Pentagon deposits unpack under gentle tapping

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We present results from simulations of regular pentagons arranged in a rectangular box. The particles are subjected to vertical tapping. We study the packing fraction, number of contacts, and arch size distribution as a function of the tapping amplitude. Compared with disks, pentagons show peculiar features. As a general rule, pentagons tend to form fewer arches than do disks. Nevertheless, as the tapping amplitude is decreased, the typical size of the pentagon arches grows significantly. As a consequence, a pentagon packing reduces its packing fraction when tapped gently, in contrast with the behavior found in rounded particle deposits.

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I. INTRODUCTION

The study of compaction of granular matter under vertical tapping is a subject of much debate and consideration. Setting apart all issues related to the slow relaxation shown by these systems, and considering only the steady state regime whenever achieved, the investigated granular deposits attain rather high packing fractions when tapped very gently. Moreover, these systems display a rapid reduction in the packing fraction as tapping intensity is increased. This decrease in packing fraction has been observed in simulation of spheres [1], in experiments with glass beads [2,3], and in simulation of disks [4,5]. In some cases, the steady state may be obtained by extended constant-intensity tapping; however, other experimental configurations may require a suitable annealing in order to achieve the so-called reversible branch [3].

Few studies of this type have been carried out on sharp objects. An experimental investigation uses assemblies of spheres to build up more complex objects which, however, retain the smooth edges of the constituents [6].

Here, we show that packings of pentagons simulated through a pseudo-molecular-dynamics method (PMDM) present a response to vertical tapping which is significantly different from that observed in packings of rounded grains like disks or spheres. We base our assertions on the comparisons with disk packings obtained with an analogous method.

It is worth mentioning that studies on pentagon assemblies do exist [7–9]. These put special emphasis on the crystallization of these systems. However, these experiments and simulations consider systems that relax continuously under the effect of a background vibration (either thermal or mechanical agitation).

II. THE MODEL

The main stages of our simulations consist in (a) the generation of an irregular base, (b) sequential deposition of pentagons to create an initial packing, (c) vertical tapping obtained through vertical expansion followed by small random rearrangements, and (d) nonsequential (simultaneous) deposition of the pentagons using a PMDM.

We sample 1000 regular pentagons from a uniform size distribution (5% dispersion). A number of them are placed at the bottom of a rectangular box in a disordered 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. Each grain falls following a steepest descent 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. If a particle has reached two contacts such that the x coordinate of its center of mass lies between and above them, the pentagon is considered stable. Otherwise, the pentagon will be allowed to rotate around the contact point with lower y coordinate. Sidewalls are considered without friction.

Once the initial configuration is obtained, a tapping process is carried out by using an algorithm that mimics the effect of a vertical tap. The system is expanded by 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 upward with this simple rule, overlaps between some of them occur. This happens, for example,

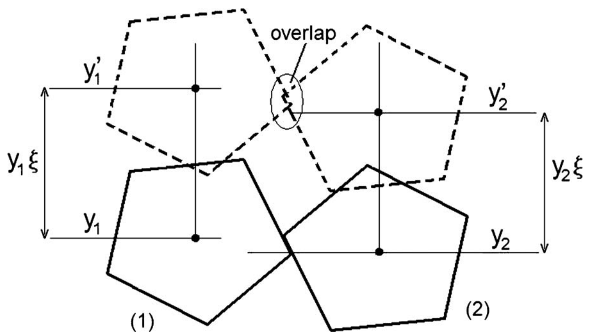

FIG. 1. Example of an overlap promoted by homogeneous upward expansion. See text for details.

when a pentagon has a vertex above a second pentagon while the center of the first pentagon is below the center of the second. In Fig. 1, we show an example of this situation. Pentagons 1 and 2 rest in contact and have vertical coordinates y_1 and y_2, respectively. After expansion, their coordinates change to $y_1'=Ay_1$ and $y_2'=Ay_2$, the net displacement for each particle being ξy_1 and ξy_2, respectively, where $\xi = A-1$. Because of the fact that initially $y_2 < y_1$, the expansion raises particle 1 more than particle 2, giving as a result an overlap as indicated in Fig. 1. For this reason, 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 expansion, we introduce a horizontal random noise for those particles touching any of the walls of the box. This is done by attempting to displace each of these particles a random distance in the range $[0, A-1]$ toward the center of the box in the x direction. Only if the new position of a pentagon does not originate an overlap with neighbor pentagons is the move accepted. Each of these particles has only one chance to move. This process mimics in some way the shaking that grains suffer in a real experiment because of the collisions with the walls. Notice that the amplitude of the random moves is proportional to the amplitude of the expansion.

Following expansion and random rearrangements, the particles are allowed to deposit nonsequentially (i.e., simultaneously rather than one at a time) following an algorithm similar to that designed by Manna and Khakhar for disks [10,11]. In brief, this is a pseudodynamic method that consists in small falls and rolls of the grains until they come to rest by contacting other particles or the system boundaries. Particles are moved one at a time but they perform only small moves that do not perturb to a significant extent the subsequent motion of the other particles in the system. For very small particle displacements, this method yields a realistic simultaneous deposition of the grains. Results obtained through the PMDM are of course dependent on the step δ used to update the particle coordinates as they fall and roll. We have carried out a series of simulations to find the dependence of the final packing fraction on δ. The system was tapped 10^4 times at constant amplitude ($A=1.10$) for various values of δ. The final steady state packing fraction was calculated by averaging over the last 1000 taps. We found that results agree within statistical uncertainties for all values of the step size as long as $\delta \lesssim 0.01$. We then took $\delta = 0.01$ as a convenient choice for the PMDM simulations since the CPU time required decreases with increasing δ.

Once all pentagons come to rest, the system is vertically expanded again and a new cycle begins. After a large number of taps, the packing attains a steady state whose characteristic parameters fluctuate around equilibrium values. Each realization (10^4 taps) takes 50 h of CPU time for the minimum tapping amplitude explored ($A=1.1$) and 240 h for the maximum amplitude ($A=3.0$) in a PC with an Intel Centrino processor.

The nonsequential deposition of grains consists in choosing a pentagon at a time and allowing 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 through an arc of length δ around the point of contact with its supporting particle [12]. On rolling, any collision is identified if after the small roll of arclength 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 to the 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 transiently stable position. If no new rearrangements of the supporting particles of a transiently stable pentagon occur in future PMDM steps, the pentagon will remain stable in position and its 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 when 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.

It is worth mentioning that, when trying to attain equilibrium positions, particles like pentagons show much more constrained movements than do disks. This fact introduces special configurations that are not commonly observed in disk packings. For instance, a pentagon may be supported by two others whose centers are at higher positions [see Fig. 2(a)]. Also, a pentagon may have two contacts with another single pentagon. This situation corresponds to the particles shearing part of a side of the polygons. If the center of mass lies between the two contacts, the upper pentagon is said to lie flat on the bottom pentagon [see Fig. 2(b)] no matter how steep is the inclined plane. Effectively, this assumes that the pentagon surfaces have a static friction coefficient μ

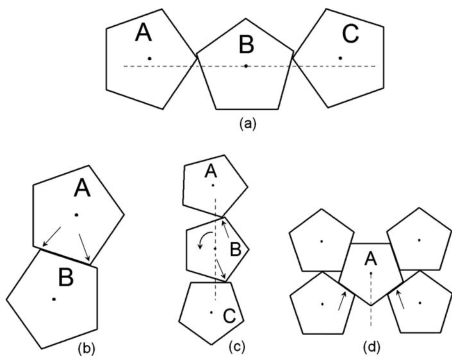

FIG. 2. Examples of unusual (compared with disks) stable configurations of pentagons. Arrows indicate contacts between particles, and bold points represent the center of mass of the pentagons. (a) The central pentagon B is supported by particles A and C whose centers of mass are in higher positions. (b) Pentagon A lies flat on top of 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 x coordinate of its center of mass lies at the left of both supporting contacts. (d) Theoretical crystal unit for pentagons, taken from Ref. [7].

$>\tan(\pi/5)\approx 0.72$ [13]. Another peculiarity is that pentagons may be locked during rolling by pentagons 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 [see Fig. 2(c)]. In this case, the particle stops rolling and attains this stuck position until a rearrangement occurs in a future PMDM step. If this does not occur, this position is the final position of that particle. 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. 2(d) later.

We study the packing fraction ϕ, coordination number $\langle z\rangle$, and arch size distribution $n(s)$ of the deposits. To identify arches one first needs to identify the two supporting particles of each pentagon in the packing. Then, arches can be identified in the usual way [5]: first we find all *mutually stable particles*—which we define as directly connected—and then we find 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 the PMDM, pentagon packings present capriciously shaped arches.

III. RESULTS AND DISCUSSION

The packing fraction of the pentagon deposits is plotted against the number of taps for various tapping amplitudes in Fig. 3. Each curve corresponds to a single run. Since density fluctuations are large, we have used running averages to make the plot clearer. The sizes of the fluctuations are indicated by error bars. The packing fraction is measured in a rectangular region far from the irregular base, the walls, and the free surface of the bed. From Fig. 3 we see that, as the amplitude is increased, compaction is enhanced. This trend is

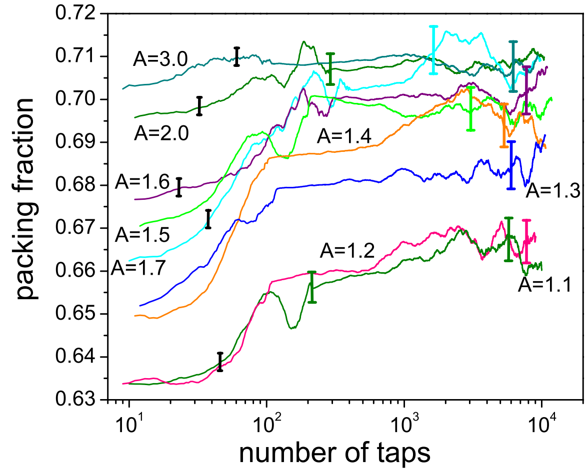

FIG. 3. (Color online) Packing fraction of pentagons as a function of the number of taps. The different curves correspond to different amplitudes A as indicated. Running averages have been taken of the raw data to make the plot clearer. The error bars indicate the size of the fluctuations in the raw data.

similar to the one found by Knight *et al.* [14]. They observed an increase in the packing fraction with tapping intensity. However, our system reaches a clear plateau after a moderate number of taps, irrespective of the tapping amplitude, while in Ref. [14] the steady state was hardly achieved for high tapping amplitudes and definitely not for low intensities. Experiments in two-dimensional (2D) packings of disks [15] show a much faster equilibration than the 3D packings of Ref. [14].

We show snapshots of part of two packings in Fig. 4. Figure 4(a) shows a picture of part of the whole assembly of a deposit of 1000 pentagons after being shaken 5×10^3 times at $A=1.2$. Figure 4(b) shows the same situation but for $A=1.7$. Arches are indicated by segments. It can be seen that the final equilibrium positions of the particles in each case are quite different. At low A, the creation of long arches due to blocked rolls of the particles gives as a result a lower ϕ compared with that shown by a packing tapped at higher amplitudes. Moving the particles farther apart during expan-

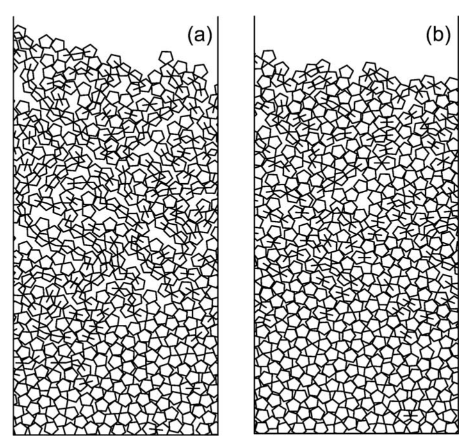

FIG. 4. Examples of two packings tapped 5×10^3 times. We show only part of the 1000-particle assembly. Arches are indicated by segments. (a) $A=1.2$ and (b) $A=1.7$.

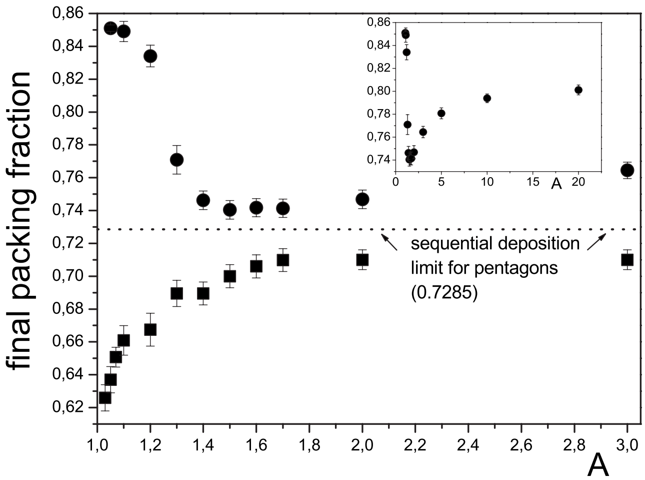

FIG. 5. Steady state packing fraction obtained by averaging over the last 1000 taps as a function of the tapping amplitude for disks (circles) and pentagons (squares). The horizontal dotted line corresponds to the sequential deposition limit for pentagons (see text for details). The inset shows results for disks up to very large tapping amplitudes.

sion allows them to rearrange better and to increase side-to-side contacts.

In Fig. 5 we plot the final values of ϕ, obtained when the system attains the steady state regime (averaging over the last 1000 taps), as a function of the tapping amplitude. We compare results with those of the same experiment carried out on disks [5] (using the same size dispersion, number of particles, and box size) and with a pentagon limiting case obtained as follows. We raise all pentagons up to a large height and let them fall one at a time and in order of height (the lowest particle first). This process leads to the highest compaction. The tapped deposits approach this value of ϕ when A is increased, as seen in Fig. 5. Since the deposition is sequential, pentagons do not form arches at all in the limiting case. Some simulations carried out on different irregular bases showed that the particular realization of the base has negligible impact on the steady state density.

There are two clear distinctions between the behavior shown by disks and that displayed by pentagons. First, disks attain larger packing fractions at all tapping amplitudes. This is to be expected since pentagons, if not carefully arranged, tend to leave large interstitial spaces. This is also explained by the fact that pentagons can hardly attain compact crystalline structures like the one sketched in Fig. 2(d) spanning all over the system. Second, while disks present a nonmonotonic dependence of ϕ versus A, pentagons show a monotonic increase in the packing fraction. At high values of A both systems increase ϕ with increasing tapping amplitudes and eventually reach a maximum plateau value. In the inset of Fig. 5 we extend the range of values of A studied for disks since the increase in ϕ is rather smooth. For low A, we find that disks tend to order and so increase ϕ as A is decreased [5]. A minimum in the packing fraction of disks is then located at intermediate values of A. However, this feature is not present in pentagon packings. Pentagons seem not to order at low A, and ϕ does not present a minimum as in disk packings.

It is worth mentioning that in Ref. [9] the authors show a pentagon system that displays crystallization. However, the Monte Carlo (MC) protocol used in [9] allows particles to explore positions and orientations only constrained by the proximity of other particles. In our model, particles can only move downward due to the action of gravity, and the exploration of positions and orientations during deposition is not driven by a stochastic process but by the dynamics of falls and rolls. After a pentagon reaches a stable position in our model, it is not possible for it to search for “more favorable” configurations. Tapping is not able to drive crystallization in these systems since the number of configurations explored is still reduced by the deposition algorithm compared with a MC simulation in a system at zero gravity.

Realistic molecular dynamic simulations of the tapping of pentagon packings yield higher densities overall [16] since, in general, the restitution coefficient is greater than zero and bouncing promotes rearrangements of already deposited grains. In our simulations the effective restitution coefficient is zero and hence bouncing is avoided. The higher compaction in realistic molecular dynamics resembles the high compaction of packings obtained in Ref. [7]. The same effect is observed when realistic molecular dynamics of disks [4] are compared with corresponding PMDM results [5]. However, the PMDM has been shown to yield the same general trends observed in realistic molecular dynamics (compare Ref. [4] with Ref. [5]).

In pentagon packings, we find that the number of arches presents a monotonic decrease with increasing A. In contrast, disks present a maximum at the same tapping amplitude where the minimum packing fraction is achieved. It is particularly interesting that at $A < 1.1$ disks enter an ordered phase [5] where arches are largely eliminated from the system, whereas pentagon deposits remain in a disordered state with an increasing number of arches down to very small tapping amplitudes.

We observe that, in general, pentagons form fewer arches than disks (about 40% fewer arches). This seems to be in contradiction to the fact that we found that pentagons show a lower coordination number. However, this effect is explained by the wider arch size distribution found in pentagons. In Fig. 6 we show the distribution of arch sizes for pentagons and disks at two values of A. We confirm here that for low A pentagons have a larger tendency to form large arches (up to 20 particles), whereas disks form arches of fewer than ten particles. A detailed study of the particle-particle contacts and the formation of arches will be presented elsewhere.

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 to compare with constant tapping. We start from a sequentially deposited packing and then tap the system at variable amplitude. The amplitude was increased from $A=1.1$ to 1.7 in steps of 0.1, and 5000 taps were applied at each amplitude value. Then the same protocol was followed but for decreasing amplitudes. No evidence of hysteresis or irreversibility was found in the results. We also found that the annealing curves coincide with the constant tapping results of Fig. 5. Both disks and pentagons attain a unique packing fraction value for a given tapping amplitude, no matter the history of the tapping protocol.

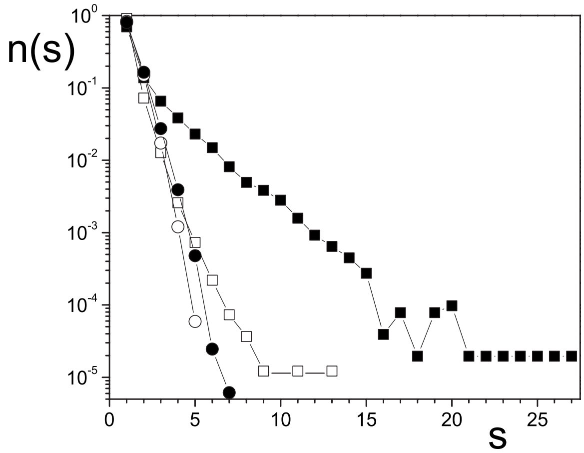

FIG. 6. Distribution of arch sizes for disks (circles) and pentagons (squares) at $A=1.2$ (filled symbols) and 3.0 (open symbols).

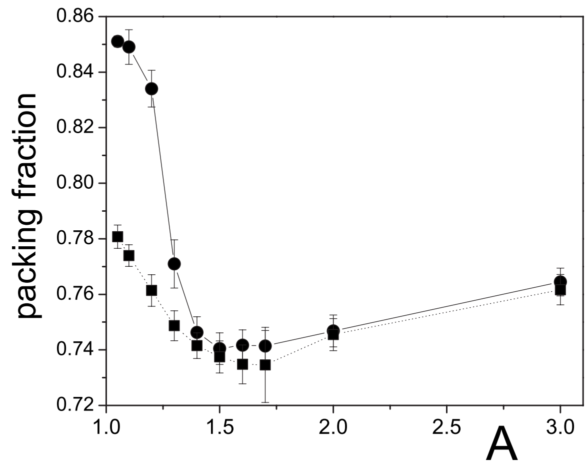

FIG. 8. Steady state packing fraction of disks as a function of A for two values of size dispersion: 5% (circles) and 50% (squares).

Previous simulations on disks [5] and experiments on glass beads [2] do show an irreversible branch in this type of experiment. It is important to note that in the case of previous simulations [5] the annealing was conducted in a different manner since the tapping amplitude was increased in a quasicontinuum fashion and a single tap was applied at each value of A. This prevented the disk packing from reaching the steady state at each value of A. In the present work we give sufficient time for the system to reach the steady state at each amplitude. The annealing experiments of Nowak *et al.* [2] 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 each tapping amplitude.

To get a closer insight into the "peculiar" behavior of pentagons (i.e., the reduction of packing fraction as A diminishes) we show in Fig. 7 the evolution of a pentagon deposit after a sudden reduction in tapping amplitude. After 5000 taps applied to the system with $A=1.5$, we set the tapping amplitude to $A=1.1$ and continue to tap the deposit for 1000 taps. As we can observe, the reduction in A induces a rapid reduction in packing fraction associated with an increase in the size of the arches formed (see insets in Fig. 7), in contrast with the behavior generally observed in deposits of disks. This seemingly paradoxical effect is in fact simple to explain. Arches—which are the main void-forming structures—are more easily created when particles start deposition from an initial high-density expanded configuration. At low A, the expanded configuration leaves particles very close to each other and this make particles meet each other more often during deposition, enhancing the probability of arch formation. This has been discussed recently by Roussel *et al.* [17] and it has been observed by Blumenfeld *et al.* [18] in experiments of compaction in two-dimensional granular systems.

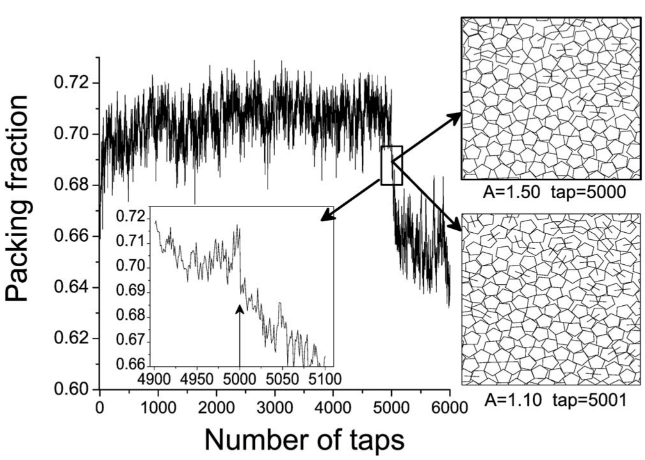

FIG. 7. Packing fraction of pentagons as a function of the number of taps before and after a sudden reduction in tapping amplitude. From $t=1$ to 5000 the packing is tapped with $A=1.5$; from $t=5001$ the amplitude is set to $A=1.1$. The insets show snapshots of parts of the system (with arches indicated by segments) before and after the change in tapping amplitude, and a magnification of the point where the sudden change is induced.

IV. CONCLUSIONS

We have shown that, for pentagons, through either constant tapping or annealing, the steady state of the packing presents a monotonically increasing packing fraction with tapping intensity. However, disks and spheres display a clear reduction in the packing fraction as tapping intensity is increased [1–5]. Moreover, we have shown that our model disks present a smooth increase in packing fraction at large tapping amplitudes. Such findings reveal that the complexity of pentagon deposition leads to an unexpectedly simpler behavior of the packing fraction compared with simpler systems.

The behavior of rounded particles—which increase density on reduction of tapping intensity—is indeed puzzling; while pentagons seem to behave as expected. If grains fall from a highly compact expanded configuration they should form more arches, and hence reduce packing fraction. Rounded particles do not follow this pattern, as has been observed in experiments and simulations of various kinds. Although the behavior of rounded particles seems to be considered reasonable by most workers, no thorough discussion on this has been given in the literature. Most authors explain the effect on the basis that large taps create voids but do not explain how these voids are created from a mechanical point of view. According to the detailed discussion presented by Roussel *et al.* [17], large taps should destroy arches (and thus voids). We believe that the "reasonable" behavior is that large taps eliminate arches and voids; however, at low tapping amplitudes, we presume that this phenomenon competes with the crystal-like ordering that reduces arch formation in disk packings in our simulations.

We have tested the hypothesis that partial ordering leads to the nonmonotonic behavior of disks and spheres. However, some trial simulations carried out with rather polydisperse disks that are known to show frustration of order still present the same nonmonotonic features, although less marked than in monosized disks (see Fig. 8). A sensible explanation for the formation of large arches of pentagons at low tapping amplitude should in principle shed light on this issue. At present, we can only suggest that pentagons (and any other sharp particles) have a larger tendency to multiparticle collisions. Multiparticle collisions are necessary (although not sufficient) to form large arches. These multiparticle collisions are enhanced by two factors: (a) the fact that pentagons may approach each other more closely 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 vertices. A recent model based on collisional probabilities [17] for the formation of arches may help to quantify these effects.

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