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Random packing of elliptical disks

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We have studied two-dimensional random packings of ellipses. When the aspect ratio is varied, a maximum packing fraction of 0.895 is found. We discuss the detailed dependence of packing fraction on aspect ratio. The results are qualitatively similar to those of Donev *et al*. [Science **303** 990 (2004)], recently reported for the random packing of ellipsoids in three dimensions.

1. Introduction

The dense packing of hard objects is a recurrent paradigm in physics, for example in early models of crystallinity, and also in theories of granular materials which are under active debate today [1, 2]. Generally speaking the objects are taken to be spheres, leading to the formulation of the Kepler Problem (what is their closest packing?) and the investigations begun by Bernal on disordered packings (what is the nature of their random packing?).

Even for spheres the subject is surprisingly rich in interesting questions, some answered, some remaining open, and some difficult even to define [3]. There is no precise definition of "densest random packing" of spheres; nevertheless it is a concept to which we have become accustomed and one that is supported by the approximate reproducibility of the density found in a variety of experimental and computational procedures. It may be estimated as $\Phi = 0.64 \pm 0.02$, where the stated uncertainty reflects a small variation in dense packings prepared by one procedure to another. While significant, this variation is small in relation to the difference between random and ordered packing, which has $\Phi = \pi/(3\sqrt{2}) \simeq 0.74$.

Most granular materials do not consist of spherical particles, and their shapes must play a role in their properties — even the most basic property, namely density. To understand this role, it is natural to deal first with particles of uniform size and a simple shape. Computer simulations for the random packing of spherocylinders (cylinders with caps of semi-spheres at both ends) were performed by Williams and Philipse [4]. They found that the packing fraction reaches a maximum

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of $\Phi \simeq 0.70$ for an aspect ratio $\alpha = 0.4$ of cylinder length to diameter, for larger values of α it decreases continually (it is below the Bernal value for $\alpha > 1.5$). Another obvious non-spherical packing candidate is the ellipsoid. Hence Chaikin has recently chosen the confectionery known as M&M's® for packing experiments [5].

Our own study was motivated in part by the desire to better understand the remarkable results of Chaikin's group. These indicated a high packing density relative to sphere packings. Donev *et al.* [6] in their recent report for a packing of ellipsoids of revolution with an aspect ratio of 1.93, appropriate to M&M's®, found a higher packing fraction than the random packing of spheres. Furthermore, computer simulations of packings of ellipsoids with principal axes having three different values, lead to random packings with packing fractions close to that of fcc/hcp.

To explain this arguments of constraints and jamming have been adduced, which have long been a part of the general subject. In brief, these associate the maximum density with the exhaustion of degrees of freedom by the constraints due to contacts, in a style of argument that goes back to James Clerk Maxwell in the general context of static equilibrium of structures. For ellipsoids there are effectively more degrees of freedom than those of spheres, so it is argued that compaction can continue further, establishing more contacts and a greater density.

2. Simulation of 2D packings of ellipses

In order to reduce the computational challenge we have retreated to two dimensions and will speak of disks rather than 3d particles. In 2d there is a strong tendency for monodisperse systems to order (resulting in the hexagonal honeycomb packing), so this forces us to deal with polydisperse systems, if we wish to gain insights into the role of disorder.

Determining whether two disks are in contact or overlap is a simple task only for circles. To allow us to study the packing of arbitrarily shaped objects, we discretize the surface of the disks. Each disk is represented as a polygon with 100 surface points (vertices) [7]. This gives us a highly accurate representation of an ellipse, introducing an error in packing fraction, Φ, of less than 0.001. (Calculated as the difference in Φ between the same packings of disks using 100 and 1000 surface points).

Our simulations are carried out using 50 disks of a given aspect ratio $\lambda = b/a$ (where a and b are respectively the semi-major and semi-minor axes). We use uniformly distributed random numbers to set the initial x and y coordinates of the disk centres (within a unit square) and the initial disk orientations (angle between semi-major axis and x-axis). The values of the semi-major axes a are taken from a uniform distribution with a finite lower bound to avoid disks that are too small. The semi-minor axes are then given by $b = \lambda a$. There is no initial disk overlap. Periodic boundary conditions are employed in all simulations (figure 1).

The compaction process consists of the following steps. First the area of each disk is increased such that the packing fraction is increased by 0.0001. We then check for every disk if this has resulted in any overlap with its neighboring ellipses. If it has, it is moved in a random direction (and/or rotated by a random angle between $-\pi/2$ and $\pi/2$) that will reduce its total overlap with neighbouring disks. If it already has

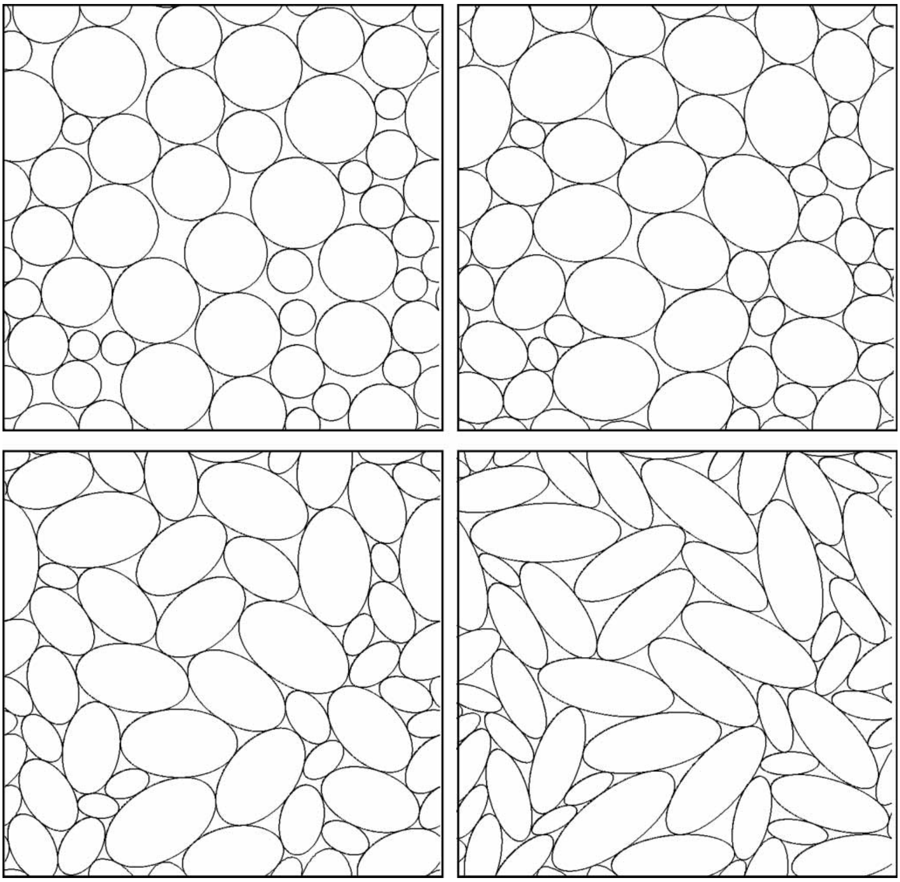

Figure 1. Computer simulations of dense packings of 50 ellipses with aspect ratio 1.0 (circles), 0.8, 0.6 and 0.4, respectively. The simulations use periodic boundary conditions.

zero overlap, then it attempts to make a random movement and rotation to another position that also represents zero overlap. This process is continued until all disks have zero overlap. Then the area of each disk is again increased such that the packing fraction is increased by 0.0001.

The process of minimization of the overlap to zero and increasing of the area of the disks is continued until it is no longer possible to obtain zero overlap. The packing fraction is then given by the ratio of the sum of all disk areas over the smallest box area at which the disks did not overlap.

Packings of ellipses of equal aspect ratios λ are produced as follows. We generate a densest packing of circles ($\lambda = 1$) using the above algorithm. For each subsequent packing, λ is reduced by 0.01, making the disks more elliptical while retaining the positions of the disk centres, and the orientation and length of their semi-major axes. The compaction of the disks then proceeds in the same way as before, resulting in a new dense packing of disks with the reduced aspect ratio. In this way, we generate packings of ellipses of equal aspect ratio λ, in the range from $\lambda = 1$ to $\lambda = 0.1$.

3. Results and conclusions

In 2d it is well established that polydisperse circular disks pack randomly with a density close to 0.84, for size distributions which involve substantial variations in size. This seems to apply quite widely, but cannot hold for extreme cases.

Figure 2 shows the variation of density Φ with aspect ratio λ. In qualitative accord with Chaikin's observations [6] and the simulations of Williams and Philipse [4], we find that as one departs from a circular shape the packing fraction increases from an initial value of 0.837 to a maximum value of 0.895 for $\lambda \approx 0.7$. We see an initial linear increase in packing fraction as we increase the ellipticity and only see the packing fraction drop below that of the circular case for $\lambda < 0.25$. Our data are well represented by a third order polynomial as shown in figure 2.

In considering these trends, we may first observe that for hard contacts there is always available to the system a structure with the same density ($\Phi \simeq 0.84$) as that of circular disks, since any degree of eccentricity may be introduced by a simple affine transformation, conserving area and the hard contacts. So in some sense both the initial linear increase and the eventual decrease of density are associated with the rotational disorder which is frozen in by the process used for compaction.

In order to shed some light on this, we have performed the following further calculation. As before, disks of a given value of were placed in a box with random

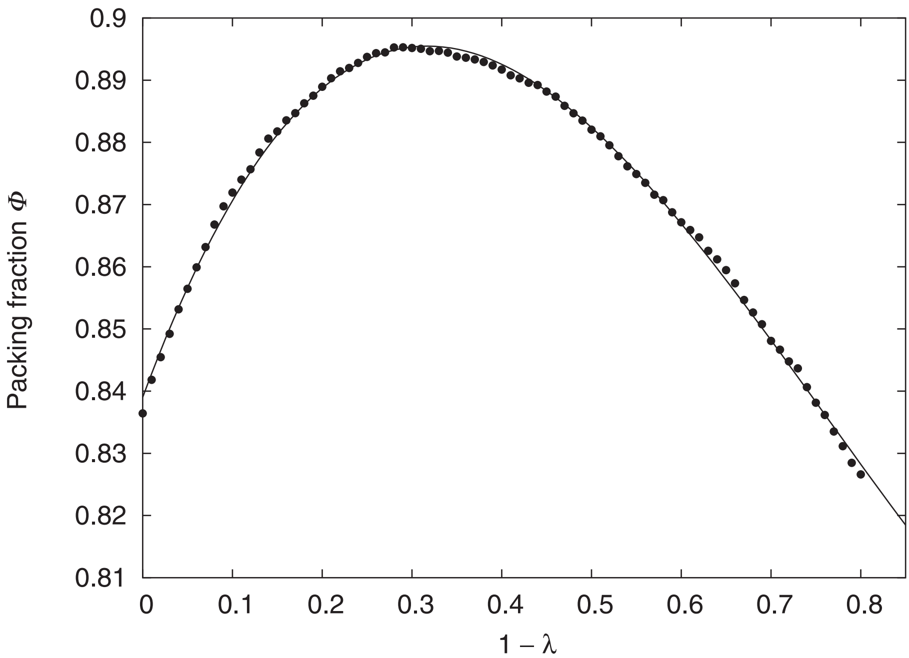

Figure 2. Variation of packing fraction Φ with $1-\lambda$, where λ is the aspect ratio. Data shown are the average of 10 simulations of 50 disks for each aspect ratio. (The average standard deviation of the packing fractions obtained is 0.004.) The solid line is a fit to a third order polynomial with a maximum $\Phi = 0.895$ at $\lambda = 0.664$ and $\Phi(\lambda = 1) = 0.839$.

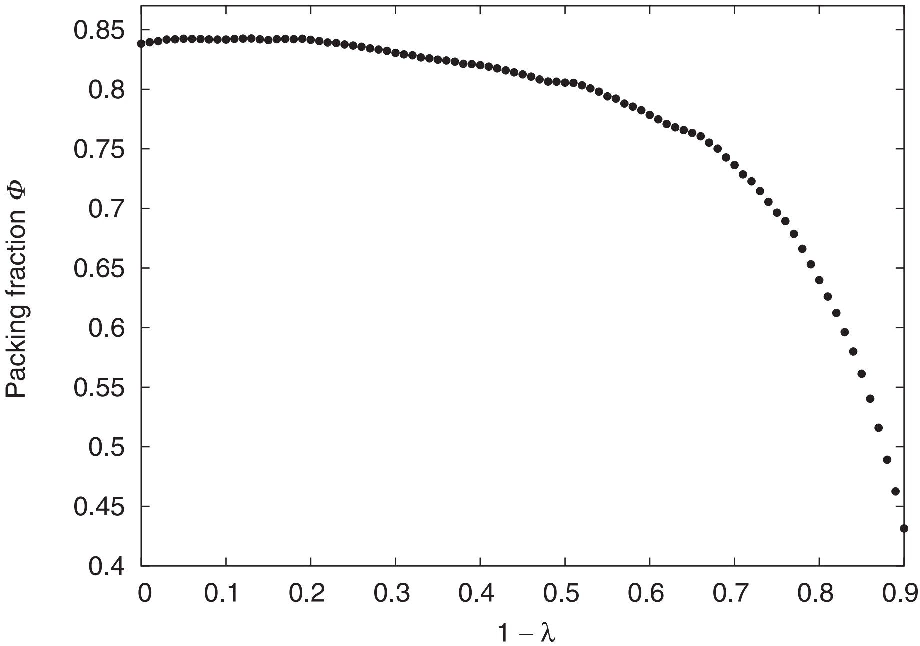

Figure 3. When we disallow disk rotations in our packing algorithm we find that the packing fraction Φ does not increase above the packing fraction of circular disks ($\Phi \simeq 0.84$). There is a sharp decrease in packing fraction for aspect ratio λ less than 0.3. Data shown are the average of 10 simulations of 50 disks for each aspect ratio.

initial locations and orientations. However, this time the disks were not allowed to rotate during the compaction process. Figure 3 shows that we no longer see the large increase in packing fraction as we increase ellipticity away from that of a circle. Instead the packing fraction remains almost constant at $\Phi \approx 0.84$ up to $\lambda \approx 0.8$. We then observe a slow decrease in packing fraction for midrange values of λ. At high values of ellipticity there is a very large decrease in packing fraction, with a packing fraction as low as $\Phi \approx 0.43$ found for an aspect ratio of 0.1. These results show that as expected, the additional rotational degree of freedom in the case of ellipses is essential for an increase in the packing fraction above that of the circular case.

The standard arguments for the mean number of contacts (due to James Clerk Maxwell [9] and Charles Bennett [8]) have been based on the concept of "jamming", that is, to constrain the system, two contacts per degree of freedom are required. Thus for a random packing of circles with two degrees of freedom (the two coordinates describing the position of the circle) one would expect a mean contact number of 4, while for the case of a random packing of ellipses one would expect a mean contact number of 6 (the extra degree of freedom being given by the angle describing the orientation of each ellipse).

The practical determination of contact numbers for computationally generated packings involves the definition of a cutoff (r_{cutoff}) distance around each particle

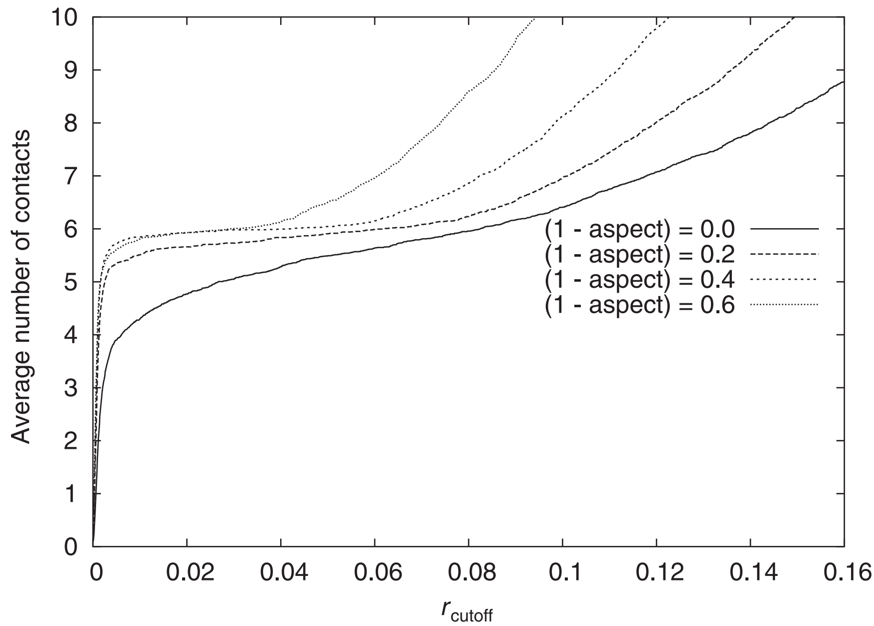

Figure 4. Variation of number of contacts, Z, with r_{cutoff} (r_{cutoff} is expressed in units of the average of the lengths of the semi-major axes, r_{avg}). We see a clear plateau region at approximately six contacts for large ellipticities.

where one considers any neighbouring particle within that distance to be in contact. Figure 4 shows the average contact number obtained for increasing values of r_{cutoff}. (This is similar to a cumulative radial distribution function.) We see that for circles there is a very sharp increase to a value of approximately 4, while at higher ellipticities there is a clear plateau region in the graph at a value close to 6. We find a value of 4.0 ± 0.1 for circles over the range $r_{\text{cutoff}} = 0.005r_{\text{avg}} \rightarrow 0.007r_{\text{avg}}$, where r_{avg} is the average semi-major length. For larger values of ellipticity a clear plateau is seen at approximately 6 and so it is appropriate to consider a larger value of $r_{\text{cutoff}} = 0.02r_{\text{avg}}$ in this case. Figure 5 shows the variation in contact number with aspect ratio where the error bars are determined from considering r_{cutoff} in the range $0.005r_{\text{avg}} \rightarrow 0.007r_{\text{avg}}$ for values of $\lambda \geq 0.6$ and $0.005r_{\text{avg}} \rightarrow 0.02r_{\text{avg}}$ for $\lambda < 0.6$.

The simple "jamming argument" is generally seen to be a very good indicator of the number contacts of particles in granular packings. However, it does imply that for an infinitesimal introduction of ellipticity there should be an immediate jump in contact number from 4 to 6. This is clearly contradicted by our simulation results, where a maximum contact number is only reached at an aspect ratio $\lambda \approx 0.7$. We find $Z = 4.0 \pm 0.1$ for circles consistent with the jamming argument, while for large ellipticities we find a value of $Z = 5.7 \pm 0.2$. This is slightly lower than the expected value of 6, consistent with the results of Donev *et al.* [6] who found a maximum value of $Z = 9.8$ for spheroids and $Z = 11.4$ for ellipsoids to be compared with values determined from the jamming argument of $Z = 10$ and $Z = 12$.

The situation is different for *periodic* densest packings of identical ellipses. A list of 54 such packings was compiled by Nowacki [11], and was extended to 58 packings

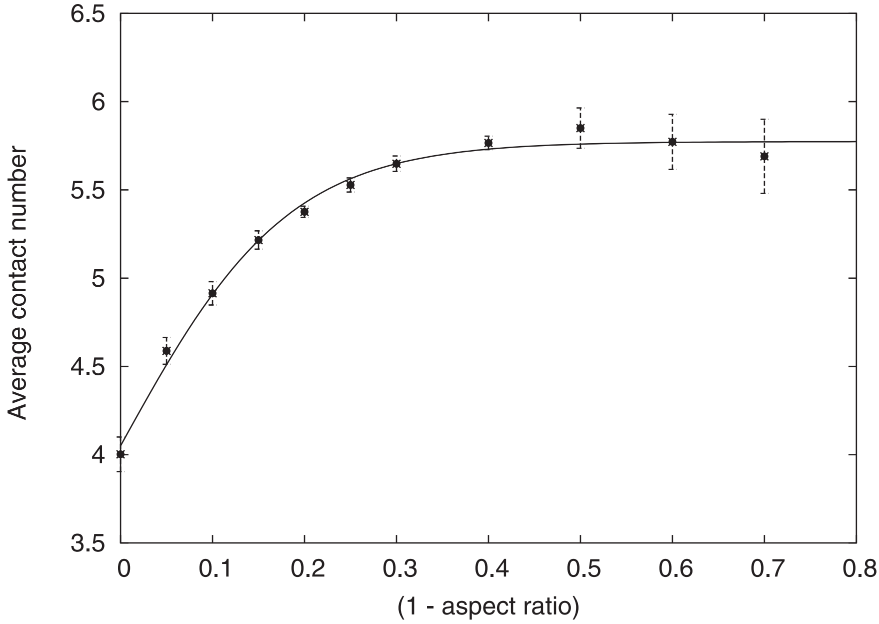

Figure 5. Variation of the average contact number with aspect ratio. The solid line is an empirical fit to $Z = a \tanh(b(1-\lambda)) + c$, with $a = 1.72 \pm 0.06$, $b = 5.5 \pm 0.3$ and $c = 4.05 \pm 0.05$.

by Grünbaum and Shephard [10]. Their book details coordination numbers and packing fractions for all these packings. The density of the closest packing of circles, $\Phi_c = \Pi/\sqrt{12}$ is the conjectured maximum density of all packings, only taken by a subset of the listed 58 packings, all with coordination number 6 [12].

In three dimensions, quite surprisingly, the packing density of ordered arrangements of ellipsoids can exceed that for ordered sphere packing, as was shown recently by Donev *et al*. [13]. This is yet another indication of the intricate nature of packings and their dependence on dimensionality and order.

Acknowledgements

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