentagon touches an already deposited particle, it is allowed to rotate about the contact point until a new contact is made or until the contact point no longer constrains the downward motion of the particle which is deemed to fall freely again. A pentagon is considered stable when it has reached two contacts such that the x-coordinate of its center of mass lies between them. Otherwise, the pentagon will be allowed to rotate around the contact point with lower y-coordinate. Side walls are considered frictionless.

2.2 Tapping

Once the initial configuration is obtained, tapping is simulated by using an algorithm that mimics the effect of a vertical tap. The system is expanded by vertically scaling all the y-coordinates of the particle centers by a factor $A > 1$. Base particles are not subjected to this expansion. When pentagons are expanded upwards with this simple rule, overlaps between some of them occur. This fact has been already pointed out in [5]. To avoid this problem we perform some additional moves for those particles presenting overlaps after the overall expansion. These additional moves consist in small upward displacements of the order of 10δ, where δ is a PMDM parameter that will be introduced below, which are repeated for overlapping particles until all overlaps are removed. We have checked that this extra moves of some particles do not affect the overall amplitude of expansion A. After a large number of taps, the packing attains a steady state whose characteristic parameters fluctuate around equilibrium values.

It has been shown [12,13] that $\sqrt{A-1}$ is proportional to the reduced acceleration Γ generally used in experiments to characterize the energy input due to a tap. This parameter Γ corresponds to the peak acceleration experienced by the container during a tap divided by the acceleration of gravity. Therefore, we use $\Gamma \equiv \sqrt{A-1}$ as a measure of the tapping intensity in the rest of this paper.

After expansion, we introduce a horizontal random noise for those particles touching any of the walls of the container. These particles are displaced toward the center of the simulation box in the x-direction by a random distance taken from a uniform distribution between 0 and Γ^2. The new position of the particle is accepted only if it does not cause any overlap with neighboring particles. This process mimics in some way the shaking that grains suffer in a real experiment because of the collisions with the walls. Note that the amplitude of the random horizontal perturbation is proportional to the expansion and each particle is tempted to be moved only once in each tapping event.

2.3 Deposition through PMDM

After expansion and random rearrangements, the particles are allowed to deposit simultaneously following an algorithm similar to that designed by Manna and Khakhar for disks [14,15]. This is a pseudo dynamic method that consists in small falls and rolls of the grains until they come to rest by contacting other particles or the system boundaries. Once all pentagons come to rest, the system is vertically expanded again and a new cycle begins.

It is worth pointing out here that more realistic simulations can in principle be used for the purposes of our investigation. However, using techniques such as molecular dynamics (MD) is rather time consuming, given that we apply of the order of 10^3 taps at each amplitude value. Indeed, previous works using MD for disks (a much simpler system) took about 10 days of cpu time to carry out 500 taps on a system with only 512 particles [20]. Besides, there is another drawback in the use of MD. Since we aim at studying arch formation, the history of the formation of each contact has to be analysed, which is a rather complex problem (see [20] for an example of the identification of arches in disk packings). In the PMDM used in this work, the stability provided by each contact is clearly defined by the simulation algorithm itself, as will be explained below.

The deposition of grains consists in choosing a pentagon and allow it to fall freely a distance δ. If in the course of a fall of length δ a pentagon collides with another pentagon, the falling pentagon is put just in contact and this contact is defined as its first supporting contact. If the pentagon has one single supporting contact we let it rotate an arc-length δ around the point of contact with its supporting particle.[1] On rolling, any collision is identified if after the small roll of arc-length δ the rolling pentagon overlaps a second particle. This overlap is negligible since δ is typically two orders of magnitude smaller than the particle diameters. We do not move this overlapping particle back at contact position but keep the small overlap. If in the course of a roll of length δ a pentagon collides with another pentagon (or a wall), a new contact is established as a potential supporting contact. The positions of the two contacts may allow the pentagon to roll further around the last contact in which case the first contact is removed from the contact list. Otherwise the pentagon is assumed to be in a transient stable position. On rolling, a pentagon may contact twice another single pentagon. In this case the pentagon is said to lay flat on the bottom pentagon if its center of mass lies between the two contacts. Notice that there is no mechanism for the pentagons to slide on top of each other. Only rolls and vertical falls are allowed. This introduces an effective static friction in the system (see next section).

If no new rearrangements of the supporting particles of a transient stable pentagon occur in future PMDM steps, the pentagon will remain stable in position and their supporting contacts will be uniquely defined. In this dynamic context, a moving pentagon can change the stability state of other pentagons supported by it; therefore, this information is updated after each move. Each particle is given a chance to move at each iteration. The deposition is over once each particle in the system has both supporting contacts defined. Then, the coordinates of the centers of the pentagons and the corresponding labels of the two supporting particles or wall, are saved for analysis.

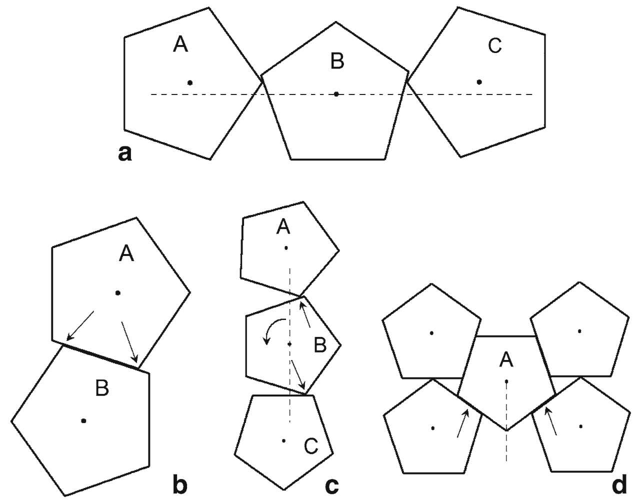

Fig. 1 Examples of unusual (as compared with disks) stable configurations of pentagons. *Arrows* indicate contacts between particles and *bold points* represent the center of mass of the pentagons. **a** The central pentagon B is supported by particles A and C whose center of mass are in higher positions. **b** Pentagon A lies side-to-side with its supporting bottom partner B. Its center of mass lies between the two indicated supporting contacts. **c** Pentagon B is locked during its rolling by the other two particles A and C. The *vertical line* indicates the fact that the x-coordinate of its center of mass lies at the $left$ of both supporting contacts. *d* Theoretical crystal unit for pentagons. *Dashed line* indicates the direction where the center of mass lay respect to the supporting particles, see [2]

3 Peculiarities of pentagon stability

Pentagons, like other pointed particles, show much more constrained movements than rounded particles like disks. Therefore, the configuration space is rather reduced. This fact introduces special configurations that are not commonly observed in disk packings. Illustration of this is presented in Fig. 1.

Figure 1a shows the case of a pentagon supported by other two whose centers are at higher positions, situation never allowed for frictionless hard disks.

A pentagon may have two contacts with another single pentagon when they share part of a side of the polygons. In this case (see Fig. 1b), if the center of mass lies between the two contacts, the upper pentagon is said to lay flat on the bottom pentagon no matters how steep the inclined plane is. Effectively, this assumes that the pentagon surfaces have a static friction coefficient $\mu > \tan(\pi/5) \approx 0.72$.[2]

[1] We call this rotation a "roll" as in the case of disks [14] even thought the contact point does not move as in real rolling. Note however that in following the steepest descent path, a pentagon can actually roll over another pentagon since the pivot contact point may change from a vertex to another or to a side of the moving particle.

[2] The maximum inclination angle of the inclined plane on which a pentagon may lay flat is $\pi/5$, since beyond this angle the center of mass lays outside the pentagon base and the particle would rotate about the lower vertex. If the particle surfaces are rough enough, the pentagon will not slide up to this point.

Figure 1c shows a pentagon that has been locked during rolling by a pentagon coming from above in such a way that the x-coordinate of the center of mass lies outside the range defined by the two contacts. This is also another peculiarity of pointed objects and, in this case, the particle stops rolling and attains this stuck position until a rearrangement occurs in a future PMDM step. If this is not the case, this position is the final position of that particle. We stress that all these configurations are not possible in disk packings and are responsible for the particular behavior found in pentagon assemblies, as we will show below. We will refer to the crystalline order shown in Fig. 1d later.

4 Arch identification

To identify arches one needs first to identify the two supporting particles of each pentagon in the packing. Then, arches can be identified in the usual way [6,7,16]: we first find all *mutually stable particles*—which we define as directly connected—and then we fin the arches as chains of connected particles. Two pentagons A and B are mutually stable if A supports B and B supports A.

Unlike disk deposits generated through PMDM, pentagon packings present capriciously shaped arches. For example, since pentagons can be locked from above on rolling, arches may bend upwards over themselves (see Fig. 2a). Also, concave up arches are common since both supporting pentagons of a given particles may be at higher y-coordinates than the supported pentagon (see Fig. 2b). These structures may extend over several particles in our model since we do not consider the instabilities caused by the weight laid on each particle. The stability of any given pentagon depends solely on the geometry defined by its supporting contacts. For example, it is allowed to lay pentagons on top of each other building up a column as illustrated in Fig 2c even though we know this is in practice impossible since the center of mass of the column soon ends up outside the base.

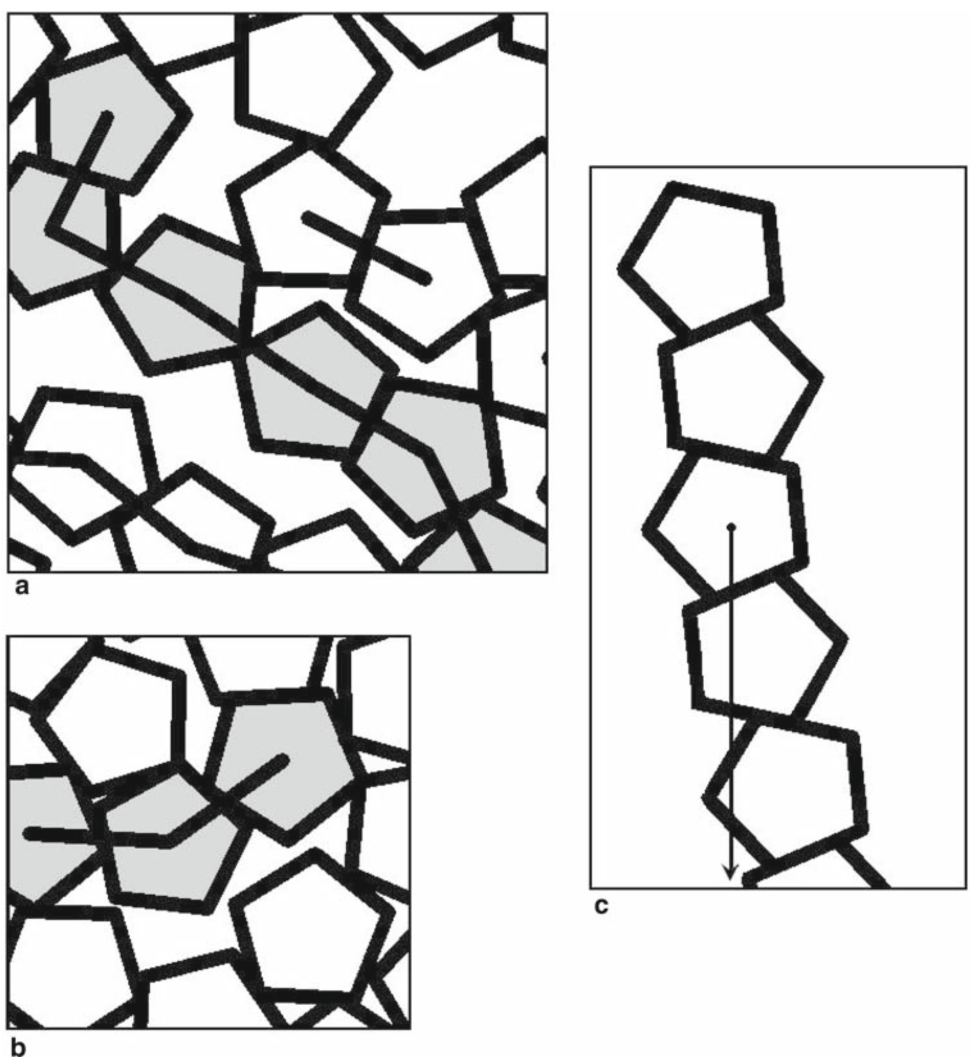

Fig. 2 Examples of unusual arches. **a** An arch that bends over itself. **b** A concave up arch. **c** A column of pentagons which is stable in the present model but unstable in real experiments. The *arrow* indicates the position of the center of mass of the column. Pentagons participating in the arching are *shaded*

5 Results on tapped beds of pentagons

5.1 Packing fraction and annealing

In pseudo dynamics protocols, results are dependent on the MD step δ used to update the particle coordinates as they fall and roll. Thus, it is mandatory to find the dependence of the properties of interest on the MD step. We have considered systems tapped 10^4 times at constant $\Gamma = 0.316$ for different values of δ. Its packing fraction was recordered after each tap. The final steady state packing fraction was calculated by averaging over the last 1,000 values. Figure 3 shows the results obtained. Since results agree within statistical uncertainties for $\delta < 0.01$ we decided to use this maximum value as a convenient choice for the PMDM simulations. Lower values of δ require larger cpu times; whereas for δ above 0.01, the results depend on δ.

Packing fraction of pentagon deposits tapped for various tapping intensities has been presented and analyzed in [5]. In that paper, the evolution of packing fraction versus the number of taps applied to the system, for different tapping intensities, was analysed. Results showed that after 2,000 taps the steady state regime is attained. This feature was the same for all the tapping intensities used in the simulations. Vidales et al. [5] also shows that the steady state values for packing fraction increased as tapping intensity increased. To summarize, compaction was enhanced as tapping intensity increased and the system reached a clear plateau after a moderate number of taps irrespective of the tapping intensity. To get an idea of the different appearance that a packing of pentagons has after suffering a large number of taps, we show in Fig. 4a a picture of an assembly of 400 pentagons after being shaken 5×10^3 times at $\Gamma = 0.316$. To compare the effect of tapping intensity, we present in Fig. 4b the same situation but for $\Gamma = 1$. On both pictures, arches are indicated by segments.

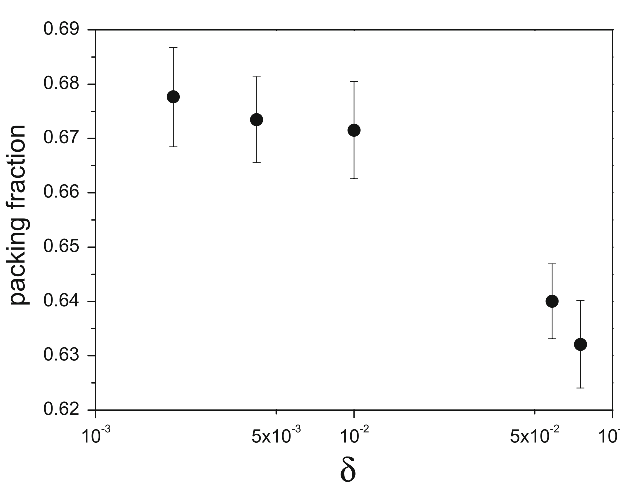

Fig. 3 Dependence of packing fraction on the PMDM parameter δ

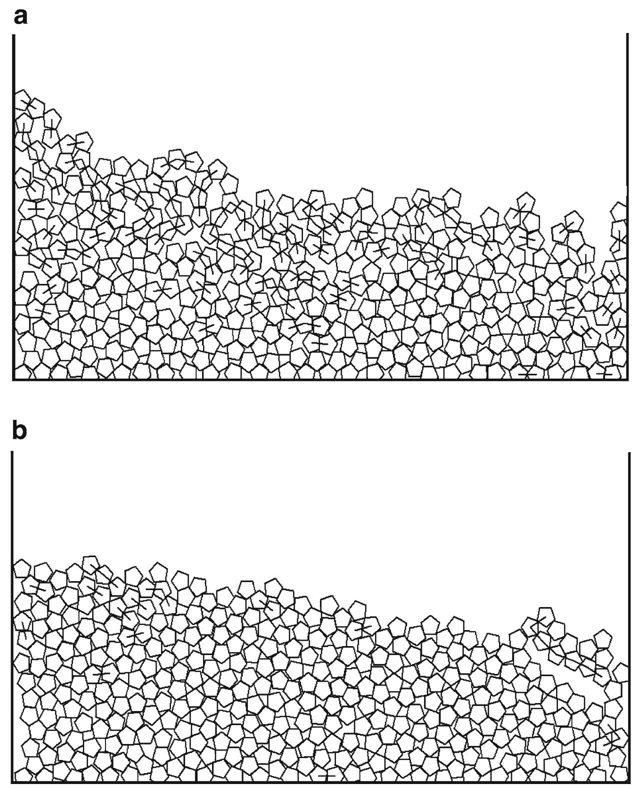

Fig. 4 Examples of two packing of 400 pentagons tapped during 5×10^3 times. Arches are indicated by *segments*. **a** $\Gamma = 0.316$, **b** $\Gamma = 1$

We will discuss this below. The final equilibrium positions of the particles in each case are quite different. The creation of long unstable chains at low Γ due to blocked rollings of the particles gives as a result a lower compaction in comparison with that shown for a packing tapped at higher intensities. Moving the particles farther apart during expansion allows them to rearrange better and to increase side-to-side contacts (see next section).

The steady state of the tapping process was evaluated over the last 1,000 taps. In Fig. 5a, we present and compare results with the same experiment carried out on disks [16] and with a pentagon limiting case obtained as explained in [5]. The limiting case is the one leading to the highest compaction value, this value being the limit to which the tapping compaction process approaches for increasing Γ.

There are two clear distinctions between the behavior shown by disks and that displayed by pentagons. Firstly, disks attain larger compaction at all tapping intensities. This is to be expected since pentagons, if not carefully arranged, tend to leave large interstitial spaces. Secondly, while disks present a non-monotonic dependence of the packing fraction versus tapping intensity [12], pentagons show a monotonic increase in the packing fraction. At high values of Γ both systems increase their packing fractions with increasing tapping intensities and eventually reach a maximum plateau value.

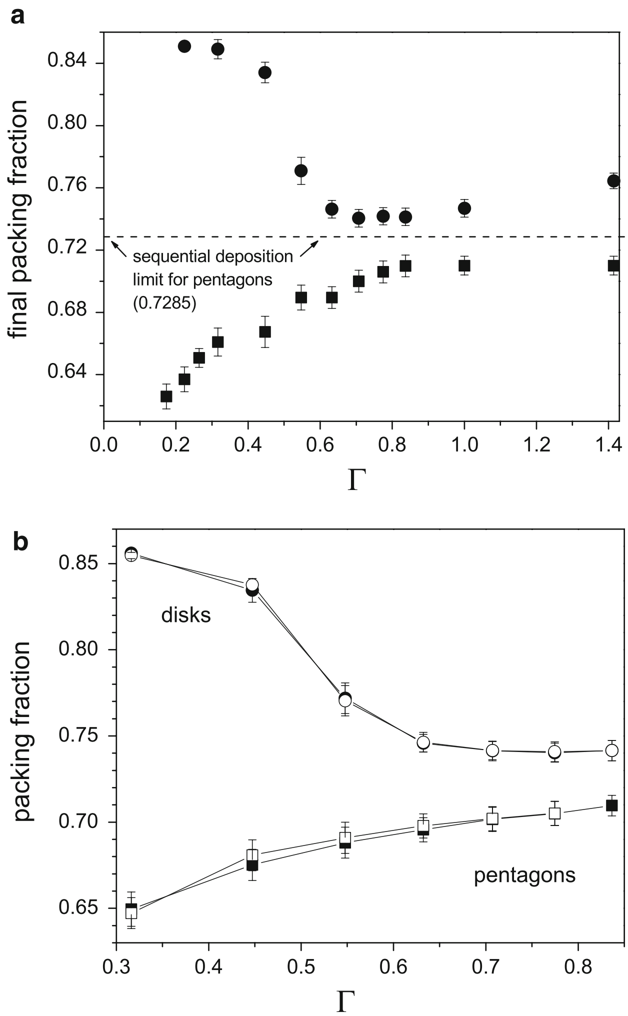

Fig. 5 **a** Steady state packing fraction obtained by averaging over the last 1,000 taps as a function of the tapping intensity for disks (*circles*) and pentagons (*squares*). The *horizontal dotted line* corresponds to the sequential deposition limit for pentagons (see [5] for details). **b** Packing fraction versus intensity Γ for ascending (*filled symbols*) and descending (*open symbols*) annealing performed on disks and pentagons. *Circles* correspond to disks and *squares* to pentagons

For low Γ we find that disks tend to order and so increase the packing fraction as Γ is decreased [16]. A minimum in packing fraction is then located at intermediate values of Γ. However, this feature is not present in pentagon packings. Pentagons seem not to order at low Γ and the packing fraction does not present a minimum as in disk packings.

In order to assess whether the tapping protocol applied to the packings is significant in the results discussed above, we have carried out an annealed tapping on our packings to compare with the constant tapping used in the previous sections. We start from a sequentially deposited packing and then tap the system at variable tapping intensity. The intensity was increased from $\Gamma = 0.316$ to $\Gamma = 0.837$ in steps of the form $0.05/\Gamma$ (smaller as Γ is larger) and 5, 000 taps where applied at each intensity value. Then, the same protocol was followed but for decreasing intensities. The corresponding annealing curves for the packing fraction as a function of Γ are shown in Fig. 5b. As we can observe, there is no hysteresis nor irreversibility in these systems. The annealing curves coincide with the constant tapping results of Fig. 5a. Both, disks and pentagons, attain a unique packing fraction value for given tapping intensity no matters the history of the tapping protocol. The same is true for arches and coordination number. This is coincident with experiments on glass beads from Philippe and Bideau [17].

Previous simulations on disks [16] and experiments on glass beads [18] do show an irreversible branch in this type of experiment. It is important to note that in the case of simulations [16] the annealing was conducted in a different manner since the tapping intensity was increased in a quasi-continuum fashion and a single tap was applied at each value of Γ. This prevented the disk packing from reaching the steady state at each value of Γ. In the present work we give sufficient time for the system to reach the steady state at each intensity. On the other hand, the annealing experiments by Nowak et al. [18] were conducted in much the same way as our simulations, however, their system presented a very slow relaxation that effectively prevented the packing from "equilibration" at low tapping intensity.

5.2 Particle–particle contacts

The mean coordination number $\langle z \rangle$ of the pentagon packings is a good indication of the formation of arches in the system [16]. In Fig. 6 we observe that as Γ is decreased pentagons reduce the coordination number all the way down to $\Gamma = 0.0$. This indicates that a progressively larger number

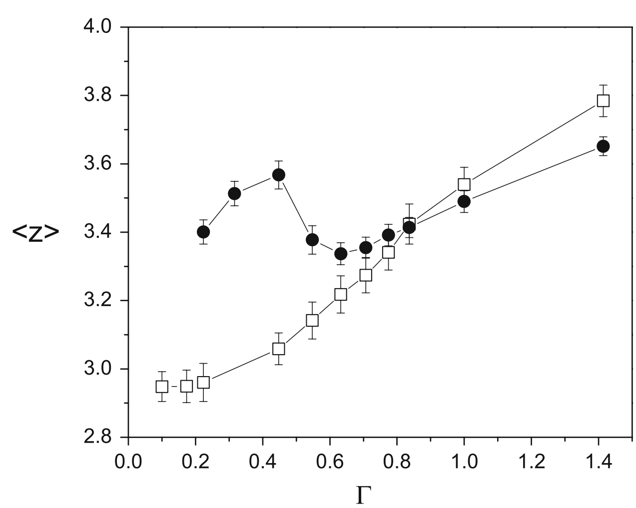

Fig. 6 Mean coordination number as a function of the tapping intensity Γ for pentagons and disks, as indicated by *open squares* and *filled circles*, respectively

of particles form mutually stable contacts. In contrast, disks show a sudden increase in ⟨z⟩ when Γ is decreased below a value that coincides with the minimum packing fraction observed (see Fig. 5a). These features suggest that the origin of the contrasting behavior in steady state packing fraction of pentagons, compared with disks, is related with the enhancement of arch formation under low tapping intensity. We will study this in detail in the next section.

Another quantity we were able to measure was N_{ss}, the relative number of pentagons that lay flat on top of a bottom partner (see Fig. 1b). This number must not be confused with the total number of side-to-side contacts between particles, which also include non-supporting contacts. In our simulations, there is a first stage of sequential deposition of pentagons to create the initial packing that will be then subjected to the tapping experiment. This sequential way of depositing particles favors the occurrence of side-to-side supporting contacts because particles do not interact with any other particle except the already stable ones on the free surface of the deposit. These configurations give rise to the development of pilings like those shown in Fig. 2c, which do not favor an efficient compaction. We find that 30% of the pentagons in the packing have this type of supporting contacts. However, after tapping, all packings reduce N_{ss} down to roughly 10% for all values of Γ. The decrease in N_{ss} implies a change in the way particles get their supporting contacts. When the system is tapped, interaction with neighbor pentagons promotes stabilization with two, rather than one, supporting particles. Since our algorithm does not allow a particle to be supported by more than one side-to-side contact, the two contacts will be of the type vertex-to-side. It has been suggested [2] that ordered structures of pentagons like those shown in Fig. 1d are the responsible of a better filling of empty space in pentagon packings. It is important to note that pentagon A in Fig. 1d has two side-to-side contacts that support it (indicated with arrows). These large ordered domains referred in [2] are not attained by tapping in our simulations. However, small crystal-like structures are indeed observed, as can be seen in Fig. 4, especially at the bottom halves of the two examples shown there.

5.3 Arches

The total number of arches per unit particle, N_{arch}, in the pentagon packings as a function of tapping amplitude Γ is shown in Fig. 7. The corresponding results for disk packings are shown for comparison. As we can see, in general, pentagons form less arches than disks. This seems to be contradictory with the fact that pentagons show a lower coordination number (see Fig. 6). We will see below that this effect is due to the wider arch size distribution found in pentagons. In pentagon packings, the number of arches presents a monotonic decrease with increasing Γ in contrast with the behavior

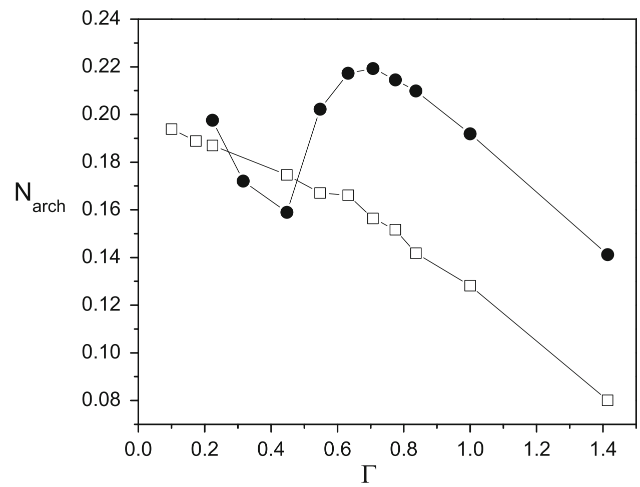

Fig. 7 Number of arches per unit particle found in the system. Here again *open squares* correspond to pentagons and *filled circles* to disks

of disks that present a maximum at the same tapping intensity where the minimum packing fraction is achieved. It is particularly interesting that at $\Gamma < 0.316$ disks enter an ordered phase [16] where arches are largely eliminated from the system whereas the pentagon deposits remain in a disordered state with an increasing number of arches up to very small tapping intensities.

A simple probe on the overall size of the arches can be obtained by plotting the number of particles, N_p, involved in arches of any type. In Fig. 8 we present such plot for pentagons and disks as a function of Γ. Given that arches are less common among pentagons we would have expected that the number of particles involved in arches would have been lower for pentagons than for disks. However, at low Γ, pentagons show a large proportion of in-arch particles

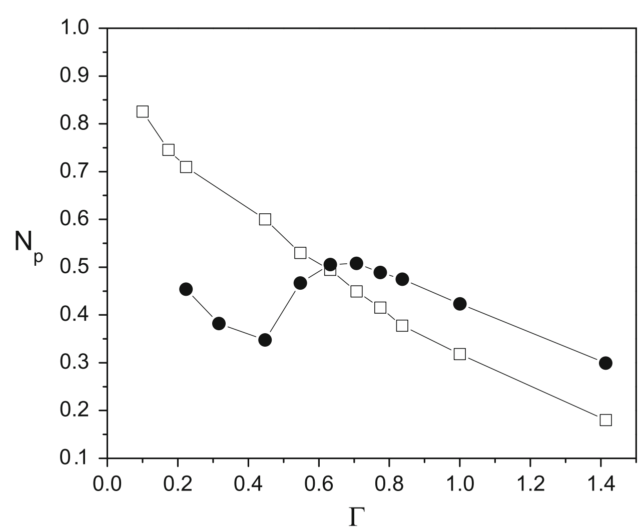

Fig. 8 Number of particles involved in arches per unit particle. *Symbols* are as in preceding figures

which implies a tendency of pentagons to form large arches if tapped gently. These are the responsible for the voids that reduce the packing fraction as Γ is decreased (see Fig. 5a) and for the relatively low coordination number at moderate and low Γ (see Fig. 6).

In Fig. 9 we show the distribution of arch sizes for pentagons and disks at two values of Γ. We confirm here that for low Γ pentagons have a larger tendency to form large arches (up to 20 particles), whereas disks form arches of less than 10 particles.

6 Conclusions and final remarks

The compaction by vertical tapping of disks and spheres has been studied to some extent in the past few years by experiments and by simulations [1,16,18–22]. Setting apart all issues related to the slow compaction shown by these systems and considering only the steady state whenever achieved—this may be obtained by extended constant intensity tapping or by a suitable annealing—all these systems display a clear initial reduction in the packing fraction as tapping intensity is increased followed by a smooth increase at large amplitudes. This behavior has been observed in simulation of spheres [22], in 3D experiments with glass beads [18,23] and in simulation of disks and spheres [12,16,20]. We have extend a previous work [5] for a deeper understanding of the unexpected behavior of pentagon deposits under tapping. We have found that—either through constant tapping or annealing—the steady state of the packing presents a monotonic increasing packing fraction with tapping intensity. Moreover, as the tapping strength is increased from zero, the steady state values for $\langle z \rangle$, N_{arch} and N_{p} vary monotonically in the case of pentagons whereas a clear non-monotonic behavior is present in disk packings. Such finding reveals that the complexity of pentagon deposition leads to an unexpectedly simpler behavior of the packing fraction as compared to simpler systems. This reinforces the idea that pentagons can achieve close packing fraction only when strong taps are applied so that the free volume introduced allows for arrangements. On the contrary, disk are able to rearrange specially well when gently tapped. This is the key to explain the finding of the simpler behavior of all steady state properties measured in pentagon packings compared with those observed in rounded objects.

We have tested the hypothesis that such simple response is induced by the frustration of order that we find in pentagon systems since partial ordering seems to lead the non-monotonic behavior of disks and spheres. Nevertheless, we checked this issue in [5] through some trial simulations on polydisperse disks that are known to show frustration of order, and still observed the same, although less marked, non-monotonic behavior. Clearly, there is more than just frustration of order to the response of pentagon packings. A sensible explanation for the formation of large arches at low tapping amplitude should in principle shed light on this issue. We have already discussed that pointed objects have a larger tendency to multiple collisions [5]. Multiple collisions are necessary (although not sufficient) to form many-particle arches. These multiple collisions are enhanced by two factors: (a) the fact that pentagons may approach each other closer than disks (recall that a side-to-side contact leaves pentagon centers separated by ≈0.8 particle diameters) which increases number density despite the lower packing fraction, and (b) the associated collisions on rolling originated by the protruding vertexes.

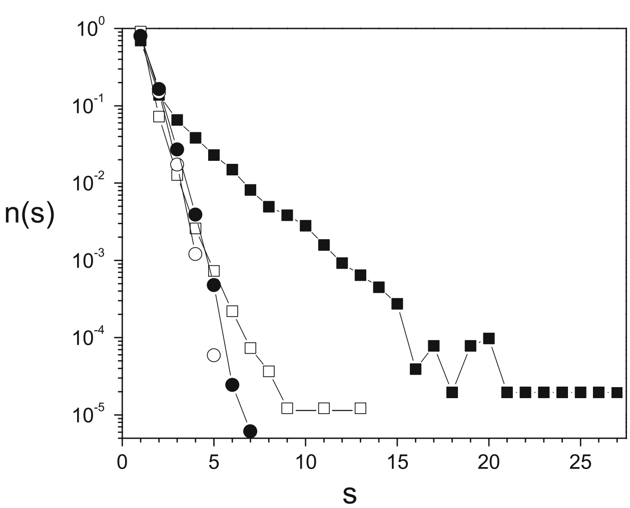

Fig. 9 Distribution of arch sizes for disks and pentagons at $\Gamma = 0.447$ (*filled symbols*) and $\Gamma = 1.414$ (*open symbols*). *Squares* represent values for pentagons and *circles* for disks

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