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PATTERNS AND STRUCTURES IN DISK PACKINGS

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Abstract

Using a computational procedure that imitates tightening of an assembly of billiard balls, we have generated a number of packings of n equal and non-equal disks in regions of various shapes. Our experiments are of three major types. In the first type, the values of n are in thousands, the initial disk configuration is random and a priori one expects the generated packings to be random. In fact, the packings turn out to display non-random geometric patterns and regular features, including polycrystalline textures with "rattlers" typically trapped along the grain boundaries. An experiment of the second type begins with a known or conjectured optimal disk packing configuration, which is then "frustrated" by a small perturbation such as variation of the boundary shape or a relative increase of the size of a selected disk with respect to the sizes of the other disks. We present such frustrated packings for both large n (~ 10,000) and small n (~ 50 to 200). Motivated by applications in material science and physics, the first and second type of experiments are performed for boundary shapes rarely discussed in the literature on dense packings: torus, a strip cut from a cylinder, a regular hexagon with periodic boundaries. Experiments. of the third type involve the shapes popular among mathematicians: circles, squares, and equilateral triangles the boundaries of which are hard reflecting walls. The values of n in these experiments vary from several tens to few hundreds. Here the obtained configurations could be considered as candidates for the densest packings, rather than random ones. Some of these conjecturally optimal packings look regular and the regularity often extends across different values of n. Specifically, as n takes on an increasing sequence of values, $n = n(1), n(2), \ldots, n(k), \ldots$, the packings follow a well-defined pattern. This phenomenon is especially striking for packings in equilateral triangles, where (as far as we can tell from our finite computational experiments), not only are there an infinite number of different patterns, each with its own different sequence $n(1), n(2), \ldots, n(k), \ldots$ but many of these sequences seem to continue indefinitely. For other shapes, notably squares and circles, the patterns either cease to be optimal or even cease to exist (as packings of non-overlapping disks) above some threshold value $n(k_0)$ (depending on the pattern). In these cases, we try to identify the values of $n(k_0)$.

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1. Introduction

Packings of non-overlapping disks or cylinders can be mechanically generated by tightening the container boundary [R]. A variant of this procedure has been implemented on a computer [L] as a discrete event "billiards" simulation algorithm., Rather than shrinking the container, in the billiards simulations we uniformly expand the disks. While growing, the disks negotiate the available area. They chaotically push each other imitating the dynamics of elastic collisions. One expects to arrive at a packed configuration when no further growth is possible.

The tool was developed and first, exercised in settings where a typical number n of disks involved was is the thousands [LS90]. The intent in [LS90] was to sample *random* particle configurations in 2D (disks) and 3D (spheres). One would expect the resulting packing to be random because the procedure in [L] involves substantial randomness and irregularity and also because the relatively large number of particles presumably precludes establishing a global order. Randomly packed spheres in 3D may be advanced as representing the short-range atomic order that exists in amorphous solids, while the disks packed in 2D model the arrangements of particles adsorbed on smooth surfaces and monolayer colloidal suspensions. Actually, the packings generated do not look random. They display, especially in 2D, many regular features and patterns, including polycrystalline textures with loose "rattler" particles which are trapped along the grain boundaries. The (visually assessed) degree of regularity in such a packing depends on the speed of disk expansion. Sufficiently slow expansion often yields packings of a high regularity some of which might be even conjectured as optimal, i.e., as having the largest possible disk diameter, given the n and the boundary shape. This is a remarkable fact in view of thousands of participating disks and local chaoticity of their motion while producing the packing.

In the random packing experiments the initial disk configuration is random and disk expansion begins with disks *of* zero diameter. We also *present* a different type of experiment where the expansion begins with an a priori regular and/or optimal disk configuration, rather than a random one. A "frustration" is introduced by varying either the boundary conditions or disk sizes and arrangements are made to let disks grow a little more. The expanding disks try to compensate for the imperfection. As before the expansion stops at a "jammed" state with "cracks" and dislocations caused by frustration. It turns out that when the expansion is slow, the structure of the cracks and dislocations is quite regular, and it depends very much on the boundary conditions. We present such frustration experiments for squares and rectangles with periodic boundaries (i.e., a torus), for a hexagonal boundary with appropriate periodic boundary conditions, and for a rectangle, two opposite sides of which are "glued" (this makes a strip cut from a cylindrical surface). The number of disks in the frustration experiments vary from about 10,000 in the impurity-perturbed crystal experiments where we increase the relative size of one disk [SL95] to under 100 in experiments where we perturb the boundary shape.

We also exercise the same billiards algorithm for small numbers of disks (n of the order of tens to few hundreds) to see how the algorithm performs in the popular problems of finding best packings in circles, squares, and equilateral triangles. Because the intent here is to produce possibly more regular packings, hoping perhaps to reach the density maximum, the disk expansion speed is set at the lowest possible level at which the emergence of the packings is not intolerably slow computationally. The packings obtained by the billiards algorithm compare very favorably with those reported in the literature obtained using other methods, see [GMPW] [G] [MFP] [NO] [IL] [S71] [S79] [V]. The algorithm not only confirms almost all reported packings but also produces many more packings, some with interesting patterns.

Sometimes the same pattern recurs as the number of disks n increases along certain sequences, $n = n(1), n(2), \ldots n(k), \ldots$, with different patterns corresponding to different sequences. The case for packing $n(k) = k^2$ disks in a square is presented in' [NO], where it is found that the obvious square pattern, while known or conjectured to be optimal for $n = 1, 4, 9, 16, 25$, and 36 disks, becomes non optimal for $n = {k_0}^2 = 49$ disks. A disk-packing of 49 disks is presented in [NO] with density higher than that of the corresponding square packing. We repeat the same steps for the other regular patterns of packings in a square identified in [NO] and [GL96] and also for the patterns identified for packings in equilateral triangle [GL95] and in a circle [GLNO]. In square and circle sequences of packings, the same pattern seems always to terminate, eventually, i.e., for each such sequence n(k) a threshold value $n(k_0)$ exists such that the packings of the pattern either are not optimal for $n \geq n(k_0)$, or the pattern cannot exist as a packing of non-overlapping disks. However, for packings in equilateral triangles one regular pattern hexagonal packing of $n(k) = k(k + 1)/2$ disks is known (proven) to exist and be optimal for *all* k. We have conjecturally identified an *infinity* of such regular patterns since for none of them were we able to find the pattern-terminating threshold.

2. Using billiards simulation to generate random packings

Figure 2.1 illustrates the work of the billiards simulation algorithm while packing 2000 equal disks in a square with periodic boundary (torus). The initial stage at time $t = 0$ is represented on the top square in the figure where 2000 points are randomly scattered. To each point an initial velocity vector is randomly assigned (not shown). Some points lie outside the square; they are periodic images of the corresponding points inside. When $t > 0$, the points grow into disks, and all disks at each time t have common diameter $d = Et$. The growth continues until the configuration "jams," at which time we expect to have a packing.

At $t = 0$ disks do not overlap because their sizes are zero. For $t > 0$ disks moves along straight lines with given velocities; their motions may conflict, with each other. At an instance of such a two-disk conflict,, we simulate an elastic collision of these disks assuming their masses are equal. At a collision both disks change their velocity vectors so as to exchange momenta and energies according to known

'The only exception is the packing of 21 disks in a square for which [MFP] provides the disk diameter 0.27181675.

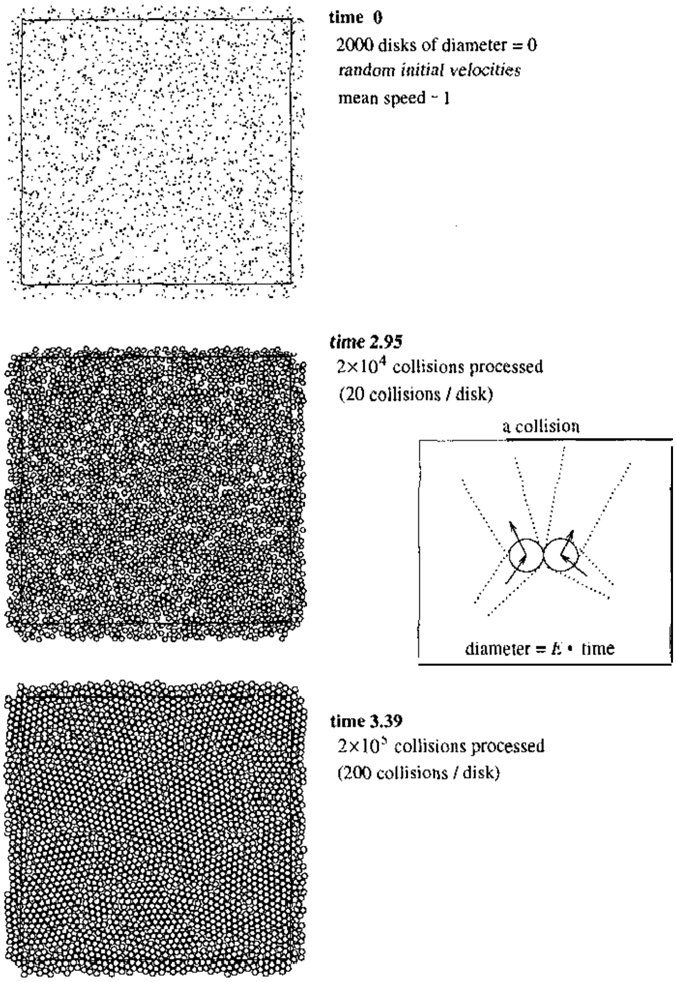


Fig. 2.1. Successive stages in an instance of disk packing by billiards algorithm

mechanical laws. Note that the evolution of the disk configuration does not change if we proportionally change both the disk expansion speed and linear disk velocities. We normalize the simulation input by assuming the unity *mean initial disk velocity.*

Increasing the size of disks introduces additional energy at collisions, which may cause the system to "overheat" computationally, i.e, to overflow, especially, if E is large. Another drawback of the "heating" is that increase over time of the average disk velocity is equivalent to the decrease of E. Such uncontrollable reduction of E is undesirable because as the experiments show the resulting configuration is sensitive to E during the entire expansion process and we would not be able to study the dependence of the resulting configuration on large E if moat of the events occur under effectively small E. We "drain" the excessive "heat" by periodically stopping the run and scaling down the velocities of all the disks.

The main processing load of the simulation algorithm is in locating and processing disk collisions. It takes roughly the same computing time for processing the same number of collisions independent of the packing phase. (When disks are very small it takes somewhat longer to process a collision than when they are larger, but this deviation from uniformity is insignificant because the initial phase is processed very fast.) The collisions become more frequent as the disks grow. Thus, it takes almost 10 times longer to reach the configuration at time $t = 3.39$ (the bottom square in Fig. 2.1) than that at time $t = 2.95$ (the middle square in Fig. 2.1). As the configuration is approaching a packed state in a finite simulated time t_0 with final disk diameter $d_0 = Et_0$, the processing time diverges. Computationally, we may never reach time t_0. Roundoff complicates the situation further. Strictly speaking not only are we unable to say that what we see on the final "jammed" picture is a rigid packing (not to mention its possible optimality), but even that the configuration presented really exists as a set of non-overlapping disks. Thinking about the statement "the configuration shown on the diagram exists" one realizes the difficulties even in assigning a precise meaning to it.

In the present, paper we do not discuss these difficulties, as that would lead us too far from the main goal of presenting the experimentally achieved packings. Some methods of convincing oneself of the existence and rigidity of a shown packing are briefly discussed in [GLNO]. As a practical matter, we stop an experiment and consider the configuration as a complete packing when during, say, the last 10,000,000 collisions we detect no visible change in the structure and the relative disk diameter increase is less than, say, 10^{-8}.

We use algorithm [L] for locating and processing the collisions. The algorithm' is event driven and seems rather efficient. With this algorithm, all the packings described below are computationally within the reach of a modern personal computer. For example, each packing presented in the next section can be achieved within several hours of processing on a PC.

3. Random packings in a square with periodic boundaries

A number of packings have been produced by randomly varying initial configuration of points, their initial velocity, and the expansion speed E. Stepping through the sequence of packing diagrams in Fig. 3.1 to Fig. 3.5 one notices the increase of regularity of the packing as expansion speed changes from $E = 100$ to $E = 0.001$. For large E the pattern is a combination of hexagonally packed fragments, "grains," with each grain having generally different orientation. Irregularity concentrates along the grain boundaries, as do the "rattlers," the disks that are not rigidly fixed in their positions but trapped in the cages formed by their fixed rigid neighbors or boundary walls if any.

The size of the grains increases (and their number for a fixed n decreases) as the E decreases. For a sufficiently small E, a single hexagonal "crystal" emerges.

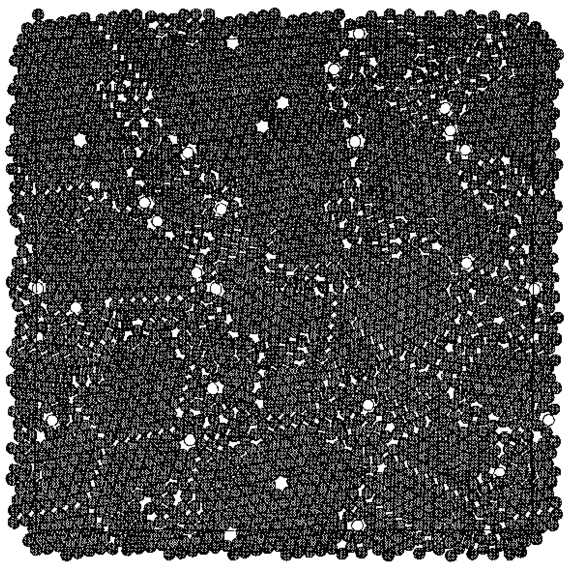


Fig. 3.1. A packing of 2000 disks in a square with periodic boundary. The packing is obtained under a fast disk expansion, $E = 100$. The packing consists of crystalline grains with many rattlers represented as unshaded disks concentrated along the grain boundaries. Monovacancies occur within the hexagonally packed grains.

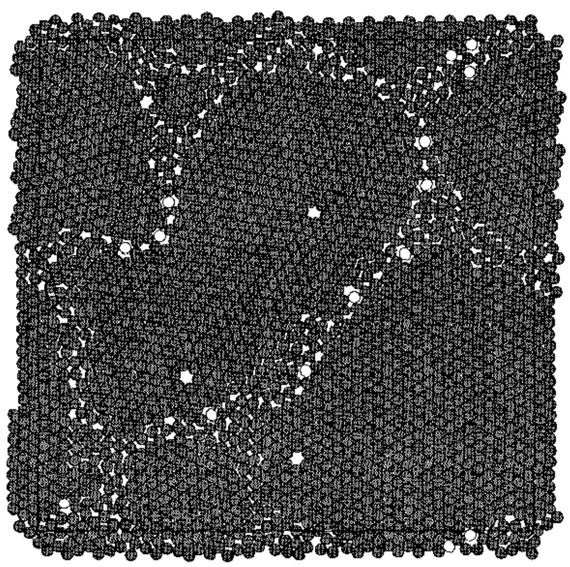


Fig. 3.2. A packing of 2000 disks in a square with periodic boundary. The packing is obtained under a moderately fast disk expansion, $E = 3.2$, and consists of grains that are larger than those in Fig. 3.1. As in Fig. 3.1, the rattlers concentrate along the grain boundaries but their number and that of the monovacancies is smaller than in Fig. 3.1.

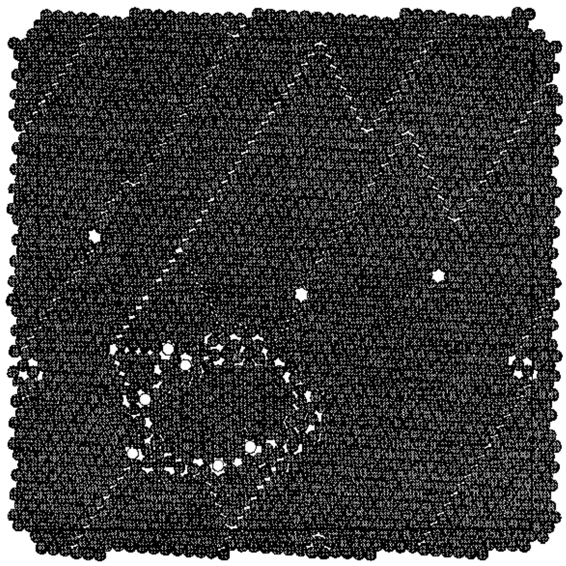


Fig. 3.3. Another packing of 2000 disks in a square with periodic boundary. The packing is obtained under a moderate disk expansion, $E = 1$. Besides crystalline grains and rattlers it also displays shear fractures.

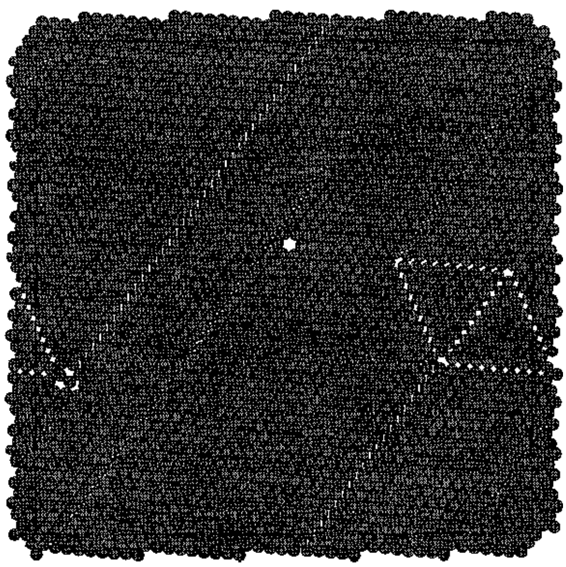


Fig. 3.4. A packing of 2000 disks in a square with periodic boundary. The packing is obtained under a slow disk expansion, $E = 10^{-3}$. The entire structure is oriented along the same axes, it includes shear fractures and two perfectly packed triangles at the right. A single monovacancy is seen hut no rattlers.

The array of hexagonally packed disks contains interesting structural deviations and insertions. Sometimes the symmetry of the packing coupled with the high value of achieved density suggests that perhaps we have achieved the optimum, as might be the case in Fig. 3.5.

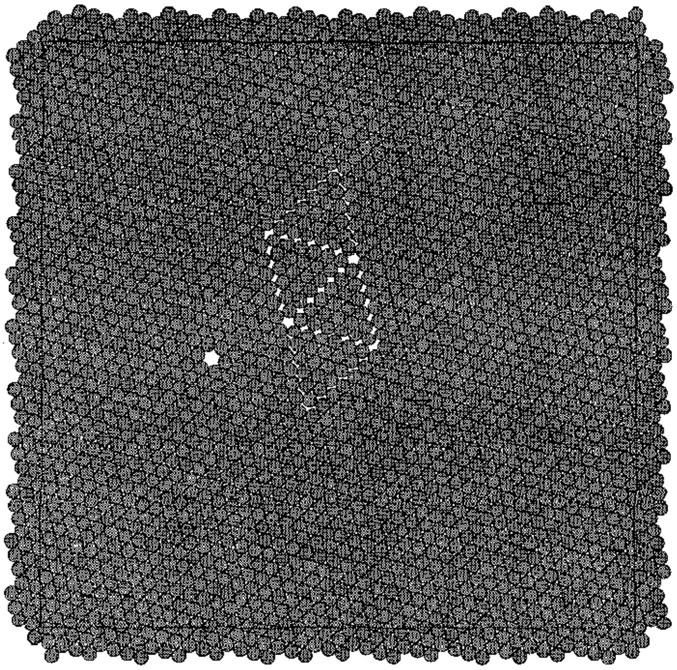


Fig. 3.5. Another *packing of 2000 disks in* a square with periodic boundary *obtained under* a slow disk *expansion*, $E = 10^{-3}$. If *the monovacancy near the center* is filled with the 2001-st disk, the obtained packing seemingly becomes perfectly symmetric. Might that be the best packing of 2001 equal disks in a square with periodic boundary? Its experimentally computed density (when the 2001-th disk is inserted) is 0.901635...

4. Frustrated packings

56 equal disks stacked hexagonally **in 8 alternating columns, 7 disks in a column,** constitute the best packing *in a rectangle* with periodic boundary conditions if the ratio of the height of the rectangle to its width is $\sqrt{1+\frac{1}{48}} = 1.01036...$ We frustrate the packing Ly increasing the width of the rectangle and making it equal to the height. In the new shape, previously jammed disks become loose (we help to loosen the disks by reducing them slightly). They can grow further to exploit the extra space. We provide the disks with random initial velocities in the usual manner. As the disks grow, a new jamming is achieved with a larger disk diameter.

We repeated this experiment several times, each time starting with a different assignment of initial disk velocities. Many runs achieved the highest density and they all

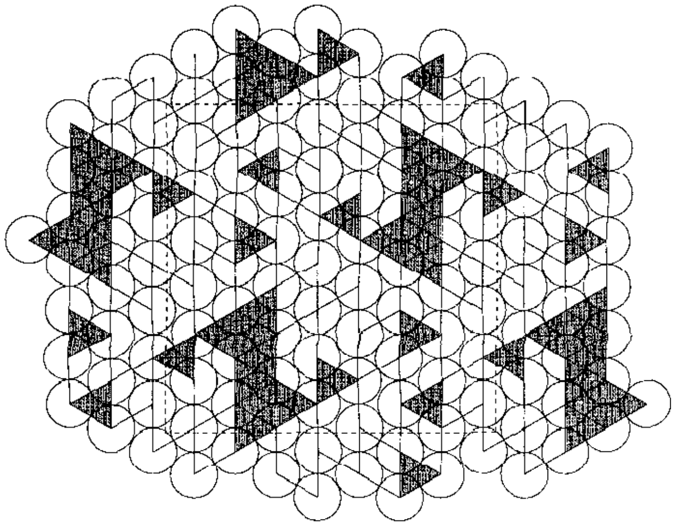


Fig. 4.1 The best found packing of 56 disks in a square with periodic boundary conditions. (The square perimeter is dashed). Pairs of disks that are in contacts are indicated by line segments connecting their centers. Triangles formed by such lines an: shaded. Tha shading helps to see the structure of the packing: the plane is tiled with 4 x 7 blocks, each block having pattern "'Z," shaded on it. The density of the packing is 0.898059591...

ended with the final configuration that is shown in Fig. 4.1. Moreover, the best packings found, if we start with zero initial disk diameters, arc also identical to the packing presented in Fig. 4.1 which we hence conjecture to bc the optimum.

To better see the structure of the packing in Fig. 4.1, the centers of disks that contact each other are connected by straight line segments. Computationally, two disks are declared as being in contact if the distance between their centers does not exceed $d(1 + 10^{-12})$, where d is the disk diameter. For comparison: the distance between the centers of any pair of disks that are not in contact in this packing is larger than $d(1+10^{-5})$. Some of the connecting segments form triangles and all such triangles are shaded. With the shading one easily sees the structure: the tiling of the plane by center-symmetric 4 X 7 blocks, each block having pattern "'Z," shaded on it.

Another example of a frustrated packing, also conjecturally optimal, is presented in Fig. 4.2. To generate this type of packing we start with two positive integers k and p, $k = 7$ and $p = 4$ in the example, and form a *rectangle with width* kp *and height* $k\frac{\sqrt{3}}{2} + 1$. Assuming the top and bottom side of the rectangle are reflecting walls while left and right side are glued with the same orientation, WC obtain, as thc boundary condition, a strip cut from a cylinder. We place $pk(k + 1)$, here 224, unit diameter disks inside this strip in a perfectly hexagonal order. The placement contains $k + 1$ alternating rows with pk disks in each. This conjecturally optimal packing is frustrated by increasing the width of the rectangle. As before the structure of the frustration is "developed" by letting the disks grow until they jam again. The best packing thus obtained is a set of $2p$ alternating triangles with k disks on their sides, as seen in Fig. 4.2.

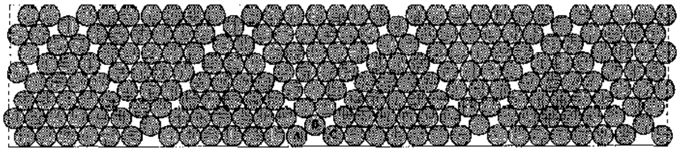


Fig. 1.2. The best found packing of 224 disks in a strip with top and bottom sides reflecting, and left and right boundaries periodic. The ratio of the height to tha width of the strip is 0.2165063509461... which corresponds to values $k = 7$, $p = 4$, $\alpha = \pi/6$ in formula (1), where α is the angle at disk A in the triangle formed by centers of disks *A, B, C.*

The magnitude of perturbation to the original strip can be quantified by angle α at disk A in the *triangle* formed by centers *of* disks A, B, and C as labeled in Fig. 4.2. If $0 \leq \alpha \leq \frac{\pi}{3}$, the hoi&t-to-width ratio of the rectangle is

$$\frac{(k-1)\frac{\sqrt{3}}{2} + 1 + \sin\alpha}{(k + 2\cos\alpha - 1)p} \tag{1}$$

For two extremes, $\alpha = 0$ or $\alpha = \frac{\pi}{3}$, the configuration is a hexagonal packing. Specifically it is the packing with $k+1$ rows, pk disks in each, for a $= \frac{\pi}{3}$. We have started the experiment with this packing which wc have frustrated by increasing the width of the strip. Wc could have started with the other *extreme*, the packing *with k rows with $p(k+1)$* disks in each, for $\alpha = 0$, and increased the height, The result would have been the same.

Several sets (k, p, α) have been tried. 'I'he best found packing has always had the pattern as described above. If somebody can present an instance of $(k, p,$ a) as described (k, p positive integers, $0 \leq \alpha \leq \frac{\pi}{3}$) and pack $pk(k+1)$ disks in a strip with the height-to-width ratio as in (1) better than the packing we describe, wc would bc surprised.

In the following two examples of a frustration we increase the size of a single disk. Specifically we begin with a perfectly hexagonally packed configuration of disks of unit diameter each. We uniformly decrease the size of all the disks but, one. The **diameter** of the latter is increased. Let the diameter of the smaller disks become d and that of the larger one $(1+\lambda)d$. The d and λ are chosen so that $(2+\lambda)d < 2$, which assures initial non-overlap of the disks. In the usual manner random initial velocities are assigned to the disks and then the disks grow until they jam. At any time during the expansion the ratio of the larger disk diameter to that of the smaller ones remains fixed at $1+\lambda$. The value of $d < 1$ must be sufficiently large and the value of $\lambda > 0$ sufficiently small so as to prevent "melting" or "forgetting" the pattern in the process of the chaotic disk negotiations. The sot of such admissible (d, λ)is not empty, but it depends on the number of disks n and the boundary shape.

We experimented with two regions: a rectangle with both periodic boundaries *(torus), and a regular hexagon where each of the three pairs of opposing* sides are "glued" without orientation change. The latter boundary conditions arc illustrated in Fig. 4.4 in the box at the right top corner, where a fragment of the infinite plane tiled with hexagonal cells is shown. Each cell is a periodic image of the same cell. In particular, all points labeled a are the periodic images of each other; so are the points labeled *b*.

For the rectangle: the height-to-width ratio of a hexagonally packed configuration with 112 alternating rows, 97 disks in a row, is $\sqrt{1 - \frac{1}{9409}} = .9999468579779\ldots$ so we choose the rectangle with such ratio, as it closely approximates a square, and we place hexagonally $10{,}864 = 112 \times 97$ disks in it, For the hexagon: $3k^2$ equal disks can be placed in a regular hexagon in the optimal arrangement (hexagonal packing) for the described above periodic boundary conditions; we take $k = 60$ and use $n = 10, 800$ disks. When $d = 0.999 \times \frac{2}{2+\lambda}$, for the chosen values of n, melting does not occur in our experiments for $\lambda = 0.2$ in the hexagon and $\lambda = 0.1$ in the rectangle.

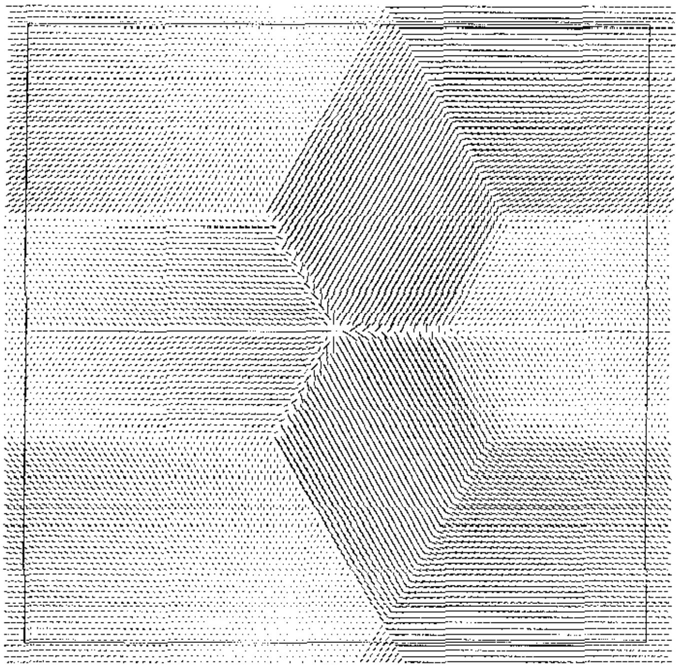
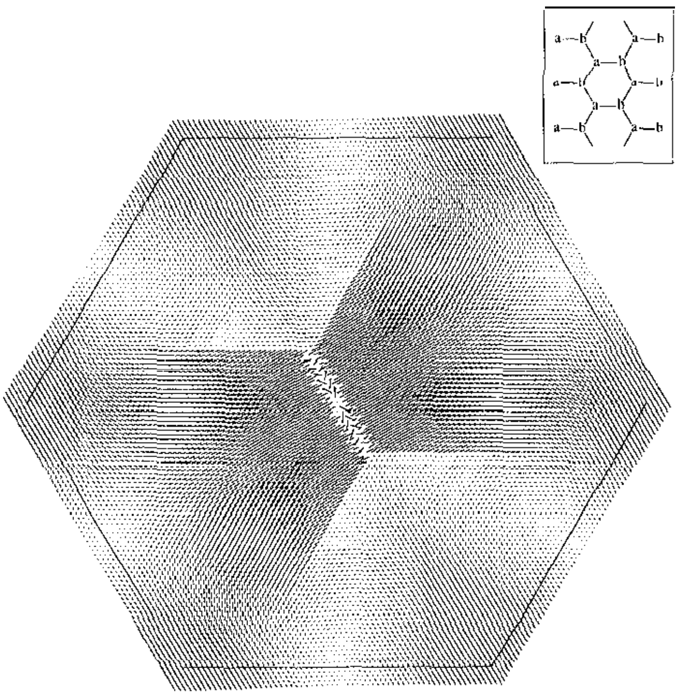


Fig. 4.3. Displacement vectors of centers of 10864 disks packed in a rectangle with height-to-width ratio close to 1 as described in the text. Boundary conditions are periodic. If all disks were of the same size ("pure" crystal), the packing would be perfectly hexagonal with 112 rows and 97 disks in a row. Displacements from this perfect order are caused by the central "impurity" disk being 10% larger than the others. Displacement vector of the central disk is 0 by definition, each other displacement vector begins at the perfect order position and its length is magnified 30 fold to enhance the resolution

We have tried several methods of enhancing visually the structure of the frustration obtained. The best method seems to be displaying disk displacements. Bach disk has the "ideal" position of its center p_0 in the original non-frustrated packing and the final position of the center p_1 in the frustrated packing. Vector $p_1 - p_0$ is thr displacement. Accumulation of the roundoff error may cause the entire configuration to shift during the expansion. We "calibrate" the displacement vectors by subtracting from each of them the displacement of thr larger disk. The latter displacement becomes zero by definition. Thus calibrated displacement vectors are shown in Fig. 4.3 and Fig. 4.4 originating at point p_0 and magnified in length 30 fold in Fig. 4.3 and 20 fold in Fig. 4.4.

We have performed several experiments with the same parameter values and boundary conditions but different initial velocities of the disks. The resulting samples of the



Fig, 4.4. Displacement vectors of centers of 10800 disks packed in a regular hexagon. Boundary conditions are periodic as shown in tha right top corner box where the same letter, a or b, marks identical points. If all disks were of the same size ("pure" crystal), the packing would be perfectly hexagonal. Displacements from this perfect order are caused by the central "impurity" disk being 20% larger than the others. Displacement vector of the central disk is 0 by definition, each other displacement vector begins at the perfect order position and its length is magnified 20 fold to enhance the resolution.

frustrated packing are different in small details (and, expectedly, some differ in orientation with respect to the boundary), but, on a large scale, they exhibit the same "crack" near the central large disk and the same arrays of displacement vectors. We suspect that the optimal packings under those conditions would look roughly the same when considering them on a large scale. Note that disk expansion speed ***E*** is kept at the lowest tolerable level $E \approx 10^{-3}$ to 10^{-4} in those experiments. Substantial increase of E also substantially changes the final packing pattern and substantially reduces thr density of the packing, see [SL95].

5. Repeated patterns in packings in equilateral triangle, square, and circle with hard walls

It has been established [0] [FG] that the best packing of $\Delta(k) = k(k+1)/2$ equal disks in an equilateral triangle is the hexagonal arrangement and that the optimality holds for all $k = 1, 2,$ Are the triangle numbers $\Delta(k)$ the only such lucky sequence? We conjecture the existence of an infinite number of such sequences.

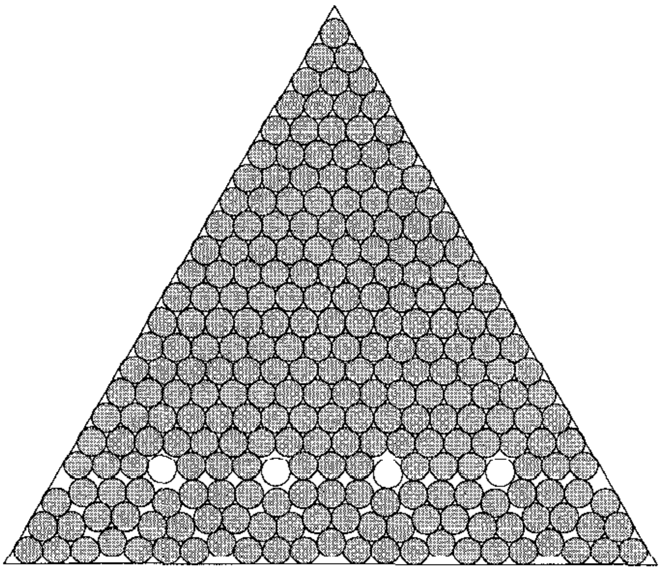


Fig. 5.1. The conjectured densest packing of $n_p(k)$ = 256 disks inside an equilateral triangle, where p = 5 and k = 3, and where $n_p(k)$ is defined by formula (2). The densest packings of n disks for all checked values of the form $n = n_p(k), p = 1, 2, \ldots. k = 1, 2, \ldots.$ have this pattern consisting of one triangle of side $(k+1)p - 1$ and $2p + 1$ alternating triangles of side k with $p - 1$ rattlers that are "falling off" the larger triangle

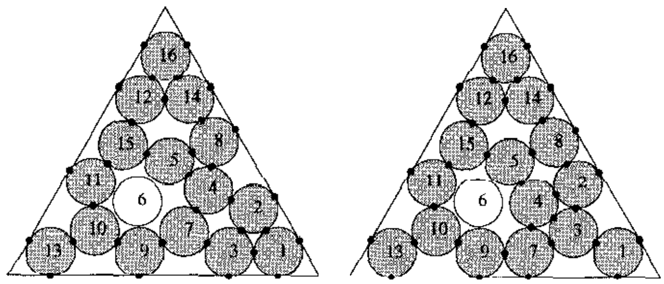
For each $p = 0, 1, 2, \ldots$ consider sequence

$$n_p(k) = \Delta((k+1)p - 1) + (2p+1)\Delta(k), \; k = 1, 2, \qquad (2)$$

For $p = 0$ sequence (2) is identical with the sequence of triangle numbers $\Delta(k)$ with known optimal packings. For each $p > 0$, we conjecture thr optimal packing of n,(k) disks as the pattern that consists of $n - p + 1$ solid disks and $p - 1$ rattlers; it includes one triangle of side $(k+1)p - 1$ and $2p + 1$ alternating triangles of side k each as shown in Fig. 5.1 for the case $p = 5$ and $k = 3$.

Suppose we rearrange the pattern in Fig. 5.1 by pushing the alternating triangles A(k) into their proper place in the would-bc perfect hexagonal order. We would align one triangle after another working, say, from left to right. At the end of the procedure extra space would emerge at the bottom of the triangle, on top of which we would have a triangle hexagonally filled with $\Delta((k+1)(p+1) - 2)$ disks, and k disks would be pushed off out of the right side boundary. It follows (and can be easily verified independently of this rearrangement argument) that $n_p(k)$ of the form (2) can also bc written as

$$n_p(k) = \Delta((k+1)(p+1) - 2) + k \qquad (3)$$



t16a33.1
density = 0.718174807623

t16a33.2
density = 0.718174807623

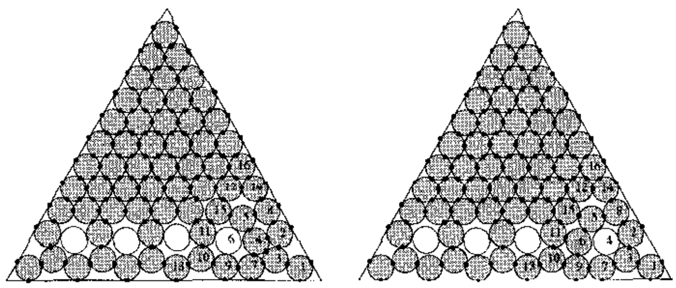
Fig. 5.2. Two equivalent best found packings of 16 equal disks in an equilateral triangle. Little black dots indicates contacts. Integer labels 1,...16 are assigned so that disks that occupy similar positions in both packings have the same label. The only difference between the packings are positions of disks 2, 3, 4, and 7.

Thus, the dense packing of $n_p(k)$ disks can be considered as a frustration of a perfect hexagonal crystal of $\Delta((k+1)(p+1)-2)$ disks packed in an equilateral triangle when k disks are added to the packing. Our experiments reveal other patterns of frustration when we add extra disks to an otherwise perfect hexagonal packing of A(n) disks in an equilateral triangle. For example, suppose we add just one extra disk to A(n) disks. For even $n = 2p$ the generated packing is of the form just considered, since $\Delta(2p) + 1 = n_p(1)$. For odd $n = 2p + I$, we have a somewhat different pattern which exists and is optimal for all sufficiently large p (as far as we have checked experimentally). The complications exist on the initial segment of p. Fig. 5.2 presents two equivalent best packings of 16 = A(5) +1 disks (p = 2). Similar disks are labeled using the same integer indices to emphasize the similarity and differences in the patterns. Little black dots indicate contact points, and each packing in Fig. 5.2 has 33 contacts. The label provided with each packing is inherited from [GL95] where such labeling is essential to distinguish among the many packings presented.

As far as we have checked, the same two optimal equivalent modifications exist for $p \geq 5$ ($n = 67, 92, 121...$). Fig. 5.3 presents one of these two best packings for $n = 67$ (labeled t67a161.2 to conform with labeling in [GL95]; it has 161 contacts), the other one also exists and has the same quality. The next beat packing (labeled t67b) is also shown in Fig. 5.3. It appears in our experiments that patterns as in t67a161.2 and in t67b coexist for $p \geq 3$ and together they occupy the places of the best and next-best packings. However, the pattern of t67a161.2 is not always better than that of t67b. For $n = 29$ ($p = 3$) and $n = 46$ ($p = 4$) the pattern as in t67b wins over the pattern as in t67a161.2 and its equivalent modification

The shape of an equilateral triangle conforms to the task of dense packing of equal disks in that the optimal packing of a "natural," i.e., a triangle number n of disks inside this shape is a fragment of the optimal packing on thr infinite plane. Our experiments show that even for "non-natural" numbers of disks n certain fragmented and frustrated variants of the basic hexagonal packing apparently may exist for infinite sequences of n.

Given any $k > 0$ we can place k^2 disks in a square in the $k \times k$ orthogonal fashion.



t67a161.2 density = 0.811959863130

t67b density = 0.811951836945

Fig. 5.3. A best and the next-best found packings of 67 equal disks in an equilateral triangle. As in Fig. 5.2, little black dots indicate contacts. 16 disks in the lower right, corner in both packings are also labeled with indices I,... 16. The disks with the same indices on both diagrams occupy similar positions and their position is also similar to the that of disks in Fig. 5.2.

This is a "natural" square packing in the same spirit as hexagonal disk arrangement yields a natural packing in an equilateral triangle. Unlike the triangular packings, square packings *become* non-optimal *for a* sufficiently large k. The shape of a square does not conform to the task of best packing. The natural square packing is not a fragment of the optimal packing on the infinite plane. What we observe in the best found packings in the square, can be described as an interplay between two patterns. square and hexagonal. For a sufficiently large number of disks n the hexagonal pattern becomes dominant. With the billiards simulation algorithm we were able to examine details of this interplay for small n.

The following sequences were recently identified as candidates for pattern repetitions (see [NO] [GL96]): $k^2 - 3$, $k^2 - 2$, $k^2 - 1$. These are "frustrations" of thr "natural? square pattern. Sequences $k(k+1)$ and $k^2 + \lfloor k/2 \rfloor$ were also identified; they can be considered as "frustrations" of a hexagonal pattern adjusted to the square boundaries.

Sequence $k^2 - 3$ yields optimal packings of the pattern exemplified in Fig. 5.4, top row, by its two members at $k = 5$ and $k = 8$. The pattern has both square and hexagonal elements in it. For $k = 9$, while the packing of the pattern still exists, it is possible to find a better packing.

Sequence k^2 -2 yields optimal packings of the pattern exemplified in Fig. 5.4, middle row, by two equivalent packings at $k = 6$. Different equivalent packings, total of four for $k = 6$, can be obtained by differently inserting two hexagonally arranged rows and two columns (lighter shaded) among $k - 2$ rows and k 2 columns arranged in the square orthogonal fashion. Only one other member of the sequence, for $k = 5$, is optimal when having this pattern For $k = 7$ a better packing of a different pattern exists.

Sequence k^2 -1 yields optimal packings of the pattern exemplified in Fig. 5.4, bottom row, by two equivalent packings at $k = 6$. Different equivalent packings, total of three for $k = 6$, can be obtained by differently inserting the shorter row and the shorter column (lighter shaded) among $k - 1$ rows and $k - 1$ columns arranged in the square orthogonal fashion. There also three equivalent, packings of this pattern far $k = 5$, and one packing

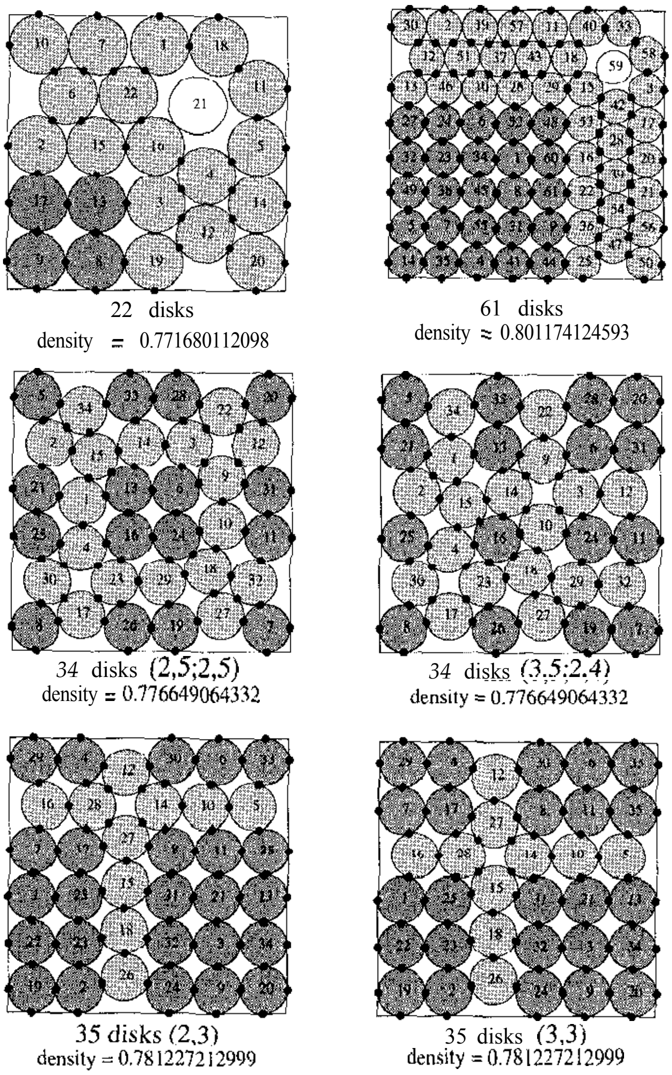


Fig. 5.4. Best found packings of equal disks in a square. *Top row:* first ($k = 5$) and last ($k = 8$) members of sequence k^2 -3. The packings consist, of a heavier shaded $(k-3) \times (k-3)$ square packing in the bottom left corner and three lighter shaded alternating rows and columns and one unshaded rattler. *Middle row: two out* of four existing best, packings of 34 disks, a member of sequence $k^2 - 2$ for $k = 6$. Each packing consists of a $(k - 2) \times (k - 2)$ heavier shaded square pattern with two lighter shaded hexagonally arranged rows and two columns. Two pairs of insertion indices identifies a packing. *Bottom row:* two *out* of three existing best packing of 35 disks, a member of sequence $k^2 - 1$ for $k = 6$. Each packing consists of a (k- 1) $\times$ $(k - 1)$ heavier shaded square pattern with one lighter shaded inserted row and one column. A pair of insertion indices identifies a packing,

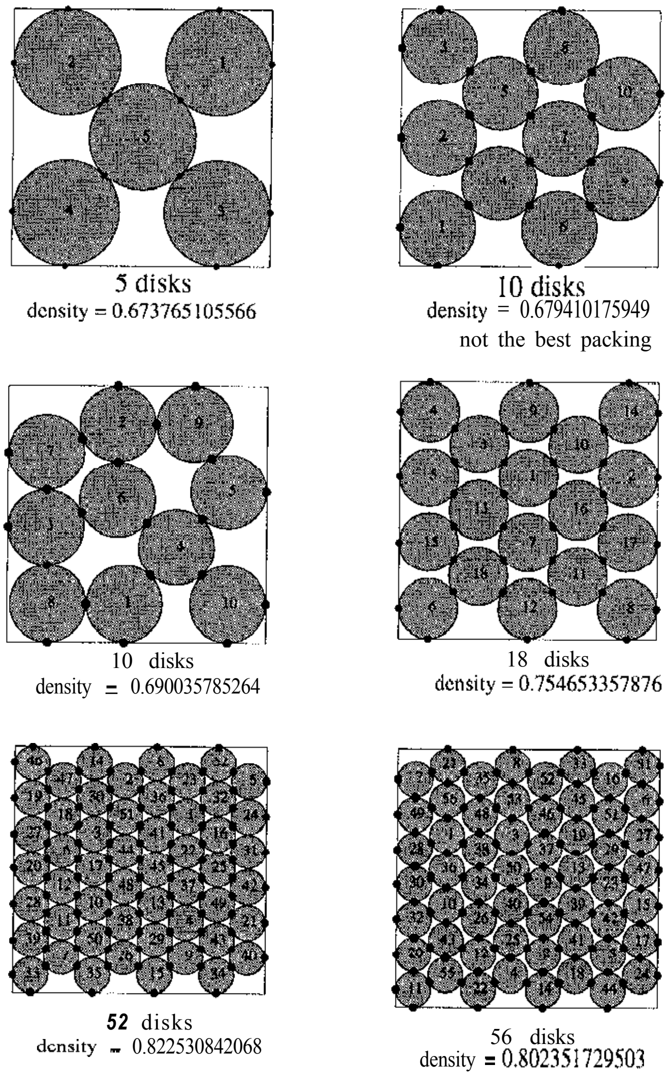


Fig. 5.5. Members of sequences $k(k+1)$ (56 disks) and $k^2 + \lfloor k/2 \rfloor$ (5, 10, 18, and 52 disks). Optimal packing of 10 disks (middle row, left) does not follow the common pattern of the latter sequence. The inferior packing of 10 disks that follows the pattern is also shown (top row, right)

for each of $k = 3$ and $k = 4$. For $k = 7$ a better packing of a different pattern exists.

Sequence $k(k+1)$ yields the pattern with $k+1$ alternating columns of k disks in each as an optimal packing for $k \geq 4$. The pattern is an adjustment of the hexagonal one for the square boundary. The pattern becomes non-optimal for $k = 8$, if we compare its quality with the best packing of 72 disks obtained in our experiments. In Fig. 5.4; bottom row, right, appears the last member of this sequence, which is still apparently optimal.

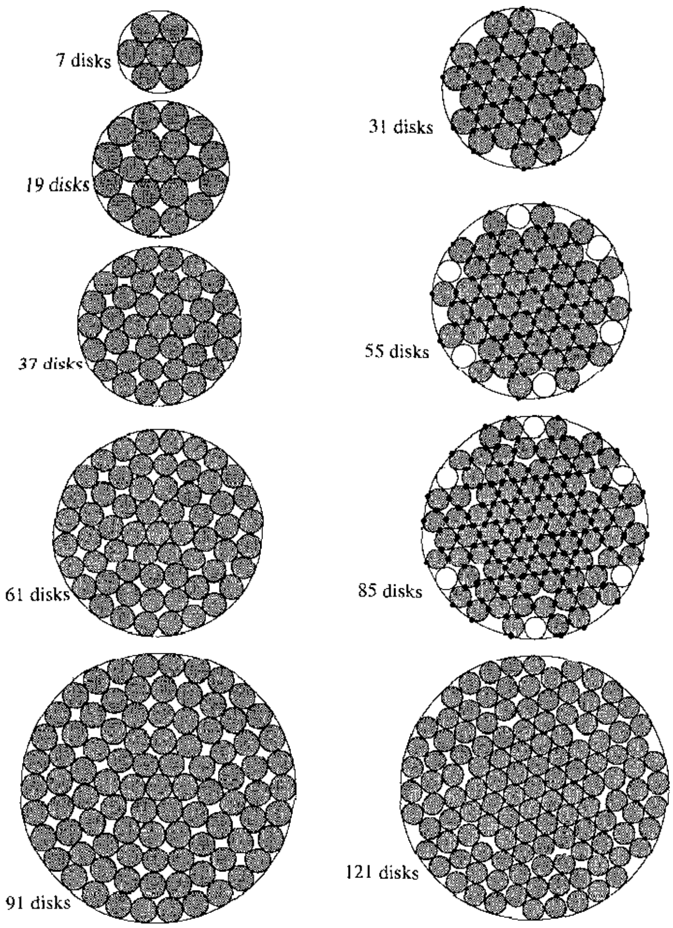


Fig. 5.6. Left: best found packings of $3k(k + 1) + 1$ equal disks in a circle for $k = 1, 2, 3, 4$, and 5. Right; best found packings of $3k(k + 3) + 1$ equal disks in a circle for $k = 2, 3$, and 4 and the highest obtained density configuration of 121 disks ($k = 5$).

Sequence $k^2 + \lfloor k/2 \rfloor$ demonstrates a different way of adjusting a hexagonal arrangement to the square boundary with $k + 1$ alternating columns whose length alternates also. The pattern begins as optimal at $k = 2$, then for the value $k = 3$ its optimality is preempted by a different, pattern and then is resumed as optimal for $k = 4$ and continues as such for $k = 5, 6$, and 7 The relative gap between consecutive disks in columns decreases (for example the gap between disks 1 and 3 in the packing of 5 disks, or between disks 1 and 7 in the packing of 18 disks) with the increase of k. For $k > 7$ the gap becomes negative, i.e., disks in the configuration constructed according to the pattern overlap.

As in the case of a square, a circle boundary shape does not conform to the hexagonal disk arrangement. Unlike the case of a square or equilateral triangle, no obviously "natural" packings of equal disks has been proposed. Perhaps, the *curved hexagonal* packings [LG95] can be taken as such. Fig. 5.6 shows five curved hexagonal packings (left column) which are also the best packings found in the experiments. There is a well-defined synthetic method to arrive at a curved hexagonal packing of $3k(k+1)+1$ disks for any $k>0$ as described in [LG95]. Exact positions of disks can be computed as well as disk diameter and density. $(k-1)!/2$ different equally good curved hexagonal packings are known for $k \geq 4$. Thus, there are three different equal quality such packings for $n=61$ disks and 12 packings for $n=91$ disks. Fig. 5.6 presents only one of these for each n. In our experiments we found a packing for 127 disks ($k=6$) that, is bettor than the corresponding curved hexagonal packing.

The right column in Fig 5 6 presents best found packings for the sequence $3k(k+3)+1$. Those demonstrate a different way of adjusting hexagonal packing to the circular-wall boundary conditions: hexagonal "core" and some loose disks on the periphery. For the specific $n=31$, 55, and 85 the adjustment produces perfect six-fold symmetrical patterns as the (conjecturally) best packings. The pattern apparently is trying to realize itself for $n=121$ ($k=5$) but we have not been able to generate a clear-cut packing: the resolution required is higher than the one offered by the double precision, i.e., with relative error of the order of 10^{14}. The algorithm stalls in this configuration without advancing further the time and the disk expansion, and for several pairs of disks we do not know whether or not they are in contact. Perhaps if the computations were done with a higher precision the best packing of 121 disks could be obtained by a small additional growth of disks starting from the presented configuration Packings of 31 and 55 disks can be easily constructed looking at their diagrams, including contacts, and their parameters can be easily calculated. (Such synthetic construction also prows their existence). The density computed in the simulation of the packing of 85 disks is 0.82293502752... and that of the presented configuration of 121 disks is larger than 0.82305172.

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