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Instability of 2D random gravitational packings of identical hard discs

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Abstract. In this paper, we consider 2D random packings of hard discs under gravity. We address the question of the nature of the typical packing of identical discs in the thermodynamic limit. We present numerical results on packings built by gravitational deposition of discs with random radii. Our results suggest that, in the limit of zero randomness: (i) the convergence of the system towards its thermodynamic limit becomes extremely slow; (ii) the limit packing fraction seems to increase drastically. We show in particular that if round-off errors are the only source of randomness of the system, the asymptotic regime cannot be reached because of the huge number of discs needed (at least 10^{16} discs using single precision floating-point arithmetic).

1. Introduction

In this paper we consider random packings of discs under gravity: the model is two-dimensional. In 3D (which is most often the experimental situation) it is well known that experimental packings of identical spheres give rise to disordered packings which exhibit a reproducible value of compacity [1], definitely different from the maximum value obtained in the case of the perfectly compact, centred cubic lattice. To our knowledge there is no explanation for this (almost) reproducible value of the packing fraction, but the origin of the disorder is well understood. Disorder originates from the frustration which occurs as soon as one tries to add new layers of identical spheres to a packing having the centred cubic geometry. In dimension 2, frustration plays a much less preponderant role; in particular, adding new layers of identical discs (or parallel cylinders, since those are most often used in experiments) over a 2D packing having the maximum packing fraction (triangular lattice) automatically expands the triangular lattice. Thus one can wonder [1] whether, in 2D, the randomness induced by frustration is sufficient to ensure a thermodynamic limit (in the sense of infinite heights) to random packings of identical discs (thus, a reproducible asymptotic value of packing fraction), as seems to occur in 3D.

On the other hand numerical simulations [1-3] and experimental studies of real systems [4] have shown typical random packings of discs with a packing fraction of about 0.82; some theoretical approaches assess for this value [5]. But the question remains open: does there exist a typical two-dimensional random packing of identical discs? Typical in this case has an experimental meaning: this packing should be stable with respect to small random fluctuations of (for instance) the radii of the discs, or the geometry of the walls.

We have processed numerical simulations of gravitational packings of discs. The radii of the discs are random (fluctuations between 0.1 and 0.001). We observed that,

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as the randomness goes to zero, the asymptotic packing fraction increases drastically; but, as randomness decreases, the amount of calculation needed to reach the asymptotic regime increases so rapidly that it was impossible to get accurate information about the limit of zero randomness.

We have recorded the coordinates of the discs' centres; these data do not exclude that the high values of packing fraction we observed might be a hint of the existence of a limiting triangular lattice.

2. The model

Our model has already been considered in previous works (see e.g. [6]). Rather than a semi-infinite rectangle we consider a semi-infinite cylinder: the base is a one-dimensional torus (the left-hand side of the packing is also its right-hand side). At each step of the simulation we drop a new disc at a random abscissa; no overlap of discs is allowed. As the disc reaches the top of the packing it rolls down the packing, according to gravity, until it finds a (statically) stable place in equilibrium over two other discs; then it sticks to the packing (it will not move any more) and a new disc may be dropped. If the disc rolls down to the bottom of the box, its abscissa is taken to be random. For the purpose of particular tests, we have built some packings over a first, regularly spaced, bottom layer.

Furthermore, we can choose two different values R and r for the radii of the discs ($R > r$): for any new disc the radius is chosen at random between these two values with probabilities p and $1-p$. Obviously, the only important quantities are p and the radii ratio R/r.

Periodically we record the geometry of the top layer of the packing in order to compute the packing fraction and the statistical distribution of the angles of the 'associated lattice'. We call the associated lattice the lattice with its vertices at the centres of the discs and with its bonds joining the centres of any two discs in contact.

We have considered packings with as many as 10^8 discs. The difference from the previous simulations is that we use an explicit control of the randomness of the radii. As we shall see, the evolution of the packing (as more and more layers are added) is so slow that the fluctuation introduced by round-off errors alone is insufficient to reach the thermodynamic limit within reasonable computation times.

The randomness that we introduce in our simulation is theoretically very important. Indeed, as we shall see in section 4, if all discs have exactly the same radius R, the asymptotic packing fraction of the packing is strongly related to the configuration of the bottom layer. In particular, depending on the choice for the bottom layer, one can get packing fractions from $\pi/4$ (≈ 0.785, value for the square lattice, observed if any two neighbouring discs of the bottom layer are $2\sqrt{2}\,R$ apart) to $\pi/2\sqrt{3}$ (≈ 0.907, value for the triangular lattice, if the space between bottom discs is $2R$, or if it is $2\sqrt{3}\,R$): the problem is highly degenerated. We expect the randomness to suppress this degeneracy and to result in a unique thermodynamic limit (thus, a unique packing fraction value).

3. The experimental results

Our experimental results are summarized in figures 1 and 2. We have used R as the unit length. We have used the following values for the box width: 200, 400, 800 and

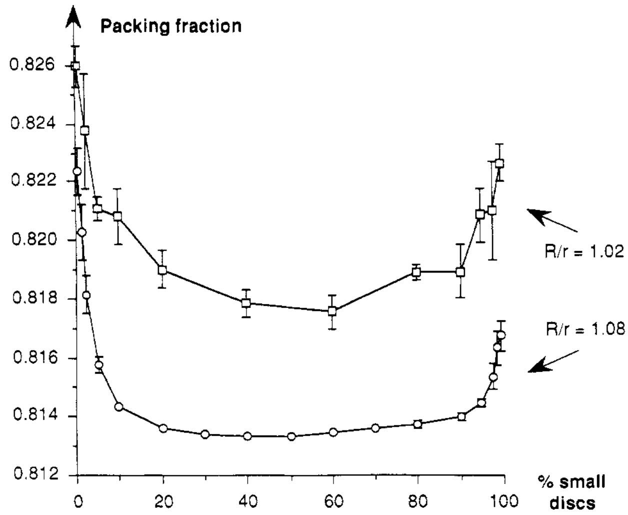

Figure 1. Plot of the asymptotic packing fraction of the packings against the percentage of small discs for two values of the radii ratio. The points of the case $R/r = 1.02$ for the extremal values of p (0.625% and 99.375%) are obtained from five samples of 50 000 000 discs each. Each other point of the graph is obtained from five samples made of 1 000 000 discs. The box width is equal to $200R$.

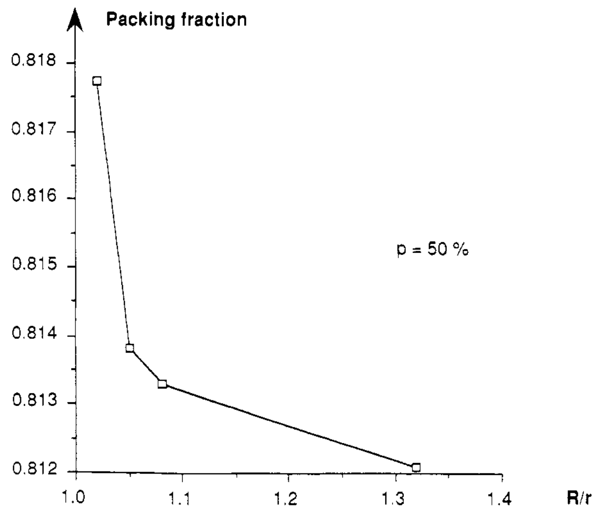

Figure 2. Plot of the asymptotic packing fraction of the packings against the radii ratio for a 50% percentage of small discs. Each value is obtained from five samples made of 1 000 000 discs. The box width is equal to $200R$. The error bars are smaller than the plot symbols.

1600; moreover, we have also used special values (multiples of 2, of $2\sqrt{2}$, of $2\sqrt{3}$), and we have checked that the asymptotic behaviour does not depend at all on the precise value of the width.

If the radii ratio is not too close to 1 and p is significantly different from both 0 and 1 the system exhibits a satisfactory convergence: the packing fraction converges rapidly to a limit value, independently of the width of the box. But as randomness decreases (radii ratio going to 1 or p going to 0 or 1), things go wrong: the convergence strongly slows down and as we approach these singular values, the asymptotic packing fraction increases rapidly. For instance, for $R/r = 1.08$, we were able to obtain with sufficient accuracy the packing fraction for values of p in [0.006 25, 0.993 75] by dropping 5×10^6 discs (five samples of approximately 10^6 discs) for each case; for a more singular radii ratio, ($R/r = 1.02$), the same number of discs provided good convergence only for p in [0.025, 0.975], and we had to drop 25×10^7 discs (five samples of approximately 5×10^7 discs) in order to deal with the extremal values of p.

We give now some geometrical observations. By studying the statistics of the orientations of the bonds of the associated lattice, we observed that, at large disorder, the angles are regularly distributed, mainly between $\pi/6$ and $\pi/3$. As randomness decreases, the distribution seems to become peaked, its average decreasing towards $\pi/6$. This would be the case if the limiting lattice was the triangular lattice with orientations of the bonds equal to $\pi/6$ mod $\pi/3$ ('vertical' triangular lattice). If this was the case, the limiting packing fraction would be $\pi/2\sqrt{3}$ (≈ 0.907); in fact, we observed neither such a value nor a Dirac distribution of the bonds' orientations.

Remark 1. In figure 1, we see that the packing fraction is minimum for $p = \frac{1}{2}$, whereas one expects generally that the diagram p versus packing fraction of a binary mixture be concave, minimum for $p = 0$ and $p = 1$, and maximum for an intermediate value of p. The explanation of this contradiction is that figure 1 was plotted for values of the radii ratio very close to 1. If this ratio becomes significantly larger than 1, the usual concavity appears for the intermediate values of p; but the ghost of the convex curve obtained in the limit $R/r = 1$ seems to remain near the values $p = 0$ and $p = 1$: the packing fraction reaches minimum values very close to $p = 0$ and $p = 1$, and seems to go abruptly but still continuously to the maximum value $\pi/2\sqrt{3}$ for p exactly equal to 0 or 1.

Remark 2. Even for the smallest randomness with which we were able to compute ($R/r = 1.001$), the packing fraction is not at all close to 0.907, and the orientations distribution is widely spread. A test of the stability of the triangular lattice would be valid only if the limiting lattice was a slightly distorted triangular lattice; this can happen only for very small randomness, which makes the test impossible since the needed amount of computation is prohibitive, as we shall see below. This explains why previous authors concluded that the asymptotic lattice is random; in particular, usual round-off errors are very small compared with 0.1%, which is the smallest amount of disorder for which our system could reach under reasonable computation times the asymptotic regime.

4. Discussion

4.1. Packings of equal discs without defects are periodic

For simplicity, let us first describe the simplest packings of equal discs (with radius unity). Suppose that the first layer has n discs and is horizontal, and that the distance between centres of successive bottom discs is never more than $2\sqrt{3}$. It is easy to see that no frustration occurs. The order in which the discs are successively deposited is irrelevant for the geometry of the packing; each pair of neighbouring bottom discs will be covered by one disc of the next layer, and so on; the concept of layer remains valid for all the packing and each disc of the packing may be indexed by the number of the layer it belongs to. Each disc is in contact with two discs of the layer above it and with two discs of the layer below it; consider now the set made of two neighbouring discs of the same layer (denoted W and E for West and East), and of the two discs in contact with these two (one above denoted N, one below denoted S). These discs form a lozenge, so that SE (i.e. the line joining the centres of S and E) is parallel to WN (and WS is parallel to NE); of course, a WN bond of layer i is a SE bond of layer $i+1$, in other words SE orientations propagate towards the North-West direction. Thus, the set of the orientations of all the, say, SE bonds of layer $i+1$ is the same as that for layer i: this set is conserved (figure 3). The same is true for the WS bonds, which propagate towards the North-East direction.

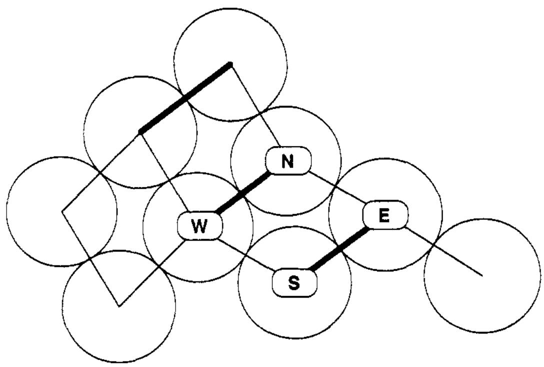

Figure 3. Detail of a packing having the lozenge structure. Although the packing is random, the three bonds drawn in bold have the same orientation.

We recall that we consider horizontally periodic packings, as if the packings were built, not on a semi-infinite rectangle, but on a semi-infinite vertical cylinder. A packing built in a box, i.e. in a semi-infinite rectangle, would slightly complicate the description, since the propagating orientations would experience reflection on the walls. The sets of the orientations of SE and WS bonds shift in opposite directions each time a new layer is deposited. Thus, layers 1 and $n+1$ are identical, up to a translation, so that the packing is periodic, with an oblique wavevector; the vertical extent of the vector describing the spatial period is the height of n layers. In particular, the asymptotic packing fraction C of the packing is the packing fraction of any subset made of n successive layers, and is given by:

$$C = \frac{\pi}{4}\left(\frac{1}{n^2}\sum_{i=1}^{n}\sum_{j=1}^{n}\sin(\alpha_i+\alpha_j)\right)^{-1}$$

where α_i is given as a function of the successive abscissae $x_1 \ldots x_n$ of the centres of the discs of the first layer by:

$$\alpha_i = \cos^{-1}((x_{i+1}-x_i)/4).$$

Thus, depending on the positions of the bottom discs, C can take any value from $\pi/4$ (≈ 0.785) (all $x_{i+1}-x_i$ equal to $2\sqrt{2}$) to $\pi/2\sqrt{3}$ (≈ 0.907) (all $x_{i+1}-x_i$ equal to $2\sqrt{3}$, or all equal to 2).

4.2. *Packings of equal discs with defects seem eventually periodic*

Suppose now that, all discs being still perfectly identical, we allow distances between centres of successive bottom discs to be more than $2\sqrt{3}$ (e.g. as in our algorithm). We use hereafter the following definitions: α (respectively β) is the generic notation for the angle (with respect to the horizontal direction) of SE and WN (respectively WS and NE) bonds; α and β are in $]-\pi/2, \pi/2]$ (e.g. for the two bottom layers, the α angles are in $]0, \pi/3]$ and the β angles are in $[-\pi/3, 0[$). According to the previous description, α and β angles propagate upwards (α going left and β going right); in the previous situation, the meeting of an α and a β created a lozenge with angle $\alpha-\beta$. This will remain the case if $\alpha-\beta$ is in $[\pi/3, 2\pi/3]$, otherwise a defect is created to the lozenge's lattice.

Here is a rough description of the simplest cases of creation of defects. Of course, more complicated cases may occur, especially if $\alpha-\beta$ is far from $[\pi/3, 2\pi/3]$. If $\alpha-\beta<\pi/3$ ('flat defect', figure 4(a)), S prevents N from touching simultaneously W and E, so that N forms an equilateral triangle with S and, either W, or E. If $\alpha-\beta>2\pi/3$ ('sharp defect', figure 4(*b*)), W and E cannot both be in contact with S: only the first of them (W, say) to be deposited will touch S. In the simplest cases, E will be deposited on W, so that N will form an equilateral triangle with W and E.

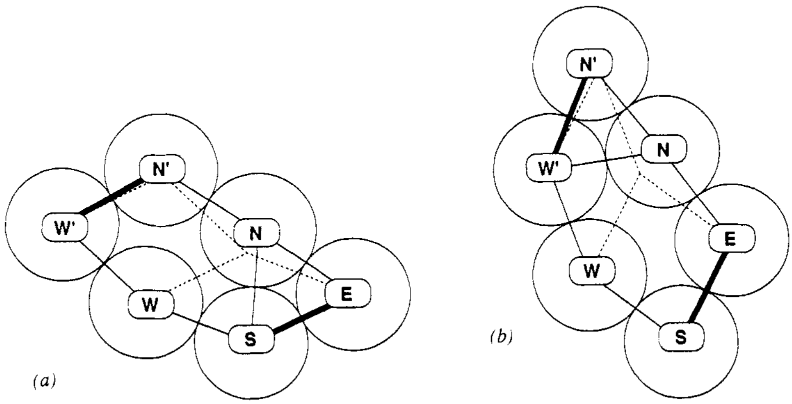

Figure 4 (*a*) Since the orientations of SE and WS are too close to the horizontal direction, a flat defect is created. The two frustrated lozenges (dotted lines) are replaced by one equilateral triangle and one pentagon. The defect somehow suppresses pathologies, since W'N' and NE are less close to the horizontal direction than, respectively, SE and WS. (*b*) Since the orientations of SE and W'W are too close to the vertical direction, a sharp defect is created. Again in this example, the defect improves things on the average: W'N' is slightly more vertical than SE but N'N is significantly less close to the vertical direction that W'W.

Since the bottom layer is horizontal, flat defects are created before sharp ones. As far as the asymptotic properties of the packing are concerned, we need know what is the effect of the defects on the previously described propagation of the orientations. Although we are not able to give rigorous statements, we can describe the main effect of defects. We have made the geometrical calculations in the simplest cases, i.e. for defects which can be seen as perturbation of the regular (lozenge) case. In this framework, the defect is the perturbation of two neighbouring lozenges (one of which is the limit lozenge, i.e. it has angles $\pi/3$ and $2\pi/3$) into one equilateral triangle and one neighbouring pentagon. Thus, we still can use the concept of propagation of α and β (the propagation through such a defect corresponds to two steps of the regular propagation), except that transmitted angles are now not exactly equal to incident ones (figure 4).

It is easy to see that the modification of the angles associated with these defects tends to suppress pathologies, in the sense that, if $\alpha-\beta<\pi/3$ (respectively $\alpha-\beta>2\pi/3$), the transmitted angles α' and β' satisfy $\alpha'-\beta'>\alpha-\beta$ (respectively $\alpha'-\beta'<\alpha-\beta$). Through this effect, initial α and β angles are corrected each time they are involved in a defect, until all possible $\alpha-\beta$ angles are in $[\pi/3, 2\pi/3]$; for a sufficiently large system, this implies that α and $(-\beta)$ angles are in $[\pi/6, \pi/3]$: we are back to the previous, flawless, situation.

We cannot make a rule that such a mechanism always takes place, leading after a finite number of layers to a periodic packing. Indeed, the rigorous rules of the propagation of α and β angles are much more intricate than what the perturbative approach provides, in particular they involve neighbouring α and β angles, and they are sensitive to the deposition order (which is governed by the random sequence of the dropping abscissae). Nevertheless, our numerical simulations are in agreement with this description of the effect of the defects since in this situation ($R/r=1$, horizontal random bottom layer), we have always seen the flawless, periodic packing settle after a finite height.

4.3. 'Large' fluctuations of the radii yield reproducible packing fractions

(Here, large means approximately above 1%). Let us introduce now a fluctuation of the radii, namely a ratio $R/r\neq 1$ and a rate p. As we are interested in the typical packing of identical discs, we restrict discussion to values of R/r close to 1. Still, we can consider the situation as a perturbation of the regular case; orientations still propagate through the packing, but they experience small variations when N, W, E and S have not all identical radius. If one considers that the variability of the radii is the main mechanism which governs the evolution of the angles, this diffusive process leads to an *a priori* regular equilibrium distribution of the angles, whence a non-singular asymptotic packing, and a typical packing fraction of such packings, as previously guessed [5], around 0.82.

In figure 5, we compare the statistics of $\alpha-\beta$ for large and (relatively) small randomness. These plots were obtained by recording the value of the angle between WN and NE as the disc N is deposited onto its neighbours W and E, for a large number of dropped N discs. Note that these statistics provide information about the defects; indeed, values of $\alpha-\beta$ around $\pi/3$ (up to an uncertainty of the angle of order $R/r-1$) or over $2\pi/3$ are the signatures of the defects. We observe indeed that, at large disorder ($R/r=1.08$, $p=0.5$), the distribution is quite flat, and almost symmetrical with respect to $\pi/2$. The bump around $\pi/3$, which is due to the N discs which deposit on contacting W and E (yielding triangles in the associated lattice), is quite important: as randomness is (relatively) large, the process of generation of defects (due to the random evolutions of the angles) is rather active. In some sense, this is the high-temperature phase of the system.

4.4. The zero-randomness limit seems singular

Unexpectedly enough, for a smaller disorder, the trend seems to be the creation of a peak near $\pi/3$, which is compatible with the higher values of packing fraction recorded at small disorder (as has been checked). Note that the defects seem much rarer: the bump around $\pi/3$ is less important. If the diffusive process described above was still preponderant, only the convergence speed would be modified, not the limit equilibrium. As this is not the case, we are led to assume that the dynamics induced by the occurrence

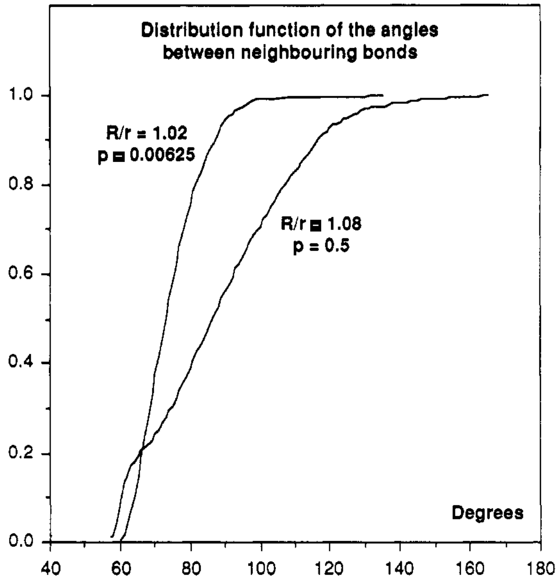

Figure 5. Plot of the distribution functions of the angles between neighbouring bonds for two values of the randomness. At small disorder, angles gather towards 60°. The jump of the curve around 60° is the signature of the population of triangular defects.

of the defects become relevant. Unfortunately, this occurs only for very small disorder, when the dynamics are very slow, so that it is numerically impossible to monitor the system for a value of the disorder small enough to enhance the effects of the defects with respect to the diffusive evolution of the angles; only such an enhancement would allow a conclusive observation of a sharp angle distribution. The next section provides some figures about the convergence speed.

4.5. Calculation of the dynamics in the simplest case

In general, it is not possible to compute analytically the evolution of the packing as its height increases. This computation is made possible if we restrict to a system with no defect, in the limit where R/r is close to 1. It becomes easy if we start the packing with a regular bottom layer with inter-disc spacing equal to $2\sqrt{2}\,R$ (which would yield, for $R/r = 1$, the square lattice with all bond orientations equal to $\pi/4$), and if we focus on the first step of the evolution, i.e. the destruction of the (square lattice) order. Of course, we have checked that this first step is followed by a second one which leads to the same asymptotic properties as indicated above, in particular (at small disorder) the trend towards a (triangular lattice) order.

For simplicity of calculation, let us now take the radii of the discs equal to:

$$r = 1 + \mathrm{d}r \qquad \mathrm{d}r = \pm a \text{ with equal probability} \qquad a \ll 1.$$

As we restrict consideration to values of the height for which the lattice is still a small perturbation of the square lattice, we can index each disc by the number n of the layer it belongs to, the bottom layer being layer 1. At the first order in a (and omitting the terms which become negligible for n large) we can compute the shift of the position of a disc belonging to layer n, with respect to its position for $a = 0$. The projection of this shift onto the North-West direction is

$$2 \sum_{i=1}^{n} \mathrm{d}r_i$$

where the indices refer to the 'path' of the sucessive SE neighbours, down to the bottom, starting from the considered disc. Then, it is easy to see that the shift of an $\alpha - \beta$ (we denote this lozenge angle now as θ) belonging to layer n is:

$$\mathrm{d}\theta = 2\left(\sum_{i=1}^{n} \mathrm{d}r_i^1 + \sum_{i=1}^{n} \mathrm{d}r_i^2 - \sum_{i=1}^{n} \mathrm{d}r_i^3 - \sum_{i=1}^{n} \mathrm{d}r_i^4 \right)$$

where the upper indices $1, \ldots, 4$ refer to four different paths. If n is small with respect to the width of the packing, these four paths do not intersect: all $\mathrm{d}r_i^j$ are independent random variables, so that $\mathrm{d}\theta^2$ is of order $4na^2$. This estimate is enough to derive the value of the local packing fraction around layer n (for a sufficiently large system):

$$C(n) = C(0)(1 + 2na^2)$$

where $C(0) = \pi/4$ (≈ 0.785).

We make a remark about the independency assumption. If n is large with respect to the box width, the paths intersect, but an easy calculation shows that the correlations induced by this finite-length effect cancel at the first order. Figure 6 shows the good fit of this estimate with the numerical results.

More generally (for an arbitrary bottom layer), the diffusion of the angles at height h is of order ha^2. In order to reach the asymptotic equilibrium, we need $\mathrm{d}\theta$ to be at least 0.1 rad. Moreover, in order to get rid of the finite-width effect, this width must

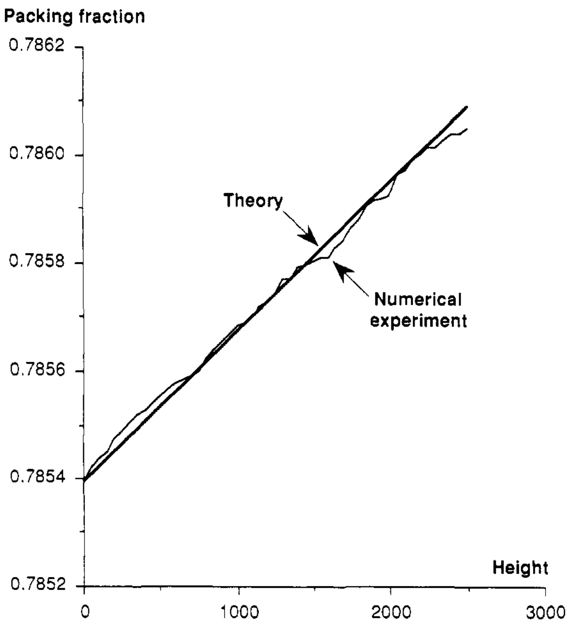

Figure 6. Evolution of the local packing fraction as a function of the height of the packing; the bottom layer has a regular interdisc spacing equal to $2\sqrt{2}\,R$ (square lattice). Here, $R/r = 1.001$, $p = 50\%$ and the box width is an integer multiple of $2\sqrt{2}\,R$, close to $1600R$.

be at least of order $1/a$. Thus the number of discs to be dropped is at least of order $1/(100a^3)$; this is why we did not use values of a below 5×10^{-4}. In fact, some works have been done in the past on boxes of width around 1000, for which the round-off errors were used as the only source of randomness. In the best case (single precision, $a\approx10^{-7}$), the limit cannot be reached before having dropped about 10^{13} layers of discs; this means packing approximately 10^{16} discs, a prohibitive amount. (A hypothetic specialized machine able to build 10^6 discs per second would have to run for 300 years to achieve this packing.)

5. Conclusion

We were interested in the typical geometry of gravitational packings of identical discs. As we have seen, fluctuations were necessary in order to reach a unique limit system. These fluctuations need to be large enough to trigger the dynamics of the defects and make it significant within the computation time limitations, but small enough not to mask it under the diffusion they generate. Due to restrictions of calculation power, we have built packings with up to 10^8 discs. The packing fraction we found (up to $0.826\pm7\times10^{-4}$) is actually still far from the maximum value 0.907; yet (see figure 1) we suggest that the limit of zero randomness is singular, and that the typical gravitational packing of identical discs may be triangular. In other terms, this limit behaves like a zero-temperature phase transition.

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