The Pursuit of Perfect Packing

# **The Pursuit of Perfect Packing**

Tomaso Aste

Istituto Nazionale per la Fisica della Materia, Genoa, Italy

and

Denis Weaire

Trinity College, Dublin, Ireland

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# Preface

There are many things which might be packed into a book about packing. Our choice has been eclectic. Around the mathematical core of the subject we have gathered examples from far and wide.

It was difficult to decide how to handle references. This is not intended as a heavyweight monograph or an all-inclusive handbook, but the reader may well wish to check or pursue particular topics. We have tried to give a broad range of general references to authoritative books and review articles. In addition we have identified the original source of many of the key results which are discussed, together with enough clues in the text to enable other points to be followed up, for example with a biographical dictionary.

Thanks are due to many colleagues who have helped us, including Nicolas Rivier (a constant source of stimulation and esoteric knowledge), Stefan Hutzler and Robert Phelan. Rob Kusner and Jörg Wills made several suggestions for the text, which we have adopted.

Denis Weaire benefited from the research support of Enterprise Ireland and Shell during the period in which this was written, and Tomaso Aste was a Marie Curie Research Fellow of the EU during part of it.

> Tomaso Aste Denis Weaire December 1999

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# How many sweets in the jar?

The half-empty suitcase or refrigerator is a rare phenomenon. We seem to spend much of our lives squeezing things into tight spaces, and scratching our heads when we fail. The poet might have said: *packing and stacking we lay waste our days*.

To the designer of circuit boards or software the challenge carries a stimulating commercial reward: savings can be made by packing things well. How can we best go about it, and how do we know when the optimal solution has been found?

This has long been a teasing problem for the mathematical fraternity, one in which their delicate webs of formal argument somehow fail to capture much certain knowledge. Their frustration is not shared by the computer scientist, whose more rough-and-ready tactics have found many practical results.

Physicists also take an interest, being concerned with how things fit together in nature. And many biologists have not been able to resist the temptation to look for a geometrical story to account for the complexities of life itself. So our account of packing problems will range from atoms to honeycombs in search of inspiration and applications.

Unless engaged in smuggling, we are likely to pack our suitcase with miscellaneous items of varying shape and size. This compounds the problem of how to arrange them. The mathematician would prefer to consider identical objects, and an infinite suitcase. How then can oranges be packed most tightly, if we do not have to worry about the container? This is a celebrated question, associated with the name of one of the greatest figures in the history of science, Johannes Kepler, and highlighted by David Hilbert at the start of the 20th century.

1



Figure 1.1. Stacking casks of Guinness.

## Hilbert's 18th problem

In 1900, David Hilbert presented to the International Mathematical Congress in Paris a list of 23 problems which he hoped would guide mathematical research in the 20th century. The 18th problem was concerned with sphere packing and space-filling polyhedra.

I point out the following question (...) important to number theory and perhaps sometimes useful to physics and chemistry: *How one can arrange most densely in space an infinite number of equal solids of given form,* e.g. spheres with given radii or regular tetrahedra with given edges (or in prescribed positions), *that is, how can one so fit them together that the ratio of the filled to the unfilled space may be as great as possible?* 

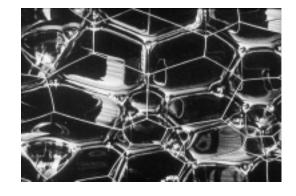


Figure 1.2. Soap bubbles.

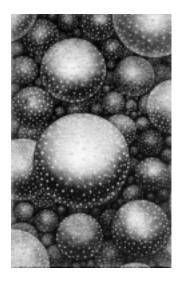


Figure 1.3. Packing on a grand scale: Wright T 1750 The Cosmos.

More subtle goals than that of maximum density may be invoked. When bubbles are packed tightly to form a foam, as in a glass of beer, they can adjust their shapes and they do so to minimize their surface area. So in this case, the total volume is fixed and it is the total area of the interfaces between the bubbles that is minimized.

The history of ideas about packing is peopled by many eminent and colourful characters. An English reverend gentlemen is remembered for his experiments in squashing peas together in the pursuit of geometrical insights. A blind Belgian scientist performed by proxy the experiments that laid the ground rules for serious play with bubbles. An Irishman of unrivalled reputation for dalliance (at least

#### 4 How many sweets in the jar?

among crystallographers) gave us the rules for the random packing of balls. A Scotsman who was the grand old man of Victorian science was briefly obsessed with the parsimonious partitioning of space.

All of them shared the curiosity of the child at the church bazaar: *how many sweets are there in the jar?* 

# Loose change and tight packing

## 2.1 A handful of coins

ρ

An ample handful of loose change, spread out on a table, will help us understand some of the principles of packing. This will serve to introduce some of the basic notations of the subject, before we tackle the complexity of three dimensions and the obscurities of higher dimensions.

Let us discard the odd-shaped coins which are becoming fashionable; we want hard circular discs. Coins come in various sizes, so let us further simplify the problem by selecting a set of equal size. About ten will do. The question is: *how could a large number of these coins be arranged most tightly?* 

If we do it in three-dimensional space, then obviously the well known bankroll is best for any number of coins. But here we restrict ourselves to twodimensional packing on the flat surface of the table.

Three coins fit neatly together in a triangle, as in figure 2.1. There is no difficulty in continuing this strategy, with each coin eventually contacting six neighbours. A pleasant pattern soon emerges: the triangular close packing in two dimensions.

The fraction of table covered by coins is called the packing fraction, which is

$$= \frac{\text{Area covered}}{\text{Total area}} = \frac{\pi}{\sqrt{12}} = 0.9068....$$
(2.1)

This must surely be the largest possible value. But can we prove it? That is often where the trouble starts, but not in this case. A proof can be constructed as follows.

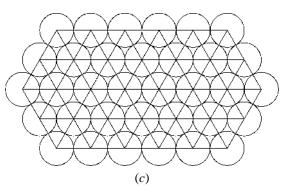
5



(a)







**Figure 2.1.** Three equal discs fit tightly in an equilateral triangle (*a*). This configuration can be extended to generate the triangular close packing (*b*). This is the densest possible arrangement of equal discs, having packing fraction  $\rho = 0.9068...$  The regular pattern drawn by joining the centres of touching discs is the triangular lattice (*c*).

## 2.2 When equal shares are best

There is a general principle which helps with many packing problems: it says that, under certain circumstances, *equal shares* are best. (We shall resist any

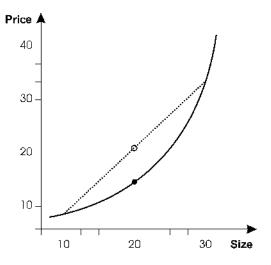


Figure 2.2. What is the best price for two fields, of a total area of 40 hectares?

temptation to draw moral lessons for politicians at this point.) A parable will serve to illustrate this principle in action.

A farmer, attracted by certain European subsidies, seeks to purchase *two* fields with a total area of 40 hectares. The prices for fields depend on the field size as shown in the diagram of figure 2.2. What is he to do?

Playing with the different possibilities quickly convinces him that he should buy two fields of 20 hectares each. The combination of ten and 30 hectares is more expensive; its price is twice that indicated by the open circle on the diagram, which lies above the price of a 20 hectare field.

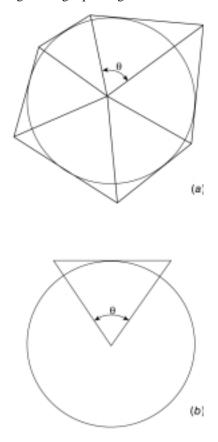
What property of the price structure forces him to choose equal-sized fields? It is the *upward curvature* of figure 2.2, which we may call *convexity*.

#### Packing a single disc

A packing problem may be posed for a single disc of radius R by requiring it to fit into a polygonal boundary—a sheep-pen—which is as small as possible. The sheep-pen has n sides: what shape should it be?

The answer is: a regular polygon (that is, totally symmetric with equal edges and equal angles between edges).

To demonstrate this we note that the area of a polygon can be divided into sectors, as shown in figure 2.3(*a*). Each sector corresponds to an angle  $\theta$  and the angles must add up to  $2\pi$ . We need to share this total among *n* angles. But the area of each sector must be greater or equal than that shown in figure 2.3(*b*) (isosceles triangle) and this is a *convex* function of  $\theta$ .



**Figure 2.3.** (*a*) A polygon with a disc inside can be divided into triangular sectors with angles  $\theta$ . (*b*) The isosceles triangle that touches the disc is the sector that minimizes the area for a given  $\theta$ . The area of such a sector is a convex function of  $\theta$ , therefore a division in equal sectors is best.

So equal angles are best, and the strategy of equal shares results in n such isosceles triangles.

#### Packing many discs

We are ready to complete the proof of the disc-packing problem in two dimensions: *what is the most dense arrangement of equal discs, infinite in number?* The answer will be the triangular close packing of figure 2.1.

In his book, which covers many such problems<sup>1</sup>, Fejes Tóth attributes the

<sup>&</sup>lt;sup>1</sup> Fejes Tóth L 1953 Lagerungen in der Ebene auf der Kugel und im Raum (Die Grundlehren der Math. Wiss. 65) (Berlin: Springer).

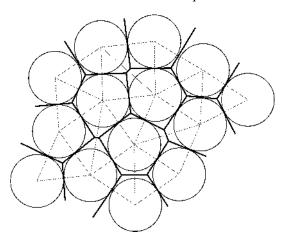


Figure 2.4. A Voronoï partition around the centres of a disordered assembly of discs.

first proof of this result to the Scandinavian mathematician Thue, who in 1892 discussed the problem at the Scandinavian National Science Congress and in 1910 published a longer proof. C A Rogers expresses some objections to these proofs: 'it is no easy task to establish certain compactness results which he takes for granted'<sup>2</sup>.

What we present here is based on one of the proofs given by Fejes Tóth.

First, we assign to each disc in any given packing its own territory, a polygonal shape which surrounds it (as in figure 2.4). This is done by drawing a line bisecting the one which joins the centres of neighbouring discs. This is the *Vorono ï construction*, to which we will return several times in this book.

We can assume that all these boundaries meet at a triple junction. (If not, just introduce an extra boundary of zero length to make it so.) For an infinite number of circles in the whole plane, a theorem of Euler<sup>3</sup> states that for such a Voronoï pattern the average number of sides of the polygons is *exactly six*<sup>4</sup>

$$\langle n \rangle = 6. \tag{2.2}$$

The triangular pattern has n = 6 for all the polygons: they are regular hexagons. If we introduce some polygons with *more* sides than six, they must be compensated by others with *less*. Now we can use the result of the last section. The area of the *n*-sided polygons cannot be less than that of the regular polygon which touches the disc. This is a convex function of *n* (figure 2.5), so that once again we can use the principle of 'equal shares', this time of polygon sides. *The total area cannot be less than what we can obtain with* n = 6 for all polygons.

<sup>&</sup>lt;sup>2</sup> Rogers C A 1964 *Packing and Covering* (Cambridge: Cambridge University Press).

<sup>&</sup>lt;sup>3</sup> See Smith C S 1981 A Search for Structure (Cambridge, MA: MIT Press) p 5.

<sup>&</sup>lt;sup>4</sup> There are certain kinds of tilings where this equation does not hold. See Grünbaum B and Rollet G C 1986 *Tilings and Patterns* (New York: Freeman).

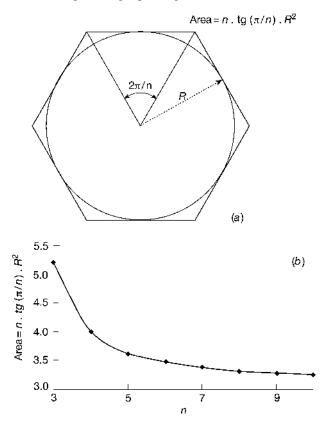


Figure 2.5. The area of regular polygons with a circle inscribed is a *convex* function of the number of sides of the polygons (n).

Here we have a pattern which, were we not to construct it in the imagination, presents itself to us in daily life, in the packing and stacking of drinking straws and other cylindrical objects, or the layout of eggs in a carton. It would even form spontaneously, at least locally, if we shuffled our coins together for long enough.

There is a research group in Northern France which does just this sort of experiment, using a gigantic air table. This is a surface with small holes through which air is pumped, so that flat objects can glide upon it without friction.

Later we will encounter other problems which look very similar to this one, but few of them submit to such a straightforward argument. Indeed a false sense of security may be induced by this example. It turns out that almost any variation of the problem renders it more mysterious.

So what is so special about the packing of these discs? It is the convenient fact that there is a best *local* packing which can be extended without variation to the whole structure. If we restore our handful of mixed change, or try to stack



**Figure 2.6.** The giant air table machine (4.5 m high) constructed, in Rennes by D Bideau and others, in order to investigate two-dimensional packings. The two men in the photograph are the builders of the system.

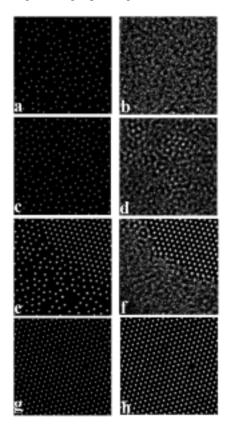
oranges in three dimensions instead, no such elementary argument will work.

The problem becomes one of a *global* optimization, which cannot always be achieved by *local* optimization. It takes its place alongside many others which practical people have to face. Under specified conditions how do we maximize some global quantity? Given life and liberty how do we best pursue happiness, allowing for the limitations of human nature and the competing demands of individuals?

As every democrat knows, global optimization is a matter of difficult compromise. Perfection is rarely achieved, and how do you know when you have it?

#### 2.3 Regular and semi-regular packings

In the previous section we learned that dividing space into equal, regular shapes is often the most convenient strategy. In the densest packing of equal discs, each disc is in contact with six others. Upon joining the centre of each disc with the centres of the ones in contact with it, there emerges a tessellation (or tiling) of



**Figure 2.7.** Spontaneous clustering into the triangular lattice for bearings on a plane shaken vertically from high (top) to low accelerations (bottom). Single images (right column) and second averaged images (left column). (Courtesy of J S Olafsen and J S Urbach.)

the plane made with equal, regular triangular tiles. This tessellation has three properties:

- (1) all the vertices are identical, that is, lines come together in the same way at each of them;
- (2) all tiles are regular (that is, completely symmetrical) polygons;
- (3) all polygons are identical.

This is called a *regular tessellation*. How many tessellations with such regularity exist? The answer is three: they correspond to the *triangular*, *square* and *hexagonal* cases, which are shown in figure 2.9. In these three packings the discs are locally disposed in highly symmetrical arrangements and the whole packing can be generated by translating on the plane a unique local configuration, as in the simplest kinds of wallpaper.

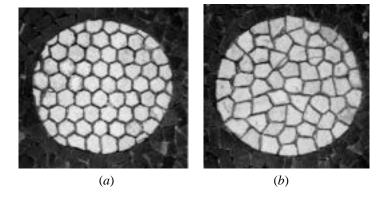


Figure 2.8. Ordered and disordered tessellations, from the pavements of Lisbon.

By relaxing the third condition, and allowing more than one type of regular polygon as tiles, eight other packings can be constructed. These tessellations are named *semi-regular* or *Archimedean* by analogy with the names used for finite polyhedra in three dimensions. Figure 2.10 shows these eight semi-regular packings and their packing fractions. Note that the lowest packing fraction among these cases ( $\rho \simeq 0.391$ ) is attained by the structure made with triangular and dodecagonal tiles. This brings us back to the equal shares principle, used this time in the opposite way: very different shares give bad packing fractions.

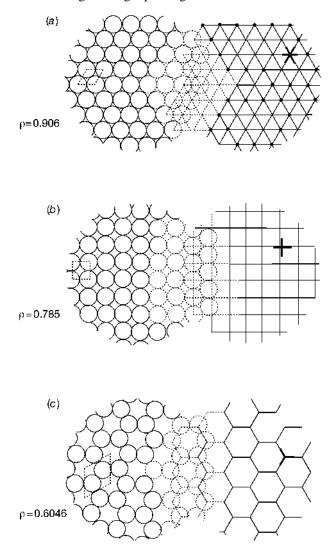
In these semi-regular packings the whole structure can again be generated by translating a unique local configuration (indicated by lines in figure 2.10). Such structures are called *lattices* or *crystalline structures*. In metals, in quartz, in diamond, and in many other solids, atoms are disposed regularly in space as in the two-dimensional arrangements of discs previously discussed. These solids are named *crystals*.

But nature is rich and diversified, and other types of packings different from the simple crystalline ones are also found.

#### 2.4 Disordered, quasi-ordered and fractal packings

We know that when equal coins are placed tightly on the table, an ordered, regular configuration emerges: the triangular lattice. What happens if coins of different sizes are used instead? Let us try to construct this packing: start with equal coins packed regularly in the tightest way, then insert a coin of a different size. If the coin is much smaller than the others (relative diameter less than 15% <sup>5</sup>), it can be inserted in one of the holes of the regular packing without modifying the whole structure. In the technical jargon of the subject, this is sometimes called a 'rattler',

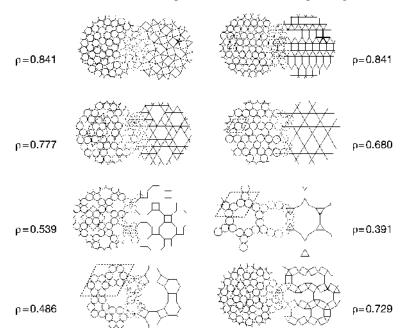
<sup>&</sup>lt;sup>5</sup> Inside the hole between three coins of diameter d, packed in the tightest way, a fourth coin of diameter equal or smaller than  $d = (2/\sqrt{3} - 1)d = (0.154...)d$  can be inserted.



**Figure 2.9.** Regular packings of equal discs. Here the patterns formed by joining the centres of the circles mutually in contact have identical vertices and regular, identical polygons as tiles. These are triangles (*a*), squares (*b*) and hexagons (*c*). The packing fractions are respectively  $\rho = \pi/\sqrt{12} = 0.906 \dots (a), \rho = \pi/4 = 0.785 \dots (b)$  and  $\rho = \pi/\sqrt{27} = 0.604 \dots (c)$ .

since it is free to rattle around the space available.

On the other hand, if the inserted coin is very large it requires the removal of the original coins to accommodate it and, in the tight packing around this inter-



**Figure 2.10.** Semi-regular packings of equal discs. Here the patterns formed by joining the centres of the circles mutually in contact have identical vertices and tiles which are different kinds of regular polygons.

loper, the whole structure is modified.

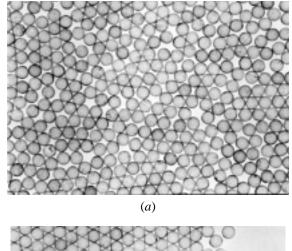
In general, it turns out that when differently sized discs are packed tightly together there is a strong tendency towards disorder. This is especially true when there is a marked difference in the disc sizes (at least 25%) and the effect is stronger when a few large discs are mixed with small ones<sup>6</sup>.

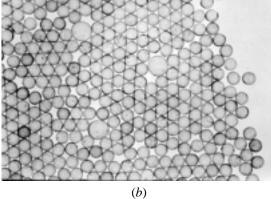
When discs with special size ratios are chosen, beautiful arrangements can be created. This, for instance, is the case when equal quantities of discs with two diameters in the ratio  $\sqrt{(3-\tau)}/\tau$  are chosen (here  $\tau = (1+\sqrt{5})/2 = 1.618...$ , is the 'golden ratio', which is the ratio between the base and the height of the *golden rectangle*: the shape with perfect proportion for the ancient Greeks). In figure 2.12 different arrangements obtained by using this mixture are shown. (The diameter ratio of the US cent and quarter coins is very close to this ratio  $\tau$ , and their contrasting colours make nice figures.)

The packing fraction can be arbitrarily increased by taking a variety of discs with sizes in an arbitrarily large range. This, for instance, is the case in the packing

<sup>&</sup>lt;sup>6</sup> See, for instance, Nelson D R, Rubinstein M and Spaepen F 1982 Order in two dimensional binary random arrays *Phil. Mag.* A **46** 105–26; Dodds J A 1975 Simplest statistical geometric model of the simplest version of the multicomponent random packing problem *Nature* **256** 187–9.

16 Loose change and tight packing





**Figure 2.11.** A disordered assembly of equal discs (*a*), and a packing of discs with two different sizes (*b*).

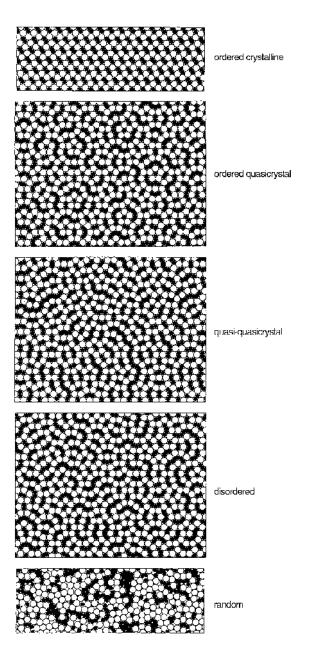
illustrated in figure 2.13 which is known by the name of Apollonian packing (to which we return in chapter 9).

Such structures are typical examples of a fractal<sup>7</sup>. The structure repeats similar patterns on each length scale. Looking at it through a microscope one would see much the same structure for any degree of magnification.

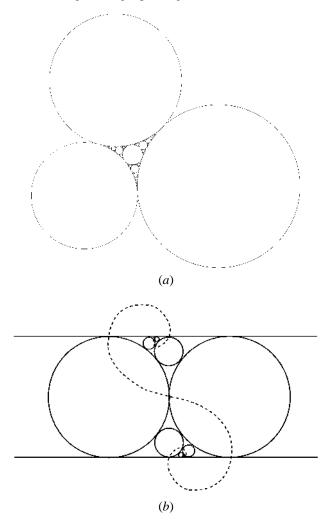
## 2.5 The Voronoï construction

We have already encountered a geometrical construction which will recur throughout this book. This has become attached to the name of Voronoï (1868–

<sup>&</sup>lt;sup>7</sup> Mandelbrot B B 1977 The Fractal Geometry of Nature (New York: Freeman).



**Figure 2.12.** Various tilings obtained using a binary mixture of discs. (From Lançon F and Billard L 1995 Binary tilings tools for models *Lectures on Quasicrystals* ed F Hippert and D Gratins (Les Vlis: ed. de physique) pp 265–81.)



**Figure 2.13.** Two examples of fractal packings: the Apollonian packing (*a*), the loxodromic sequence of circles (*b*). (See Coxeter H S I 1966 Loxodromic sequences of tangent spheres *AEQ*. *MATH* **1** 104–21.)

1908) but the primary credit probably belongs to Dirichlet, in 1850. Both he and Voronoï used the construction for a rather abstract mathematical purpose in the study of quadratic forms. Since then, it has played a supporting role in many important theories.

The modern use of Voronoï diagrams in physical science (in two, three or in many dimensions) began with crystallography but has since become much more general. In geography and ecology, indeed everywhere that spatial patterns are

analysed, this construction has proved useful.

The German term 'Wirkungsbereich' for a Voronoï cell is particularly apt; it refers to a region of activity or influence. It has often been considered to be a good basis for dividing political territories, given a set of pre-existing centres in major towns. Indeed, the division of France into Departments, laid down by Napoleon, corresponds rather well to the Voronoï regions around their principal cities.

In solid state physics the name Wigner–Seitz cell has been used instead, since 1933, and it was used to calculate the changes in the energy of electrons when atoms were packed together.

A recent monograph on the subject, although confined largely to two-dimensional patterns, ran to over 500 pages, so it evidently has many ramifications<sup>8</sup>.

<sup>&</sup>lt;sup>8</sup> Okabe A, Boots B and Sugihara K 1992 Spatial Tessellations: Concepts and Applications of Voronoï Diagrams (Chichester: Wiley).

# Hard problems with hard spheres

## 3.1 The greengrocer's dilemma

Now we will exchange our coins for a heap of oranges or a bag of ball bearings. It is much more difficult to see the possibilities that they present, in the mind's eye or in reality. But one thing becomes quite clear at an early stage: no amount of shaking the bag will cause the balls to come together in an elegant ordered structure. By the same token, the greengrocer must take time and care to stack his oranges neatly. Is his stacking the densest possible? Of course, this is not his objective. For our greengrocer, considerations of stability and aesthetics are paramount. If he is an amateur mathematician perhaps he might just wonder....

### **3.2** Balls in bags

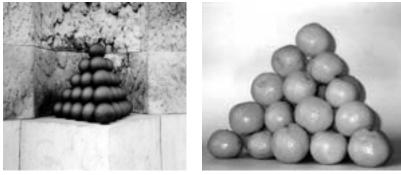
Let us look more closely at the ball bearings in the bag. In order to fix their positions, wax may be poured in and the contents then dissected. The first person to undertake this experiment systematically was J D Bernal, or rather his student John Finney, in the 1950s<sup>1</sup>. The random packing of balls became known as Bernal packing. One might wonder why it was not done before. Certainly it is tedious, but such tedium is often part of the price of a PhD.

The preceding century, in which the detailed atomic arrangements of crystals were hypothesized and powerful theories of symmetry applied to them, was one in which perfect order was the ideal (as one might expect in an imperial age).

<sup>&</sup>lt;sup>1</sup> Bernal J D 1959 A geometrical approach to the structure of liquids *Nature* **183** 141–7.

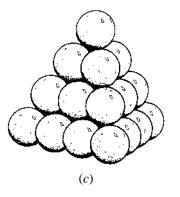
Balls in bags

21



*(a)* 

(*b*)



**Figure 3.1.** This is the sphere packing commonly found on fruit stands, in piles of cannon balls on war memorials and in the crystalline structures of many materials.

Order and beauty were often interchangeable in the sensibility of the admirer of nature.

*Là, tout n'est qu'ordre et beauté* Charles Baudelaire (1821–67)

At the century end, as the old order fell into decay, the mood began to change. The poet Hopkins gloried in 'dappled things', the commonly observed disarray of the real world. Nevertheless, words like 'impurity' and 'defect', applied to departures from perfect order, still carried a prejudicial overtone in physics, even as they eventually emerged as the basis of the semiconductor industry.

Those whose curiosity centred on the structure of liquids still tended to picture them as defective crystals or construct elegant formal theories that had little to do with their characteristically random geometry.

Eventually Bernal, perhaps because of his biological interests, saw the necessity to examine this geometry more explicitly, to confront and even admire its

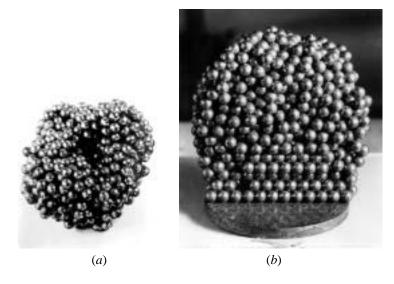


Figure 3.2. Bernal packing of spheres.

variety. He also recognized the difficulty of doing so, other than by direct observation of a model system. Why not ball bearings? He called this unsophisticated approach 'a new way of looking' at liquids.

Hence the shaking and kneading of ball bearings in a bag, the pouring in of wax, the meticulous measurement of the positions of balls as the random cluster was disassembled. The packing fraction of the Bernal packing was found to be roughly 0.64; or slightly less if the balls are not kneaded to encourage them to come together closely. Although particular local arrangements recur within it, they are variable in shape and random in distribution<sup>2</sup>.

Subsequently, the chief scientific interest of the Bernal structure has been in its application to describe the structures of amorphous (i.e. non-crystalline) metals.

Si l'ordre satisfait la raison, le désordre fait les délices de l'imagination. Paul Claudel (1868–1955)

#### 3.3 A new way of looking

Desmond Bernal, born in 1901 on an Irish farm, was one of the prime movers of modern crystallography and biophysics. He is thought to have narrowly missed a Nobel Prize for his work on sex hormones. This would have been singularly appropriate for a man whose sexual appetite was rumoured to be prodigious. This

<sup>&</sup>lt;sup>2</sup> Bernal J D and Mason J 1960 Co-ordination of randomly packed spheres *Nature* **385** 910–11.

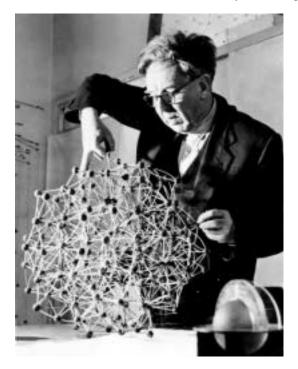


Figure 3.3. Desmond Bernal (1901–71).

is unusual in a scientist, as Bernal himself found out when curiosity moved him to check the historical record for the exploits of others. He found that typically they had less adventurous erotic *curricula vitae* than his. Certainly, few can have enjoyed the excitement of being pursued down the street by a naval officer with a revolver after a brusque interruption of an amorous interlude.

His intellectual brilliance is better documented. It would have found more positive expression if it had not been deflected into political channels (he was an ardent Communist—some of his sociopolitical writings are still highly regarded). Despite such distractions, he gathered around him in London an outstanding international research group.

Among the thoughts that most fascinated him from the outset were ideas of packing. They eventually found expression in his study of the structure of liquids, which proceeded directly along the down-to-earth lines advocated by Lord Kelvin, the founder of the 'hands-on' school of British crystallography whose crowning achievement was the discovery of the spiral structure of DNA.

Bernal used his hands and those of his students to build large models or take apart packings of ball bearings. He showed that geometrical constraints impose organization and local order on such random structures.

#### **3.4** How many balls in the bag?

The Bernal packing falls well short of the maximum density that can be achieved in an ordered packing. Nevertheless it has acquired its own significance as the best *random* packing. It is difficult to give to this notion any precise meaning, but many experiments and computer simulations of different kinds do reproduce the same value (to within a percent or so). For example, spheres may be added to a growing cluster, according to various rules, and the eventual result is a random packing not very different from that of Bernal. This was the finding of Charles Bennett, who wrote various computer programs for such 'serial deposition' at Harvard University in the mid-1960s. (Bennett has gone on to be one of the most authoritative and imaginative theoreticians in the science of computation.)

From the outset, this was called *dense random packing*, to distinguish it from looser packings of spheres which were found in some experiments. Attempts to define a unique density for random *loose* packings are probably futile, because it must depend on the precise circumstances, and physical effects (such as friction) which contribute to it. For instance, G D Scott poured thousands of ball bearings into spherical flasks of various sizes<sup>3</sup>. When the flask was gently shaken to optimize the packing, the density was found to be  $\rho = 0.6366 - 0.33N^{-1/3}$ , with N being the number of balls. When the flask was not shaken, the loosest random packing was found to have  $\rho = 0.60 - 0.37N^{-1/3}$ . Lower values for the packing fraction can be obtained by eliminating the effect of gravity. The lowest densities which can be experimentally obtained are around  $\rho \simeq 0.56^4$ .

Although his approach was an original one, Bernal's investigations followed in the footprints of an eminent English scientist of the 19th century.

#### 3.5 Osborne Reynolds: a footprint on the sand

It is seldom left for the philosopher to discover anything which has a direct influence on pecuniary interests; and when corn was bought and sold by *measure*, it was in the interest of the vendor to make the interstices as large as possible, and of the vendee to make them as small (...).

If we want to get elastic materials light we shake them up (...) to get these dense we squeeze them into the measure. With corn it is the reverse; (...) if we try to press it into the measure we make it light—to get it dense we must shake it—which, owing the surface of the measure being free, causes a rearrangement in which the grains take the closest order<sup>5</sup>.

<sup>&</sup>lt;sup>3</sup> Scott G D 1960 Packing of spheres Nature 188 908–9; 1969 Brit. J. Appl. Phys. 2 863.

<sup>&</sup>lt;sup>4</sup> Onoda G Y and Linger E G 1990 Random loose packing of uniform spheres and the dilatancy onset *Phys. Rev. Lett.* **64** 2727–30.

<sup>&</sup>lt;sup>5</sup> Reynolds O 1886 Experiment showing dilatancy, a property of granular material, possibly connected with gravitation *Proc. Royal Institution of Great Britain* Read 12 February.

With these words Osborne Reynolds described this 'paradoxical' property of granular packings.

When granular material, such as sand or rice, is poured into a jar its density is relatively low and it flows rather like an ordinary fluid. A stick can be inserted into it and removed again easily. If the vessel, with the stick inside, is gently shaken the level of the sand decreases and the packing density increases. Eventually the stick can no longer be easily removed and when raised it will support the whole jar. This conveys a strong sense of the ultimate jamming together of the grains, in the manner described by Bernal.

Such procedures have been the subject of research in physics laboratories in recent years<sup>6</sup>, but they can be traced back to the words of Osborne Reynolds.

At the present day the measure for corn has been replaced by the scales, but years ago corn was bought and sold by measure only, and measuring was then an art which is still preserved. (...) The measure is filled over full and the top struck with a round pin called the strake or strickle. The universal art is to put the strake end on into the measure before commencing to fill it. Then when heaped full, to pull the strake gently out and strike the top; if now the measure be shaken it will be seen that it is only nine-tenths full.

J J Thomson, the discoverer of the electron, called Reynolds 'one of the most original and independent of men', having attended his lectures at Owens College, Manchester. Thomson described Reynolds' chaotic lecturing style which, though it failed to impart much actual knowledge, 'showed the working of a very acute mind grappling with a new problem'. His rambling and inconclusive manner of teaching was due in part to his failure to consult the existing literature before developing his own thoughts. He was fond of what Thomson called 'out-of-door' physics, including the calming effect of rain or a film of oil on waves, the singing of a kettle and—in the episode that concerns us here—the properties of 'sand, shingle, grain and piles of shot'. He noted that 'ideal rigid particles have been used in almost all attempts to build fundamental dynamical hypotheses of matter', yet it did not appear 'that any attempts have been made to investigate the dynamical properties of a medium consisting of smooth hard particles (...)', although some of these had 'long been known by those who buy and sell corn'.

While consistent with his love of out-of-door physics, this preoccupation with sand arose in a more arcane context. Like many others, he had set out to invent an appropriate material structure for the ether of space. The ether was a Holy Grail for the classical physicist, which was also pursued by Lord Kelvin at about the same time, as we shall recount in chapter 7.

<sup>&</sup>lt;sup>6</sup> Similar experiments are reported by: Jenkin C F 1931 The extended pressure by granular material: an application of the principles of dilatancy *Proc. R. Soc.* A **131** 53–89; Weighardt K 1975 *Ann. Rev. Fluid. Mech.* **7** 89; Dahmane C D and Molodtsofin Y 1993 *Powders & Grains 93* ed C Thornton (Rotterdam: Balkema) p 369; Horaváth V K, Jánosi I M and Vella P J 1996 Anomalous density dependence of static friction in sand *Phys. Rev.* E **54** 2005–9.

#### 26 Hard problems with hard spheres

Could the electromagnetic properties of space be somehow akin to the mechanical properties of sand? Reynolds somehow convinced himself of this, asserting the 'ordinary electrical machine' then in use as a generator 'resembles in all essential particulars the machines used by seedsmen for separating two kinds of seed, trefoil and rye grass, which grow together (...)'.

So inspired was he by this notion that his last paper was entitled 'The Submechanics of the Universe'. But he hedged his bets by saying that his work also offered 'a new field for philosophical and mathematical research quite independent of the ether'. Most of his readers probably agreed with J J Thomson that this 'was the most obscure of his writings, as at this time his mind was beginning to fail'. Oliver Lodge diplomatically wrote that 'Osborne Reynolds was a genius whose ideas are not to be despised, and until we know more about the ether it is just as well to bear this heroic speculation in mind'.

In his speech at the British Association Meeting (Aberdeen 1885)<sup>7</sup> Reynolds explained that a granular material in a dense state must expand in order to flow or deform

As the foot presses upon the sand when the falling tide leaves it firm, that portion of it immediately surrounding the foot becomes momentarily dry (...). The pressure of the foot causes dilatation of the sand, and so more water is (drawn) through the interstices of the surrounding sand (...) leaving it dry....

Lord Kelvin spoke admiringly of this observation:

Of all the two hundred thousand million men, women, and children who, from the beginning of the world, have ever walked on wet sand, how many, prior to the British Association Meeting in Aberdeen in 1885, if asked, 'Is the sand compressed under your foot?' would have answered otherwise than 'Yes'?<sup>8</sup>

What Reynolds observed he called *dilatancy*, since the sand dilates. An expansion is required to allow any deformation (typically the distance between grains increases by about 1%).

In public lectures he dramatically demonstrated dilatancy (his 'paradoxical or anti-sponge property') by filling a bag with sand and showing that if only just enough water was added to fill the interstices, the sealed bag became rigid.

Reynolds was remembered thereafter for his contributions to the dynamics of fluids (including the Reynolds number) but his work on granular materials enjoys belated celebrity today. It has become a fashionable field of physics, one in which fundamental explanations are sought for phenomena long known to engineers.

In one practical example, dry cement is stocked in large hoppers from which it is dispensed at the bottom. Normally, the cement comes out with a constant

<sup>&</sup>lt;sup>7</sup> Reynolds O 1885 *British Association Report* Aberdeen p 897; 1885 On the dilatancy of media composed of rigid particles in contact. With experimental illustrations *Phil. Mag.* **20** 223.

<sup>&</sup>lt;sup>8</sup> Lord Kelvin 1904 *Baltimore Lectures* p 625.

flux independent of the filling of the hopper (which is not what a normal liquid would do). Occasionally, when it is not been allowed enough time to settle, the cement behaves in a much more fluid manner. A disaster ensues when the hopper is opened<sup>9</sup>.

### 3.6 Ordered loose packings

Ordered loose packings sometimes occur in the study of crystal structures. Here our question may be turned on its head: what is the lowest possible density for a packing of hard spheres which is still mechanically stable or 'rigid'? For such rigidity, each sphere needs at least four contacts and these cannot be all in the same hemisphere. Many loose crystalline packings have been proposed. For instance, the structure shown in figure 3.4(a) has  $\rho = 0.1235$ . It was proposed many years ago by Heesch and Laves and has been long considered to be the least dense stable sphere packing. Recently a packing with  $\rho = 0.1033$  (figure 3.4(b)) was obtained by decorating, with tetrahedra, the vertices of the CdSO<sub>4</sub> net<sup>10</sup>.

The lowest known density for stable packing is  $\rho = 0.0555...^{11}$ . This value is about ten times smaller than the one for the loose random packing. But this is not surprising, since structures such as those in figure 3.4 are highly symmetric and cannot be obtained or approximated by simply mixing spheres at random.

#### 3.7 Ordered close packing

What about dense ordered packings of spheres, the central question, from which we have digressed?

Back at the greengrocer's shop, the proprietor, unconcerned about theory, has stacked his oranges in a neat pyramidal pile. He proceeds by first laying out the fruit in the manner of the coins of chapter 2, and observes that this creates resting-places for the next layer, and so on. The packing fraction is  $\pi/\sqrt{18} = 0.74048...$  Is this the best that can be done?

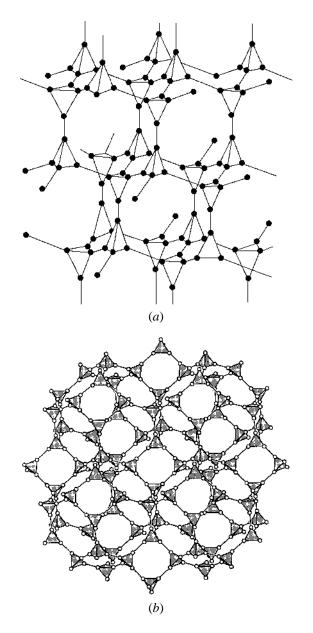
It has been remarked that *all mathematicians think and all physicists know that this is the best*. Some metallurgists have gone one step further by declaring in textbooks that such an assertion has been *proved*. At least prior to August 1998, such a statement was quite incorrect. This is the longstanding Kepler Problem.

Let us resort to theoretical argument, following the line of chapter 2. In three dimensions the counterpart of the trio of coins in mutual contact is the regular tetrahedron (figure 3.5). If these fourfold units could be tightly assembled we might well expect them to give us the best possible structure in three dimensions, and its packing fraction would be  $\sqrt{18}[\cos^{-1}(\frac{1}{2}) - \pi/3] = 0.7797...$ 

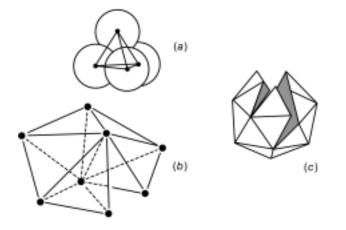
<sup>&</sup>lt;sup>9</sup> Duran J 2000 Sands, Powders and Grains (New York: Springer).

<sup>&</sup>lt;sup>10</sup>O'Keeffe M and Hyde G B 1996 Crystal Structures (Washington, DC: Mineralogical Society of America).

<sup>&</sup>lt;sup>11</sup>Gardner M 1966 Packing spheres *Martin Gardner's New Mathematical Diversions from Scientific American* (New York: Simon and Schuster).



**Figure 3.4.** (*a*) A structure (called D4) of stable equal-sphere packing with low density (the circles indicate the centres of the spheres and the lines connect neighbours in contact). (*b*) This structure (called W4) is obtained by replacing the vertices of the CdSO<sub>4</sub> net with tetrahedra.



**Figure 3.5.** Four spheres can be assembled mutually in contact on the vertices of a regular tetrahedron (*a*). This disposition is the closest possible with packing fraction  $\rho = 0.7797...$  But regular tetrahedra cannot be combined to fill the whole Euclidean space. The angle between two faces of the tetrahedron is  $\theta = \cos^{-1}(\frac{1}{3}) = 2\pi/5.104...$ , which means that around a common edge one can dispose five tetrahedra, but an interstice of  $2\pi - 5\cos^{-1}(\frac{1}{3}) = 0.128...$  will remain (*b*). Twenty tetrahedra can be disposed around a common vertex; the 12 external vertices make an irregular icosahedron (*c*).

But they cannot be so combined. This strategy fails.

Such a packing would necessarily involve tetrahedra which share a common edge, but the angle between two faces (dihedral angle,  $\theta = \cos^{-1}(\frac{1}{3})$ ) does not allow this, as figure 3.5 shows. Local desiderata are incompatible with global constraints, and this is sometimes categorized by the apt term 'frustration'<sup>12</sup>.

One strategy to relieve this frustration would be to relax the condition that the tetrahedra be regular (perfectly symmetric), as they must be if all four balls are in contact with each other. We shall return to this possibility in chapter 8.

# 3.8 The Kepler Conjecture

Science is notoriously dependent on military motives. In 1591 Walter Raleigh needed a formula to count the number of cannonballs in a stack. His friend Thomas Harriot<sup>13</sup>, who was his surveyor/geographer on the second expedition to Virginia, developed a formula without much difficulty and made a study of close packing. He was an accomplished mathematician, later credited with some of the theorems of elementary algebra still taught today.

He was also active in promoting the atomic theory, which hypothesized that

<sup>&</sup>lt;sup>12</sup>Sadoc J-F and Mosseri R 1997 Frustration Géométrique (Paris: Éditions Eyrolles).

<sup>&</sup>lt;sup>13</sup>See Rukeyser M 1972 *The Traces of Thomas Harriott* (London: Gollanz)



Figure 3.6. Thomas Harriot (1560–1621). Courtesy of Trinity College Oxford.

matter was composed of atoms. In a letter in 1607, he tried to persuade Kepler to adopt an atomic theory in his study of optics. Kepler declined, but a few years later in his *De Nive Sexangula* (1611) he adopted an atomistic approach to describe the origin of the hexagonal shape of snowflakes. To do this he assumed that the snowflakes are composed of tiny spheres<sup>14</sup>.

Kepler recognized the analogy with the bee's honeycomb. He therefore studied the shape resulting from compressing spheres arranged in the closest way. The construction of the 'most compact solid' is described as follows:

For in general equal pellets, when collected in any vessel, come to a mutual arrangement in two modes according to the two modes of arranging them in a plane.

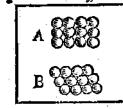
If equal pellets are loose in the same horizontal plane and you drive them together so tightly that they touch each other, they come together either in a three-cornered or in a four-cornered pattern. In the former case six surround one; in the latter four. Throughout there is the same pattern of contact between all the pellets except the outermost. With a five-sided pattern uniformity cannot be maintained. A six-sided pattern breaks up into three-sided. Thus there are only the two patterns as described.

<sup>&</sup>lt;sup>14</sup>See Leppmeier M 1997 Kugelpackungen von Kepler bis heute (Wiesbaden: Vieweg).

#### SEXANGVLA.

Ram fierrantes in oodem plano horiZontali globulos aqualescoegeris in ang flum, vs fe mutuo contingant; aut triangulari forma count, ant quadrangulari; ibi fex vuum circumflant, bic quatuor: vtrinque eadem estratio contactus per omnes globulos, demptis extremis. Quanquanguli forma nequit retineri aqualitas, fexangulum refoluitur in triangula: vt ita dicti duo ordines foli fint.

Uam fi ad fir utturam folidorum quam poteft fieri arttiffimam progredioris, ordinesą, ordinibus fuperponas, in plano prius coaptatos,



aut ijerunt quadrati A aut trigonici: 5 fiquadrati, aut finguliglobi ordinis fuperioris fingulis fuperstabunt ordinis inferioris aut contra finguli ordinis fuperioris fedebunt inter quaternos ordinis inferioris. Priori modo tangitur quilibet globus à quatuor circumstantibus in eodem plano, ab

vno fupra fe, & ab vzo infra fe: & ficin vninerfum à fex alijs, erit à ordo cubicus, & compreffione facta fient cub: : fed non crit arctiffima constatio. Posteriorimodo praterquam quod quilibet globus à quatuor circumftantibus in codem plano tangitur ctiam à quatuor infra fe, & à quatuor fupra fe, & fic in univer fum à duo decim tangetur; fientge compressione ex globofis Rhombica. Or do bie magis affimilabitur offaedro & Pyramidi, Cosptatio fiet artifima: vt nullo prateren ordine plures globuli in idem vas compingi que ant. Rurfum fi ordines in plano fructi fuerint trigonici tuncin conplatione folida aut finguli globi or dinis fuperi . Superfant fingulis inferioris, coaplationerurfum laxa, aut finguli superioris, fedent inter ternes inferioris Priori mode tangitur quilibet globus à fex circumffantibus in codem plino, ab uno supra, & ab uno infra fe, & fic in uniner sum ab octo alijs. Ordo afimilabitur l'rifmati , & copreffione fattafient pro globulis columna fenum laterum quadragulorum, duarumá bafum Jexangularum. Posteriori modo fiet idë, quod prius posteriori modo in R 984-

**Figure 3.7.** The original page of 'De Nive Sexangula' where the two regular packings of spheres in the plane are drawn. Square (A) and triangular (B).

Now if you proceed to pack the solid bodies as tightly as possible, and set the files that are first arranged on the level on top of others, layer on layer, the pellets will be either in squares (A in diagram), or in triangles (B in diagram). If in squares, either each single pellet of the upper range will rest on a single pellet of the lower, or, on the other hand, each single pellet of the upper range will settle between every four of

#### 32 Hard problems with hard spheres

the lower. In the former mode any pellet is touched by four neighbours in the same plane, and by one above and one below, and so on throughout, each touched by six others. The arrangement will be cubic, and the pellets, when subjected to pressure, will become cubes. But this will not be the tightest packing. In the second mode not only is every pellet touched by it four neighbours in the same plane, but also by four in the plane above and by four below, and so throughout one will be touched by twelve, and under pressure spherical pellets will become rhomboid. This arrangement will be more comparable to the octahedron and pyramid. *This arrangement will be the tightest possible, so that in no other arrangement could more pellets be packed into the same container*<sup>15</sup>.

The structure here described by Kepler is cubic close packing, also called face-centred cubic (fcc). It has the greengrocer's packing fraction  $\rho = 0.7404...$  It is a regular structure: the local configurations repeat periodically in space like wall paper but in three dimensions. Such a periodic structure is now often called *crystalline* because it corresponds to the internal structure of crystals.

Kepler's work was the first attempt to associate the external geometrical shape of crystals with their internal composition of regularly packed microscopic elements. It was very unusual for his time, when the word 'crystal' was applied only to quartz, which was thought to be permanently frozen ice.

Kepler asserted that the cubic close packing 'will be the tightest possible, so that in no other arrangements could more pellets be packed into the same container'. Despite Kepler's confidence this conjecture long resisted proof and became the oldest unsolved problem in discrete geometry.

# 3.9 Marvellous clarity: the life of Kepler

Kepler was born in Weil der Stadt (near Leonenberg, Germany) in 1571. He was originally destined for the priesthood, but instead took up a position as school teacher of mathematics and astronomy in Graz.

When Kepler arrived in Graz he was 25 years old and much occupied with astrology. He issued a calendar and prognostication for 1595 which contained predictions of bitter cold, a peasant uprising and invasions by the Turks. All were fulfilled, greatly enhancing his local reputation.

Kepler was an enthusiastic Copernican. Today he is chiefly remembered for his three laws on planetary motion but his search for cosmic harmonies was much broader, ranging from celestial physics to sphere packings.

Kepler's personality has been described as 'neurotically anxious'. Certainly he had an unhappy personal life. The story goes that, in seeking to optimize the partner for his second marriage, he carefully analysed the merits of no less than

<sup>&</sup>lt;sup>15</sup> Quoted from: Kepler 1966 *The Six-cornered Snowflake* translated by C Hardie (Oxford: Clarendon).



Figure 3.8. Johannes Kepler (1571–1630).

11 girls—before choosing the wrong one. The word 'nerd' may be inappropriate for a giant of the Renaissance but it springs to mind.

On the other hand Kepler's scientific writing presents us with what he called a 'holy rapture' of compelling power. One young scientist in this century who was inspired by its fusion of scientific insight and religious mysticism was L L Whyte<sup>16</sup>. This is his translation of the breathless cadenza from Kepler's *Harmony of the Worlds*.

But now, since eighteen months ago the first light dawned, since three moons the full day, and since a few days the sunshine of the most marvellous clarity now nothing holds me back: now I may give in to this holy rapture. Let the children of men scorn my daring confession: Yes! I have stolen the golden vessels of the Egyptians to build from them a temple for my God, far from the borders of Egypt. If you forgive me, I am glad; if you are angry I must bear it. So here I throw my dice and write a book, for today or for posterity. I care not. Should it wait a hundred years for a reader, well, God himself has waited six thousand years for a man to read his work.

Whyte suggested that there should be a verb 'to kepler, meaning to identify a conceivable form of order as an aim of search'. Perhaps it could have the secondary meaning 'to over-idealize real systems, in an attempt to scientifically analyse them', as in Kepler's search for a wife.

<sup>&</sup>lt;sup>16</sup>Whyte L L 1963 Focus and Diversions (London: Cresset Press).

# 3.10 Progress by leaps and bounds?

While the Kepler problem remained unsolved, many mathematicians contributed to this study by offering something less than the full theorem that is required.

Gauss contributed to the problem by demonstrating that the face-centred cubic structure is the densest *crystalline*<sup>17</sup> packing in three dimensions. But this is not sufficient since denser local configurations exist (such as the tetrahedral configuration of four spheres mutually in contact) and therefore non-crystalline structures could conceivably have packing fractions higher than that of the cubic close packing.

Fejes Tóth reduced the problem to a finite but impossibly large calculation: 'It seems that the problem can be reduced to the determination of the minimum of a function of a finite number of variables' <sup>18</sup>.

Often mathematicians set themselves the task of proving that the highest density must be lower than some value X. This is an *upper bound*. With no thought at all we can offer X = 1.0 for an upper bound of  $\rho$ , and with some subtlety much better values may be found. Obviously if we could show that 0.7404... is an upper bound, then, we would also know we can reach it by the method of the greengrocer. The ball game would be over, apart from questions of uniqueness.

A particularly nice bound is that of C A Rogers (1958); it is precisely the packing fraction that we recognized as appropriate to a perfect tetrahedral packing (which cannot exist), that is, 0.7797... Better bounds have followed: 0.77844... (Lindsey 1987), 0.77836... (Muder 1988), 0.7731 (Muder 1993) and others. There are older ones as well 0.828 (Rankin 1947), 0.883... (Bichfeldt 1929)<sup>19</sup>.

This was progress by bounds but hardly by leaps. A proof of the original proposition still seemed far off, until recently.

<sup>&</sup>lt;sup>17</sup> In which each sphere is in an equivalent position. The term *lattice* packing is also used as a synonym.

<sup>&</sup>lt;sup>18</sup>Fejes Tóth L 1964 Regular Figures (New York: Pergamon).

<sup>&</sup>lt;sup>19</sup>Conway J H and Sloane N J A 1988 Sphere Packings, Lattices and Groups (Berlin: Springer).

# **Proof positive?**

# 4.1 News from the Western Front

It may be safely assumed that quite a few experts have devoted some small fraction of their time to looking for a solution to the Kepler problem, rather as the punter places a small bet on a long-odds horse. One would not want to stake a whole career on it, but the potential rewards are attractive enough to compel attention.

The problem was included in a celebrated list drawn up by David Hilbert at the dawn on this century, which was like a map of the mathematical universe for academic explorers and treasure hunters. We have already cited his challenge to posterity in chapter 1. Some of his treasures were found from time to time, but the key to Kepler's conjecture lay deeply buried. As D J Muder said, 'It's one of those problems that tells us that we are not as smart as we think we are'.

In 1991 it seemed that the key had finally been found by Wu-Yi Hsiang. The announcement of the long awaited proof came from the lofty academic heights of Berkeley, California. Hsiang had been a professor there since 1968, having graduated from Taiwan University and taken a PhD at Princeton. Few American universities enjoy comparable prestige, so the mathematical community was at first inclined to accept the news uncritically. When Ian Stewart told the story in 1992 in his *Problems of Mathematics*, he described Hsiang's work in heroic terms, but wisely added some cautionary touches to the tale.

Many mathematical proofs are long and involved, taxing the patience of even the initiated. There has to be a strong element of trust in the early acceptance of a new theorem. So the meaning of the word *proof* is a delicate philosophical and practical problem. The latest computer-generated proofs have redoubled this difficulty. In the present case, most of the mathematics was of an old-fashioned variety, close to that of school-level geometry. Indeed Hsiang claimed that a retreat

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from sophistication to more elementary methods was one secret of his success. Nevertheless his preprint ran to about 100 pages and was not easily digested even by those hungry for information. As his colleagues and competitors picked over the details, some errors became apparent.

This is not unusual. Another recent claim, of an even more dramatic result the proof of Fermat's Last Theorem—has required some running repairs, but is still considered roadworthy and indeed prizeworthy. However, Hsiang did not immediately succeed in rehabilitating his paper.

Exchanges with his critics failed to reach a resolution. A broadside was eventually launched at Hsiang by Thomas Hales in the pages of the splendidly entertaining *Mathematical Intelligencer*. Hales' piece lies at the serious end of that excellent magazine's spectrum but nevertheless it grips the reader with its layers of implication and irony, most unusual in a debate on a piece of inscrutable academic reasoning.

Despite the inclusion of some conciliatory gestures ('promising programme', 'improves the method') the overall effect is that of a Gatling gun, apparently puncturing the supposed proof in many places. Hales begins with the statement that 'many of the experts in the field have come to the conclusion that [Hsiang's] work does not merit serious consideration' and ends with a demand that the claim should be withdrawn: 'Mathematicians can easily spot the difference between hand-waving and proof'.

Hsiang replied at length in the same magazine, protesting against the use of a 'fake counter example'. Meanwhile Hales and others were themselves engaged in defining programmes for further work, as the explorer stocks supplies and makes sketch-maps for a hopeful expedition. Indeed he was already at base camp.

# A comment by Kantor on Hilbert's 18th problem

Hilbert's text gives the impression that he did not anticipate the success and the developments this problem would have.

The hexagonal packing in plane is the densest (proof by Thue in 1892, completed by Fejes in 1940). In space, the problem is still not solved. Although there is very recent progress by Hales. For spheres whose centres lie on a lattice, the problem is solved in up to eight dimensions. The subject has various ramifications: applications to the geometry of numbers, deep relations between coding theory and sphere-packing theory, the very rich geometry of the densest known lattices. (Kantor J M 1996 *Math. Intelligencer* Winter, p 27)

# 4.2 The programme of Thomas Hales

Mathematicians often speak of a 'programme' <sup>1</sup> upon whose construction they are engaged, and do not mean a computer *program*. Rather, it is a tactical plan designed to achieve some objective. Like mountaineers who wish to conquer Everest, they define in advance the route and various camps which must be established along the way. It is in this spirit that Thomas Hales has attacked the Kepler problem. He had established base camp when we set out to write this book. He had proved a number of intermediate results and felt that the summit could be reached.

Hales' programme was based on reducing the Kepler problem to certain *local* statements about packing. Earlier we pointed to the impossibility of packing regular tetrahedra (chapter 3), and saw the Kepler problem as one of 'frustration', for this reason. But this does not mean that the global packing problem cannot be reduced to a local one, in some more subtle sense.

Hales considers a *saturated* packing, which is an assembly of non-intersecting spheres where no further non-intersecting spheres can be added. He uses *shells*: local configurations made of a sphere and its surrounding neighbours. He calculates the local density and a *score*, this quantity is associated with the empty and occupied volume in the local packing around the sphere. The programme of Hales was to prove that all the possible local configurations have scores lower or equal than 8.0, that is, the one associated with Kepler's dense packing. This is enough to prove Kepler's conjecture.

Hales started the implementation of this programme around 1992. He soon proved that a large class of local packings score less than eight, but there remained a few local configurations for which this proof was extremely tricky. In spring 1998 one could read on his home-page on the Internet: 'When asked how long all this will take, I leave myself a year or two. But I hope these pages convince you that the end is in sight!'. He estimated that would take until year 2000 to finish the proof.

The main problem in this kind of proof is to find a good way to partition a packing into local configurations. This is a key issue: *how does one properly define 'shells' in the packing?* All the major breakthroughs in the history of the Kepler conjecture (including the Hsiang attempt) are associated with different ways of partitioning space. In particular, there are two natural ways to divide the space around a given sphere in a packing.

The first is the *Vorono' decomposition* (chapter 2). The Vorono' cell is a polyhedron, the interior of which consists of all points of the space which are closer to the centre of the given sphere than to any other. This was the kind of decomposition adopted by Fejes Tóth to reduce the Kepler problem to the 'determination of the minimum of a function of a finite number of variables'. But this method meets with difficulties for some local configurations, such as when a sphere is surrounded by 12 spheres with centres on the vertices of a regular

<sup>&</sup>lt;sup>1</sup> Only east of the Atlantic are there extra letters which maintain a useful distinction between these two spellings.



Figure 4.1. The assembly of 12 spheres around a central one in a pentahedral prism configuration.

icosahedron. In this case the local packing fraction associated with the Voronoi cell is  $\rho = 0.7547...$  which is bigger than the value of the Kepler packing ( $\rho = 0.7404...$ ) and its score is bigger than eight.

The second natural way of dividing space is the *Delaunay decomposition*. Here space is divided in Delaunay simplexes which are tetrahedra with vertices on the centres of the neighbouring spheres chosen in a way that no other spheres in the packing have centres within the circumsphere of a Delaunay simplex. The local configuration considered is now the union of the Delaunay tetrahedra with a common vertex in the centre of a given sphere (this is called the *Delaunay star*). This was the kind of decomposition first adopted by Hales in his programme. For instance, the Delaunay decomposition succeeds in the icosahedral case, giving a score of 7.999 98. But there exists at least one local configuration with a higher score. This is an assembly of 13 spheres around a central one, which is obtained by taking 12 spheres centred at the vertices of an icosahedron and distorting the arrangement by pressing the 13th sphere into one of the faces. This configuration scores 8.34 and has local packing fraction  $\rho = 0.7414$ . Another nasty configuration which has a score dangerously close to eight is the 'pentahedral prism'. This is an assembly of 12 spheres around a central one, shown in figure 4.1.

The Voronoï and Delaunay decompositions can be mixed in infinitely many ways. This is what Hales attempted by decomposing space in 'Q-systems' and associated stars. This decomposition was successful to establish the score of the pentahedral prism at 7.9997. However, new and nasty configurations remained to be considered....

# 4.3 At last?

On 10 August 1998, as one of the authors of this book was picking his fishing tackle out of the back of his car, his eye fell on a headline in a British newspaper. All thoughts of angling were dismissed for a while.

#### **KEPLER'S ORANGE STACKING PROBLEM QUASHED**

In a short report Simon Singh announced Thomas Hales' success, and quoted John Conway, a leading expert and mentor of Hales: 'For the last decade Hales's work on sphere packings has been painstaking and credible. If he says he's done it, then he's quite probably right'.

Back at the office an email message had been received, which must have disturbed quite a few other summer holidays as well.

From Thomas Hales Date: Sun, 9 Aug 1998 09:54:56 To: Subject: Kepler conjecture

Dear colleagues,

I have started to distribute copies of a series of papers giving a solution to the Kepler conjecture, the oldest problem in discrete geometry. These results are still preliminary in the sense that they have not been refereed and have not even been submitted for publication, but the proofs are to the best of my knowledge correct and complete.

Nearly four hundred years ago, Kepler asserted that no packing of congruent spheres can have a density greater than the density of the face-centred cubic packing. This assertion has come to be known as the Kepler conjecture. In 1900, Hilbert included the Kepler conjecture in his famous list of mathematical problems.

In a paper published last year in the journal 'Discrete and Computational Geometry', (DCG), I published a detailed plan describing how the Kepler conjecture might be proved. This approach differs significantly from earlier approaches to this problem by making extensive use of computers. (L. Fejes Toth was the first to suggest the use of computers.) The proof relies extensively on methods from the theory of global optimization, linear programming, and interval arithmetic.

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The full proof appears in a series of papers totalling well over 250 pages. The computer files containing the computer code and data files for combinatorics, interval arithmetic, and linear programs require over 3 gigabytes of space for storage.

Samuel P. Ferguson, who finished his Ph.D. last year at the University of Michigan under my direction, has contributed significantly to this project.

The papers containing the proof are:

An Overview of the Kepler Conjecture, Thomas C. Hales A Formulation of the Kepler Conjecture, Samuel P. Ferguson and Thomas C. Hales

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Sphere Packings I, Thomas C. Hales
(published in DCG, 1997)
Sphere Packings II, Thomas C. Hales
(published in DCG, 1997)
Sphere Packings III, Thomas C. Hales
Sphere Packings IV, Thomas C. Hales
Sphere Packings V, Samuel P. Ferguson
The Kepler Conjecture (Sphere Packings VI),
Thomas C. Hales
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Postscript versions of the papers and more information about this project can be found at

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http://www.math.lsa.umich.edu/~hales
```

Tom Hales

A month later, after Hales had enjoyed his own holiday, he kindly consented to answer a few emailed questions that might illuminate this account of his achievement. His answers were as follows, with some minor editing:

Date: Wed, 30 Sep 1998 08:42:12
From: Tom Hales
Reply-To: Tom Hales
To:
cc:
Subject: Re: your mail
> Dear Thomas
>

> - when were you first attracted to the problem?

In 1982, I took a course from John Conway on groups and geometry.

> - what was the hardest part?

The problem starts out as an optimization problem in an infinite number of variables. The original problem must be replaced by an optimization in a finite number of variables. It was extremely difficult to find a finite-dimensional formulation that was simple enough for computers to handle.

> - in what your method is different from the > previous approaches?

This approach makes extensive use of computers, especially interval arithmetic and linear programming methods. Most previous work was based on the Voronoi cells. This approach creates a hybrid of Voronoi cells and Delaunay simplices.

```
- did you follow the lead/style of anyone inparticular?
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My greatest source of inspiration on this problem was L. Fejes Toth. He was the first to propose an optimization problem in a finite number of variables and the first to propose the use of computers. But my proof differs from the program he originally proposed.

>	-	is it correct	to say that	this is a "trad	ditional"
>		proof with no	significant	elements of	
>		computer-based	l proof?		

Not at all. The computer calculations are an essential part of the proof.

> - what was your first reaction when Hsiang claimed > a proof?

I have followed his work closely from the very start. My doubts about his work go back to a long discussion we had in Princeton in 1990. I discuss my reaction to his work further in my Intelligencer article.

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> - have you always been confident in success?

In the fall of 1994, I found how to make the hybrid decompositions work, combining the Voronoi and Delaunay approaches. I have been optimistic since then.

> - your proof fill 10 papers and about 250 pages, > why does it need so much?

This is a constrained nonlinear optimization problem involving up to 150 variables with many local maxima that come uncomfortably close to the global maxima. Rigorous approaches to problems of this complexity as generally regarded as hopelessly difficult.

>	-	do you think that in the future a different	
>		approach might be able to reduce the size and	
> complexity of this proof?			

This is not an optimal proof. I have concrete ideas about how the proof might be simplified. Although I'm quite certain the proof can be simplified, it will require substantial research to carried this out. There could also be other proofs along completely different lines, but I do not have any definite ideas here.

>	-	can you calculate the maximum size of a cluster
>		of spheres with a given density
>		(larger than the Kepler one)?

This is an interesting question that a number of people would like to understand. I would be curious to know whether my methods might lead to something here.

As things stand in 2000, it would appear that the credit for solving this centuries-old question may well go to Hales. But only time (and much toil by colleagues) will yield the eventual guarantee of proof. Or will it start another chapter of debate?

# 4.4 Who cares?

This is a fair question, often addressed to startled scientists and mathematicians by puzzled journalists. Particularly in this case, why does proof matter, if we know the truth anyway?

One answer is that some people did admit to a tiny sliver of doubt insinuating itself into the certainty of their conviction. These were usually not physical scien-

tists, who would assert that if there was a better structure they would have spotted it by now, written somewhere in the book of nature. This may be insufficiently humble: surprises do occur from time to time, even in crystallography. They often result in Nobel Prizes. As Alfred North Whitehead said, 'in creative thought common sense is a bad master. Its sole criterion for judgement is that the new ideas shall look like the old ones, in other words it can only act by suppressing originality.'

Another answer is that mathematicians have to prove things, as birds fly and fish swim. It is silly to ask why, since it is in the very nature of their profession to create these elegant cultural artefacts. It is not that mathematics consists entirely of theorems. There is a rough texture of conjecture and useful approximation, held up here and there by a rigorous proof, serving the same purpose as the concrete framework of a building. The more of these the better, to stop the whole thing collapsing under the weight of loose speculation.

Rigorous proofs and exact results are like the gold bars in the vaults of the Federal Reserve, guaranteeing the otherwise unreliable monetary transactions of the world. They are apparently useless since they are not put to any direct use, and yet they have real value. (Since the first draft of this book was written there has been much debate on the abandonment of gold reserves, so the simile may soon be a feeble one. The value of a proof is more durable.)

# 4.5 The problem of proof

In 1967 the announcement in the *New York Times* of a computer proof of the fourcolour conjecture by Kenneth Appel and Wolfgang Haken sparked off a lively debate on the acceptability of such methods. Thirty years on they are much less controversial, as we continue to accommodate ourselves to the ever greater role of computers in our lives. It would be more provocative to debate, say, the limits of artificial intelligence or the possibilities of computer consciousness than to dispute the validity of computer proofs. Nevertheless, since we have encountered them in packing theorems, particularly in the work of Hales, let us rehearse the arguments as presented by, for example, Davis and Hersh in *The Mathematical Experience* (1981).

The traditional view has held that it must be possible to check every step in a proof, in order for it to be acceptable. In some cases, such as that of the proof of Fermat's last theorem by Wiles, few will ever be able to accomplish this. Those that do so (who may include the referees for publication, if they are conscientious) will be the guarantors upon which the rest of us can rely. But modern computer proofs generate such a multitude of logical operations within the machine that it is beyond any human capacity to follow them, even if they are made manifest.

There is no getting away from the necessity to rely on the correct functioning of the machine and its software, in response to the programmer's instructions. They can be checked only at the level of programming, or in terms of the repro-

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ducibility of the result on a quite different machine, rather as some experimental results are tested. If these precautions are taken, today's generation is quite happy to accord the same status to the proof as in days of old. They will say: There was always a tiny element of uncertainty in any elaborate traditional proof. Human beings are susceptible to error, as are computers. Rather more so, perhaps?

Some of us would still sigh. We point to economy, elegance and transparency as cardinal virtues of a *good* mathematical proof, award low scores to the new methodology on those criteria, and call for renewed efforts to be more explicit<sup>2</sup>.

# 4.6 The power of thought

In one of many important articles on polyhedra and packings, the eminent Canadian mathematician H S M Coxeter chose to begin with a poem by Charles Mackay:

Cannonballs may aid the truth, But thought's a weapon stronger, We'll win our battles by its aid; Wait a little longer.

To this we might add a verse to bring it up to date:

If you fail to reach your end, your siege has come to nought, call on your electronic friend, to spare a microsecond's thought.

Whether computers can really 'think' is a deeper problem than the merely technical one of proof-checking. We may someday accept an even stranger role for these machines in mathematics. Will they write books as well?

 $<sup>^2</sup>$  For a further exploration of this ongoing debate, see the article by: Horgan J 1993 The death of proof *Sci. Am.* October 75, and the responses and discussion that followed in later issues.

# Peas and pips

# 5.1 Vegetable staticks

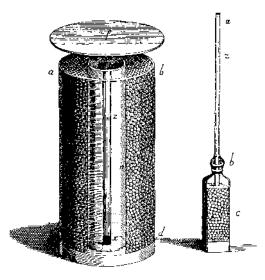
When soft objects are tightly packed, they change their shapes to eliminate the wasted interstitial space. Even if they begin as spheres they will develop into polyhedra. The question is: *which types of polyhedra will be formed?* The formation of foam by bubbles is an example of such a process; another is to be found in the familiar insulating material of polystyrene, formed by causing small spheres to expand and fill a mould. But the most famous early experiment was carried out with peas.

The Reverend Stephen Hales performed this classic experiment, in an age when science was practiced as much in the parlour or the kitchen as in the laboratory. Hales compressed a large quantity of peas (or rather expanded them under pressure by absorption of water) and described what he observed in a book with the charming title of *Vegetable Staticks*.

I compressed several fresh parcels of Pease in the same Pot, with a force equal to 1600, 800, and 400 pounds; in which Experiments, tho' the Pease dilated, yet they did not raise the lever, because what they increased in bulk was, by great incumbent weight, pressed into the interstices of the Pease, which they adequately filled up, being thereby formed into pretty regular Dodecahedrons<sup>1</sup>.

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<sup>&</sup>lt;sup>1</sup> Published in 1727 by Stephen Hales, with the title 'Vegetable Staticks: or An Account of some Statistical Experiments on the Sap Vegetables: being an essay towards a Natural History of Vegetation. Also, a Specimen of An Attempt to Analyse the Air, By great Variety of Chymio-Statical Experiments; Which were read at several Meetings before the Royal Society' and dedicated to His Royal Highness George Prince of Wales.



**Figure 5.1.** The experimental apparatus used by Hales to demonstrate the force exerted by dilating peas. When the lid was loaded with a weight, the dilated peas fill the interstices, developing polyhedral forms.

At this point the reverend gentleman's report is misleading. We will see later in this chapter that when soft objects are closely packed in a disordered fashion, they form polyhedral grains with irregular shapes. Only a few of them have 12 faces. Moreover, regular dodecahedral cells<sup>2</sup> cannot fill three-dimensional space, so Hales purported to observe something which is plainly impossible. But this mistake probably has a simple explanation: in such packings the majority of faces are pentagons and the dodecahedron is the regular solid made with pentagonal faces. The history of science is full of such cases in which the observer tries to draw a neat conclusion from complex and variable data. Too determined a search for a simple conclusion can lead to an erroneously idealized one.

Rob Kusner (a mathematician currently at the University of Massachusetts at Amherst) tells us that a modern version of Hales' experiment with peas was carried out in New England a few summers ago by a group of undergraduates using water-balloons, greased with vegetable oil and stuffed into a large chest freezer. Some balloons burst from being pierced by sharp ice crystals, and others did not freeze, but it was still possible to see the packing patterns since the low temperature folding on the balloon rubber left permanent marking (lighter colour) at the folds.

 $<sup>\</sup>overline{}^2$  The reader unfamiliar with their polyhedra should turn to figure 5.6.

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Figure 5.2. Stephen Hales (1677–1761).

# 5.2 Stephen Hales

At first sight, the pea-packing experiments of Stephen Hales might seem to be the dabblings of a dilettante. Not so. Hales was a significant figure in the rapid development of science after Newton. He is much mentioned, for example, in the work of Lavoisier, and has been the subject of several biographies and many portraits.

Belonging to the gentry of the south of England, he had no difficulty in gaining access to undemanding positions as a clergyman, many of which were in the gift of members of his class. The research that he carried out over many years forms part of the foundation of today's science of the physiology of plants and animals—the study of function as opposed to mere form, as in anatomy and taxonomy. He was also something of a technologist, being credited with the invention of forced ventilation. It has not always been self-evident that fresh air is good for us! The navy, in particular, enthusiastically adopted his recommendations in an attempt to improve the health of sailors.

It was in a physiological spirit that Hales performed his experiment with dried peas. The pressure associated with their uptake of water was at issue: what we would today call 'osmotic pressure'. The fact that the peas, swelling while under pressure, were compressed into polyhedral forms, was really incidental. This may be offered as an excuse for the unfortunate inaccuracy of Hales' description of their polyhedral form.

It would be pleasing to establish some family connection between this man and his modern namesake (chapter 4). Alas, Thomas Hales reports that none has been established, and reminds us that Stephen died without issue.

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# 5.3 Pomegranate pips

About one century before Hales, Kepler had studied the shape of the pips inside a pomegranate. These seeds are soft juicy grains with polyhedral shapes. Kepler was trying to understand the origin of the hexagonal shapes of snowflakes, so the pomegranate grains were used as an example of the spontaneous formation of regular geometrical polyhedral shapes in a packing. Kepler observed that these grains have rhomboidal faces and he remembered that the same rhomboidal faces are present in the bottom of bees' cells and make up the interface between the two opposite layers of cells in the honeycomb (see chapter 6).

Attracted by these rhombes, I started to search in the geometry if a body similar to the five regular solids and to the fourteen Archimedean could have been constituted uniquely of rhombes. I found two (...). The first is constituted of twelve rhombes, (...) this geometrical figure, the closest possible to the regularity, fill the solid space, as the hexagon, the square and the triangle fill the plane.

(...) if one opens a rather large-sized pomegranate, one will see most of its loculi squeezed into the same shape, unless they are impeded by the peduncles that take food to them.

(...) What agent creates the rhomboid shape in the cells of the honeycomb and in the loculi of the pomegranate?

Kepler argues that the key to the honeycomb and pomegranate is the problem of packing equal-sized spherical objects into the smallest possible space; and he finds the answer in a conjecture for the closest sphere packing (chapter 3). Indeed, if one takes this packing and expands the spheres, grains with 12 rhombic faces are obtained.

Kepler carefully warns the readers that one must take a 'rather large-sized pomegranate' to find many rhombohedral grains inside. Indeed, in a typical pomegranate the rhombohedral grain shape is not so common. The packing is not so perfect and the grains take different shapes. Just like Stephen Hales, Kepler was oversimplifying his conclusions.

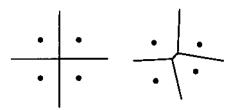
# 5.4 The improbable seed

An example will be useful to show why the shape observed by Kepler in the pomegranate seeds is quite unusual in disordered packings.

Take a world atlas and put your finger on a continent, then follow the border between two states. This line follows mountains, rivers or other features for geological or historical reasons. The set of states in the continent can be seen as a two-dimensional packing, or a jigsaw puzzle, where each state is a tile with an irregular complex shape different from the others. These tiles fit perfectly together filling the continent without leaving any empty space. This is an irregular packing



Figure 5.3. A pomegranate.



**Figure 5.4.** Voronoï partitions are made here from four points in the plane. The whole space is subdivided into four domains which are the regions of space closest to each point. The full lines mark the boundary between these four domains. These lines intersect in one common four-connected vertex only when the points are symmetrically placed on the vertices of a rectangle. Any other configuration generates a couple of three-connected vertices.

of very different elements but with an important common property: everywhere *only three states meet in a common vertex*. In other words, in such a packing the *vertex connectivity* is equal to three. This is true all around the world for national states or provinces, with—as for any good rule—at least one exception that we will leave the reader to find in the world atlas.

If there is no special symmetry, the threefold vertex is the type of intersection that is automatically generated in two-dimensional space-filling packings. Consider, for example, four cells in a Voronoï partition as shown in figure 5.4. The cells meet at the same four-connected vertex only in the case when the centres of the cells are on the vertices of a rectangle; in all the other—infinite—possibilities the cells meet on two three-connected vertices. Only an infinitesimal displacement of the original points of the Voronoï construction is needed to split the four-

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fold vertex into two threefold ones.

Patterns with vertex connectivity three are not only found in the political division of territory but are also present in a very large class of natural packings and patterns. Some examples are given in figure 5.5.

In three dimensions the most probable configuration has four cells that meet at a common vertex. This is the minimal vertex connectivity and—again—configurations with higher connectivity can be split into two or more minimally connected ones by infinitesimal rearrangements.

The Kepler rhombic dodecahedra pack together in such a way as to produce vertices of connectivity six. This is therefore an improbable configuration and it will not be naturally formed in disordered packings. A Voronoï partition from the centres of the spheres in the Kepler packing generates a space-filling assembly of rhomboid dodecahedra, but when the position of the spheres is slightly deformed by infinitesimal displacements the vertex connectivity becomes four and the average number of faces in the Voronoï cells increases to a value of around 14.

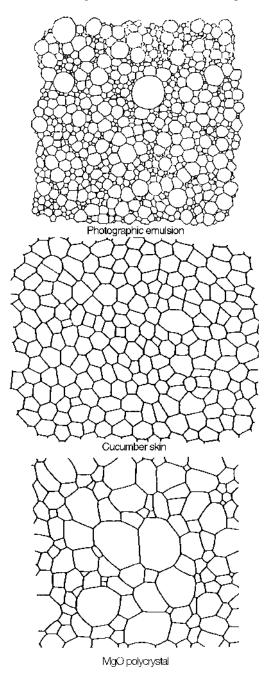
# 5.5 Biological cells, lead shot and soap bubbles

From the beginning of microscopy, anatomists were impressed by the similarities between the shape of biological cells in undifferentiated tissues and that of bubbles in foam. Robert Hooke includes in his *Micrographia* (1665) an observation on the 'Schematism or Texture of Cork, and the Cells and Pores of some other such frothy Bodies' and describes the pith of a plant as 'congeries of very small bubbles'. For centuries, with almost no exceptions, cells in undifferentiated tissues were described as regular dodecahedra (the impossible peas of Hales) or as rhombic dodecahedra (the improbable pomegranate seed of Kepler). Then, at the end of the 19th century a new type of cell with 14 faces emerged. It was the *tetrakaidecahedron*, a polyhedron that Lord Kelvin proposed in 1887 as the structure that divides space 'with minimum partitional area'. (We will follow Kelvin's line of thought in chapter 7.)

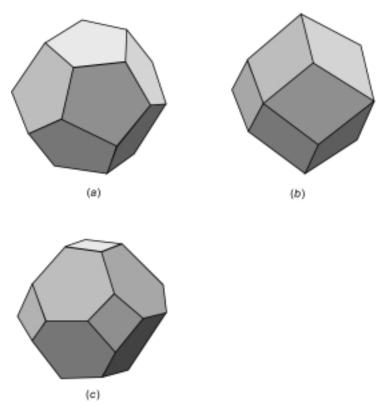
It was only at the beginning of this century that careful and extensive studies of the shape of bubbles in foams and cells in tissues were undertaken. In particular, a large series of biological tissues was meticulously studied by F T Lewis of Harvard University between 1923 and 1950<sup>3</sup>. He concluded that cells in undifferentiated tissues have polyhedral shapes with about 14 faces on average and he inferred that they tend to be approximated by Kelvin's ideal polyhedron. Further investigation now indicates that the cells have about 14 faces on average but a large variety of shapes contribute to form the cellular structure. The Kelvin polyhedron is rarely observed<sup>4</sup>.

<sup>&</sup>lt;sup>3</sup> See, for example, Lewis F T 1950 Reciprocal cell division in epidermal and subepidermal cells *Am. J. Bot.* **37** 715–21.

<sup>&</sup>lt;sup>4</sup> Dormer K J 1980 Fundamental Tissue Geometry for Biologists (Cambridge: Cambridge University Press).



**Figure 5.5.** Two-dimensional cellular patterns (from Weaire D and Rivier N 1984 Soap, cells and statistics—random patterns in two dimensions *Contemp. Phys.* **25** 59).



**Figure 5.6.** A pentagonal dodecahedron (a); a rhombic dodecahedron (b) and a tetrakaidecahedron (c).

The experimental study of the form of biological cells inspired experiments in which cellular structures were created by compressing together soft spheres to fill all the space (as Reverend Hales did with peas). In this way, the resulting structure can be disassembled and the shapes of the individual cells easily studied. A classical experiment of this kind is the one by Marvin<sup>5</sup>, who compressed 730 pellets of lead shot in a steel cylinder. When the spheres are carefully packed layer by layer in the closest way, then—not surprisingly—the cells take Kepler's rhombic dodecahedral shape. Totally different shapes are observed when the spheres are packed in a disordered way, for instance by putting the shot in the container at random or by shaking it before compression. In this case, the cellular structures have polyhedral cells with faces that vary from triangles to octagons with the great majority being pentagons and, less abundantly, squares and hexagons. The average number of neighbours was reported to be 14.17 in a set of 624 internal lead

 $<sup>^5</sup>$  Marvin J W 1939 The shape of compressed lead shot and its relation to cell shape Am. J. Bot. **26** 280–8.

pellets. No Kepler cells were observed in these experiments.

One may look for similar structures in deformed bubbles of foam, but looking at bubbles inside a foam is quite difficult, if we wish to observe the properties of *internal* bubbles. In 1946, Matzke<sup>6</sup> reported the study of the shapes of 600 central cells (which he claimed to be of equal volume) in a soap froth. This research is still the most extensive study of the structure of foam bubbles up to the present time. He found an average number of faces per bubble of 13.7 and a predominance of pentagonal faces, with 99.6% of all faces being either quadrilateral, pentagonal or hexagonal. Kepler's cell never appeared, nor was that of Kelvin observed. This disappointing tale is told in more detail in chapter 7.

Biological cells, peas, lead shot and soap bubbles are quite different systems, although all consist of polyhedral cells packed together to fill the whole space. A biological tissue is generated by growth and mitosis (division) of cells. The shape of a cell is therefore continuously changing following the mitotic cycle. In contrast to this, when lead shot is compressed the shapes of the cells are mostly determined by the environment of the packed spheres. Indeed, during the compression, rearrangements are very rare. In foams the structure is strictly related to the interfacial energy and bubbles assume shapes that minimize the global surface area. The great similarity in the polyhedral shapes of the cells in these very different systems can therefore be attributed only to the inescapable geometrical condition of filling space.

<sup>&</sup>lt;sup>6</sup> Matzke E B 1946 The three-dimensional shape of bubbles in foam—an analysis of the role of surface forces in three-dimensional cell shape determination *Am. J. Bot.* **33** 58–80.

# **Enthusiastic admiration: the honeycomb**

# 6.1 The honeycomb problem

We have encountered various cases of *cellular structures*, which divide space into cells. How can this be done most economically, in terms of the surface area of the cells? It is not clear that this has any relevance to the squashed peas of Hales or the lead shot of Marvin, but it certainly is the guiding principle for foams (the subject of the next chapter), for which the cell interfaces cost energy. The bubble packing which we call a foam is not alone in minimizing surface area. Emulsions, such as that of oil and vinegar shaken to make a salad dressing, conform to the same principle.

For centuries this principle has also been supposed to govern the construction of the honeycomb by the bee. The bee, it has been said, needs to make an array of equal cells in two dimensions, using a minimum of wax, and hence requires a pattern with the *minimum perimeter per cell*.

Although the perfection of the honeycomb is a very proper object for admiration, it may be naive to impute to the bee the single mathematical motive of saving of wax, just as it can hardly be said that the greengrocer cares much about the maximum density of oranges. There really aren't many reasonable alternatives to the two-dimensional hexagonal structure for the honeycomb. Other considerations surely impose themselves, such as simplicity and mechanical stability, in the evolutionary optimization of the hive.

A full account of the arguments that have raged over the shape of the bee's cell would read like a history of Western thought. We can find one of the first attempts at an explanation in Pliny (*Naturalis Historia*) who associated the hexago-

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Figure 6.1. The Hungarian mathematician L Fejes Tóth has been a leader in the mathematics of packings for many years, and his son G Fejes Tóth now follows in his footsteps.

nal shape of the cell with the fact that bees have six legs. Among the other notable minds that have been brought to bear on it, we must count at least those of: Pappus of Alexandria (*Fifth Book*), Buffon (*Histoire Naturelle*), Kepler, Koenig, Maraldi, Réamur, Lord Brougham, Maurice Maeterlinck (*La Vie des Abeilles*), Samuel Haughton, Colin MacLaurin, Jules Michelet (*L'insecte*), and Charles Darwin (*The Origin of Species*). 'He must be a dull man' said Darwin, who could contemplate this subject 'without enthusiastic admiration'. Not surprisingly, he attributed 'the most wonderful of all known instincts' to 'numerous, successive, slight modifications of simpler instincts'.

Darwin's account of the process by which the honeybee achieves its precise constructions, by forming rough walls and refining them, is instructive, but he is not quite correct in saying that 'they are absolutely perfect in economizing wax' as we shall shortly see, when we turn to the three-dimensional aspect of the hive, that is, the structure of the interface between the two opposed honeycombs. For the moment we address only its two-dimensional aspect, the arrangement of the elongated cells which is visible on the surface. Does this two-dimensional pattern of cells of equal area have the least possible perimeter?

Of course it does: it is well known that this pattern is the best. What has remained hidden from general appreciation is that this proposition has not until now been fully proved! This was rarely stated, probably because most authors cannot believe there is no proof hidden somewhere in the unfathomable depths of the technical literature. We saw in chapter 2 that a proof exists for the closely related problem of optimal packing of equal discs, but this should not be confused with the question posed by the honeybee.

This should take its rightful place alongside Kepler's problem as a notable frustration for the mathematician, both in the personal sense and in the technical one (a circle being the best form for a single cell if we ignore the rest). Frank

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Morgan has drawn attention to the problem<sup>1</sup>.

There does exist a proof of a lesser theorem, once again attributed to Fejes Tóth. It imposes certain restrictions, of which the most important is the requirement that all the sides of the cells are straight. This follows from the convexity principle which was described in chapter 2. But in general it is very natural for them to be curved, so this is a much weaker result than one would like.

At the time of writing, Thomas Hales has informally announced that he will shortly publish such a full proof. If confirmed this will complete, together with his analysis of the Kepler conjecture (chapter 4), a remarkable double.

```
Date: Mon, 7 Jun 1999 12:37:27 -0400 (EDT)
From: Tom Hales
To: Denis Weaire
cc:
Subject: honeycombs
```

Dear Denis Weaire,

If all goes well, I'll announce a solution to the honeycomb conjecture in a few days. (I don't make any assumptions about the convexity or topology of the cells.) I've shown it to Frank Morgan and John Sullivan, and they didn't find any obvious problems with my proof.

I hope you don't mind that in my acknowledgements, I quote from your email message to me from October, 'Given its celebrated history, it seems worth a try...'. Thanks for attracting my attention to the problem.

Of course, I'm fascinated by the Kelvin problem too, but I don't think that will be solved anytime soon...

Best,

Tom

# 6.2 What the bees do not know

As we have warned, it turns out that bees (even Hungarian ones) are not so smart after all, when the three-dimensional aspect of their construction is considered.

<sup>&</sup>lt;sup>1</sup> Morgan F 1999 The hexagonal honeycomb conjecture *Trans. Am. Math. Soc.* **351** 1733. See also Morgan F 2000 *Geometric Measure Theory: A Beginners Guide, 3rd Edition* (New York: Academic).

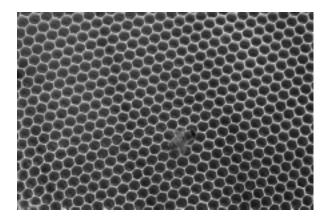


Figure 6.2. The beehive.

The enthusiastic admiration of the scientific community for the pattern of the beehive has often extended to the *internal* structure of the honeycomb. It has two sides from which access is possible, with a partition wall in the middle.

A flat wall would be wasteful of wax. Instead the bee chooses a faceted wall which neatly fits the two halves of the honeycomb, when the cells are staggered with respect to each other. The edges of the facets meet each other and the side walls of the hexagonal cells at the same angle (the Maraldi angle) of approximately 109° that, as we will see in the next chapter, Plateau recognized in foams as a consequence of the minimization of surface energy. So the parsimony of the bee apparently extends even to this internal structure. (Nowadays the bee has no real choice, since the wall is provided by the keeper as a preformed 'foundation'.)

There is a close connection between this strategy and the successive optimal stacking of close-packed planes of spheres. The Voronoï construction (section 2.5) applied to two such layers gives, for the partition between them, precisely the form of the bee's wall.

Indeed, the bee's faceted wall can be shown to minimize area and hence the expenditure of wax, in the limited sense that any small change will increase the area. The occurrence of the Maraldi angle signals this: indeed it gained its name in this context.

Learned academies have sung the praises of the bees for basing their construction on the Maraldi angle and, in so doing, have exaggerated its precision. This has caused some speculation as to whether the Almighty has endowed these creatures with an understanding of advanced mathematics.

The whole story is told in detail in D'A W Thompson's *On Growth and Form*<sup>2</sup>. Dismissing earlier follies (including Darwin's) he is driven to the extreme conclusion that 'the bee makes no economies; and whatever economies lie in the

<sup>&</sup>lt;sup>2</sup> Thomson D'A W 1942 On Growth and Form 2nd edn (Cambridge).

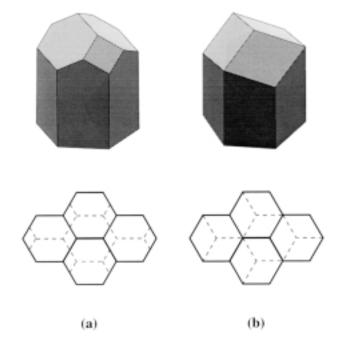


Figure 6.3. The alternative of Fejes Tóth (a) to the bee's design (b).

theoretical construction, the bee's handiwork is not fine or accurate enough to take advantage of them'. Where Darwin had invoked slow changes in response to a marginal advantage of design, Thompson looked for physical forces at work, supposing the thin wax film of the hive to be more or less fluid at the same time in their construction, and so forming the angles dictated by surface tension.

Where precisely the truth lies in this old and muddled dispute about angles we do not know, but Thompson would clearly have been delighted to learn of Fejes Tóth's startling conclusion, many years later: there is an entirely different arrangement which is better than the design of the bee! This was published in a charming paper entitled 'What the Bees Know and What They Do Not Know'<sup>3</sup>.

The bee's design can be improved, with a saving of 0.4% of the surface area of the wall, by using a different arrangement of facets, again constructed with the angles dictated by surface tension. The alternative presented by Fejes Tóth is shown in figure 6.3 and is closely related to the Kelvin structure described in chapter 7.

Bees do sometimes create the Hungarian mathematician's design locally, whenever they are left to build the wall themselves, and then make a mistake, so that the two parts of the honeycomb are misaligned.

<sup>&</sup>lt;sup>3</sup> Fejes Tóth L 1964 Bull. Am. Math. Soc. **70** 468–81.

# Toils and troubles with bubbles

# 7.1 Playing with bubbles

Foams and bubbles have fascinated scientists of all ages, in all ages. Most have devoted some time to admiration of what Robert Boyle called 'the soap bubbles that boys are wont to play with'. Part of their charm and mystery lies in the colours produced by the interference of light in thin films. Small clusters of bubbles, or the extended ones we call foams, have elegant structures which call for explanation.

The poet and philosopher may point to the ephemeral nature of these things as a metaphor for our own mortality or the transience of fame and fortune, but the first interest of the scientist is in making relatively stable foams. This is not difficult with a little ordinary detergent solution shaken in a sealed container. Looking into it, one can see that, though disordered, it shows clear evidence of some principles of equilibrium at work. What are they?

When spherical bubbles pack together to form a foam (as when they rise out of a glass of beer) they are forced into polyhedral shapes as gravity extracts most of the liquid from their interstices. What began as a sphere packing, in conformity to the rules of previous chapter, now presents a different paradigm for pattern in nature. In this case the density is fixed and surface area is to be minimized<sup>1</sup>.

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<sup>&</sup>lt;sup>1</sup> See for general reference: Sadoc J F and Rivier N (ed) 1999 *Foams and Emulsions* (Dordrecht: Kluwer); Ball P 1999 *The Self-made Tapestry: Pattern Formation in Nature* (Oxford: Oxford University Press); Hildebrandt S and Tromba A 1996 *The Parsimonious Universe* (Berlin: Springer).



Figure 7.1. Playing with soap bubbles.

# 7.2 A blind man in the kingdom of the sighted

The man who most clearly saw the principles of bubble-packing was blind. Joseph Antoine Ferdinand Plateau caused irrecoverable damage to his eyes by staring at the sun in an experiment on the retention of vision. The 1999 eclipse brought many public reminders of the extreme danger of doing so. He began to go blind in 1841 and had lost all vision by 1844.

Michael Faraday wrote consolingly and prophetically to him:

Well may you and your friends rejoice that though, in the body, you have met with a heavy blow and great discouragement, still the spirit makes great compensation, and shines with glorious light across the bodily darkness.

Today Plateau is remembered for his later researches, undertaken with the help of family, friends and students, leading to his great work *Statique experimentale et théorique des liquides soumis aux seules forces moléculaires* (1873).

As a hero of Belgian science, he was elevated to the rank of 'Chevalier' in the Order of Léopold. His extraordinary dedication to science did not preclude a happy family life but he was often preoccupied. It is recorded that he disappeared for six hours while on honeymoon in Paris, returning eventually to his distraught bride, to say that he had forgotten that he had just been married. A similar case is to be found in the Irish mathematician George Gabriel Stokes, whose love-letters contained too much mathematical physics to be fully effective.

At the heart of Plateau's classic text were those experiments with wire frames dipped in soap solution which are still commonly used in lecture demonstrations. They were popularized as such by C V Boys in his *Soap-Bubbles, their Colours and the Forces which mould them, being the substance of many lectures delivered to juvenile and popular audiences*, published by the Society for Promoting Chris-



Figure 7.2. A Plateau frame.

tian Knowledge in 1911<sup>2</sup>. The tradition of Plateau's experiments continues today in the hands of Cyril Isenberg<sup>3</sup> and others, and one can purchase the frames at modest cost from Beevers Molecular Models.

Plateau's book was well received. J C Maxwell reviewed it in *Nature*, first asking ironically—*Can the poetry of bubbles survive this?*—then replying with this encomium:

Which, now, is the more poetical idea—the Etruscan boy blowing bubbles for himself, or the blind man of science teaching his friends to blow them, and making out by a tedious process of question and answer the condition of the forms and tints which he can never see?

The meaning of the book's title is not self-evident. It may be taken to mean *the laws of equilibrium of liquids under surface tension, when gravity is negligible.* Or, plainly put, *what are the shapes and connections of soap films?* 

Plateau's laws which answer this question are as follows:

- (1) Films can only meet three at a time and they do so symmetrically, so that the angles between them are  $120^{\circ}$ .
- (2) The lines along which they meet are themselves joined in vertices at which only four lines (or six films) can meet. Again they are symmetric, so that the angle between the lines has the value cos<sup>-1</sup>(-<sup>1</sup>/<sub>3</sub>) or approximately 109° (the tetrahedral, or Maraldi, angle).
- (3) The films and the lines are curved in general: the average amount by which the films are bowed in or out is determined by the difference in pressure between the gas on either side (Laplace's law).

Note that the third law does not dictate that a zero pressure difference implies a flat film. Saddle-shaped surfaces can have zero mean curvature.

<sup>&</sup>lt;sup>2</sup> A later edition is Boys C V 1959 Soap Bubbles (New York: Dover).

<sup>&</sup>lt;sup>3</sup> Isenberg C 1992 The Science of Soap Films and Soap Bubbles (New York: Dover).

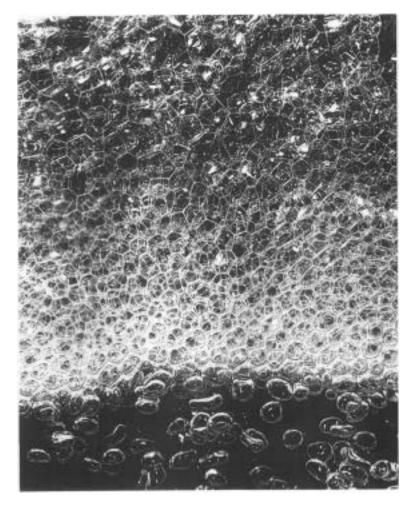


Figure 7.3. Soap foam (courtesy of J Cilliers, UMIST).

If soap films are trapped between two glass plates in order to create a twodimensional structure, only first and third laws are needed.

These laws were inspired by observation, but most of them are easily rationalized by theory. Soap films have energies proportional to their surface area, and they therefore tend to contract and pull with a force (the surface tension) on their boundaries. Plateau's laws express the conditions for stable equilibrium of these forces and the gas pressures which act on the films.

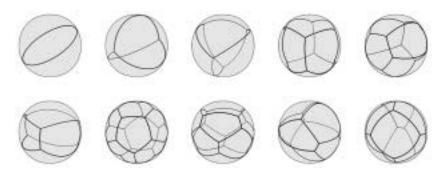


Figure 7.4. Different equilibrium vertex configurations, in terms of geodesics. (Redrawn from Almgren F Jr and Taylor J 1976 *Sci. Am.* 235 82–93.)

#### 7.3 Proving Plateau

Although he was not averse to mathematical analysis, Joseph Plateau's essential method was that of generalization from observation—he was content to leave it to others to find theoretical justifications of his laws.

Ernest Lamarle, a Belgian mathematician who was expert in differential geometry, provided some of this mathematical underpinning in the 1860s. He showed that the principle of minimal area implied everything that Plateau had reported. In particular he gave a justification of the rule that states that only four soap films can meet at a point. A foam cannot have stable vertices formed by more than this number of films.

The proof runs to many pages. It begins with the classification of every possible form of vertex, consistent with the balance of the surface tension forces acting in the adjoining films. This in itself does not guarantee stability: most of these turn out to be unstable equilibria.

One might expect to encounter a great difficulty at this point, if there are infinitely many possibilities for such a vertex. But it turns out that there are only a few.

A small sphere centred on the vertex must have intersections with the soap films which form a pattern on its surface as follows:

- (1) The lines are geodesics: that is, each lies in a plane which cuts the sphere in half.
- (2) The lines intersect at  $120^{\circ}$ , three at a time.

The possible patterns of this type are highly reminiscent of the earliest stages in embryonic development.

Lamarle proceeded to devise ways in which each of the more complicated vertices could be deformed and dissociated into combinations of the elementary one, while lowering the total surface area. These define modes of instability of the vertex, hence disqualifying it as a possible stable configuration.

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For serious mathematicians, the story does not end here. In particular, it reappeared on the agenda of Fred Almgren, 100 years after Lamarle.

Just as Lamarle had performed, at one level, a clean-up operation on Plateau's arguments, so Fred Almgren set out to perfect the proofs of Lamarle and others in the study of minimal surfaces<sup>4</sup>. Their work contained hidden or explicit assumptions of smoothness in the minimal structures that they purported to describe.

Mathematicians can conceive all sorts of strange entities with surfaces which are the opposite of smooth—not just rough, but perhaps infinitely so. In recent years Benoit Mandelbrot has taught us that these monstrous constructions are not really alien to our world. Previously, we have projected on to nature a vision of rounded smoothness and continuity which is only one extreme of reality. Much of nature is better described as rough and ragged, jagged and jerky. The romantic landscapes and seascapes, which are the subject of so much of our art, display such fractal forms, but scientists somehow ignored them for rather too long. Cyril Stanley Smith (chapter 14) was a rare exception. He complained that 'scientists have tended to overlook the form of the world and concentrate on forces', and attacked the smooth, periodic idealizations of material science in his time.

This said, it can hardly be maintained that much real doubt should be entertained about the assumption of smoothness in the particular case of soap films. Almgren's quest was for completeness and rigour, to eliminate nasty possibilities, however hypothetical, from the proof. Much of his fastidious work in this vein over a 35-year career at Princeton was compiled in a 1720-page paper, unpublished at the time of his death in 1997.

Another part of Almgren's legacy is to be found in successive generations of graduate students. One of these was Jean Taylor, who became his wife. It fell to her to construct the new version of Lamarle's proof, which she published in 1976<sup>5</sup>. It is of comparable length to the 19th century paper, but couched in the inscrutable language of geometric measure theory.

Almgren and his successors have leavened their rather impenetrable studies with a lively sense of the more accessible and practical facets of their subject. In particular, Ken Brakke emerged from that school to write the Surface Evolver software, the fruits of which we will see later in this chapter.

<sup>&</sup>lt;sup>4</sup> Almgren F Jr 1976 Existence and regularity almost everywhere of solutions to elliptic variational problems with constraints *Mem. Am. Math. Soc.* 165; Almgren F Jr and Taylor J 1976 *Sci. Am.* **235** 82–93.

<sup>&</sup>lt;sup>5</sup> Taylor J 1976 The structure of singularities in soap bubbles-like and soap-film-like minimal surfaces *Ann. Math.* **103** 489–539.

#### **Minimal surfaces**

The theory of minimal surfaces has continued to be an active focus of research in this century. Several Fields Medals (a particularly prestigious mathematical prize) have acknowledged great achievements in that area. In particular, Jesse Douglas received the first medal in 1936 for his contribution to the 'Plateau problem', which is concerned with a single soap film spanning a loop of wire of arbitrary shape.

#### 7.4 Foam and ether

Plateau's rules apply to any foam in equilibrium. They place restrictions on, but do not define in full, the answer to our question: *which structure is best?* This we have already answered for two dimensions; and, indeed, experiments with foams of equal bubbles do reproduce the honeycomb.

But just as ball bearings are uncooperative in the search for ideal structures, so are soap bubbles in three dimensions. A foam of equal-sized bubbles remains disordered, in practice. This did not stop Sir William Thomson (later Lord Kelvin) attacking the theoretical problem of the ideal ordered foam, in 1887. Indeed he does not seem to have tried to make such a 'monodisperse' foam, despite his credo (stated later) that theory must be anchored in reality.

At that time Kelvin was the pre-eminent, if ageing, figure of British science. He still had a strong appetite for scientific endeavour—in the end he published over 600 papers, a score worthy of the most competitive (and repetitive) of today's careerists. They stretch across the spectrum of physics from telegraphy and electrical technology to the second law of thermodynamics, for which we honour his name in the scientific unit of temperature. Quite a man.

#### Ether

Apollonius of Tyana is said to have asked the Brahmins of what they supposed the cosmos to be composed.

'Of the five elements'.

'How can there be a fifth' demanded Apollonius 'beside water and air and earth and fire?'

'There is the ether' replied the Brahmin 'which we must regard as the element of which the gods are made; for just as all mortal creatures inhale the air, so do immortal and divine natures inhale the ether.' (From Sir Oliver Lodge 1925 *Ether and Reality* (London: Hodder and Stoughton) p 35.)



Figure 7.5. Sir William Thomson (Lord Kelvin) (1824–1907).

One of the great quests of Victorian science was the search for a physical model for light waves. In the centuries-old debate between the advocates of particle and wave interpretations of light, the wave enthusiasts had gained the upper hand by the middle of the 19th century. It remained to specify the substance—the ether—the vibrations of which, like those of sound in air, constituted the light waves. We have already encountered the fanciful ideas of Osborne Reynolds, concerning the nature of the ether (chapter 3). The word itself came down to us from the Greeks, for whom it represented a fiery heaven into which souls were received.

British natural philosophers were determinedly realistic in their outlook, always trying to relate the world of microscopic and invisible phenomena to everyday experience. This may be the reason that neither relativity nor quantum mechanics, both of which conflict with everyday experience, can be listed among the achievements of that school.

Lord Kelvin, together with P G Tait, wrote in the preface to their textbook:

Nothing can be more fatal to progress than too confident reliance on mathematical symbols; for the student is only too apt to take the easier course, and consider the *formula* and not the *fact* as the physical reality.

In common with others, Kelvin was not easily impressed by formalism and abstraction, despite being a first-rate mathematician. He did not even join the growing band of Maxwellians who fully accepted the theory of James Clerk Maxwell, in which light emerges not as a mechanical vibration but rather as a variation in electric and magnetic fields. The implication of the equations of Maxwell, which



Figure 7.6. Kelvin's palatial residence on the Scottish coast.

required a whole generation of debate to clarify, was triumphantly vindicated in 1887 by the experiment of Heinrich Hertz in Germany. In this climactic moment of the history of science, man 'won the battle lost by the giants of old, has snatched the thunderbolt from Jove himself and enslaved the all-pervading ether'. These are the words of George Francis Fitzgerald, addressing the British Association.

It was a little too late to convert Kelvin, who went on cooking up material ether models until he died, insisting that the elusive substance was 'a real thing'. 'Nothing' said Fitzgerald later 'will cure Sir William Thomson, short of the complete overthrow of the whole idea'. Nothing indeed was going to deflect this gallant knight from tilting at a favourite windmill.

On 29 September 1887, Kelvin woke up, sat up, and wrote in his notebook 'rigidity of foam'. He had conceived the notion that the ether might be a foam, a wild idea that Gibbs politely called 'the audacity of genius', after complaining about the proliferation of published speculations on the ether. (Amazingly, the latest speculation on the nature of space-time now seems headed in the same direction.)

Kelvin turned to Plateau's book for inspiration in trying to decide what structure the foam should have, and was soon playing with wire frames. His niece Agnes King wrote on 5 November:

When I arrived here yesterday Uncle William and Aunt Fanny met me at the door, Uncle William armed with a vessel of soap and glycerine prepared for blowing soap bubbles, and a tray with a number of mathematical figures made of wire. These he dips into the soap mixture and a film forms or adheres to the wires very beautifully and perfectly regularly. With some scientific end in view he is studying these films.

By then Kelvin had already solved the problem that he had set himself, i.e. to define the ideal structure of equal bubbles: *what partitioning of space into equal volumes minimizes their surface area?* Or rather, he had come up with a reason-

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able conjecture, a masterful design which he thought nature must be compelled to follow. He recorded it in his notebook on 4 November.

Since Kelvin's first words on the subject—rigidity of foam—were written in early September at 7.15am while in bed, we may presume that his foam ether model was conceived during the night. This is a common enough phenomenon. The scientist who retires, his brain feverishly obsessed with a single problem, is likely enough to spend the night attacking it in that semi-conscious state which is ideal for unbridled yet directed thought. Helmholtz gave as the requirement for mathematical reasoning that 'the mind should remain concentrated on a single point, undisturbed by collateral ideas on the one hand, and by wishes and hopes on the other'.

Maxwell described such an experience in a poem;

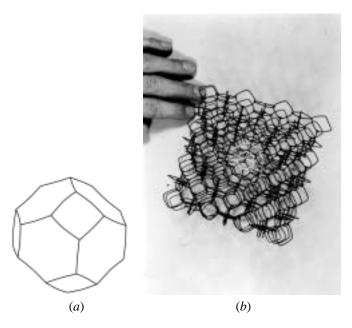
What though Dreams be wandering fancies, By some lawless force entwined, Empty bubbles, floating upwards Through the current of the mind, There are powers and thoughts within us (...).

Kelvin's thought indeed consisted of empty bubbles, for it was a foam without gas that he saw as a possible ether model. Such a thing cannot be stable but he convinced himself otherwise. So, when he had succeeded in describing an appropriate structure for the ether foam, he rushed into print with it in the *Philosophical Magazine*. The speed of this publication (not much more than a month later) rivals or exceeds that of the printed journals of today. It may have helped that the great man himself was editor of the journal, but one presumes that reviewers would hardly have questioned his insights.

#### 7.5 The Kelvin cell

The cell described by Kelvin may be described as a modified form of a truncated octahedron, a term used by Kepler. Kelvin chose to call it the 'tetrakaidecahedron'. Coxeter has called this name 'outrageous'; and it does seem unnecessary. It was one of the 13 Archimedean solids and was familiar, for example, to Leonardo. It plays an important role in modern solid state theory and crystallography, but it was not so well known to physicists in the 1880s as it is today<sup>6</sup>. Kelvin's ability to visualize it derived in part from his contributions to crystallography, to which he applied his characteristically down-to-earth approach, advising students to buy 1000 wooden balls and study their possible arrangements. He saw that this polyhedron can be packed to fill all space. Furthermore, only a little curvature of the hexagonal faces is necessary to bring it into complete conformity with Plateau's requirements (Maraldi angles, etc). He adroitly calculated this subtle curvature

<sup>&</sup>lt;sup>6</sup> See: Weaire D (ed) 1997 *The Kelvin Problem* (London: Taylor and Francis).



**Figure 7.7.** The Kelvin cell (*a*). 'Kelvin's Bedspring' (*b*) (courtesy of the University of Glasgow).

but had difficulties in drawing it. True to form, he made a wire model so that it could be seen in concrete form. This survives in the University of Glasgow and is known as 'Kelvin's bed-spring'. Visitors to what remains of the Lisbon EXPO can admire the large Kelvin cells at the centre of a framework of cables, designed as a climbing frame for children.

Kelvin's various attempts to bring forth an acceptable model for the material ether were greeted with limited and diminishing enthusiasm. This particular version was called 'utterly frothy' by a Cambridge don. When Fitzgerald tried to be conciliatory by suggesting that Kelvin's models were at best allegories, he received a spirited retort in the words of Sheridan's Mrs Malaprop: 'certainly not an allegory on the banks of the Nile'.

It is curious that Kelvin said nothing about a direct experimental test, although he described a way of making his structure with wire frames (which begs the question). Perhaps he was unaware of the ease with which equal bubbles can be made, simply by blowing air through a thin nozzle immersed in a soap solution. Unfortunately his unconfirmed conjecture was accepted too readily as the established truth by others. It was as if, as John Ziman once said of another theoretical model, 'the Word had been made Flesh'. Uncritically accepted, his conjecture remained unchallenged for quite some time.

In one unfortunate sequel, a Russian mathematician posed the same prob-

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lem as Kelvin, and developed the same conjecture, in 1992. He was apparently oblivious of the work of his illustrious predecessor.

#### Most beautiful and regular

There has never been much doubt that Kelvin's is the correct solution if all foam cells are restricted to have an identical shape and orientation. The doubt arises when they are given more freedom than this, as they have in nature, while maintaining equal volumes.

It is part of the physicist's faith that things are simple. (But not too simple, as Einstein warned.) There is always a provisional prejudice in favour of a neat solution rather than a complicated one. Or, put in grander language by D'Arcy Wentworth Thompson, 'the perfection of mathematical beauty is such (as Colin MacLaurin learned of the bee), that whatsoever is most beautiful and regular is also found to be most useful and excellent'.

Such a precept would be greatly improved by the addition of 'generally speaking' but the imperious sweep of this superlative prose stylist would not admit it. The Kelvin problem was for him solved 'in the twinkling of an eye', presumably that of Kelvin. Thus was the Word made Flesh, at least in the mind of the succeeding generation.

Kelvin's favourite polyhedron also played a large role in his research on space-filling structures in relation to general crystallography. In 1893 he wrote to Rayleigh about this, in the midst of filing patents, worrying about Home Rule and other preoccupations. Referring decorously to his wife as 'Lady Kelvin', as befits a correspondence between two members of the House of Lords, he said that she had begun to make a tetrakaidecahedral pin-cushion, which 'will make all clear'. Kelvin always brought his work home.

#### 7.6 The twinkling of an eye

The American botanist Edwin Matzke used Thompson's phrase as the title of a lecture he gave to the botanical club at Columbia University in 1950. He poured scorn on the widespread acceptance of Kelvin's conjecture, together with the erroneous conclusions of Buffon and Hales, also repeated uncritically by Thompson. They were relegated to the 'limbo of quaint and forgotten dreams'.

It had led him and other biologists to undertake fruitless searches for the Kelvin cell in natural cellular structures. It was nowhere to be found. He had been driven to perform the experiment so long overlooked, by making an actual foam of equal bubbles.

He did so in a manner which now looks foolish. It should have been known to him that such bubbles may be created simply by blowing air steadily through a fine nozzle beneath the surface of a soap solution. Instead he and his assistants blew every bubble individually with a syringe and added it carefully to the foam. This was a great labour and probably a labour of Sysiphus, because foam experiments must be completed quickly to avoid effects due to diffusion of gas between cells.

'Is this an indictment of twinkling eyes?', asked Matzke in the end, after failing to find a single Kelvin cell, and generously answered 'no' but not before condemning the naivety of his predecessors.

Despite reservations about the validity of Matzke's methods, there is nothing wrong with his general conclusion: the cells remain disordered in an equilibrium structure which is not optimal (like the bag of ball bearings), and there are no Kelvin cells to be seen within the foam.

All this heavy labour and even heavier irony discouraged others, but the mathematical question remained. Was Kelvin's solution the best, at least in principle? Some authorities, for example Hermann Weyl, were inclined to believe that it was, while others had an open mind. Fred Almgren of Princeton said in 1982 that 'despite the claims of various authors to the contrary it seems an open question'. A few mathematicians<sup>7</sup> and especially the Almgren group kept the Kelvin problem alive. One of Almgren's graduate students (John Sullivan) has said: 'I think most people assumed this partition was best. But Fred alone was convinced it could be beaten'.

Rob Kusner maintains that many people were also convinced that it could be beaten. Indeed he was among them. In 1992 he proved that an assembly of equal-pressure bubbles can minimize the interfacial surface area in a foam with an average number of faces greater or equal to  $13.39733...^8$ . The inequality did not exclude the Kelvin solution, but Kusner (following ideas from Coxeter and Bernal) was inclined to think that a minimal partition must have an average number of faces close to 13.5.

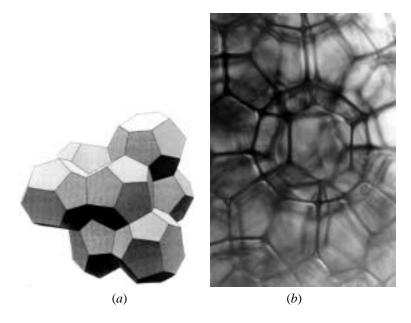
#### 7.7 Simulated soap

Today's mathematicians can ease their frustration with the solution of difficult problems and with the illustration of abstract results by the use of powerful computer simulations and advanced graphics. A leading exponent of such techniques is Ken Brakke of Susquehanna University in Pennsylvania. A former student of the Princeton school of Fred Almgren, he set out to develop a new and flex-ible computer code for producing surfaces of minimum area (Brakke's Surface Evolver). Once completed, it was generously offered to the world at large<sup>9</sup>. It has been continuously updated ever since, and used for many things, from the shape of a pendant liquid drop to the modelling of solder connections in semiconductor circuits. It is, in particular, ideal for the Kelvin problem and it was set to work on it around 1990.

<sup>&</sup>lt;sup>7</sup> Choe J 1989 On the existence and regularity of fundamental domains with least boundary area *J. Diff. Geom.* **29** 623–63.

<sup>&</sup>lt;sup>8</sup> Kusner R 1992 The number of faces in a minimal foam Proc. R. Soc. A 439 683-6.

<sup>&</sup>lt;sup>9</sup> http://www.susqu.edu/FacStaff/b/brakke/



**Figure 7.8.** (*a*) The Weaire–Phelan structure. (*b*) The observation of these cells in a real form.

Kelvin's conjecture at first survived this first onslaught by modern technology: no better structure could be found.

#### 7.8 A discovery in Dublin

In late 1993 Robert Phelan began his research at Trinity College Dublin. His task was to explore the Kelvin problem and variations upon that theme, using Brakke's Surface Evolver.

Phelan had joined a computational physics group which had a broad background in solid state and materials science. Hence there was no question of a blind search for an alternative structure. An idea was formed of the type of structure which might be competitive with that of Kelvin, essentially one with a lot of pentagonal faces. What structures in nature have such a form?

There is one class of chemical compounds in which covalent bonds create suitable structures: the bonds are tetrahedral. The compounds are called clathrates, a reference to the fact that they are made up of polyhedral *cages* of bonds. Usually they form because they create convenient homes for guest atoms or molecules. Gas pipelines in the Arctic are sometimes clogged up with clathrate crystals of ice.

The cages of bonds can be visualized as foam cells. Most of the rings of

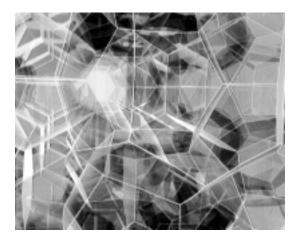


Figure 7.9. The Weaire–Phelan structure in a computer-generated image by J M Sullivan.

bonds on the sides of the cages are fivefold, creating pentagonal faces, as seemed to be required. The suggestion therefore was to explore the clathrates, particularly the two simplest ones, Clathrate I and II. The first of these was fed into the Evolver as a foam structure with equal cell volumes. Such a structure is a regular assembly of two types of cell with, respectively, 12 and 14 faces and results in a foam with 13.5 faces in average.

When the first output emerged, it was immediately evident that it was going to defeat Kelvin. When fully equilibrated, it turned out to have a surface area 0.3% less than that of the venerable conjecture. This does not sound like very much but endeavours in optimization always have to strive for quite small differences, in horse-races and elsewhere. The margin of success in this case was recognized as quite large<sup>10</sup>.

```
Date: 9 December 1993 03:25:03.13
From: "brakke@geom.umn.edu"
Reply-To: "brakke@geom.umn.edu"
To: "dweaire@vax1.tcd.ie", "rphelan@alice.phy.tcd.ie"
cc:
Subject: kelvin
```

I confirm your results. I got the area down to 21.156. As soon as I saw the picture on the screen, I was sure you had it. I always figured the way to beat Kelvin was to use lots of pentagons, since pentagon vertex angles

<sup>&</sup>lt;sup>10</sup>Later, Almgren, Kusner and Sullivan provided a rigorous proof that the Weaire–Phelan structure is of lower energy than that of Kelvin's.

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are very close to the tetrahedral angle. So when I saw you had almost all pentagons, I knew you'd done it.

Congratulations.

Ken Brakke

It was, according to Almgren, a 'glorious day for surface minimization theory' but, strictly speaking, it provides no more than a counter-example to Kelvin's conjecture and hence a replacement for it. The problem of proof that it is optimal in an absolute sense remains, though confidence grows that this structure will not in turn be surpassed: many related candidates have already been tried, mostly from the wide class of clathrate structures<sup>11</sup>.

<sup>&</sup>lt;sup>11</sup>See: Weaire D (ed) 1997 *The Kelvin Problem* (London: Taylor and Francis); Rivier N 1994 Kelvin's conjecture on minimal froths and the counter-example of Weaire and Phelan *Phil. Mag. Lett.* **69** 297–303.

# The architecture of the world of atoms

### 8.1 Molecular tactics

Another book which appeared in the same year as that of Plateau (1873) was *L'architecture du monde des atomes* by Marc-Antoine Gaudin, from which we borrow the title for this chapter on the role of packing ideas in crystallography.

Gaudin sought to reconcile the laws of chemistry with the findings of early crystallography, the experimental part of which comprised the study of the external forms of crystals. He constructed molecules of various shapes, consistent with the symmetry of the corresponding crystal. The molecules were composed of atoms in the required proportions. These atoms were, in turn, considered to be made up of particles of ether but it sufficed for his purpose that they were assumed to be roughly spherical and packed together with roughly constant separations. His illustrations were delightful (figure 8.1) but his speculations were no more than a shot in the dark, one small chapter in a confused story not concluded until the early 20th century.

That crystals owe their beautiful angular forms to regular arrangements of atoms or molecules was a very old hypothesis, but only in the late 19th century was it at last pursued with rigour and related to properties: this was the birth of solid state physics, which grew to be the dominant sector of modern physics, at least in terms of the active population of researchers<sup>1</sup>.

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<sup>&</sup>lt;sup>1</sup> See for general reference: Smith C S 1981 A Search for Structure (Cambridge, MA: MIT Press); Burke J G 1966 Origin of the Science of Crystals (University of California Press); Weaire D L and Windsor C G (ed) 1987 Solid State Science, Past, Present and Predicted (Bristol: Institute of Physics Publishing).

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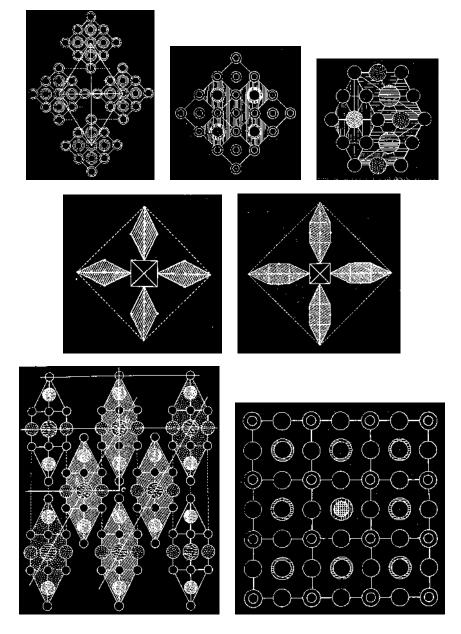
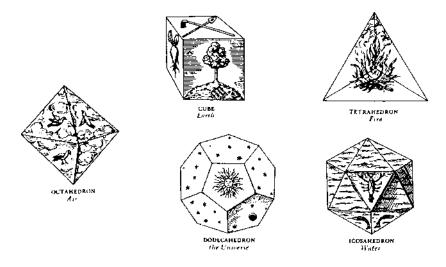


Figure 8.1. Gaudin's drawings of hypothetical molecular structures (1873).

Identifying what Kelvin called the 'molecular tactics of a crystal' remained a hesitant and erroneous process until x-rays provided the means to determine these



**Figure 8.2.** The four elements and the Universe in Plato's conception (from a drawing by J Kepler).

arrangements reliably if not quite directly, early in the 20th century. Today we can finally see (or, more accurately, feel) the individual atoms on the surface of a crystal, using the scanning tunnelling or atomic force microscope.

#### 8.2 Atoms and molecules: begging the question

Whether matter is discrete or continuous has been a subject of debate at least since the time of the ancient Greek philosophers. The first detailed atomistic theory was that of Plato (in the *Timaeus*) who described matter to be 'One single Whole, with all its parts perfect'. He associated the four 'elements'—*earth*, *water*, *fire* and *air*—with the form of four regular polyhedra—*cube*, *icosahedron*, *tetrahedron* and *octahedron*—and with the *dodecahedron* he associated the *Universe*. Plato attempted to match the properties of the elements with the shapes of the constitutive atoms. For instance water, being fluid, was associated with the icosahedron, which is the most spherical among the five regular solids. This theory was able to offer an ad hoc explanation of phase transitions (for instance the transition solid-to-liquid-to-vapour, which means earth-to-water-to-air and corresponds to cube-to-icosahedron-to-octahedron).

The atomistic theory of Plato was dismissed by Aristotle. He argued that if the elements are made up of these particles then the copies of each regular polyhedra must fill the space around a point and this operation cannot be done with the icosahedron and the octahedron (he thought erroneously that it was possible to fill space with regular tetrahedra).

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In other periods atoms have been reduced to mere points, or considered to be hard or soft spheres, or to have more exotic shapes endowed with specific properties inspired by chemistry. As Newton said, the invention of such 'hooked atoms' by followers of Descartes often begged the question.

Christian Huygens in his *Traité de la lumière* (1690) suggested that the Iceland spar (at that time very much studied for its birefringence) may be composed of an array of slightly flattened spheroids (see figure 8.3(c)). In this way he explained in one stroke the birefringence and the cleavage properties of these crystals.

Haüy's celebrated constructions begged the question, in as much as he explained the external form of crystals as being due to the packing of small components which were identical to the crystal itself. Haüy's 1784 *Essai d'une theorie sur la structure des crystaux* was nevertheless the most perspicacious of early attempts to make sense of crystals, in that he recognized that their angles are not arbitrary but follow certain rules, still used today.

#### **8.3** Atoms as points

The Newtonian vision was taken to an extreme by Roger Joseph Boscovitch, early in the 18th century. He postulated that 'matter is composed of perfectly indivisible, non-extended, discrete points' which interacted with one another.

Boscovitch published his *Theory of Natural Philosophy* on 1758, when he was a professor at the Collegium Romanum. He has been described as a philosopher, astronomer, historian, engineer, architect, diplomat and man of the world. Given all this, the book is a disappointingly dry exposition in which he attempts to deduce much of physics from a 'single law of forces'. This means a mutual force between each pair of points. Boscovitch struggled to describe a possible form for this, drawing illustrations which resemble modern graphs of interatomic interactions.

Half a century later, French mathematicians such as Navier and Cauchy developed powerful theories of crystal elasticity based on this idea but independent of any particular form for the interaction. Their elegant analysis of the effect of crystal symmetry on properties has provided one of the enduring strands of physical mathematics. However, they were little concerned with the origins of crystal structure itself.

Late in the 19th century, the Irish physicist Joseph Larmor reduced the role of matter still further, to a mere mathematical singularity in the ether. His view was enshrined in the book *Aether and Matter*, to which contemporaries jokingly referred as 'Aether and No Matter'. It was published in 1900, a date after which Larmor declared that all progress in physical science had ceased. He was probably not serious—it is, in fact, the date of the inception of quantum theory, which finally told us what atoms are really like.

Today's quantum mechanical picture of a nucleus surrounded by a cloud

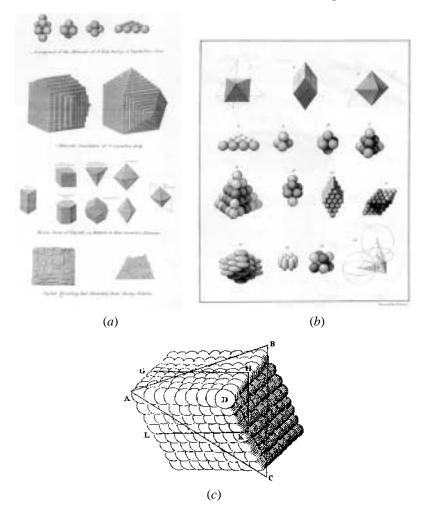


Figure 8.3. Various atomic models for crystals: Haüy (a), Wollaston (b), Huygens (c).

of electrons is a subtle one: it taxes the resources of the largest computers to predict what happens when these clouds come into contact. The day has not yet come when older, rough-and-ready descriptions are completely obsolete. It is still useful for some purposes to picture atoms as hard balls with relatively weak forces of attraction pulling them together. In particular the structures of many metals can be understood in this way.



Figure 8.4. All the snow crystals have a common hexagonal pattern and most of them show a hexagonal shape.

#### 8.4 Playing hardball

Among the manifold older ideas about atoms, the elementary notion of a hard sphere has endured as a useful one, even today.

Spherical 'atoms' were adopted by Kepler to explain the hexagonal shape of snowflakes (chapter 3). Kepler assumed that they were composed of tiny spheres arranged in the plane in the triangular packing. He did not consider these spheres to be atoms in the modern sense but more as the smallest particle of frozen water.

Of the later re-inventions of this type of theory, one of the most influential was that of William Barlow, writing in *Nature* in 1883.

Barlow is a prime example of the self-made scientist. His paper 'On the probable nature of the internal symmetry of crystals' is remarkable for its total lack of any reference to previous work. He happily ignored centuries of speculations, particularly those of his compatriot William Wollaston (see figure 8.3) early in the same century. His influence, particularly on and through Lord Kelvin, may be attributed in part to his clear writing style, his choice of the simplest cases and his use of attractive illustrations (figure 8.5).

Barlow's method was to look for dense packings of spheres, with no attempt at proof that they were the densest. This he left for mathematicians to consider later. He mentioned the possibility that soft spheres might make more realistic atoms but did little with this.

His down-to-earth commonsense approach might be regarded as a reaction against the refined mathematics of the French school, which many British natural philosophers, such as Tait, had found rather indigestible. John Ruskin, venturing into science in a manner which was then fashionable, had said in his *Ethics of the Dust* (1865), which consisted of 'ten lectures to little house wives on the elements of crystallization', that the 'mathematical part of crystallography is quite beyond girls' strength'. One might suppose that it would be beyond Barlow's strength as

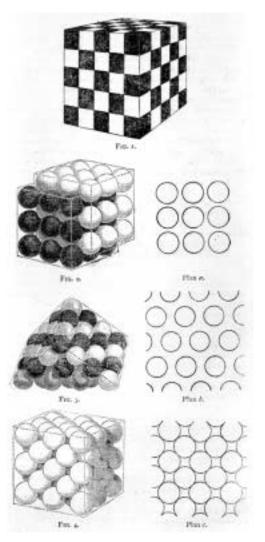


Figure 8.5. Some illustrations from Barlow's papers.

well, but in fact he took it up avidly, and absorbed the full mathematical theory in later years. Indeed he published in that area (albeit with some further disregard for the precedents).

By 1897 he was ready to expound a more mature version of the theory in a more erudite style. He described many possible stackings for hard spheres, of equal or unequal sizes.

Barlow's intuitive attack scored a number of notable hits, particularly in pre-



Figure 8.6. One of the earliest x-ray photographs (1896).

dicting the structures of the alkali halides. His place in the history of science was then assured by a contemporary and apparently unrelated discovery.

On 8 November 1895 a professor of physics in Würzburg realized that a new type of ray was emanating from his discharge tube. The Röntgen ray, named after its discoverer but eventually to be called the x-ray, was an immediate popular sensation, much to Röntgen's distaste. The potential for medical science and the challenge to the modesty of Victorian ladies was clear—the implications for physics were not. One of the most extraordinary of these, which took two decades to emerge, was the determination of crystal structures using x-rays, vindicating much of the guesswork of Barlow and others.

It should not be thought that all crystal structures are dense packings of balls. In the structure of diamond, each atom has only four atoms as neighbours. And this does not even qualify as a stable loose packing. This structure too was presaged before it was observed—this time by Walter Nernst (1864–1941), better known for his Heat Theorem (the Third Law of Thermodynamics).

#### 8.5 Modern crystallography

In a crystal the structure repeats a local configuration of atoms as in a threedimensional wall paper. There are 14 ways to construct such periodic structures in three dimensions, the *Bravais lattices*, but 230 different types of internal symmetry. This 'crushingly high number of 230 possible orderings', as Voigt called it, was both challenging and depressing to the theorist, until x-ray diffraction offered the means to use the theory in every detail.

When x-rays (electromagnetic radiation with a typical wavelength between 0.1 and 10 Ångstroms, i.e. between 0.000 000 01 and 0.000 001 mm) are incident on a crystal, they are diffracted and form a pattern with sharp spots of high intensity corresponding to specific angular directions. On 8 June 1912 at the Bavarian Science Academy of Munich, a study entitled 'Interference effects with Röntgen rays' was presented<sup>2</sup>. In this work Max von Laue developed a theory for the diffraction of x-rays from a periodic packing of atoms, associating the spots of intensity in the diffraction pattern with the regularity of the positions of the atoms in the crystal structure. One year later Bragg reported the first determination of crystal structures from x-ray diffraction for such systems as KCl, NaCl, KBr and KI, confirming Barlow's models<sup>3</sup>.

#### 8.6 Crystalline packings

In many crystal structures one or several types of atom are in positions corresponding to the centres of spheres in a sphere packing, as Barlow had supposed. It has been noted by O'Keeffe and Hyde<sup>4</sup>, two experts in crystal structures, that 'it is hard to invent a simple symmetric sphere packing that does not occur in nature'.

Of these, the most important family is that of packings with the maximal density  $\rho = 0.740\,48\ldots$  of which the face-centred cubic (fcc) is a member. This maximal density can be realized in infinitely many ways, all of which are based on the stacking of close-packed layers of spheres (figure 8.8), as practised by the greengrocer.

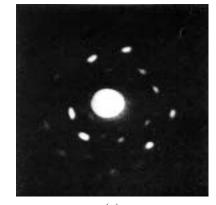
Two possibilities present themselves for the relative location of the next layer, if it is to fit snugly into the first one. Each successive layer offers a similar choice, and only by following a particular rule will the fcc structure described by Kepler result, with a cubic symmetry, which is not at all apparent in this building procedure. A different rule produces the hexagonal close-packed (hcp) structure, also described by Barlow, the next in order of simplicity. These two structures occur widely among the structures formed by the elements of the Periodic Table. More complex members of the same family—for example the double hexagonal close-packed structure—are found in alloys.

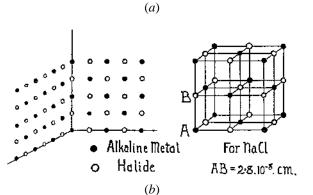
The original appeal of crystals lay in their external shapes, and these provided clues to their internal order. However, the precise shape of a crystal in equilibrium cannot be deduced from this order alone. According to a principle enunciated by Gibbs and Curie in 1875, the external shape of a crystal minimizes

<sup>&</sup>lt;sup>2</sup> Friedrich W, Knipping P and Laue M 1912 Interferenz-Erscheinungen bei Roentgenstrahlen S. B. Bayer. Akad. Wiss. pp 303–22.

<sup>&</sup>lt;sup>3</sup> Bragg W L 1913 The structure of some crystals as indicated by their diffaction *Proc. Roy. Soc.* A **89** 248–77.

<sup>&</sup>lt;sup>4</sup> O'Keefe M and Hyde G B 1996 *Crystal Structures* (Washington, DC: Mineralogical Society of America).





**Figure 8.7.** X-ray diffraction pattern (*a*) and the relevant crystalline structure (*b*) for NaCl, as reported by Bragg (1913).

the total surface energy. This is made up of contributions from each facet but different types of facet are more expensive in terms of energy.

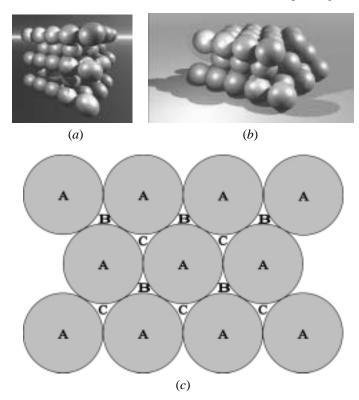
Some of the observed shapes can be realized by a rule developed by Bravais: *the largest facets have the densest packing of atoms* (which might be expected to have the lowest surface energy).

If the packing fraction is decreased a little from its maximum value, allowing the hard spheres some room to move, and they are given some kinetic energy, what can be said about the competition between these structures? This is a very delicate question for thermodynamics, and it has only been settled recently by extensive computations. The winner (as the more stable structure) is fcc<sup>5</sup>.

Some natural elements which have an fcc or hcp crystalline structure are given in table 8.1.

<sup>&</sup>lt;sup>5</sup> Woodcock L V 1997 Entropy difference between the face-centred cubic and hexagonal closepacked crystal structures *Nature* **385** 141–3.

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**Figure 8.8.** The hexagonal closed-packed (hcp) (*a*) and cubic closed-packed (fcc) (*b*) structures. These lattices are generated by a sequence of layers of spheres in the triangular packing configuration (*c*). Suppose that the first layer of spheres has centres in position A, the second layer can be placed in position B (or equivalently C), and for the third layer we have two alternatives: (i) placing the centres of the spheres in position A generating the sequence ABABAB... (which corresponds to the hcp lattice); (ii) placing the centres in position C generating the sequence ABCABCABC... (which corresponds to the fcc lattice).

### 8.7 Tetrahedral packing

Regular tetrahedra cannot pack together to fill space but irregular ones may do so. Of special interest for crystal chemistry are packings in which neighbouring atoms are on the vertices of such a system of closely packed tetrahedra. These structures are called 'tetrahedrally packed'.

A very important tetrahedrally-packed structure is the *body-centred cubic lattice* (bcc). This is the crystalline structure of many chemical elements. The bcc structure is the only tetrahedrally packed structure where all tetrahedra are identical.

fcc	hcp
Al	Be
Ag	Cd
Ar (20 K)	Co
Au	He (He <sup>4</sup> , 2 K)
Ca	Gd
Ce	Mg
$\beta$ -Co	Re
Cu	Ti
Ir	Zn
Kr (58 K)	
La	
Ne (20 K)	
Ni	
Pb	
Pd	
Pt	
$\delta$ -Pu	
Rh	
Sr	
Th	
Xe (92 K)	
Yb	

**Table 8.1.** Some natural elements which have an fcc or hcp crystalline structure. These are at room temperature unless otherwise indicated.

A special class of structures consists of those in which the packing is restricted to configurations in which five or six tetrahedra meet at an edge. These are the crystal structures of some of the more important intermetallic phases. Such structures are known as tetrahedrally close packed (tcp) and were described in the 1950s by Frank and Kasper<sup>6</sup>. These two eminent crystallographers were inspired to produce their classification of complex alloy structures by a visit to Toledo, where the Moorish tiling patterns incorporate subtle mixtures of coordination and symmetry, particularly fivefold features such as the regular pentagon. In the Frank–Kasper structures the packed spheres have various combinations of 12, 14, 15 and 16 neighbours, and the average is between 13.33... and 13.5.

Each tetrahedron of a tetrahedrally-packed structure has four other tetrahedra sharing its faces, so the dual structure, derived by placing the vertices in the centre of the tetrahedra (i.e. in the holes between spheres), forms a four-connected network. Such a network can be regarded as the packing of polyhedra which are

<sup>&</sup>lt;sup>6</sup> Frank F C and Kasper J S 1958 Acta Crystallogr. **11** 184; 1959 Acta Crystallogr. **12** 483.

restricted to pentagonal and hexagonal faces only. These networks also represent significant structures in chemistry—the clathrates (section 7.8).

#### 8.8 Quasicrystals

We have seen in the previous paragraphs how, starting from such clues as the regular angular shapes of crystals, scientists constructed a theory—crystallography in which the intrinsic structure of crystals was described as a periodic assembly of atoms, in an apparently complete system of ordered structures in the solid state. But in November 1984 a revolution took place: Shechtman, Blech, Gratias and Chan identified, in rapidly solidified AlMn alloys, an apparently new state of condensed matter, ordered but not periodic. The scientific journal *Physics Today* headlined 'Puzzling Crystals Plunge Scientists into Uncertainty'. Marjorie Senechal, a mathematician who has been one of the protagonists of this revolution, described this climate of astonishment in her book *Quasicrystals and Geometry*<sup>7</sup>:

It was evident almost immediately after the November 1984 announcement of the discovery of crystals with icosahedral symmetry that new areas of research had been opened in mathematics as well as in solid state science. For nearly 200 years it had been axiomatic that the internal structure of a crystal was periodic, like a three-dimensional wallpaper pattern. Together with this axiom, generations of students had learned its corollary: icosahedral symmetry is incompatible with periodicity and is therefore impossible for crystals. Over the years, an elegant and far-reaching mathematical theory had been developed to interpret these 'facts'. But suddenly—in the words of the poet W B Yeats *all is changed, changed utterly*.

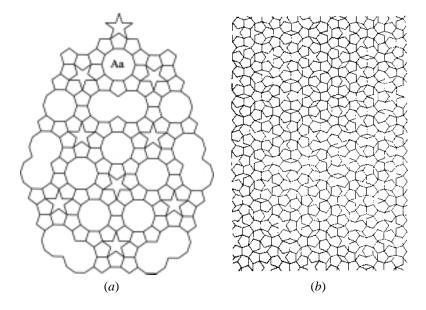
What terrible beauty was born? These new solids, with diffraction patterns which exhibit symmetries which are forbidden by the crystallographic restrictions, have been called *quasicrystals*. The internal structure of a quasicrystal is an ordered packing of identical local configurations with non-periodic positions in space.

With this perspective, it is a shock to realize that the seed of quasi-crystallinity was already there in Kepler's work<sup>8</sup>. In his book *Harmonices Mundi* (1619) Kepler described a repetitive structure with the 'forbidden' fivefold symmetry, but with 'certain irregularities'.

If you really wish to continue the pattern, certain irregularities must be admitted, (...) as it progresses this five-cornered pattern continually introduces something new. The structure is very elaborate and intricate.

<sup>&</sup>lt;sup>7</sup> Senechal M 1995 *Quasicrystals and Geometry* (Cambridge: Cambridge University Press).

<sup>&</sup>lt;sup>8</sup> Or even older instances in Islamic architecture: see Makovicky E 1992 *Fivefold Symmetry* ed I Hargittai (Singapore: World Scientific) p 67.



**Figure 8.9.** Two non-periodic tilings: that proposed by Kepler in 1619 (*a*) and that proposed by Penrose in 1974 (*b*). Note that Kepler's one is finite whereas Penrose's can be continued on the whole plane.

Hundreds of years later, in 1974, Roger Penrose produced a tiling that can be considered the realization of the one described by Kepler (see figure 8.9)<sup>9</sup>.

The Penrose tiling covers the entire plane; it is non-periodic but repetitive. *Non-periodic* means that if one takes two identical copies of the structure there is only one position where these two structures superimpose perfectly. In other words, sitting in a given position, the landscape around, up to an *infinite* distance, is unique and cannot be seen from any other point. *Repetitive* means that any local part of the structure is repeated an infinite number of times in the whole structure.

Exactly ten years after Penrose's work, this pattern was first observed in nature.

What most surprised the researchers after the discovery of quasicrystals was that these structures have diffraction patterns with well-defined sharp peaks that were previously considered to be the signature of periodicity. How can aperiodic structures have sharp diffraction peaks? Let us just say that the condition to have diffraction is associated with a strong form of repetitiveness, which is typical of these quasicrystalline structures.

Mathematically, these quasiperiodic patterns can be constructed from a crystalline periodic structure in a high-dimensional hyperspace by cutting it with a plane oriented with an irrational angle in respect to the crystalline axis. This con-

<sup>&</sup>lt;sup>9</sup> Penrose R 1974 Pentaplexity Bull. Inst. Math. Appl. 10 266–71.

struction explains the existence of diffraction peaks but does not give any physical understanding.

Why has nature decided to pack atoms in these non-periodic but repetitive quasicrystalline configurations? This is a matter of debate, unlikely to be quickly resolved<sup>10</sup>.

As a consequence of this revolution it was necessary for the scientific community to ask: *what is to be considered to be a crystal?* 

The International Union of Crystallography established a commission on Aperiodic Crystals that, in 1992, proposed for 'crystal' the following definition:

A crystal is any solid with an essentially discrete diffraction diagram.

According to this edict, the definition of a crystal which we have given earlier is too restrictive but the new one will, alas, be a mystery to many.

#### 8.9 Amorphous solids

Since ancient times, the distinction has been made between crystals and noncrystalline or amorphous (shapeless) solids. But the first category was reserved for large crystals such as gemstones. It was not realized until the present century that most inanimate materials (and quite a few biological ones as well) consist of fine crystalline grains, invisible to the eye and not easy to recognize even under a microscope. Hence they were wrongly classified as amorphous. Despite important clues, such as the fracture surface of typical metals, crystallinity was regarded as the exception rather than the rule<sup>11</sup>.

It remains difficult to distinguish an aggregate of very fine crystals from an amorphous solid using x-ray diffraction, and careers have been founded on an increasingly meaningless distinction. Today such amorphous materials as window glass are accepted as having a random structure, just as John Tyndall suggested with typical lyricism in *Heat—A Mode of Motion* (1863):

To many persons here present a block of ice may seem of no more interest and beauty than a block of glass; but in reality it bears the same relation to glass that orchestral harmony does to the cries of the marketplace. The ice is music, the glass is noise; the ice is order, the glass is confusion. In the glass, molecular forces constitute an inextricably entangled skein; in ice they are woven to a symmetric texture (...)

Amorphous metals, usually obtained by very rapid cooling from the liquid state, also have a random structure, in this case approximated by Bernal's random

<sup>&</sup>lt;sup>10</sup>See, for instance, Steinhardt P, Jeong H-C, Saitoh K, Tanaka M, Abe E and Tsai A P 1998 Experimental verification of the quasi-unit-cell model of quasicrystal structure *Nature* **396** 55–7; 1999 *Nature* **399** 84.

<sup>&</sup>lt;sup>11</sup>See for general reference: Lines M E 1994 *On the Shoulders of Giants* (Bristol: Institute of Physics Publishing).

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sphere packings (chapter 3). This structure gives them exceptional properties, useful in magnetic devices or as a coating on razor blades and in the manufacture of state-of-the-art golf clubs. What was once a mere academic curiosity now caresses the chin of the aspiring executive and adds several yards to his drive into the bushes from the first tee.

#### 8.10 Crystal nonsense

Old errors cast long shadows in our conception of the natural world. Astrology still commands copious column-inches in the daily papers, spiritualists ply a busy trade, and books abound on the mystical power of crystals. A suitable crystal, we are told, can radiate its energy to us and influence our aura, in a harmonious vibration of happiness. If only it were so easy.... Solid state physicists would go around with permanent smiles on their faces.

This strange attribution of a hidden potency is derived from the time when crystals were regarded as rare exceptions to the general disorder of inanimate nature. Their strange perfection of form must have led primitive man to wonder at them: it is known that Peking Man collected rock crystals. Perhaps in modern times the renewed fascination with 'crystal energy' also derives from the period of early radio when 'crystal sets', consisting of little besides a point contact to a crystal, acting as a rectifier, could be used to listen to radio broadcasts. Magic indeed!

The more sophisticated may have been aware that the details of the process of growth of a crystal proved intractable to any convincing explanation for some time. The problem was, for example, mentioned by A E H Tutton (1924) *The Natural History of Crystals*:

One of the most deeply interesting aspects of a crystal (...) concerns the mysterious process of its growth from a solution (...). The story of the elucidation, as far as it has yet been accomplished, of the nature of crystallization from solution in water is one of the most romantic which the whole history of science can furnish.

It is, by its very nature, a delicate problem of surface science, where minute amounts of impurities, or defects, can do strange things to help or hinder growth. But, by and large, crystallization is no longer such a mystery—otherwise the semiconductor industry could hardly be engaged in making huge silicon crystals of extraordinary perfection, every day.

The progress of physics did not, however, deflect Rupert Sheldrake from using the assumed intractability of the explanation of crystallization as a pretext for his provocative theory of 'morphic resonance', according to which crystallization is guided by a memory from the past. As a botanist of impeccable pedigree, he was then able to generalize his principle to the living world, creating a considerable following and almost unbearable irritation in the orthodox scientific community.

## **Apollonius and concrete**

#### 9.1 Mixing concrete

Any builder knows that to obtain compact packings in granular mixtures such as the 'aggregate' used to make concrete, the size of the particles must vary over a wide range. The reason is evident: small particles fit into the interstices of larger ones, leaving smaller interstices to be filled, and so on. A typical recipe for very dense mixtures starts with grains of a given size and mixes them with grains of smaller and smaller sizes in prescribed ratios of size and quantity, as already mentioned in chapter 2. The resulting mixture has a density that can approach unity.

Such recursive packing was already imagined around the 200 BC by Apollonius of Perga (269–190 BC), a mathematician of the Alexandrine school. He is classified with Euclid and Archimedes among the great mathematicians of the Greek era. His principal legacy is the theory of those curves known as conic sections (ellipse, parabola, hyperbola). He brought it to such perfection that 1800 years passed before Descartes recast it in terms of his new methods.

The method of recursive packing reappeared more recently in a letter by G W Leibniz (1646–1716) to Brosses:

Imagine a circle; inscribe within it three other circles congruent to each other and of maximum radius; proceed similarly within each of these circles and within each interval between them, and imagine that the process continues to infinity. (See figure 9.1.)

Something similar also arose in the work of the Polish mathematician, Waclaw Sierpiński (1887–1969), who wrote a paper in 1915 on what has come to be called the 'Sierpiński Gasket', and well known as a good example of a fractal

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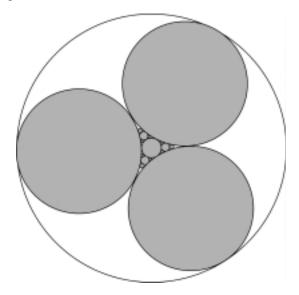


Figure 9.1. Apollonian packing.

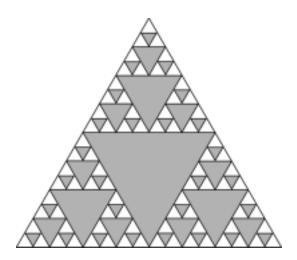


Figure 9.2. Sierpiński Gasket.

structure (see figure 9.2). Ian Stewart has called it the 'incarnation of recursive geometry'.

The aim of Sierpiński was to provide an example of a curve that crosses itself at every point, 'a curve simultaneously Cartesian and Jordanian of which every point is a point of ramification'. Clearly this curve is a *fractal*, but this word was coined by Benoît Mandelbrot<sup>1</sup> only in 1975.

Sierpiński was exceptionally prolific—he published 720 papers and more than 60 books. He called himself an 'Explorer of the Infinite'.

#### 9.2 Apollonian packing

In the packing procedure known as 'Apollonian Packing', one starts with three mutually touching circles and puts in the hole between them a fourth circle which touches all three. Then the same procedure is iterated.

Apollonius studied the problem of finding the circle that is tangent to three given objects (each of which may be a point, line or circle). Euclid had already solved the two easiest cases in his *Elements*, and the other (apart from the three-circle problem) appeared in the *Tangencies* of Apollonius. The three-circle problem (or the kissing-circle problem) was finally solved by Viète (1540–1603) and the solutions are called Apollonian circles. A formula for finding the radius ( $r_4$ ) of the fourth circle which touches three mutually tangent circles of radii ( $r_1, r_2$  and  $r_3$ ) was given by René Descartes in a letter in November 1643 to Princess Elisabeth of Bohemia:

$$2\left[\left(\frac{1}{r_{1}}\right)^{2} + \left(\frac{1}{r_{2}}\right)^{2} + \left(\frac{1}{r_{3}}\right)^{2} + \left(\frac{1}{r_{4}}\right)^{2}\right] \\ = \left[\left(\frac{1}{r_{1}}\right) + \left(\frac{1}{r_{2}}\right) + \left(\frac{1}{r_{3}}\right) + \left(\frac{1}{r_{4}}\right)\right]^{2}.$$
(9.1)

This formula was rediscovered in 1936 by the physicist Sir Frederick Soddy who expressed it in the form of a poem, 'The Kiss Precise'<sup>2</sup>:

Four pairs of lips to kiss maybe Involves no trigonometry. 'Tis not so when four circles kiss Each one the other three. To bring this off the four must be As three in one or one in three. If one in three, beyond a doubt Each gets three kisses from without. If three in one, then is that one Thrice kissed internally.

Four circles to the kissing come, The smaller are the benter, The bend is just the inverse of The distance from the centre.

<sup>1</sup> Mandelbrot B B 1977 *The Fractal Geometry of Nature* (New York: Freeman).

 $^2~$  Soddy F 1936 The kiss precise Nature 137 1021.

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Though their intrigue left Euclid dumb. There's now no need for the rule of thumb. Since zero bends a straight line And concave bends have minus sign, The sum of the squares of all four bends Is half the square of their sum.

To spy out spherical affairs An oscular surveyor Might find the task laborious, The sphere is much the gayer, And now besides the pair of pairs A fifth sphere in the kissing shares. Yet, signs and zero as before, For each to kiss the other four The square of the sum of all five bends Is thrice the sum of their squares

In the Apollonian procedure, the size of the circles inserted inside the holes become smaller and smaller and the packing fraction approaches unity in the infinite limit. For example, one can start from three equal tangent unit circles which pack with a density of 0.907... Inside the hole one can insert a circle with radius 1/6.46... = 0.15... and the density becomes 0.95... Now there are three holes where one can insert three circles with radius 1/15.8... = 0.063... and the density rises to 0.97....

#### 9.3 Packing fraction and fractal dimension

Pursued indefinitely, Apollonian packing leads to a dense system with packing fraction  $\rho = 1$ . But how is this limit reached? Suppose for instance that we start with circles of radii  $r_{\text{large}}$  and stop the sequence when the radii arrive at the minimum value  $r_{\text{small}}$ . The packing fraction is

$$\rho = 1 - \left(\frac{r_{\text{small}}}{r_{\text{large}}}\right)^{(2-d_{\text{f}})} \tag{9.2}$$

where  $d_{\rm f}$  is the fractal dimension. Indeed the Apollonian packing is a classical example of a fractal, in which the structure is composed of many similar components with sizes that scale over an infinite range. Numerical simulations give  $d_{\rm f} = 1.305...^3$ . The analytical determination of  $d_{\rm f}$  is a surprisingly difficult problem. Exact bounds have been calculated by Boyd who found  $1.300\,197 < d_{\rm f} < 1.314\,534^4$ . The fractal dimension can be calculated in the two

<sup>&</sup>lt;sup>3</sup> Manna S S and Hermann H J 1991 Precise determination of the fractal dimension of Apollonian packing and space-filling bearings J. Phys. A: Math. Gen. 24 L481–90.

<sup>4</sup> Boyd D W 1973 Mathematica 20 170.



**Figure 9.3.** 'So we may image similar rings of spheres above and below (...) and then being all over again to fill up the remaining spaces and so on *ad infinitum*, every sphere added increasing the number that have to be added to fill it up!' [Soddy F 1937 The bowl of integers and the hextet *Nature* **139** 77–9.]

interesting models for packings with triangles and hexagons which have  $d_{\rm f} = 1$  and  $d_{\rm f} = 1.585$  respectively<sup>5</sup>.

#### 9.4 Packing fraction in granular aggregate

The Apollonian packing procedure can be extended to three dimensions. In this case, four spheres are closely packed touching each other and a fifth one is inserted in the hole between them. Then the procedure continues infinitely as in two dimensions.

Descartes' theorem (equation (9.1)) was extended to three dimensions by Soddy in the third verse of his poem and to d dimensions by Gosset in another poem also entitled 'The Kiss Precise'<sup>6</sup>.

And let us not confine our cares To simple circles, planes and spheres, But rise to hyper flats and bends Where kissing multiple appears. In n-ic space the kissing pairs Are hyperspheres, and Truth declares— As n + 2 such osculate

<sup>&</sup>lt;sup>5</sup> Bidaux R, Boccara N, Sarma G, de Seze L, de Gennes P G and Parodi O 1973 Statistical properties of focal conic textures in smetic liquid crystals *J. Physique* **34** 661–72; Eggleton A 1953 *Proc. Camb. Phil. Soc.* **49** 26.

<sup>&</sup>lt;sup>6</sup> Gosset T 1937 The kiss precise *Nature* **139** 62.

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Each with n + 1 fold mate The square of the sum of all the bends Is *n* times the sum of their squares.

Gosset's equation replaces the factor 2 in front of equation (9.1) with a factor d (the space dimension, n in Gosset's poem). In three dimensions it gives, for example, a radius of 0.2247... for the maximum sphere inside the hole between four touching spheres.

The relation for the packing density can also be extended to three and higher dimensions<sup>7</sup>.

$$\rho = 1 - \left(\frac{r_{\text{small}}}{r_{\text{large}}}\right)^{(d-d_t)}.$$
(9.3)

This expression is not limited to the Apollonian case but is valid for any fractal packing in the limit of very wide polydispersity  $(r_{\text{large}} \gg r_{\text{small}})$  with power law in the size distribution.

The fractal dimension for Apollonian sphere packings has been less studied than in the two-dimensional case. However, the two models of packings with hexagons and triangles can be easily extended to three dimensions giving  $d_{\rm f}$  =  $1.26 \text{ and } d_{\rm f} = 2.$ 

Engineers have long known<sup>8</sup> that the porosity p of the grain mixture is a function of the ratio between radii of the smallest and the largest grains utilized. They empirically use the equation

$$p = 1 - \rho = \left(\frac{r_{\text{small}}}{r_{\text{large}}}\right)^{\frac{1}{5}}.$$
(9.4)

A comparison with equation (9.3) gives the fractal dimension as  $d_{\rm f} = 3 - \frac{1}{5} = 2.8$ .

<sup>&</sup>lt;sup>7</sup> Herrmann H J, Mantica G and Bessis D 1990 Space-filling bearings *Phys. Rev. Lett.* **65** 3223–6. <sup>8</sup> Caquot M A 1937 Le role des matériaux inerts dans le béton Société des Ingeniéurs Civils de France

pp 563-82.

## The Giant's Causeway

#### **10.1** Worth seeing?

The Giant's Causeway is a columnar basalt formation on the north coast of Ireland. It has been an object of admiration for many centuries and the subject of continual scientific debate<sup>1</sup>. Although it still draws tourists from afar, Dr Johnson's acid remark that it was 'worth seeing but not worth going to see', echoed by the irony of Thackeray's account of a visit, may be justified, since similar geological features occur throughout the world. Among the more notable examples are those of the Auvergne in France, Staffa in Scotland and the Devil's Postpile in the Sierra Nevada of California.

The primary historical importance of the debate on the origins of the Causeway lies in it being a focus of the intellectual battle between the Neptunists and the Vulcanists in the 18th century. The history of geology delights in giving such titles to its warring sects: others have been classed as Plutonists, Catastrophists and Uniformitarians.

To the convinced Neptunist the origin of rocks lay in the sedimentary processes of the sea, while a Vulcanist would argue for volcanic action. As in most good arguments, both sides were right in certain cases. But in the case of basalt the Neptunists were seriously wrong.

Why should this concern us here? Simply because the story is intertwined with many of the strands of ideas on packing and crystallization in the understanding of materials which emerged over the same period.

What was so fascinating about the Causeway?

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<sup>&</sup>lt;sup>1</sup> Herries Davies G L 1981 A Geology of Ireland ed C H Holland (Edinburg: Scottish Academic).



Figure 10.1. Sketch of the Giant's Causeway (from *Philosophical Transactions of the Royal Society* 1694).

#### 10.2 Idealization oversteps again

As with the bee's cell, but even more so, sedentary commentators on the Causeway have generally overstated the perfection of order which is to be seen in the densely packed basalt columns. They have been described as 'hexagonal', implying that the pattern is a perfect honeycomb. This is not at all the case (see figure 10.2).

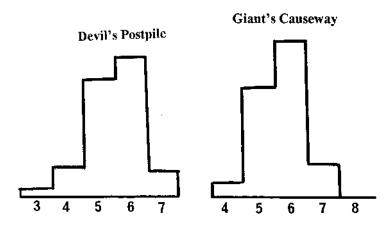
Eyewitness reports, especially by unscientific visitors, were generally more accurate. The Percy family of Boston reported in their *Visit to Ireland* (1859):

Do they not all look alike?

Yes, just as the leaves are alike in general construction, but endlessly diverse, just as all human faces are alike, but all of them possessed of an individual identity.

But as the story was passed around, idealization constantly reasserted a reg-

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**Figure 10.2.** Distribution of the number of sides of basalt columns in two of the most famous sites where these occur (after Spry A 1962 The origin of columnar jointing, particularly in basalt flans *J. Geol. Soc. Australia* **8** 191).

ular hexagonal pattern for the Causeway, instead of the elegant random pattern in which less than half of the polygons are six-sided, as one can verify from figure 10.2.

'Hexagonal' was an evocative word, calling to mind the form of many crystals. It was natural therefore to call the Causeway 'crystalline'; and see the columns as huge crystals, even though their surfaces were rough in appearance. Alternatively, it was suggested that the columns are formed by compaction or by cracking. The latter was the choice of the Vulcanists, who saw the basalt as slowly cooling and contracting, until it cracked.

That random cracking should have this effect seems almost as unlikely as crystallization, at first glance, yet it has come to be accepted, as we explain later. This has not stopped the continued generation of wild theories, even late in the 20th century.

#### **10.3** The first official report

In 1693 Sir Richard Bulkeley made a report of the Causeway to the Royal Society in London. Like many who were to follow, he offered an account of the phenomenon without troubling himself to go to see it. He relayed the news from a scholar and traveller well known to him, that it 'consists all of pillars of perpendicular cylinders, Hexagones and Pentagones, about 18 to 20 inches in diameter'.

While offering no promise to make a visit himself, he offered to answer any queries. In the following year Samuel Foley published answers to questions forwarded by Bulkeley. Already the similarity to crystalline forms was noted. A more scholarly and verbose account by Thomas Molyneux of Dublin followed,

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complete with classical references, and containing some intemperate criticisms of the original reports. Despite his superior tone, the author confesses that 'I have never as yet been upon the place myself'. He noted a similarity to certain fossils described by Lister but found the difference of scale difficult to explain away.

For a time the arguments lapsed, but a number of fine engravings with detailed notes were published. Art served science well, in providing an inspiring and accurate picture for the armchair theorists of geology. The correspondence resumed around 1750. Richard Pockock had spent a week at the Causeway, and settled on a Neptunist mechanism of precipitation.

In 1771, N Desmarest published a memoir which was to be central to the Vulcanist/Neptunist dispute. In his view the 'regular forms of basalt are the result of the uniform contraction undergone by the fused material as it cooled and congealed'. This was countered by James Keir, who reasserted the crystalline hypothesis, drawing on observations of the recrystallization of glass. Admittedly there was a great difference of scale, but 'no more than is proportionate to the difference observed between the little works of art and the magnificent operations of nature'. Here 'art' means craft or industry, for recrystallization was a matter of intense commercial interest in the attempt to reproduce oriental porcelain.

The Reverend William Hamilton added further support to crystallization with published letters and a dreadful 100-page poem ('*Come lonely Genius of my natal shore*...'), published in 1811. This and vitriolic rebuttals of Desmarest by Kirwan and Richardson did not succeed in reversing the advance of the Vulcanist hypothesis. It was, said Richardson, an 'anti-Christian and anti-monarchist conspiracy', since it set out to 'impeach the chronology of Moses'. He favoured a model of compression of spheroidal masses to form columns, with some laboratory experiments to back it up.

It was probably fair comment when Robert Mallett summarized the state of play in 1875 by saying that 'no consistent or even clearly intelligible theory of the production of columnar structure can be found'.

Mallett was an early geophysicist, who invented the term 'seismology'. The name of his engineering works still adorns the railings of Trinity College Dublin. He undertook a thorough review of the basalt question and attempted to publish it in the *Proceedings of the Royal Society*. After five months and four referees he was told that 'it was not deemed expedient to print it at present'—a splendidly diplomatic refusal to publish the work of a Fellow of the Society.

This reversal may well have stemmed from his trenchant criticism of 'very crude and ill-thought-out notions' and a 'bad or imperfect experiment inaccurately reasoned upon and falsely applied' by his predecessors, who were 'blinded by a preconceived and falsely based hypothesis'. His own advocacy was directed in support of contraction and cracking. He gave credit for this to James Thomson (the Glasgow professor who was the father of Lord Kelvin) together with the French school of Desmarest.

He finally succeeded in publishing his article in the lesser (and less conservative) journal *Philosophical Magazine*.



Figure 10.3. Polyhedral basaltic columns in the Giant's Causeway.

#### 10.4 Mallett's model

Mallett proposed to attack the problem 'in a somewhat more determinate manner'. By this he meant that his approach would be mathematical and quantitative, in contrast to the hand-waving of the other geologists. This more modern style has made the article influential ever since.

One of his principal interests was in the energy liberated in volcanic eruptions, so it was natural for him to think in terms of the total energy of the system of cracks rather than their precise mechanism of formation. At a time when there was a general tendency to express the laws of physics as minimal principles, he appealed rather vaguely to the 'principle of least action' and 'the minimum expenditure of work'. *What crack pattern would minimize energy*?

This question makes little sense unless some constraint fixes the size of the cells of the pattern, but this was somehow ignored, and he triumphantly announced that the hexagonal pattern was best, by comparison with other simple cases.

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#### 10.5 A modern view

D'Arcy Wentworth Thompson recognized that cracks which proceed explosively from isolated centres could never form such a harmonious pattern. He failed to see the possibility that crack patterns first formed deep within a lava flow could propagate very slowly outwards as it cooled. A careful reading of Mallett's paper shows that he had already recognized this, and this part of his description is impeccable.

In their slow motion the cracks migrate until they form a balanced network which propagates unchanged. To have this property it need not be ordered: the best analogy is the arrangement of atoms when a liquid becomes a glass on cooling. There is local order only.

When precisely the realization dawned more generally that it must be so is not clear, but certainly Cyril Stanley Smith gave this explanation in 1981, when preparing the published version of a lecture to geologists. It appears very natural to the modern mind. Until full computer simulations are performed, one hesitates to state it emphatically and risk joining such a long list of unwarranted claims.

#### 10.6 Lost city?

In October 1998, an article in the British press reported the possible discovery of a lost city by a documentary film-maker in Nicaragua. The evidence consisted of 62 polygonal basalt columns. Troops had been dispatched to guard the find against looters. Geologists had expressed some scepticism....

It seems that the columnar basalt story, begun in 1693, is destined to run and run.

# Soccer balls, golf balls and buckyballs

#### 11.1 Soccer balls

A favourite close-up of the television sports director shows a soccer ball distending the net. This offers the opportunity to compare the two: for the net is nowadays made in the form of the hexagonal honeycomb, and the surface of the ball looks roughly similar. Closer examination reveals the presence of 12 pentagons among the hexagons on the ball.

The problem of the soccer ball designer was to produce a convenient polyhedral form which is a good approximation to a sphere. The presently favoured design replaces a traditional one and we are not aware of the precise arguments that brought this about. Certainly it is more aesthetic, on account of its high symmetry, which is officially described as *icosahedral*. The simplest design of this type would be that of the pentagonal dodecahedron (figure 5.6), but this was perhaps not sufficiently close to a sphere. Instead, 32 faces are used, of which 12 are pentagons and the rest are hexagons.

By a curious coincidence, this icon of modern sport has cropped up in a prominent role in modern science as well, as we shall see shortly. But first let us switch sports and examine the golf ball.

#### 11.2 Golf balls

The dynamics of a sphere immersed in a viscous fluid presents one of the classic set-piece problems of physics and engineering, dating back to the work of Newton (applied, in particular, to the motion of the Earth through the ether), and tidied

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Figure 11.1. A soccer ball.



Figure 11.2. A golf ball.

up in some respects by Sir George Gabriel Stokes more than 100 years ago. In modern times it can be safely assumed that there has been a large investment in a better understanding of the motion of a sphere in air, since it commands the attention of many important people on the golf courses of the world.

The extraordinary control of the golf ball's flight which is exercised by (some) golfers owes much to the special effects imparted by the spin which is imposed on the ball by the angled blade of the club. This can be as much as 10 000 revolutions per minute. Because of its backspin the ball is subject to an upward force, associated with the deflection of its turbulent wake. This is the Magnus Effect, also responsible for the swerve of a soccer ball. It causes the ball to continue to rise steeply until, both velocity and spin having diminished, it drops almost vertically onto its target.

It was found that marking the surface of the ball enhanced the effect, and a dimple pattern evolved over many years. Today such patterns typically consist of 300–500 dimples. All are consistent with the incorporation of a 'parting line' where two hemispherical moulds meet to impress the shape. Locally the dimples are usually close-packed on the surface of the ball.

We know of no physical theory which would justify any particular arrangement. Many are used, whether motivated by whim or the respect for the intellectual property of established designs. Titleist has favoured an essentially icosahedral ball derived from the pentagonal dodecahedron by adding hexagons, just as for the soccer ball. Note that here we are dealing with a 'dual' structure: each dimple lies at the centre of one of the polygons. A simple topological rule governs all such patterns. Indeed, to wrap a honeycomb on a sphere or other closed surface is not possible, without introducing other kinds of rings. According to Euler's theorem the minimum price to be paid is 12 pentagons. One may take the pentagonal dodecahedron, beloved of the Greeks, and expand it by the addition of any number of hexagons (except, as it happens, one). In some cases the result is an elegantly symmetric structure.

### 11.3 Buckyballs

The modern science of materials has matured to the point at which progress seems barred in many directions. One cannot envisage, for example, magnetic solids which are much more powerful than the best of today's products, because they are close to very basic theoretical limits. (The scientist who says this type of thing is always in danger of following in the footsteps of the very great men who denounced the aeroplane, the space ship and the exploitation of nuclear energy as patent impossibilities.)

Despite this sense of convergence to a state in which optimization rather than discovery is the goal, new materials continue to make dramatic entrances. Sometimes they arise because certain assortments of many elements have not previously been tried in chemical combination. There is one great exception to this trend towards combinatorial research. The sensational advance in carbon chemistry which goes by the affectionate nickname of 'buckyballs' has raised more eyebrows and opened more doors than anything else of late, with the possible exception of high-temperature superconductors.

This is not a case of a single, momentous revelation: rather one of steadily increasing knowledge and decreasing incredulity over many years, from the first tentative clues to the establishment of major research programmes throughout the world. The story up to 1994 has been compellingly recounted by Jim Baggott in *Perfect Symmetry*<sup>1</sup>.

At its conclusion Baggott wondered which of the four central personalities of his tale would be rewarded by the Nobel Prize, which is limited to a trio. The answer came in 1996: the Royal Swedish Academy of Science awarded the Nobel Prize in Chemistry to Robert F Curl, Harold W Kroto and Richard E Smalley.

The carbon atom has long been renowned as the most versatile performer in the periodic table. It is willing to join forces with other atoms either three or four

<sup>&</sup>lt;sup>1</sup> Baggott J 1994 Perfect Symmetry: The Accidental Discovery of Buckminsterfullerene (Oxford: Oxford University Press).

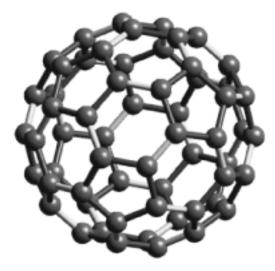


Figure 11.3. The C<sub>60</sub> buckyball.

at a time. Pure carbon with fourfold bonding is diamond, whereas graphite consists of sheets with the honeycomb structure in which there is threefold bonding. The two solids have vastly different properties; one is hard, the other soft; one is transparent, the other opaque; one is horribly expensive, the other very cheap. Nothing could better illustrate the falsity of the ancient idea that all the properties of elements spring directly from the individual atoms.

For pure carbon, that was supposed to be the end of the story, give or take a few other forms to be found under extremely high pressures. Yet we now recognize that graphite-like sheets can be wrapped to form a spherical molecule of 60 atoms—the buckyball—and buckyballs can be assembled to form an entirely new type of carbon crystal, with startling properties. And further possibilities continue to emerge in the laboratory or the fevered imagination of molecule designers: other, larger molecules, concentric molecules like onions, tubular forms called nanotubes, which may be key components of future nanoengineering. The buckyball belongs to an infinite family of possibilities which comprise the new subject of fullerene chemistry.

The buckyball has a great future, a fascinating history and even an intriguing prehistory. The existence of molecules like this had been teasingly conjectured by a columnist in the *New Scientist*, and Buckminster Fuller built most of his reputation on the architectural applications of such structures (generally containing many more hexagons than the buckyball). Hence the C<sub>60</sub> molecule was first baptised *buckminsterfullerene* in his honour. This is by no means a large mouthful by

chemical standards, but the snappier 'buckyball' has steadily gained currency at its expense<sup>2</sup>.

#### 11.4 Buckminster Fuller

Buckminster Fuller<sup>3</sup> has been described by an admirer as a 'protean maverick'. For many he is the prime source of insight into many of the structures which we have pondered in this book. Over several decades he poured forth a torrent of ideas and assertions which combined the Greek faith in geometry as lying at the heart of all nature with vague and superficially impressive notions of energy and synergy. The resulting pot-pourri is inspiring or bewildering, according to taste. When he ventures into fundamental descriptions of nature, it is reminiscent of the speculations of those 19th-century ether theorists.

One of Fuller's assertions was that all nature is 'tetrahedronally coordinated'. Here he was thinking of close-packing of spheres (although this, in part, contradicts the statement—not all arrangements are tetrahedral). He seems to have claimed to have discovered the ideal close-packed arrangement, only to find it in the work of Sir William Bragg, who he then supposed to have independently found it around 1924!

It is the practical outcome of Fuller's ruminations, in the form of the geodesic dome, that we remember today. Here again there is some question of priority. Tony Rothman, in *Science à la Mode*, has pointed out that such structures were patented by the Carl Zeiss company, for the construction of planetariums, in the 1920s. Fuller's patent is dated 1954. Rothman generously gives the protean maverick the benefit of the doubt....

#### 11.5 The Thomson problem

Another problem which involved placing points on a sphere was posed by J J Thomson in 1904 in the context of speculations about classical models of the atom, which were soon to be rendered out-of-date by quantum mechanics. But as with many other cases in this book, the problem has survived in its abstract mathematical form, and continues to intrigue mathematicians and challenge computer scientists. It is simply this: *what is the arrangement of N point electrical charges on a sphere, which minimizes the energy associated with their interactions?* This is just the sum of 1/r over all pairs of points, where r is their separation. Generally speaking the solution is neither the best packing nor the most symmetric arrangement of points. Beginning with L Foppl, around 1910, mathematicians

 $<sup>^2</sup>$  It has been suggested that, since the polyhedral structure of the buckyball and soccer ball date back to Archimides, 'archiball' might be more appropriate.

<sup>&</sup>lt;sup>3</sup> See, for reference, Marks R W 1960 *The Dymaxion World of Buckminster Fuller* (Reinhold); Rothman T 1989 *Science à la Mode, Physical Fashions and Fictions* (Princeton, NJ: Princeton University Press).

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have accepted Thomson's challenge. Kusner and Sullivan<sup>4</sup> analysed the cases N < 20, discovering that there is only one stable structure when N is smaller than 16.

The target of most researchers is to find structures of low energy using computational search procedures and identify the one which is lowest among these, for large values of  $N^5$ . Some of the structures which crop up here are similar to those of Buckminster Fuller constructions and golf balls.

This computational quest is an ideal testing-ground for new software ideas, such as simulated annealing (see section 13.11).

The minimal energy structures for small N are surprising in some cases: for N = 8 we do not find the obvious arrangement in which the charges are at the corners of a cube, but rather a twisted version of this.

For N = 12 the familiar icosahedral structure is found, with the charges at the corners of the pentagonal dodecahedron (figure 5.6). Each charge has five nearest neighbours. Thereafter this structure is elaborated to accommodate more charges. For all N which satisfies

$$N = 10(m^2 + n^2 + mn) + 2 \tag{11.1}$$

with m and n being positive integers; this can be done very neatly as in figure 11.4.

All the additional charges have six neighbours. In special cases these correspond to the buckyball or soccer ball structure which we have already admired.

That is not the end of the story. Eventually at high N these structures can be improved by modifications which introduce more charges with five or seven neighbours.

#### **11.6 The Tammes problem**

Many pollen grains are spheroidal and have exit points distributed on the surface. The pollen comes out from these points during fertilization. The position of the exit points is rather regular and the number of them varies from species to species. In 1930 the biologist Tammes described the number and the arrangement of the exit points in pollen grains of many species. He found that the preferred numbers are 4, 6, 8, 12, while 5 never appears. The numbers 7, 9 and 10 are quite rare and 11 is almost never found. He also found that the distance between the exit points is approximately constant, and the number of these points is proportional to the surface of the sphere<sup>6</sup>.

Tammes posed the following question: given a minimal distance between them, how many points can be put on the sphere? We can think of the points as

<sup>&</sup>lt;sup>4</sup> Kusner R and Sullivan J 1997 *Geometric Topology* ed W H Kazez (International Press).

<sup>&</sup>lt;sup>5</sup> Altschuler E L *et al* 1997 Possible global minimum lattice configurations for Thomson's problem of charges on a sphere *Phys. Rev. Lett.* **78** 2681.

<sup>&</sup>lt;sup>6</sup> Tammes P M L 1930 On the origin of number and arrangement of the places of exit on pollen grains *Diss. Groningen.* 



Figure 11.4. Three low-energy structures for charges on a sphere as depicted by Altschuler *et al.* 

associated with (curved) discs of a certain size, which are not allowed to overlap. Tammes attacked the problem in an empirical way by taking a rubber sphere and drawing circles on it with a compass. He found, for instance, that when the space is enough for five circles then an extra circle can always be inserted. In this case the six circles are located at the vertices of an octahedron. In this way the preference for 4 and 6 and the aversion for 5 in pollen grains may be explained. Tammes also found that when 11 points find enough space then 12 can also be placed at the vertices of an icosahedron.

The first of these results has been mathematically proved to be valid for the surface of a sphere in three dimensions and it has been extended to any dimension. If on the surface of a sphere in d-dimensional space more than d + 1 discs can be placed then 2d such discs can be placed at the extremities of the coordinate axes.

The Tammes problem is the subject of an enormous amount of literature.

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Mathematically the questions raised by Tammes can be expressed as follows: what is the largest diameter  $a_N$  of N equal circles that can be placed on the surface of a unit sphere without overlap? How must the circles be arranged, and is there a unique arrangement?

Exact solutions are known only for  $N \leq 12$  and N = 24. These and other solutions are shown in table 11.1 (taken from  $\text{Croft}^7$ ).

Ν	$a_N$	Arrangement
2	$180^{\circ}$	Opposite ends of a diameter
3	$120^{\circ}$	Equilateral triangle in the equator plane
4	109° 28'	Regular tetrahedron
5	$90^{\circ}$	Regular octahedron less one point, not unique configuration
6	$90^{\circ}$	Regular octahedron
7	77° 52'	Unique configuration
8	74° 52'	Square anti-prism
9	70°32'	Unique configuration
10	66°9'	Unique configuration
11	63°26'	Icosahedron less one point, not unique configuration
12	63°26'	Icosahedron
24	43°41'	Snub cube

Table 11.1.

Note that for N = 6 and 12,  $a_N = a_{N-1}$  which is the Tammes empirical result.

A bound for the minimum distance d between any pair of points on the surface of the unit sphere, was given in 1943 by Fejes Tóth

$$d \le \sqrt{4 - \operatorname{cosec}^2 \left[\frac{\pi N}{6(N-2)}\right]} \tag{11.2}$$

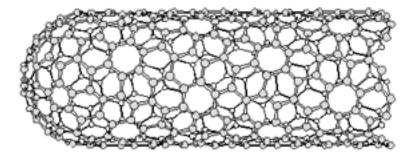
with the limit exact for N = 3, 4, 6 and  $12^8$ .

#### 11.7 Helical packings

The packing of spheres around a cylinder results in helical patterns, which may often be seen in street festivals when balloons are used to decorate lamposts. These attractive structures have an interesting history because they are found in many plants. Botanists have long been fascinated by the way in which branches or

<sup>&</sup>lt;sup>7</sup> Croft H T, Falconer K J and Guy R K 1991 Unsolved Problems in Geometry (New York: Springer) p 108.

Ogilvy C S 1994 Excursions in Mathematics (New York: Dover) p 99.



**Figure 11.5.** Carbon crystals make tubular structures called 'nanotubes'. In the tubular part carbons make a network with rings of six atoms, whereas the positive curvature is induced by rings of five atoms.

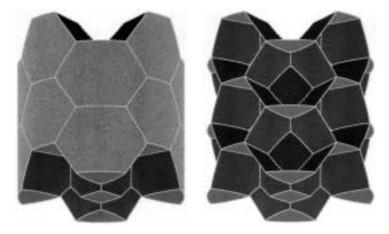
leaves are disposed along a stem, or petals in flower. They have found many different helical arrangements, but almost all have a strange mathematical property, which is the main preoccupation of much of the extensive literature on this subject, at times acquiring a mystical flavour. This dates back (at least) to Leonardo. In the 19th century, the Bravais brothers, and later Airy and Tait began a more modern study, which surprisingly continues today. The reviewer of a recent book by Roger Jean, said that it 'remains one of the most striking phenomena of biology'.

Recently the subject has recurred in an exciting new context—the creation of nanotubes, which are tiny tubes with walls which are a single layer of carbon atoms. They are first cousins to the 'buckyballs' (see section 11.3). They were first made in the 1970s by Morinobu Endo, a PhD student at the University of Orleans.

Biologists call this subject 'phyllotaxis', and obscure it further with terms such as 'parastichies', which are rather repellent to the first-time reader. But these helical structures are really quite simple things. If we are to place spheres or points on the surface of a cylinder, it is much the same as placing them on a plane. We therefore expect to find the close-packed triangular arrangement of chapter 2, which is optimal under a variety of conditions. The difference lies in the fact that the surface is wrapped around the cylinder and joins with itself. It is like wallpapering a large pillar—the packing must continue smoothly around the cylinder, without interruption.

We could think of cutting out a strip from the triangular planar packing and wrapping it around the cylinder. We might have to make some adjustments to avoid a bad fit where the edges come together. We can displace the two edges with respect to each other and/or uniformly deform the original pattern (not easy with wallpaper!), in order to have a good fit.

Let us reverse this train of thought: roll the cylinder across a plane, 'printing' its surface pattern again and again. We expect to get the close-packed pattern, or a



**Figure 11.6.** Bubbles packed in a cylinder show the familiar hexagonal honeycomb wrapped on a cylinder. This simulation by G Bradley shows surface patterns and the interior for one of these structures.

strained version of it. The three directions of this pattern, in which the points line up, correspond to helices on the cylinder. Taking one such direction, how many helices do you need to complete the pattern? This defines an integer, and the three integers k, l, m corresponding to the three directions can be used to distinguish this cylindrical pattern from all others. It is easily seen that two of these must add to give the third integer.

This is the notation of phyllotaxis, applied to plants, to nanotubes and to bubble packings within cylinders. In the last case, the surface structure is always of this close-packed form.

# Packings and kisses in high dimensions

#### 12.1 Packing in many dimensions

The world of mathematics is not confined to the three dimensions of the space that we inhabit. Mathematicians study sphere-packing problems in spaces of arbitrary dimension. Geometrical puzzles can be posed and solved in such spaces. Some practical challenges end up in such a form.

With this chapter we present a short excursion into some of the relevant points concerning packings of spheres in high dimensions and their applications. The topic is explored in a very comprehensive way by Conway and Sloane in their book *Sphere Packings, Lattices and Groups*<sup>1</sup>, which is considered the 'bible' of this subject.

Packings in many dimensions find applications in number theory, numerical solutions of integrals, string theory, theoretical physics and digital communications. In particular, some problems in the theory of communications, with a bearing on the optimal design of codes, can be expressed as the packing of *d*dimensional spheres. Indeed, in signal processing it is convenient to divide the whole information into uniform pieces and associate each piece with a point in a *d*-dimensional space (a point in a *d*-dimensional space is simply a string of *d* real numbers  $\{u_1, u_2, u_3, \ldots, u_d\}$ ). To transmit and recover the information in the presence of noise one must ensure that these points are separated by a distance larger than that at which the additional noise would corrupt the signal. Each point (encoded information) can be seen as surrounded by a finite volume, a *d*dimensional ball with a diameter larger than the additional noise. The encoded

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<sup>&</sup>lt;sup>1</sup> Conway J H and Sloane N J A 1988 Sphere Packings, Lattices and Groups (Berlin: Springer).

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information can be reliably recovered only if these balls are non-overlapping. An efficient coding, which minimizes the energy necessary to transmit the information, organizes these balls in the closest possible packing around the origin. Therefore, the problem relates back to the greengrocer dilemma: *how to arrange these balls most tightly? Which is the maximum density of a packing of solid spheres in d dimensions?* 

It might be thought that this journey into many dimensions might be uneventful: *if you've seen one such space, you've seen them all?* Surely some simple generalization of the close-packing strategy which works in three dimensions can be successfully extended? Not so. The possibilities are much richer than this and include some startling special cases. Who would have thought that dimensions 8 and 24 are very special? In these cases structures of particularly high density can be found. The eight-dimensional one is called  $E_8$  and dates from the last century, while the 24-dimensional one was discovered by J Leech of Glasgow in 1965. New dense structures, indeed whole families of them, continue to be constructed. For example, in 1995, A Vardy announced a new packing record for 20 dimensions.

We have already seen in chapter 3 how close-packed hexagonal layers of spheres may be stacked to generate the face-centred cubic lattice, the one described by Kepler as 'the most compact solid'. This is the regular packing with the highest density in three dimensions. This procedure also works in many dimensions: *d*-dimensional compact structures are often stacked one upon the other (or laminated) making an (d + 1)-dimensional packing. There are some special dimensions where these laminated lattices have remarkable properties in terms of density and symmetry. A very special one is d = 24, the laminated lattice for which is the one discovered by Leech in 1965. It has a density of  $\rho = 0.00193...$  and it is conjectured to be the densest *lattice* packing in 24 dimensions. This packing is highly symmetrical and the symmetry group associated to it has fundamental importance in the history of group theory. Indeed, the discovery of the Leech lattice in 1968 resulted in the discovery of three new simple groups.

Group theory is an abstract branch of mathematics which is closely tied to practical applications throughout physics. Simple groups make a special finite class of groups from which any finite group can be built up. The largest simple group, the 'Monster', was constructed by R L Griess in 1981 using the Leech lattice. The classification of all simple groups was finally completed in 1982 after having involved the work of many mathematicians for over 50 years.

Low-dimensional sections of the Leech packing produce laminated packing in dimensions d < 24 but curiously they also produce non-laminated ones. Among them is the K<sub>12</sub> lattice first described by Coxeter and Todd in 1954, which is likely to be the densest lattice packing in d = 12.

It has been proved that the laminated lattices ( $\Lambda_d$ ) are the densest lattice packings up to dimension d = 8. They are the densest known up to dimension 29 except for d = 10, 11, 12, 13 and it seems likely that  $K_{12}, \Lambda_{16}$  and  $\Lambda_{24}$  (the Leech

Dimension d	Density $\rho$	Lattice
0	1	$\Lambda_0$
1	1	$\Lambda_1, Z$
2	$\frac{\pi}{2\sqrt{3}} = 0.906\dots$	$\Lambda_2, A_2$
3	$\frac{\pi}{3\sqrt{2}} = 0.740\dots$	$\Lambda_3, A_3$
4	$\frac{\pi^2}{16} = 0.616\dots$	$\Lambda_4, D_4$
5	$\frac{\pi^2}{15\sqrt{2}} = 0.465\ldots$	$\Lambda_5, D_5$
6	$\frac{\pi^3}{48\sqrt{3}} = 0.372\dots$	$\Lambda_6, E_6$
7	$\frac{\pi^3}{105} = 0.295\dots$	$\Lambda_7, E_7$
8	$\frac{\pi^4}{384} = 0.253\dots$	$\Lambda_8, E_8$
12	$\frac{\pi^6}{19440} = 0.0494\dots$	$K_{12}$
16	$\frac{1}{16} \frac{\pi^8}{8!} = 0.0147\ldots$	$\Lambda_{16}$
24	$\frac{\pi^{12}}{12!} = 0.00193\ldots$	$\Lambda_{24}$

Table 12.1.

lattice) are the densest in dimensions 12, 16 and 24. (See table 12.1, courtesy of Conway.)

Note that even in the 'very dense' 24-dimensional Leech lattice, the volume occupied by the spheres is less than 0.2% of the total. Indeed the density of sphere packings tends to zero as the dimension goes to infinity.

'Packings of Spheres Cannot be Very Dense' is the title given by C A Roger to a chapter of his book *Packing and Covering* (1964) where he calculates a bound for the density of sphere packings in any dimension. His bound is calculated from the generalization to high dimensions of the three-dimensional case of four spheres in mutual contact with centres on the vertices of a regular tetrahedron (section 3.10). In *d* dimensions this configuration is made of d + 1 mutually contacting spheres. In the large *d* limit it has density

$$\sigma_d \sim \frac{d}{e} \left(\frac{1}{\sqrt{2}}\right)^d.$$
 (12.1)

These local configurations of d + 1 spheres cannot be tightly assembled in the *d*-space. Some interstices always remain and so  $\sigma_d$  is an upper bound for the density of *d*-dimensional sphere packings.

Other more restrictive bounds have been given during the years. Summarizing these results, the density of the closest d-dimensional packing is between the bounds

$$2^{-d} \lesssim \rho \lesssim (1.5146...)^{-d}$$
 (12.2)

for large d. One can see that when the dimension increases by 1, the density of the closest packing (lattice or non lattice) is divided by a number between 2 and 1.546... and therefore goes rapidly to zero when d increases.

#### Magic dimensions

To understand why there are magic dimensions for which very special lattice packings appear, let us consider the simple case of the hypercubic lattice packing. In this packing, spheres with unit radius are placed with the centres at positions  $(2u_1, 2u_2, \ldots, 2u_d)$  where  $u_i$  are integer numbers. In two dimensions this is the square lattice packing, and the elementary local configuration is a set of four spheres with the centres on the vertices of a square. In d dimensions the elementary local configuration of this packing is a *d*-dimensional hypercube with  $2^d$  spheres on its vertices. It is easy to see that infinite copies of this local configuration form the whole packing. Each interstice between the  $2^{d}$  spheres can accommodate a sphere with maximum radius  $\sqrt{d} - 1$ . In two dimensions this radius is  $\sqrt{2} - 1 \sim 0.41$ , in three dimensions it is  $\sqrt{3} - 1 \sim 0.73$ , but in four dimensions this radius is  $\sqrt{4} - 1 = 1$ , which means that the sphere inserted in the interstice inside the cube can have the same unit radius of the external ones. Now, two copies of the cubic packing can be fitted together without overlap to form a new lattice packing with a density that is double the original one. This is known as checkerboard lattice D<sub>4</sub>, and is the densest lattice in four dimensions. In this packing the spheres have centres in the points (0, 0, 0, 0), (1, 1, 0, 0), (1, 0, 1, 0).... In general in a packing  $D_d$  the spheres have centres in  $(u_1, u_2, u_3, u_4, \ldots)$  where the  $u_i$  are integers that add to an even number.

It is the doubling possibility that renders special the dimensions 8 and 24. Indeed, in d = 8 the packing D<sub>8</sub> can be doubled in two copies that fit together making the lattice packing E<sub>8</sub>, the densest in d = 8. Analogously, in 24 dimensions it is a doubling of a particular lattice packing associated with the Golay code that forms the Leech lattice packing.

#### 12.2 A kissing competition

How many spheres can be placed around a given sphere, such that they are all of the same size and touch the central one? Mathematicians often refer to such contact as 'kissing'. This was the topic of a famous discussion between Isaac Newton and David Gregory in 1694. Newton believed that the answer was 12, as in the compact packing of Kepler, while Gregory thought that 13 was possible. The problem is not simple. The solid angle occupied by an external sphere is less than 1/13 of the total and the volume around the central sphere which is available to touching spheres is, in principle, sufficient to contain the volumes of 13 spheres<sup>2</sup>. But the correct answer is 12.

 $<sup>^2</sup>$  In fact, the fraction is 1/13.397 33..., the same number which appears in the lower bound on the average number of cells in a foam of minimal surfaces (chapter 7).

Kissing number $\tau$	Dimension $d$
2	1
6	2
12	3
25	4
46	5
82	6
140	7
240	8
380	9
595	10
196 560	24

**Table 12.2.** Known lower bounds for the kissing numbers up to dimension 10 and for d = 24. Boldface indicates bounds which are realized.

Note that a configuration of 13 spheres around a central one makes a very compact packing without quite achieving contact of all spheres with the central one. This is one of the local configurations that locally pack more tightly than the Kepler bound (chapter 3).

The 12 spheres can be disposed in the rhombic dodecahedron configuration, in the icosahedral arrangement (where the 12 spheres are separated from each other and touch only the central one) or in the pentahedral prism (with two spheres at the north and south poles and five spheres around each of them). The first configuration is the most compact global packing (the Kepler close packing). The other two are packings that are *locally* more dense than the first one but that cannot be continued in the whole space.

#### 12.3 More kisses

As Newton and Gregory did for three dimensions, one can ask which is the greatest value of the kissing number ( $\tau$ ) that can be attained in a *d*-dimensional packing of spheres. In one dimension the answer is clearly two, in two dimensions it is six and in three dimensions the answer is 12. The answer is unknown for dimensions above three except for d = 8 and d = 24. In eight dimensions spheres arranged in the lattice packing E<sub>8</sub> touch 240 neighbours, and in 24 dimensions each sphere kisses 196 560 neighbours in the Leech lattice  $\Lambda_{24}$ . (See table 12.2.)

In dimension d = 4 the highest known lower bound is 25. Dimension d = 9 is the first dimension in which non-lattice packings are known to be superior to lattice packings. Here,  $\Lambda_9$  has  $\tau = 272$  whereas the best bound known is 380. Remember that the kissing number question aims to find the best *local* configu-

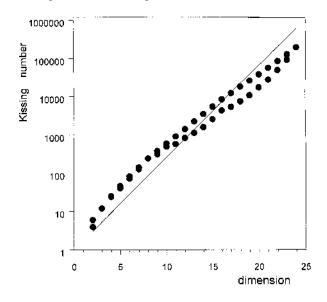


Figure 12.1. Known kissing numbers and the Kabatiansky and Levenshtein bound.

ration (one sphere and its surroundings) while the sphere packing problem is a *global* problem.

An upper bound for the attainable kissing numbers in high dimensions has been calculated by Kabatiansky and Levenshtein who showed that

$$\tau \le 2^{0.401d[1+o(1)]} \tag{12.3}$$

(where o(1) indicates and unknown number which must have a value of *order* 1).

In figure 12.1 the values of  $\tau$  for configurations with a high kissing number are reported together with the Kabatiansky and Levenshtein bound with exponent fixed at 0.802d.

## **Odds and ends**

#### 13.1 Parking cars

That parking can pose problems should come as little surprise to most of us.

For example, imagine a parking space of length x where cars of unit length are parked one by one, completely at random. What, on average, is the maximum number of cars M(x) that can find a place in this space (without overlapping between cars)?

It is always possible to obtain a packing fraction of one by systematically putting each segment (car) in contact with two others. But if the segments are disposed in a random way without overlapping and readjustment, then after a certain stage the line has no remaining spaces large enough to accommodate another segment.

When cars are parked at random, Rényi<sup>1</sup> determined an integro-functional equation that gives M(x) in an implicit form. In the limit of an infinitely large parking space the resulting packing fraction is

$$\rho \to 0.7475\dots \tag{13.1}$$

The packing fraction  $\rho$  and the average of the maximum number of cars are simply related according to  $M(x) = \rho x$ .

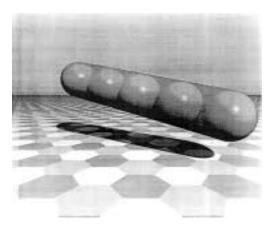
If the random packing is modified so that a car arriving can move slightly (up to half segment length) in order to create an available space, then the packing fraction increases to 0.809.

In the analogous two-dimensional problem, objects with a unit square shape are placed in a rectangular parking lot. In this case no exact results are available.

<sup>&</sup>lt;sup>1</sup> Rényi A 1958 On a one-dimensional problem concerning random space-filling *Publ. Math. Inst. Hung. Acad. Sci.* **3** 109–27.

<sup>119</sup> 

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**Figure 13.1.** Sausage packing of five balls. (Courtesy of J M Wills, University of Siegen, Germany.)

Palasti (1960) conjectured that the two-dimensional packing fraction has the same value  $\rho = 0.7475...$  as in the one-dimensional case. But this conjecture remains unproved and computer simulations suggest that the packing fraction is slightly higher than the conjectured value.

#### 13.2 Stuffing sausages

All packings in the real world are finite, even atoms in crystals or sand at the beach. Finite packing problems have boundaries. This makes their solution more difficult than for infinite packings.

#### **Optimal box for discs**

How may we arrange N unit discs so as to minimize the area of the smallest convex figure containing all discs (the convex hull)? It has been shown for all  $N \leq 120$  and for  $N = 3k^2 + 3k + 1$ , that the convex hull tends to be as hexagonal as possible<sup>2</sup>.

#### The sausage conjecture

The analogous problem in three dimensions is: how to arrange N unit spheres so as to minimize the volume of the smallest convex figure containing all spheres? For  $N \leq 56$  the best arrangements are conjectured to be 'sausages' (the centres of the spheres all along a straight line). But larger N convex hulls with minimum

<sup>&</sup>lt;sup>2</sup> Wegner G 1986 Über endliche Kreispackungen in der Ebene Stud. Sci. Math. Hungar. pp 1–28.

volume tend to be associated with more rounded clusters. This might be called the sausage-haggis transition.

For dimension d = 4 it has been shown that the 'sausage' is the best solution for N up to at least 377 000<sup>3</sup>. The Sausage Conjecture states that for  $d \ge 5$ the arrangement of hyperspheres with a minimal volume convex hull is always a 'sausage'<sup>4</sup>.

#### 13.3 Filling boxes

When objects are packed in spaces of finite size and of given shape, new questions arise. How many objects can be put inside a given box? Or equivalently, how big must a box be to contain a given set of objects? Which is the best arrangement and what is the density of this packing? Is the solution unique?

Let us consider the two-dimensional case first.

#### Discs in a circular box

Which is the smallest diameter a of a circle which contains N packed discs of diameter 1? The answer to this question is known up to N = 10 and conjectures are given for N up to 19. For N = 1 the solution is clearly a = 1. For  $2 \le N \le 6$  the answer is  $a = 1 + 1/\sin(\pi/N)$ , and it is  $a = 1 + 1/\sin(\pi/(N-1))$  for  $7 \le N \le 9$ . Whereas for N = 10 one finds a = 7.747...

#### Discs in a square

An analogous problem is to find the smallest size of the square containing N packed unit circles. Exact results are known for  $N \leq 9$  and N = 14, 16, 25, 36. Conjectures have been made for  $N \leq 27$ .

For large N one has the approximate expression  $a \simeq 1 + \frac{1}{2} 12^{1/4} N^{1/2}$ . In such a packing the density is, therefore,

$$\rho = \frac{\pi N}{4a^2} \simeq \frac{\pi}{\sqrt{12}} - \frac{\pi}{3\sqrt{\sqrt{12}N}}$$
(13.2)

which tends to the density of the hexagonal lattice for large N.

It turns out that for small N the hexagonal arrangement is not the best. Square packing is better adapted to the square symmetry of the container and it results in a denser packing certainly for  $N \le 36$  and probably up to  $N = 49^5$ .

<sup>&</sup>lt;sup>3</sup> Gandini P M and Zucco A 1992 On the sausage catastrophe in 4-space *Mathematika* **39** 274–8.

<sup>&</sup>lt;sup>4</sup> See Croft H T, Falconer K J and Guy R K 1991 *Unsolved Problems in Geometry* (New York: Springer); Wills J M 1998 Spheres and sausages, crystals and catastrophes—and a joint packing theory *Math. Intell.* **20** 16–21.

<sup>&</sup>lt;sup>5</sup> See for general reference Melisson H 1997 *Packing and Covering with Circles* (Proefschrift Universiteit Utrecht, Met lit. opy.).

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Beer distributors should look into hexagonal packings now that they sell cases of 18 or more cans: the superiority of square packing is not clear for *rect-angular* boxes<sup>6</sup>. (See table 13.1, from Croft<sup>7</sup>.)

**Table 13.1.**  $a = 1 + 1/d_N$  where is the  $d_N$  minimal separation between the N points in a unit square.

N	a (side of the square)
1	1
2	$1 + \frac{1}{\sqrt{2}}$
3	$\begin{array}{l} 1 + \frac{1}{\sqrt{2}} \\ 1 + \frac{1}{(\sqrt{2}(\sqrt{3} - 1))} \end{array}$
4	2
5	$1 + \sqrt{2}$
6	$1 + \frac{6}{\sqrt{13}}$
7	$ \begin{array}{r}1 + \frac{6}{\sqrt{13}} \\ 1 + \frac{1}{2(2-\sqrt{3})} \end{array} $
8	$1 + \frac{\sqrt{2}}{\sqrt{3}-1}$
9	3
14	$1 + \frac{3}{\sqrt{6} - \sqrt{2}}$
16	4
25	5
36	6

#### **13.4** Goldberg variations

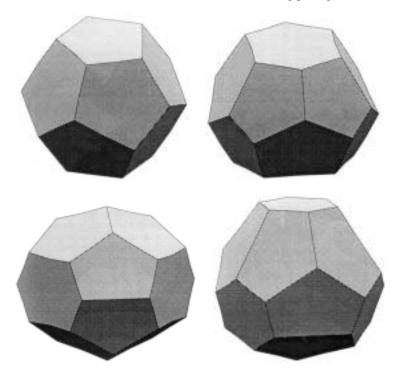
The sphere minimizes the surface area for a fixed volume, as the soap bubble teaches us. In three-dimensional packing problems we need to consider shapes which fit together to fill space, and the problem of minimizing surface area is not so easy. One interesting clue to the best strategy was provided by Michael Goldberg in 1934.

Goldberg restricted himself to the case of a single polyhedron (not necessarily space filling) with N planar sides. What kind of polyhedron is best, in terms of area?

He conjectured that the solution always has threefold (or trivalent) vertices. Bearing in mind the ideal of a sphere, it is attractive to conjecture that the solution is always a regular polyhedron, that is, one with identical faces. This is not always possible. Goldberg's conjecture, supported by a good deal of evidence, states that the solution is always at least close to being regular, in the sense of having only faces with n and n + 1 edges.

 $<sup>\</sup>frac{6}{18}$  18 discs can be hexagonally packed in a pattern made of five lines of 4, 3, 4, 3, 4 inside a rectangular box.

<sup>&</sup>lt;sup>7</sup> Croft H T, Falconer K J and Guy R K 1991 Unsolved Problems in Geometry (New York: Springer).



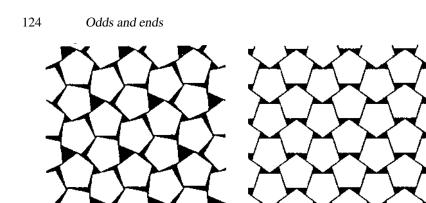
**Figure 13.2.** Goldberg polyhedra for N = 12, 14, 15 and 16. They are the building-blocks of the Weaire–Phelan and other foam structures (chapter 7).

In particular, the solutions for N = 12 and 14 are as shown in figure 13.2. Although there is no rigorous chain of logic making a connection with the Weaire– Phelan structure (chapter 7), it turns out to be the combination of these two Goldberg polyhedra.

#### **13.5** Packing pentagons

Pentagons cannot be packed together, without leaving some free space. What is the maximum packing fraction that can be achieved?

There are several obvious ways of arranging the pentagons in a periodic structure. Figure 13.3 shows two of the densest ones. The structure with packing fraction 0.92 is thought to be the densest, and it has been found in the air-table experiments of the Rennes group (section 2.2).



**Figure 13.3.** Two dense packings of pentagons, with packing fractions 0.864 65 (*a*) and 0.921 31 (*b*).

*(b)* 

#### 13.6 Dodecahedral packing and curved spaces

(a)

Consider a (not necessarily ordered) packing of equal spheres. Construct around any sphere the Voronoï cell (the polyhedron in which the interior consists of all points of the space which are closer to the centre of the given sphere than to any other, chapter 2). It was conjectured and proved very recently by Hales and McLaughlin that the volume of any Voronoï cell around any sphere is at least as large as a regular dodecahedron with the sphere inscribed. This provides the following bound for the densest local sphere packing

$$\rho \le \rho_{\text{dodecahedron}} = \frac{V_{\text{sphere}}}{V_{\text{dodecahedron}}} = \pi \frac{\sqrt{5 + \sqrt{5}}}{5\sqrt{10}(\sqrt{5} - 2)} = 0.7547\dots$$
 (13.3)

This is 1% denser than the Kepler packing but this is a local arrangement of 13 spheres that cannot be extended to the whole space. Indeed, regular dodecahedra cannot be packed in ordinary space without gaps.

The situation is similar to that for pentagons in two dimensions. Regular pentagonal tiles cannot cover a floor without leaving any interstitial space. However, in two dimensions one can immediately see that this close packing can be achieved by curving the surface. The result is a finite set of 12 closely packed pentagons that tile the surface of a sphere making a dodecahedron. Analogously, in three dimensions, regular dodecahedra can closely pack only in a positively curved space. In this case regular dodecahedra pack without gaps making a closed structure of 120 cells which is a four-dimensional *polytope* (that is a *polyhedron* in high dimensions)<sup>8</sup>.

<sup>&</sup>lt;sup>8</sup> See for general reference: Sadoc J F and Mosseri R 1997 *Frustration Géométrique* (Paris: Éditions Eyrolles).

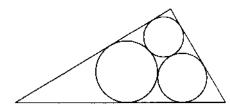


Figure 13.4. Malfatti's solution to the problem.

It started with liquids, you know. *They* didn't understand liquids. Local geometry is non-space-filling. Icosahedra. Trigonal bipyramids. Oh, this shape and that shape, lots of them. More than the thirty-two that fill ordinary space, let me tell you. That's why things are liquid, trying to pack themselves in flat space, and that's what I told *them*.

*They* couldn't deal with it. *They* wanted order, predictability, regularity. Silly. Local geometry can be packed, I said, just not in flat space. So, I said, give them a space of constant curvature and they'll pack. All *they* did was laugh. I took some liquids to a space of constant negative curvature to show *them* it would crystallize, and it sucked me up. (Tepper S S *Mavin Manyshaped* (New York: Ace Fantasy Books).)

#### **13.7** The Malfatti problem

A parsimonious sculptor wants to cut three cylindrical columns from a piece of marble which has the shape of a right triangular prism. How should he cut it in order to waste the least possible amount of marble? The problem is equivalent to that of inscribing three circles in a triangle so that the sum of their areas is maximized.

In 1802 Gian Francesco Malfatti (1731–1807) gave a solution to this problem which thereafter bore his name. Previously Jacques Bernoulli had given a solution for a special case. In due course other great mathematicians were attracted to it, including Steiner and Clebsch. Malfatti assumed that the three circles must be mutually tangent and each tangent to only two sides of the triangle. Under this assumption the Malfatti solution follows as in figure 13.4.

The problem was considered solved and for more than 100 years nobody noticed that the Malfatti arrangement shown in figure 13.4 is not the best. For instance, for an equilateral triangle, the solution of figure 13.5(a) is better than Malfatti's one shown in figure 13.5(b). Howard Eves (1965) observed that if the

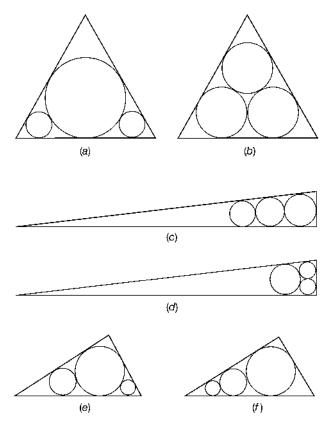


Figure 13.5. Solutions to the Malfatti problem.

triangle is elongated, three circles in line (as in figure 13.5(c)) have a much greater area than those of figure 13.5(d).

Finally in 1967, Michael Goldberg showed that the Malfatti configuration is *never* the solution, whatever the shape of the triangle! The arrangements in figure 13.5(e,f) are always better. Goldberg arrived at this conclusion by using graphs and calculations. A full mathematical proof has yet to be produced <sup>9</sup>.

#### **13.8** Microspheres and opals

Oranges do not spontaneously form close-packed ordered structures but atoms sometimes do. Where is the borderline between the static world of the oranges and the restless, dynamic one of the atoms, continually shuffled around by thermal

<sup>&</sup>lt;sup>9</sup> From Stanley Ogilvy C 1969 *Excursion in Geometry* (New York: Dover) p 145; 1932 *Periodico di Mathematiche* **12** (4th series) is a complete review.

energy-between the church congregation and the night-club crowd?

At or near room temperature, only objects of size less than about 1  $\mu$ m are effective in exploring alternatives, and perhaps finding the best. A modern industry is rapidly growing around the technology of making structures just below this borderline, in the world of the 'mesoscopic' between the microscopic and the macroscopic.

In one such line of research, spheres of diameter less than a micrometre are produced in large quantities and uniform size using the reaction chemistry of silica or polymers. Such spheres, when placed in suspension in a liquid, may take many weeks to settle as a sediment. When they do so, a crystal structure is formed—none other than the fcc packing of earlier chapters. This crystallinity is revealed by striking optical effects, similar to those which have been long admired in natural opal.

Natural opals are made of silica spheres of few hundred nanometres  $(1 \text{ nm} = 10^{-9} \text{ m})$  in size, packed closely in an fcc crystalline array. Opals are therefore made of a very inexpensive material but they are valued as gemstones because their bright colours change with the angle of view. This iridescence is due to the interference of light which is scattered by the ordered planes of silica spheres. Indeed the size of these spheres is typically in the range of visible light wavelength (430–690 nm).

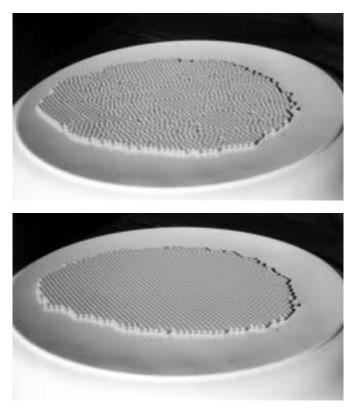
An important goal of present research in material science is the creation of artificial structures with such a periodicity, in order to tailor their optical properties. Several studies begun in the late 1980s showed that a transparent material can become opaque at certain frequencies provided that a strong and periodic modulation of the refractive index is imposed in space. Structures with these properties have been constructed for microwave radiation but, until recently, not for visible light. With conventional microelectronic techniques it is very difficult to shape structures below 1000 nm (which is 1  $\mu$ m). Artificial opals provide the right modulation in the diffraction index, opening the way to the construction of new 'photonic band gap' materials. Photonic crystals are the ingredients for future optical transistors, switches and amplifiers, promising to become as important to the development of optical devices as semiconductors have been to electronics.

#### 13.9 Order from shaking

A home-made experiment of spontaneous crystallization can easily be performed in two dimensions by putting small beads on a dish and gently shaking it. The result is the triangular arrangement shown in figure 13.6.

Large spheres in a box are not so easily persuaded to form a crystal, but nevertheless shaking them can have interesting effects.

It was observed in the 1960s that repeated shear or shaking with both vertical and horizontal motion can increase the density of the packing. Recently a density of 0.67 was obtained in a packing of glass beads of about 2 mm in diameter slowly



**Figure 13.6.** Spontaneous 'crystallization' into the triangular packing induced by the shaking of an initially disordered arrangement of plastic spheres on a dish.

poured into a container subject to horizontal vibrations <sup>10</sup>. This packing consists of hexagonal layers stacked randomly one upon the other with few defects. Spontaneous crystallization into regular fcc packing was also obtained when the starting substrate was forced to be a square lattice.

This packing has the minimum potential energy under gravity. The system spontaneously finds this configuration by exploring the possible arrangements under the shaking. The slow pouring lets the system organize itself layer upon layer. This is analogous to what happens in the microspheric suspensions of a previous section where the sedimentation is very slow and the shaking is provided by thermal motion.

<sup>&</sup>lt;sup>10</sup> Pouliquen O, Nicolas M and Weidman P D 1997 Crystallization of non-Brownian Spheres under horizontal shaking *Phys. Rev. Lett.* **79** 3640–3.

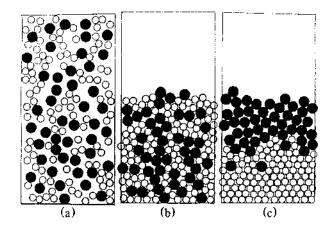


Figure 13.7. Why are Brazil nuts always on top?

### 13.10 Segregation

Sorting objects of miscellaneous size and weight is a key industrial process. Filtration, sieving or flotation may be used. With granular materials it is often enough to shake the mixture for some time. This must be done judiciously; vigorous shaking (as in a cement mixer) will produce a uniform mixture. Gentle agitation, on the other hand, can promote the segregation of particles of different sizes. The result is quite surprising: the larger, heavier objects tend to rise! This seems an offence against the laws of physics but it is not. That is not to say that it is easily explained. Numerous research papers, including the teasingly entitled 'Why the Brazil Nuts are on Top' have offered theories<sup>11</sup>.

Figure 13.7 shows a simulation of the effect. It is thought to be essentially geometric: whenever a large object rises momentarily, smaller ones can intrude upon the space beneath. Such an explanation calls to mind the manner in which many prehistoric monuments are thought to have been raised. Note that the energy increases as the Brazil nut is raised, contradicting intuition and naive reasoning. This is not forbidden, because energy is being continuously supplied by shaking.

By slowly pouring a mixture of two kinds of grain of different sizes and shapes between two narrow layers of glass, one can observe that the grains separate or, under some circumstances, stratify into triangular strips (see figure 13.8). Large grains are more likely to be found near the base of the pile whereas the smaller are more likely to be found near the top. The phenomenon is observable for mixtures of grains in a wide range of size ratios (at least between 1.66 to 6.66

<sup>&</sup>lt;sup>11</sup>Rosato A, Strandburg K J, Prinz F and Swendsen R H Why the Brazil nuts are on top: size segregation of particular matter by shaking *Phys. Rev. Lett.* **58** 1038.



**Figure 13.8.** Segregation and stratification in a granular mixture of brown and white sugar poured between two glass plates.

as reported by Makse *et al*<sup>12</sup>). When the large grains have a greater angle of repose<sup>13</sup> with respect to the small grains then the mixture stratifies into triangular strips. (This can be achieved by making the small grains smooth in shape and the large grains more faceted.) For instance, a mixture of white and brown sugar works well for this purpose.

Fineberg has suggested that Cinderella could have utilized this spontaneous separation phenomenon (instead of help from the birds) when the step-sisters threw her lentils into the ashes of the cooking fire.

#### 13.11 Turning down the heat: simulated annealing

If a suit is to be made from a roll of cloth, how should we cut out the pieces in such a way as to minimize wastage? This is a packing problem, for we must come up with a design that squeezes all the required shapes into the minimum area.

No doubt tailors have had traditional rules-of-thumb for this but today's automated clothing industry looks for something better. Can a computer supply a good design?

This type of problem, that of optimization, is tailor-made for today's powerful computers. The software which searches for a solution does so by a combination of continual small adjustments towards the desired goal, and occasional

<sup>&</sup>lt;sup>12</sup> Makse H A, Halvin S, King P R and Stanley E 1997 Spontaneous stratification in a granular mixture *Nature* **386** 379–82; Fineberg J 1997 From Cinderella's dilemma to rock slides *Nature* **386** 323–4.

 $<sup>^{13}</sup>$ The angle of repose is the maximum angle of slope in a pile of sand, beyond which it suffers instability in the form of avalanches.



Figure 13.9. Propagation of stress lines in a disordered packing of discs.

random shuffling of components in a spirit of trial and error—much the way that we might use our own intelligence by a blend of direct and lateral thinking.

A particularly simple strategy was suggested in 1983 by Scott Kirkpatrick and his colleagues at IBM. Of course, IBM researchers are little concerned with the cutting (or even the wearing) of suits, but they do care passionately about semiconductor chip design, where a tiny competitive advantage is well worth a day's computing<sup>14</sup>. The components in microchips and circuit boards should be packed as tightly as possible, and there are further requirements and desired features which complicate the design process.

The research in question came from the background of solid state physics. Nature solves large optimization problems all the time, in particular when crystals grown as a liquid are slowly frozen. Why not think of the components of the suit or the chip as 'atoms', free to bounce around and change places according to the same spirit of laws which govern the physical world, at high temperatures? Then gradually cool this imaginary system down and let it seek an optimum arrangement according to whatever property (perhaps just density) is to be maximized.

This is the method of 'simulated annealing', the second word being taken

<sup>&</sup>lt;sup>14</sup> Kirkpatrick S, Gelatt C D and Vecchi M P 1983 Optimization by simulated annealling *Science* **220** 671.

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from the processing of semiconductors, which are often heated and gradually cooled, to achieve perfection in their crystal structure.

The idea was simple and it is relatively straightforward to apply—so much so that incredulous circuit designers were not easily persuaded to try it. Eventually it was found to be very effective, and hence it has taken its place among the optimizer's standard tools. Its skilful use depends on defining a good 'annealing schedule', according to which the temperature is lowered.

The mathematical background to these large and complicated optimization problems is itself large and complicated. Complexity theory often offers the gloomy advice that the optimum solution cannot be found in any practical amount of time, by any program. But, unlike the pure mathematician, the industrial designer wants only a very good packing, not necessarily the best. Beyond a certain point, further search is pointless, in terms of profit. As Ogden Nash said: 'A good rule of thumb, too clever is dumb'.

## Conclusion

We stated at the outset that examples of packing would be drawn from a wide field of mathematics, science and technology. Have we revealed enough connections between them to justify their juxtaposition within the same covers? Recall the recurrence of the greengrocer's stacking in the search for dense lattices in higher dimensions and the threefold interconnection of metallic alloys, chemical compounds and the ideal structure of foam. Such was the doctrine of Cyril Stanley Smith (1903–92), who called himself a 'philomorph' or lover of form. He was fascinated by such similarities. This is no mere aesthetic conceit: it gives power to the method of *analogy* in science. Smith rebelled against the narrow orthodoxies of conventional science. He saw in materials a richness of form, upon which he speculated in terms of complexity, analogy, hierarchy, disorder and constraints.

If we have given offence to any specialist in this attempt to follow the example of Smith, by over-simplification or neglect, we are sorry for that. Scientists, he said, should be allowed to play, and we would rest our case on that.

Smith would have enjoyed being on a bus taking a party of physicists (which included several philomorphs) to the airport after a conference in Norway in 1999. A brief 'comfort stop' was planned at a motorway service station which included a small shop. Several of the party disappeared for a time. They had discovered something remarkable in the shop—a close packing of identical tetrahedral cartons! This clever arrangement is possible only because it uses slightly flexible cartons and the container (which has an elegant hexagonal shape) is finite. We would like to give the details but the bus had to leave for the airport...

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