A Short History of Packing Problems

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Abstract. Packing problems have arisen throughout the history of science. In particular the problem of the densest close packing of spheres has become celebrated as the Kepler Problem. The history of the subject is briefly reviewed, from both mathematical and physical (or practical) standpoints.

1. Introduction

This article is based on a recent book which reviews sphere packings of all kinds (WEAIRE and ASTE, 1999); more detailed references can be found therein.

In the story of man's search for an understanding of the constitution and structure of matter, many forms have been ascribed to its constituents. At one extreme, the followers of Descartes accepted imaginative descriptions of individual atoms, endowed with special shapes and appendages to account for their chemical properties. As Newton said, such speculations were often "Begging the Question". Physics was not sufficiently developed to test them.

At the other extreme stands the school of Boscovich, which reduced the atom to a mere mathematical point and sought to explain the properties of matter in terms of interactions between these points. Somewhere between the two lie the ideas of Haüy and others, which ascribed to each constituent, perhaps an atom or molecule, the shape of a paralleliped. This accounted for the shape of a crystal in terms of a similar shape for its basic building blocks (BURKE, 1966): Fig. 1.

One recurrent theme which had the merit of great simplicity was that of the atom as a hard sphere (Fig. 2). It led to conjectures about sphere packings which are still debated today, and it is still a useful ingredient in materials science. Atoms in solids often take up the structures which suggest themselves in a study of packed spheres. Even though we can today resort to large computers to predict equilibrium structures of solids in a reliable and respectable manner, the mental picture of packed spheres is inescapable as a simple rationalisation of many of them, and so it persists.

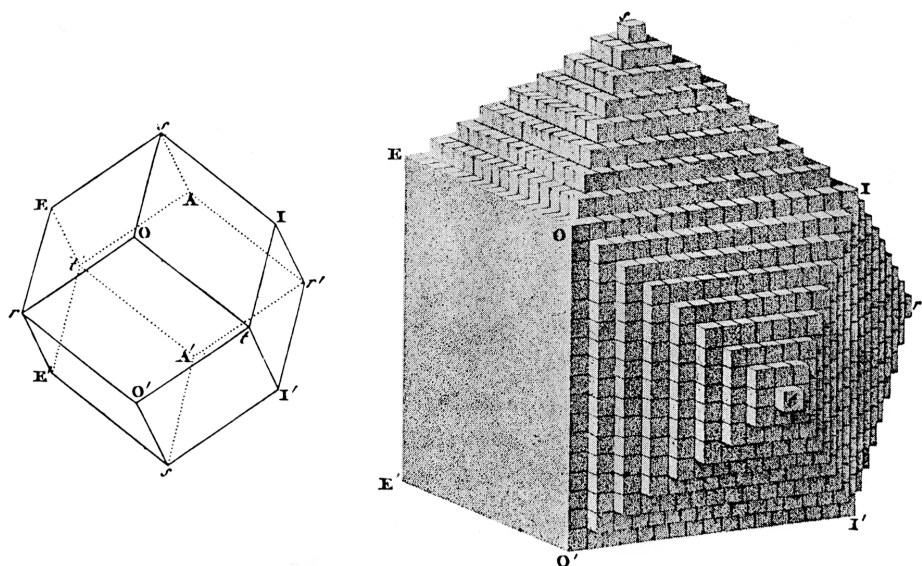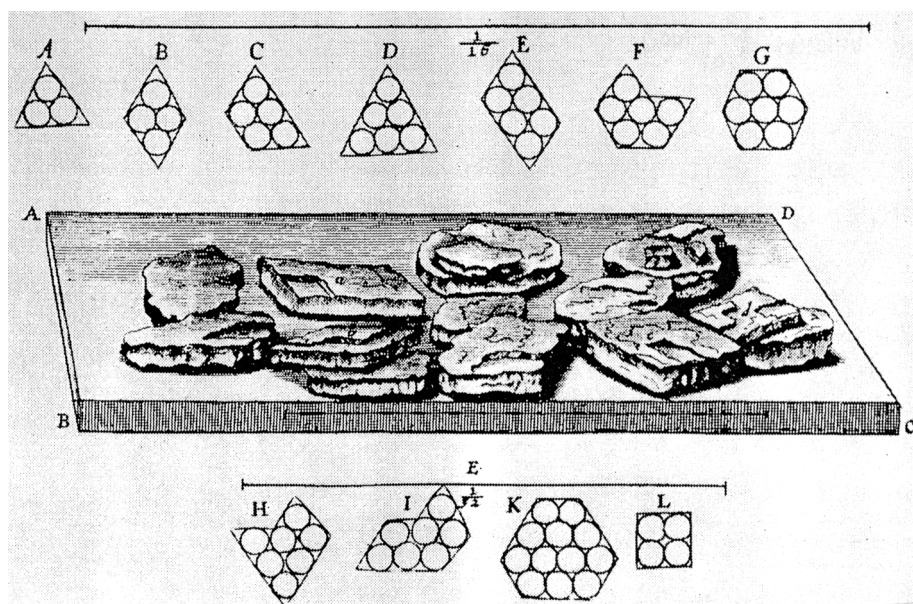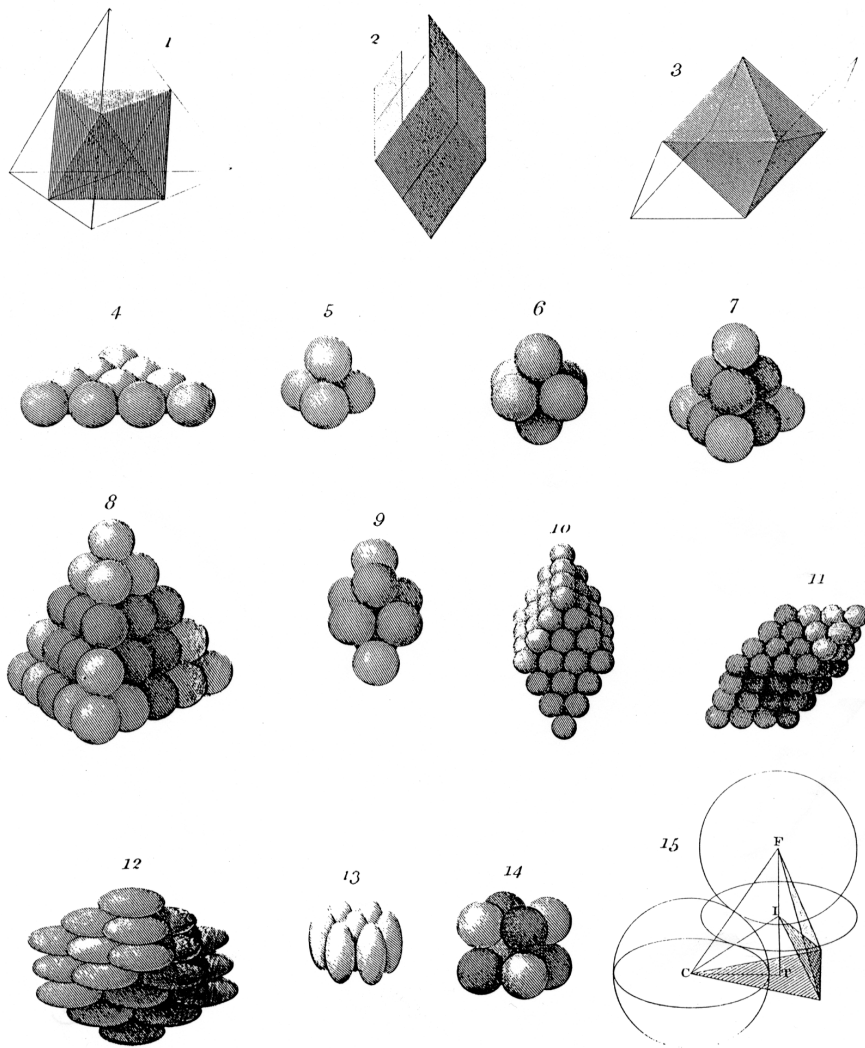In this article we attempt a broad and shallow review of such packings.

Fig. 1. Haüy's explanation of the external shape of crystals.

(a)

Fig. 2. Sphere packings invoked by Hooke (a) and Wollaston (b) in early theories of crystal structure.

(b)

Fig. 2. (continued).

2. The Kepler Problem

One of the earliest references in this subject is to the work of Kepler, who sought order and structure within solid matter, just as he did in the solar system. He was inspired by the hexagonal structure of the snowflake to study the packing of spheres, as in Fig. 2. Such a packing generates hexagonal symmetry in a very natural way. Ultimately, this notion is

misguided, for ice does not consist of identical spherical atoms, packed in such a manner. Nevertheless, as is the way in science, it led Kepler to an interesting question, which has endured in association with his name:

The Kepler Problem: *What is the arrangement of (many) identical spheres that has maximum density?*

There was an obvious answer. Close-packed layers, as in Fig. 2(a), may be stacked on top of each other so that each sphere nestles between three of the layer below. Indeed there is a twofold choice of how to do this, for each succeeding layer, so there are infinitely many alternatives. All have the packing fraction 0.747... (this being defined as the fraction of space occupied by the spheres).

But there was no immediate proof that there could be no structure more dense than this; nor has any been forthcoming in the intervening centuries, at least until very recently. In Sec. 5 we will refer to recent progress on this rather intractable problem.

Few have ever seriously doubted that Kepler's style of stacking (also that of the greengrocer) is the most dense. Those who wish to play Devil's Advocate sometimes refer to the following. In what we shall call Kepler close-packed structures, each sphere touches exactly twelve others. Focussing on just one sphere we can ask: is this the maximum number of contacts that can be made? This "kissing problem" was the subject of a celebrated debate between Newton and Gregory, which shows that the answer is not quite self-evident. It turns out that a configuration with twelve contacts is indeed the most that can be achieved, but one can *almost* bring thirteen into contact. With twelve contacts and one near-contact, this single sphere finds itself more tightly surrounded than in a Kepler structure. If only we could get many spheres to come together with that local configuration, or something close to it, we could surely "beat Kepler". But it seems that it cannot be done.

This situation is nowadays called "frustration". A desirable arrangement can be achieved in one locality, but cannot occur consistently throughout an extended structure. We are familiar with frustration in everyday life: the happiness of the individual is not always compatible with the rules of society.

Close packing in two dimensions does not suffer from frustration. The closest local arrangement of disks (or spheres confined to a plane; Fig. 2(a)) can be extended to an infinite structure. For this reason, a proof can be found with relative ease, for the 2d counterpart of Kepler's conjecture.

Kepler was not the only mathematician of his time to think about close packing. Another example is Thomas Hariot (Fig. 3), a friend of Sir Walter Raleigh, who took him to the new American colonies. In the quieter moments of his adventurous life he too wondered how spheres should be packed.

3. Other Crystalline Sphere Packings

In the context of crystal structure, many other sphere packings are of interest, whether of equal spheres or unequal. Before the modern science of crystallography arrived (following the discovery of X-rays), William Barlow speculated in these terms, and several of the structures which he described were eventually found (Fig. 4).

In creating such structures in the manner of Barlow, we do not always insist that they are stable without the addition of further forces. The hard sphere represents only the short-
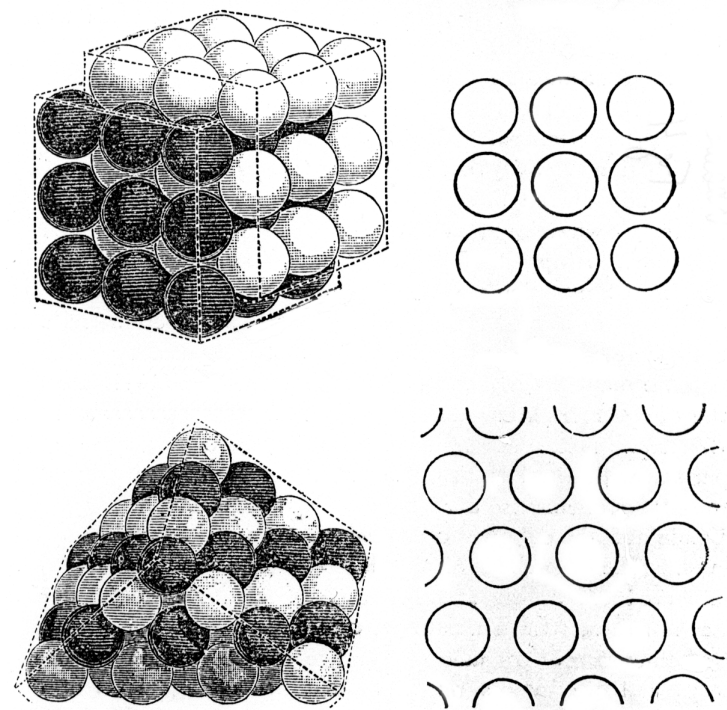
Fig. 3. Thomas Hariot.

Fig. 4. Examples of Barlow's conjectured crystal structures based on sphere packings.

range repulsive part of the interaction between atoms.

Sometimes the question of Kepler has been reversed, to ask what is the least dense stable sphere packing.

4. Order and Disorder

The Pythagorean vision of nature sought *order* in everything and such has been the watchword of many scientists ever since that time. In the more recent past, this perspective was consistent with hierarchical, imperial societies. Disorder was something to be eschewed. It had no place in nature's purest, undisturbed forms, apart from the thermal disorder which lay at the heart of thermodynamics, and was bound to obey strict laws. For example, amorphous (non-crystalline) solids were of little interest, except to the more empirically minded scientists who thought about glass in manufacture or in geological specimens. Nowadays we have a more balanced view. Ordered structures are, in a sense, as accidental as disordered ones—they occur in special circumstances only, whenever atoms are mobile enough to search for optimal structures. Here again, someone with the insight to see this was able to make a lasting contribution with the simplest of procedures. This was J. D. Bernal, who attacked the problem of the structure of liquids in the 1950's.

Up to that point, theorists had very vague ideas about the structure of liquids, expressed in "correlation functions" and concomitant mathematics. Some considered liquids to be locally crystalline. Bernal simply assumed that they were as disordered as they could be, consistent with being tightly packed, since they are almost as dense as solids. A *random* packing of hard spheres was to be his model. This has proved to be close to the truth for liquids, and even closer for some amorphous metals.

The dense random packing of spheres (which can be arrived at in various ways) is therefore still called the Bernal packing. It has a packing fraction which is about 0.64. Looser (stable) random packings are possible.

5. Problems of Proof

The proof which Kepler's question calls for has turned out to be elusive. Many other minimisation problems are similarly intractable—for example, that of the Kelvin problem, described in a previous Katachi lecture (WEAIRE, 1993). We have indicated part of the reason for this—that the obvious route to a proof, starting from local considerations, is in such cases blocked by frustration.

Faced with this mountain to climb, many mathematicians have settled in the foothills, producing instead demonstrations of upper bounds to the maximum density, which steadily advanced towards the Kepler density, but seemed unlikely to offer the means of final proof.

In 1991 a proof of the Kepler conjecture was announced by a mathematician in California. It sparked off a controversy, as colleagues began to find defects in the proof, and its author mounted his defence. It is an elaborate piece of work, making it difficult for the bystander (a category which includes the present writer) to make a judgment. The principal critic has been Thomas Hales, who has since launched his own extensive proof. It seems that the time is fast approaching when the Kepler problem will be led to rest, except perhaps for those who yearn for compact, transparent proofs without the aid of computers!

6. A Footprint in the Sand

As the pendulum has swung towards interest in disordered structures, the Bernal packing and related structures have attracted increasing attention—not so much for their static structure, which has been described here, as for the effects observed when they are disturbed by applied forces.

In this case the originator of the subject is Osborne Reynolds. In a curious parallel with the speculations of his 19th century contemporary, Lord Kelvin on foam (WEAIRE, 1993), Reynolds became fascinated by sand, because it seemed to offer a suitable model for the ether of space. He described its strange property of "dilatancy", which he noticed while walking on the beach. The dense random close-packing of sand grains cannot be compressed, and it expands when it is sheared. Nowadays this is part of the general problem of the description of the mechanics of powders, slurries, cereal grain in hoppers, and the like, in a host of important industrial contexts. Theory remains inconclusive or controversial.

7. Colloids as Hard Spheres

Another context in which hard sphere packings are enjoying the limelight again is that of colloids, which can take this form. These systems lie at a borderline of order in nature, in that their constituents are only just small enough to have enough thermal motion to search for alternative structures and seek out an ordered optimal choice.

They are of intense interest at present, because they offer a route to the fabrication of a new kind of material, to which the word "photonic" has been applied. Researchers are therefore experimenting with templates and other tricks that encourage ordering.

Figure 3 is reproduced by permission of Trinity College, Oxford.

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