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Abstract

We present a simple model to describe the response of a granular bed to a tapping-like excitation when grains can form capillary bridges due to the presence of interstitial liquid. We implement a pseudodynamic simulation of adhesive hard disks. The packing fraction and coordination number after the steady state of the tapping process has been reached are compared for different tapping intensities and liquid contents. We find some contrasting behavior with dry systems and qualitative agreement with experimental data.

Keywords (separated by '-'): Hard disks - Capillary bridges - Pseudo dynamics - Compaction - Tapping

Footnote Information

Simple model for wet granular beds subjected to tapping

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Keywords Hard disks · Capillary bridges · Pseudo dynamics · Compaction · Tapping

1 Introduction

Numerous studies have focussed on the mechanics of wet granular materials [1,2]. Although it is known that capillary bridges between particles are one of the most important mechanisms for cohesion in these systems, is still unclear how the mechanical properties of a wet granular bed can be associated to these bridges.

The use of vibration to drive dry granular matter is commonly used in the study of granular gases [3], segregation [4], and pattern formation [5]. In these systems, fluidization depends on the dimensionless acceleration Γ. For a harmonic oscillatory excitation the dimensionless acceleration is given by $\Gamma = A\omega^2/g$, where A is the amplitude of the oscillation, ω is the frequency, and g is the acceleration of gravity. When these excitations are applied over very short periods of time $[< (2\pi\omega)^{-1}]$ and repeated after the system has reached mechanical equilibrium, we say that the system is being tapped. The evolution of packing fraction as tapping progresses is a very well studied phenomenon in dry granular matter. Moreover, the steady state achieved after a large number of taps can be studied as a function of Γ. Many of these types of studies have been largely advanced by the group of Chicago [6] on the one hand, and by the group of Rennes [7] on the other.

The development of models for wet granular matter is still incipient [8–13]. We adapt a previous model [14] used for the study of dry granular disks compacted by vertical tapping in order to introduce some simple constrains that mimic the presence of capillary bridges. For dry granular disks the model consists in a pseudodynamics where disks fall and roll on top of each other until they find stable positions. The model has proved to be satisfactory in describing some qualitative features of grains having a very low restitution coefficient.

In Sect. 2, we describe the model. In Sect. 3, we present results obtained for systems tapped at various intensities and liquid contents. Finally, we draw some conclusion on the applicability of these types of models.

2 Simulation model

2.1 The reference model

As a reference, we use a model of inelastic hard disks deposited in a 2D rectangular box. Disks move according to an algorithm proposed by Manna and Khakhar [15]. In brief,

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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.

The deposition algorithm consists in picking up a disk in the system and performing a free fall of length δ if the disk has no supporting contacts, or a roll of arc-length δ over its supporting disk if the disk has one single supporting contact. Disks with two supporting contacts are considered stable and left in their positions. If in the course of a fall of length δ a disk collides with another disk (or the base), the falling disk is put just in contact and this contact is defined as its first supporting contact. Analogously, if in the course of a roll of length δ a disk collides with another disk (or a wall), the rolling disk is put just in contact. If the first supporting contact and the second contact are such that the disk is in a stable position, the second contact is defined as the second supporting contact; otherwise, the lowest of the two contacting particle is taken as the first supporting contact of the rolling disk and the second supporting contact is left undefined. If, during a roll, a particle reaches a lower position than the supporting particle over which it is rolling, its first supporting contact is left undefined. A moving disk can change the stability state of other disks supported by it, therefore, this information is updated after each move. The deposition is over once each particle in the system has both supporting contacts defined or is in contact with the base (particles at the base are supported by a single contact).

Particles are moved one at a time, but they perform only small moves that do not perturb to a significant extent the ulterior motion of the other particles in the system. An iteration consist in moving every disk in the system by a distance δ—or the amount allowed by the constrains imposed by neighboring disks. Notice that after an iteration many disks may be left in unstable positions. A number of iterations are needed before every disk finds its stable configuration. For very small values of δ, this method yields a realistic simultaneous deposition of grains with zero restitution coefficient.

The initial configuration is obtained by placing disks "in the air" at random in the simulation box with a very low packing fraction (<0.3). An initial deposition takes the system to its first stable configuration. Then, a tapping process is carried out by using an algorithm that mimics the effect of a vertical tap of amplitude A. The system is expanded by vertically scaling all the y-coordinates of the particle centers by a factor $A > 1$. Then, random rearrangements scaled with the tapping amplitude are introduced to simulate the disorder induced by particle–particle collisions. Then, a new deposition phase takes the system to the next stable configuration. After many taps, the system attains a steady state where properties such as packing fraction, ϕ, and coordination number, z, fluctuate around a plateau value. This model has been described in detail before [14]. We extend this model in such

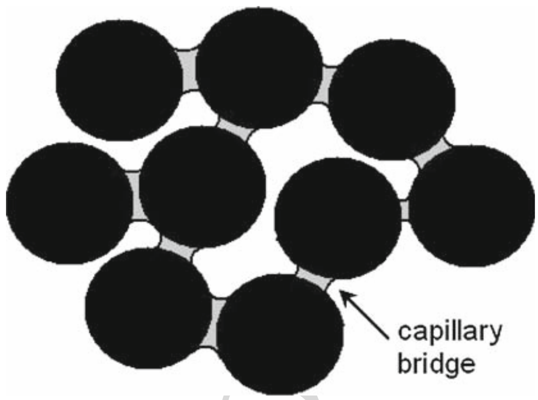

Fig. 1 Schematic diagram of a granular sample in the pendular state. Capillary bridges hold particles together

a way that the effect of capillary forces are taken into account in a qualitative fashion.

2.2 Cohesion forces

A wet granular sample at low content of liquid presents a network of capillary bridges connecting the grains. The structure of this network of bridges determines to a large extent the mechanical properties of the sample [1,2]. We consider situations where cohesion outweighs other effects of the presence of liquid in the system such as lubrication and viscosity. Our model represents a granular assembly in the so called "pendular state" according to the classification by liquid content [1]. In the pendular state particles are held together by the attraction of the capillary bridges at their contact points. Figure 1 shows a scheme of this situation.

In a wet sample, capillary bridges form when two adjacent particles have a contact point. At this point, the liquid surface of the films that wet the particles makes a sharp bend. This is in fact not an equilibrium situation. Where the liquid films meet, the curvature of the liquid surface is very large and negative. This fact generates a substantial under pressure which sucks the liquid towards the contact region. Equilibrium is reached when the liquid surface has acquired a spatially constant mean curvature. If the particles are moved away from each other by a certain distance, a so-called pendular bridge appears due to the bridge stretching [16].

As explained elsewhere [18], there are four main factors affecting the total capillary force in a static liquid bridge: (1) the separation distance between two particles, (2) the liquid bridge volume, (3) the surface tension of the liquid, and (4) the contact angle. Assuming that the contact angle is zero (complete wet) and that the surface tension of the liquid is constant all over the system, the remaining factors can be considered stochastic variables since each bridge in the system may have a different volume and separation depending on local conditions and contact history. We introduce these

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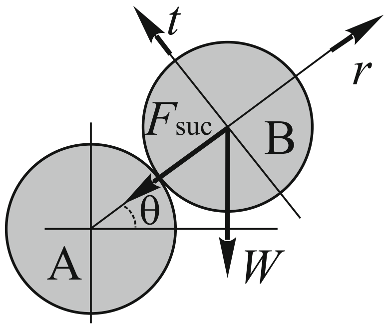

Fig. 2 Schematic diagram of forces acting on a particle B that forms a capillary bridge after contacting another grain A during deposition

two important factors through a single parameter P_0 that we describe below in this section. It is important to notice that in the pendular state some particles may be stable thanks to the geometrical constrains imposed by others. In this situation capillary bridges may exist at the contact points with the supporting grains; however, the stability of the particle is not determined by these bridges. In our model we will only count as a capillary bridge the particle–particle contacts that support the entire weight of one of the touching grains.

In Fig. 2, we show a scheme of the balance of forces on a given particle B of weight W that is in contact with a lower partner A. Assuming the suction F_{suc} [1] does not depend on the angle θ between two particles, the forces involved will be

$$\begin{aligned} \vec{F}_{\text{r}} &= \vec{F}_{\text{suc}} + \vec{W}_{\text{r}} \\ &= (F_{\text{suc}} + W\sin(\theta))\,\vec{r} \quad \text{in the radial direction} \qquad (1) \\ \vec{F}_{\text{t}} &= W\cos(\theta)\,\vec{t} \quad \text{in the tangential direction} \qquad (2) \end{aligned}$$

On the one hand, provided that particle A is fixed in its position, the radial force F_{r} is responsible for the adhesion of particle B onto the bottom partner A. On the other hand, the tangential force F_{t} provides the torque that drives particle B into rolling on top of particle A. Let us assume that the average suction is x times larger than the weight of a particle (i.e. $F_{\text{suc}} = xW$). We consider monodisperse systems where all particles have the same weight. Then we have $F_{\text{r}} = W[x + \sin(\theta)]$. This means that the total force that is responsible for maintaining the particles in contact will vary between $W(x+1)$and $W(x-1)$ as θ goes from $\pi/2$ to $-\pi/2$. For $x < 1$, negative values of F_{r} are obtained for some configurations of dangling disks ($-\pi/2 < \theta < 0$). This corresponds to the radial component of the particle weight overcoming the suction, which invariably leads to the detachment of the dangling disk.

In our model, we represent capillary bridges through a stochastic mechanism so that particles may get stuck during its rolling down over another disks due to suction. The effective sticky probability P_{sticky} is then proportional to F_{r} at each value of θ during rolling

$$P_{\text{sticky}}(\theta) = \max\left\{0,\, P_0 \frac{[x + \sin(\theta)]}{x+1}\right\}. \qquad (3)$$

In this equation we have divided F_{r} by its maximum possible value and introduced the proportionality constant P_0 to control the maximum sticky probability. For $P_0 = 1$ the stickiness is maximum whereas for $P_0 = 0$ particles do no stick, which corresponds to the dry case [14]. In this manner, we can test different overall sticky probability so as to emulate a variation in liquid content within the pendular state. The max function in Eq. (3) takes care of the situation where $x < 1$ for which the second argument may become negative indicating that the particle must detach [i.e., $P_{\text{sticky}}(\theta) = 0$]. Nevertheless, all our simulations have been carried out setting $x = 1$ (see Sect. 3).

2.3 Simulation algorithm

The pseudodynamics for the sticky disks is carried out in much the same fashion as for hard disks [14]. Every disk falls or rolls a small distance in each iteration. After a number of iterations all disks find stable positions; some do this earlier than others. There may be two situations under which a disk is considered stable: (i) the particle contacts with two others (or wall) such that its center of mass lies above the segment that joins the contact points, or (ii) the particle sticks to another disk and so becomes immobilized.

Within each iteration, we choose a disk at a time and allow it to fall freely a small distance δ. If in the course of a fall of length δ a disk overlaps another, the falling disk is put just in contact and this contact is defined as a potential supporting contact. If in a given iteration a disk already has one single potential supporting contact there are two possibilities: (1) to stick through a capillary bridge to the supporting particle and so become immobilized [probability $P_{\text{sticky}}(\theta)$], or (2) to move on by either a roll or a free fall. A particle that sticks is an example of the situation in which the strength of the capillary bridge is enough to prevent the particle from further rolling on top of its supporting disk. A particle that does not sticks to its first potential support [probability $1 - P_{\text{sticky}}(\theta)$] corresponds to the situation in which either a capillary bridge does not form at the contact or the weight of the disk overcomes the strength of the capillary bridge. For this reason the particle can roll down the surface of the lower partner. If a bridge exist, and the suction is not too weak, one expects that the particle may keep rolling without detaching from the surface of the contacting disk even after reaching a lower position with respect to its partner. All along the rolling—composed of small arcs of length δ travelled during each iteration—the disk has a chance to stick [$P_{\text{sticky}}(\theta)$] at every

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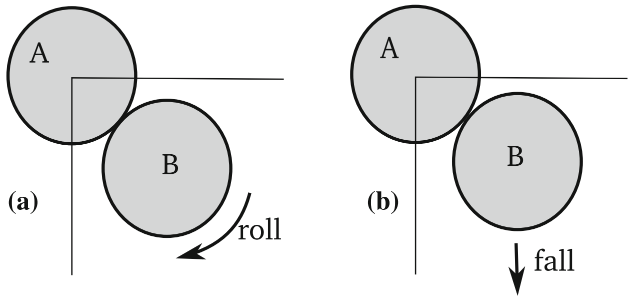

Fig. 3 Example of possible motion followed by a particle that pendulates beneath a second grain. In case **a** the particle rolls down, in case **b** the particle falls freely

iteration and become immobilized. However, once the particle has rolled to a position beneath its supporting partner, and provided that the particle does not stick, there is a probability for the particle to detach and fall freely and a probability for it to keep rolling in contact. We use again $P_{\text{sticky}}(\theta)$ to set the probability that a particle dangling beneath its support will roll in contact without detaching. This probability does not need to be the same as the sticky probability, but it has to be related to the strength of the capillary bridge. We have chosen $P_{\text{sticky}}(\theta)$ for this probability to reduce the number of control parameters in the model. Notice that in this case the disk is not stuck—i.e., it is not immobilized—but remains in contact. In the next iteration, the disk will again have the chance to stick. It is worth mentioning that, since in our simulations $P_{\text{sticky}}(-\pi/2) = 0$ (recall that $x = 1$), all particles that do not stick but roll dangling from its partner will eventually detach at the point $\theta = -\pi/2$, unless a second contact is formed during rolling. The decision of what action to take at any iteration with a given disk in contact with a potential supporting grain can be stated as follows:

1. A disk in contact with a second disk is given a probability $P_{\text{sticky}}(\theta)$ to stick (see E[illegible] If this happens, we say that the second disk fully support the first through a capillary bridge. If the supporting particle does not move further in future time steps the disk will remain in its stable position held by the capillary bridge.
2. If a disk does not stick to its supporting grain [this will happen with probability $(1 - P_{\text{sticky}})$], it will move differently depending on the relative position with respect to the potential supporting particle.
   (a) A disk which is above its supporting particle ($0 < \theta < \pi/2$) will always roll by an arc of length δ or until it touches a third disk (whatever happens first) in its way down.
   (b) A disk which is below its supporting particle ($-\pi/2 < \theta < 0$) will either roll down dangling from the other disk or detach and fall. We choose to make the disk roll with probability P_{sticky} (see Fig. 3a) and fall with probability $(1 - P_{\text{sticky}})$ (see Fig. 3b).

In summary, a particle that contacts another disk with $0 < \theta < \pi/2$ has a probability $P_{\text{sticky}}(\theta)$ to stick and a probability $[1 - P_{\text{sticky}}(\theta)]$ to roll. However, if $-\pi/2 < \theta < 0$, the particle has a probability $P_{\text{sticky}}(\theta)$ to stick, a probability $[1 - P_{\text{sticky}}(\theta)]P_{\text{sticky}}(\theta)$ to roll, and probability $[1 - P_{\text{sticky}}(\theta)]^2$ to detach.

A particle that reaches a second contact after a roll may or may not be stabilized depending on whether the center of mass of the disk lies or not above the segment that joins the contacts. If the disk is stable, and none of the supporting particles move further in future time steps, the disk will remain stable. If the contacts do not stabilize the disk the particle will further roll (or stick) on the lower contact.

After each deposition, a tap is simulated by multiplying all vertical coordinates by a factor $A > 1$ and allowing the particles to move under random displacements of length $0 < \xi < A - 1$. Typically, each particle attempts 20 random moves. Moves that lead to overlaps are rejected. All particles are effectively disconnected after a tap, with no contacts between them. Following Philippe and Bideau [19], we use $\Gamma = \sqrt{A-1}$ as a measure of the tapping intensity. This quantity is proportional to the energy input given by a realistic tap with peak acceleration Γg, with g the acceleration of gravity.

A related model [17] has considered the introduction of stickiness in the deposition of disks. However, this model is based on a deterministic approach in the sense that particles with θ greater than a given critical angle θ_c always stick as soon as they touch their partner, whereas disks that make their first contact with $\theta < \theta_c$ always roll. Moreover, the deposition is conducted in a sequential way, so as to ensure that each particle is stable before the next is released into the simulation box. The deterministic stickiness seems to be more suitable to describe adhesion due to forces such as van der Waals interactions in fine powders, which operate on every pair of grains, since capillary bridges may or may not form at contact.

3 Results and discussion

We have carried out extensive simulations with a rectangular box of width $L = 20$ where we deposit 1,000 monosized disks of radius $r = 0.1 + 1/\sqrt{2} \approx 0.807$. We have chosen the parameter x that accounts for the strength of the suction in such way that a particle dangling right beneath another disk has probability 1 of falling freely, i.e. $x = 1$. This situation corresponds to the case where the suction is just as

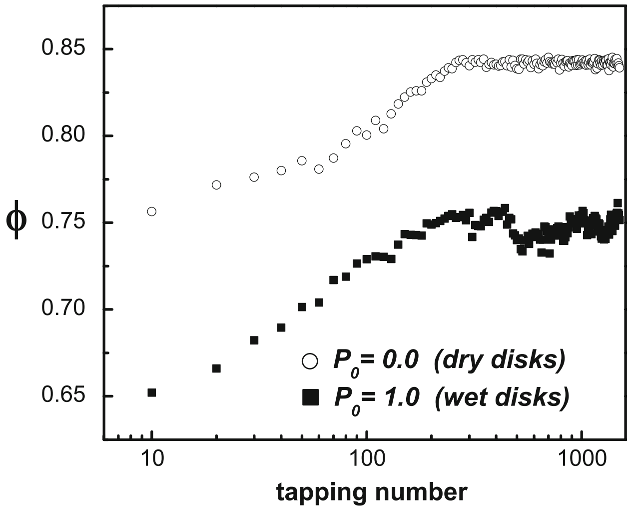

Fig. 4 Packing fraction ϕ as a function of number of taps for dry disks ($P_0 = 0.0$) and maximally wet disks ($P_0 = 1.0$). The tapping amplitude is $\Gamma = 0.224$ in both cases

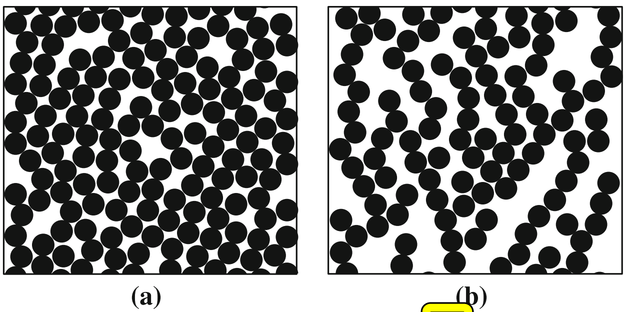

Fig. 5 Snapshots of a fully deposited bed of disk after 1,500 taps for **a** dry ($P_0 = 0.0$) and **b** partially wet samples ($P_0 = 0.125$). Both systems were tapped at $\Gamma = 0.316$. Only part of the whole assembly is shown

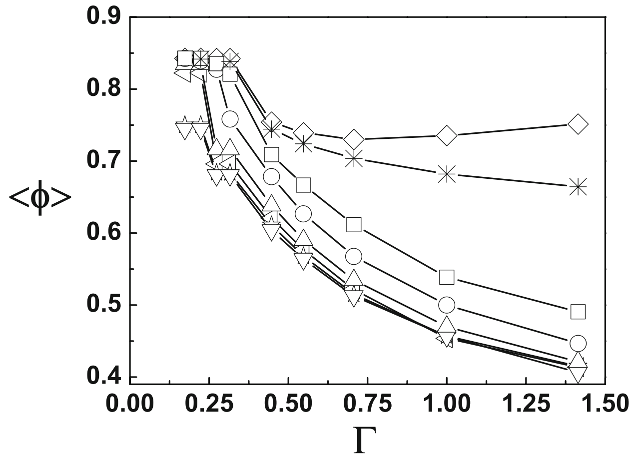

Fig. 6 Mean steady state packing fraction $< \phi >$ as a function of tapping intensity Γ at different liquid content. From top to bottom $P_0 =$ 0.0, 0.005, 0.025, 0.05, 0.125, 0.25, 0.5, 1.0

strong as the weight of the particle. Each system is tapped 1.5×10^3 times at various tapping intensities Γ and for different maximum sticky probabilities P_0. Averages have been taken over the steady state of the system; typically after 10^3 taps. The very first deposition is performed on a dispersed configuration ($\phi = 0.3$) with disks randomly placed in the simulation box.

In order to asses the main features distinguishing a dry system from a wet system we plot in Fig. 4 the packing fraction as a function of the number of taps applied from the start of the simulation for the two extreme cases, i.e., $P_0 = 0$ (dry disks) and $P_0 = 1.0$ (wet disks). In both cases tapping improves the compaction of the system. However, the steady state packing fraction of wet disks is significantly lower (13% lower than the dry system). The capillary bridges formed in the wet system prevent efficient filling of the space. Moreover, the wet system present larger density fluctuations. This is commonly observed in experiments; reproducibility in wet granular systems is hard to achieve due to these large fluctuations even in very well controlled conditions. Figure 5 shows snapshots of fully deposited configurations of a dry system ($P_0 = 0$) and a partially wet system ($P_0 = 0.25$) after 1,500 taps of amplitude $\Gamma = 0.316$. It is clear form this figure that stickiness promotes the formation of chain like structures in the deposit.

In Fig. 6, we show the steady state packing fraction $< \phi >$ of the granular beds as a function of the tapping intensity Γ. Each curve corresponds to a different value of sticky probability P_0 ("liquid content"). For the dry system ($P_0 = 0$) it has been shown [14] that, as Γ is increased, the packing fraction falls and reaches a minimum at $\Gamma \approx 0.75$ after which a mild increase is evident. The initial decrease in $< \phi >$ (between $0.3 < \Gamma < 0.4$) is rather sharp and coincides with an apparent order-disorder transition. For the wet systems the change in behavior is dramatic. A very small amount of liquid (or equivalently, a low sticky probability $P_0 = 0.025$) suffice to draw the packing fraction a monotonic function of the tapping intensity. Moreover, the wet samples show a marked reduction in packing fraction for large tapping intensities reaching as low as 0.4. Interestingly, beyond $P_0 = 0.125$ we find that all systems present the same response to tapping.

The mean coordination number $< z >$ is very sensitive to changes in the liquid content. In Fig. 7 we can see that, whereas the coordination number increases with Γ at tapping intensities beyond the order–disorder transition (see Ref. [14]) for dry systems, wet samples have a sharp decrease in $< z >$. Again, beyond $P_0 = 0.125$. All samples have a similar response to tapping. In particular, for $P_0 > 0.125$, the coordination number falls abruptly to the asymptotic value $< z > = 2.0$ which means that all disks are stable thanks to a capillary bridge. In this situation, the packing is made up of a series of vertical chains of disks.

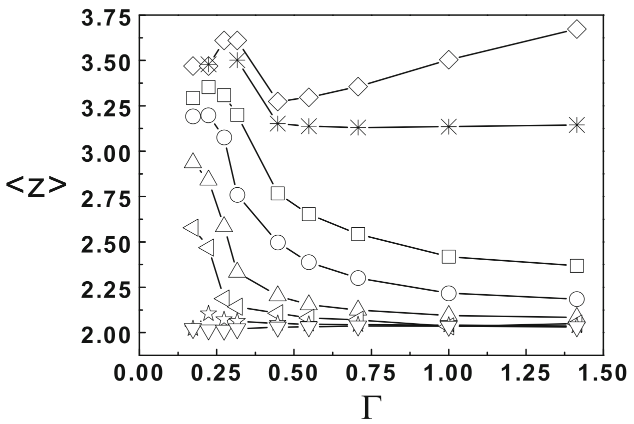

Fig. 7 Mean coordination number $< z >$ as a function of the tapping amplitude Γ for different liquid content P_0. From top to bottom $P_0 = 0.0, 0.005, 0.025, 0.05, 0.125, 0.25, 0.5, 1.0$

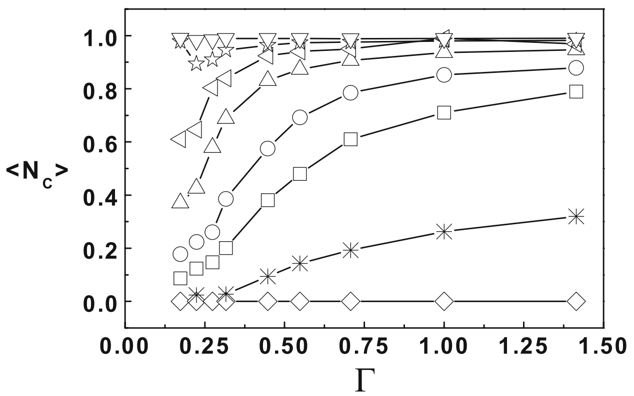

Fig. 8 Mean number of supporting capillary bridges $< N_c >$ as a function of the tapping amplitude Γ. Results for different sticky probability P_0 are shown. *Symbols* are as in Fig. 6

The drop in the coordination number is connected directly with the number of capillary bridges. In Fig. 8, we plot the mean number of capillary bridges $< N_c >$ that support a particle. For each particle the number of capillary bridges that support it is either 0 (the particle is supported by the geometrical constrain imposed by two contacts rather than a capillary bridge) or 1. As we can see, $< N_c >$ grows very rapidly from 0 to 1 as Γ is increased. For high liquid content, the rise is very sharp. This plot shows that capillary bridges, below a given liquid content, are not present for very low tapping intensities. We recall here that a contact is consider a liquid bridge if it supports a particle that would otherwise need a second contact to stay stable. Therefore, that the coordination number is high while N_c is low means that most particles are supported by two contacts capable of stabilizing the grain even in the absence of liquid.

The results shown are consistent with experimental observations within the pendular state. The addition of liquid to the system leads to the formation of liquid bridges between the grains. The capillary forces restrict the motion of the particles during deposition, giving, as a result, a rather inefficient packing and a low packing fraction. In the region where the liquid content is low (wetting region) increasing humidity will cause the increase of the number of particle–particle contacts that develop a capillary bridge [9]. As a consequence, packing fraction and coordination number decrease with liquid content. However, beyond a given liquid content, a further increase in liquid does not promotes the appearance of more bridges. This last scenario corresponds with the so-called filling region, where ϕ is almost constant and saturation plateau appears in N_c. Finally, if liquid content is increased further, forces related to capillary bridges becomes smaller as the amount of liquid in the bridges increases [1,8,9]. This leads to less restriction to the motion of grains that form capillary bridges which drives to an eventual increase in packing fraction. This last effect is not observed in the present model because we restrict ourselves only to simulate the pendular regime [8].

Let us consider now the effect of tapping intensity. For high tapping intensities, each tap increases considerably the free space in the system [20]. During deposition, particles rolling down along the surface of another disk will unlikely find other disks to rest over. Therefore, grains spend more time steps rolling over the surface of the supporting disk increasing the probability of getting stuck. Moreover, after the random moves, particles have a greater chance to collide with each other with an angle θ near $\pi/2$ where sticky probability P_{sticky} is maximum (see Eq. 3, Fig. 2). This gives place to the formation of open structures where particles stick to each other in long chain-like clusters. Consequently, a low packing fraction is obtained with low coordination number. When the tapping intensity is low, expansion introduces a very limited free space in the system. This implies that random moves are small and the structure evolves very slowly from tap to tap. A disk supported by a capillary bridge may detach after a tap and contact the same supporting disk roughly at the same point on deposition, with great chances of forming a new bridge further down on its rolling. Even at high liquid content, particles may find highly compact structures in the presence of many capillary bridges because each tap drives a particle to make a capillary bridge slightly below the point where it was the tap before. Packing structures are then closer and the final relaxation of the system allows a better compaction.

For the sake of completeness, we plot in Figs. 9, 10 and 11 the packing fraction, mean coordination number and mean number of supporting capillary bridges as a function of maximum sticky probability. All trends described above are observed again in these plots. It is worth mentioning that the packing fraction in Fig. 9 is consistent with the density observed in wet expanded polystyrene beds [21,22] and glass beads [8] (note that in these experimental studies the distance to the maximum density is reported as porosity).

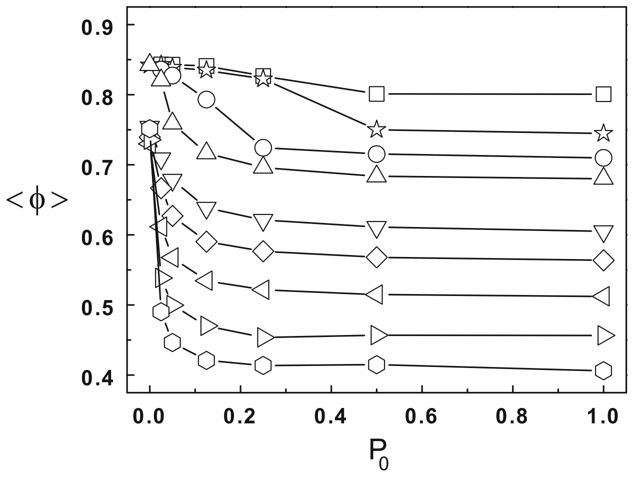

Fig. 9 Packing fraction $< \phi >$ as a function of liquid content (as measured by the sticky probability P_0. Each curve corresponds to a different tapping intensity Γ as follows: 0.173 (*squares*), 0.224 (*stars*), 0.274 (*circles*), 0.316 (*up triangles*), 0.448 (*down triangles*), 0.548 (*diamonds*), 0.707 (*left triangles*), 1.000 (*right triangles*), 1.414 (*hexagons*)

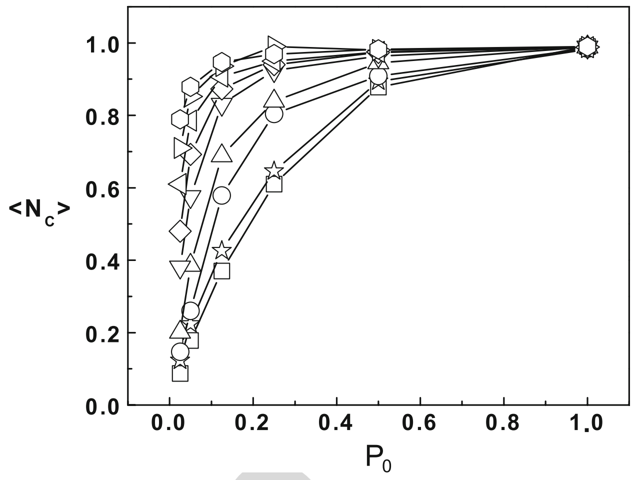

Fig. 11 Mean number of supporting capillary bridges $< N_c >$ as a function of the sticky probability P_0. Results for different tapping intensities are presented as in Fig. 9

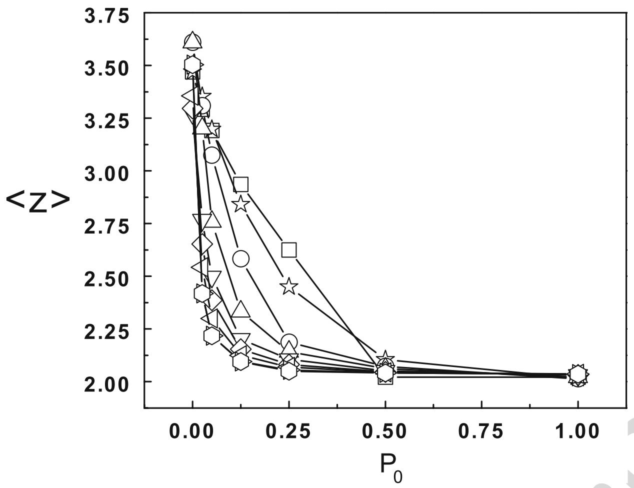

Fig. 10 Mean coordination number $< z >$ as a function of the sticky probability P_0. Results for different tapping intensities are presented as in Fig. 9

The coordination number shows a fast decrease when liquid content is increased for samples tapped at not very low intensities. However, at very low tapping amplitudes $< z >$ falls somewhat slowly towards the universal limit reached for all samples at very high liquid content (i.e. $< z > = 2$). In this limit, all samples present chain-like structures [10,21,23].

The number of supporting capillary bridges follows a trend inverse to the coordination number (see Fig. 11). In the limit of high liquid content all particles are supported by a capillary bridge. This behavior is observed in experiments with glass beads where the addition of water promotes a rapid increase in the total number of capillary bridges that soon reaches a plateau [2].

4 Conclusions

We have shown that a very simple model of hard inelastic adhesive disks displays many of the features seen in wet granular materials within the pendular state. These type of models may help to understand the general and more robust features of wet granular samples that are driven by geometrical constrains as well as effective attractive short range interactions.

In our model the maximum sticky probability P_0 is a measure of the chances that a capillary bridge forms between two touching grains. We can tune this probability within the pendular state. At larger liquid contents, the number of bridges stay relatively constant while their strength changes. This last regime cannot be modeled in the simple approach presented here.

The results show that the increase of P_0 promotes the formation of open chain like structures with very low packing fractions (below 0.5 at high tapping intensities) and low coordination numbers. However, the effect of the increase of P_0 levels off beyond $P_0 = 0.125$. At low tapping intensities it is possible to reach relatively high packing fractions even with large liquid contents.

Our results prove that a simple model accounting for the cohesion forces present in wet granular media within the pendular state can explain the observed experimental trends at least qualitatively.

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