Cambridge University Press
978-0-521-61770-3 — Dense Sphere Packings
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Excerpt
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1

Close Packing

1.1 History

This section gives a brief history of the study of dense sphere packings. Further details appear at [43] and [20]. The early history of sphere packings is concerned with the face-centered cubic (FCC) packing, a familiar pyramid arrangement of congruent balls used to stack cannonballs at war memorials and oranges at fruit stands (Figure 1.1).

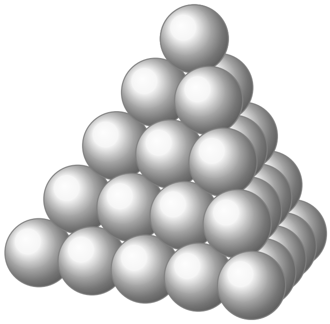

Figure 1.1 The face-centered cubic (FCC) packing.

1.1.1 Sanskrit sources

The study of the mathematical properties of the FCC packing can be traced[1] to a Sanskrit work (the Āryabhaṭīya of Āryabhaṭa) composed around 499 CE. The following passage gives the formula for the number of balls in a pyramid

[1] I am obliged to Plofker [35].

pile with triangular base as a function of the number of balls along an edge of the pyramid [40].

> *For a series [lit. "heap"] with a common difference and first term of 1, the product of three [terms successively] increased by 1 from the total, or else the cube of [the total] plus 1 diminished by [its] root, divided by 6, is the total of the pile [lit. "solid heap"].*

In modern notation, the passage gives two formulas for the number of balls in a pyramid with n balls along an edge (Figure 1.2):

$$\frac{n(n+1)(n+2)}{6} = \frac{(n+1)^3 - (n+1)}{6}. \tag{1.1}$$

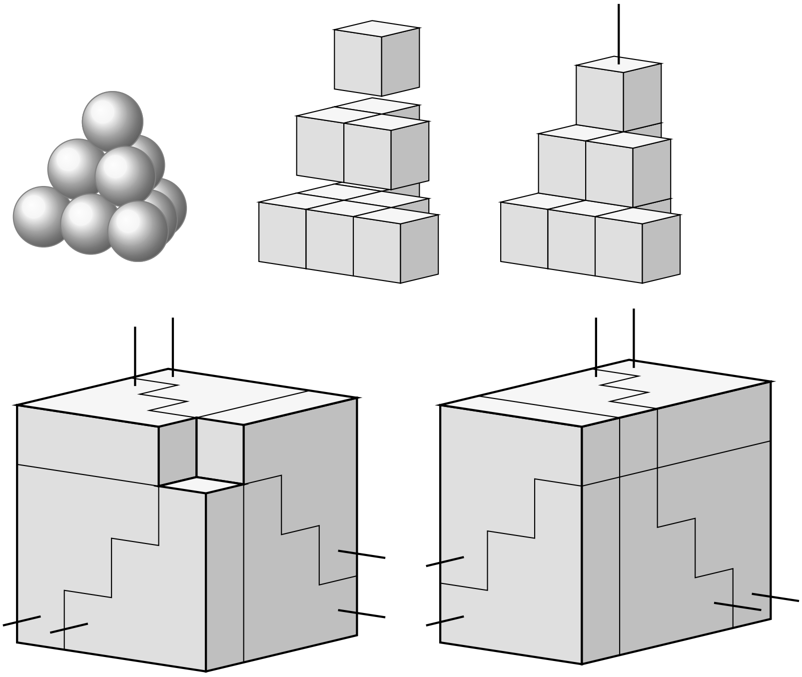

Figure 1.2 Derivation of Sanskrit formula (1.1). A cannonball packing can be converted to unit cubes in a staircase aligned along the rear column. Six staircase shapes fill an $(n+1)^3$ cube without its diagonal of $n+1$ unit cubes, or a rectangle of dimensions n by $n+1$ by $n+2$.

1.1.2 Harriot and Kepler

The modern mathematical study of spheres and their close packings can be traced to Harriot. His work – unpublished, unedited, and largely undated – shows a preoccupation with sphere packings. He seems to have first taken an interest in packings at the prompting of Sir Walter Raleigh. At the time, Harriot was Raleigh's mathematical assistant, and Raleigh gave him the problem of determining formulas for the number of cannonballs in regularly stacked piles. Harriot interpreted the number of balls in a pyramid as an entry in Pascal's triangle[2] (Figure 1.3). Through his study of triangular and pyramidal numbers, Harriot later discovered finite difference interpolation [3]. Shirley, Harriot's biographer, writes that it was his study of cannonball arrangements in the late sixteenth century that "led him inevitably to the corpuscular or atomic theory of matter originally deriving from Lucretius and Epicurus" [39, p. 242].

Kepler became involved in sphere packings through his correspondence with Harriot around 1606–1607 on the topic of optics. Harriot, the atomist, attempted to understand reflection and refraction of light in atomic terms. Kepler favored a more classical explanation of reflection and refraction in terms of what Kargon describes as "the union of two opposing qualities – transparence and opacity" [27, p.26]. Harriot was stunned that Kepler would be satisfied by such reasons.

Despite Kepler's initial reluctance to adopt an atomic theory, he was eventually swayed and published an essay in 1611 that explores the consequences of a theory of matter composed of small spherical particles. Kepler's essay describes the FCC packing and asserts that "the packing will be the tightest possible, so that in no other arrangement could more pellets be stuffed into the same container" [28]. This assertion has come to be known as the Kepler conjecture. This book gives a proof of this conjecture.

1.1.3 Newton and Gregory

The next episode in the history of this problem, a debate between Isaac Newton and David Gregory, centered on the question of how many congruent balls can be arranged to touch a given ball. The analogous question in two dimensions is readily answered; six pennies, but no more, can be arranged to touch a central penny. In three dimensions, Newton said that the maximum was twelve balls, but Gregory claimed that thirteen might be possible.

The Newton–Gregory problem was not solved until centuries later (Figure 1.4). The first proper proof was obtained by van der Waerden and Schütte in

[2] Harriot was well-versed in Pascal's triangle long before Pascal.

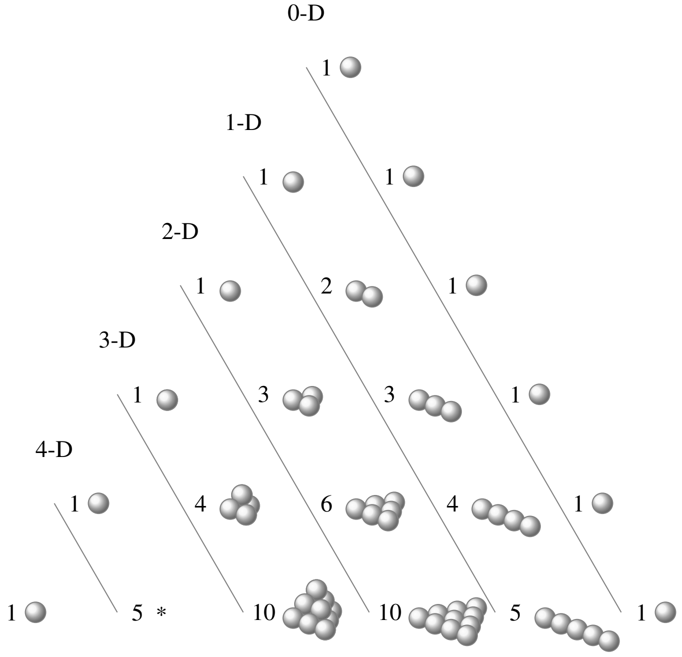

Figure 1.3 The binomial coefficient $\binom{d+n}{n}$ gives the general formula for the number of balls in a d-dimensional pyramid of side $n+1$. As Harriot observed, the recursion of Pascal's triangle $\binom{d+n}{n} = \binom{d+(n-1)}{n-1} + \binom{(d-1)+n}{n}$ can be interpreted as a partition of a pyramid of side $n+1$ into a pyramid of side n resting on a pyramidal base of side $n+1$ in dimension $d-1$.

1953 [38]. An elementary proof appears in Leech [30]. Although a connection between the Newton–Gregory problem and Kepler's problem is not obvious, Fejes Tóth successfully linked the problems in 1953 [12].

1.2 Face-Centered Cubic

The FCC packing is the familiar pyramid arrangement of balls on a square base as well as a pyramid arrangement on a triangular base. The two packings differ only in their orientation in space. Figure 1.5 shows how the triangular base packing fits between the peaks of two adjacent square based pyramids.

Density, defined as a ratio of volumes, is insensitive to changes of scale. For convenience, it is sufficient to consider balls of unit radius. This means that the distance between centers of balls in a packing is always at least 2. We identify

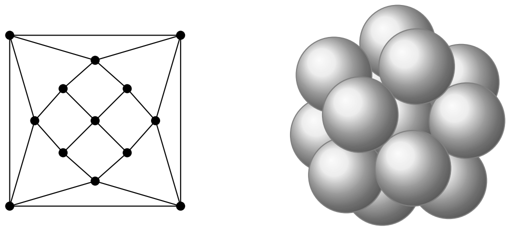

Figure 1.4 Newton's claim – twelve is the maximum number of congruent balls that can be tangent to a given congruent ball– was confirmed in the 1953. Musin and Tarasov only recently proved that the arrangement shown here is the unique arrangement of thirteen congruent balls that shrinks the thirteen by the least possible amount to permit tangency [32]. Each node of the graph represents one of the thirteen balls and each edge represents a pair of touching balls. The node at the center of the graph corresponds to the uppermost ball in the second frame. The other twelve balls are perturbations of the FCC tangent arrangement.

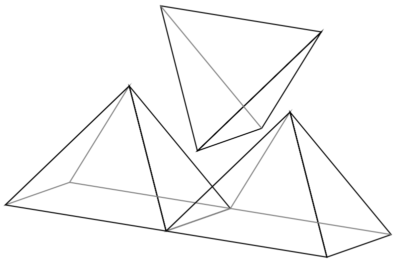

Figure 1.5 The pyramid on a square base is the same lattice packing as the pyramid on a triangular base. The only differences are the orientation of the lattice in space and the exposed facets of the lattice. Their orientation and exposed facets are matched as shown.

a packing with its set V of centers. For our purposes, a packing is just a set of points in $\mathbb{R}^3$ in which the elements are separated by distances of at least 2.

The density of a packing is the ratio of the volume occupied by the balls to the volume of a large container. The purpose of a finite container is to prevent the volumes from becoming infinite. To eliminate the distortion of the packing caused by the shape of the its boundary, we take the limit of the densities within an increasing sequence of spherically shaped containers, as the diameter tends to infinity.

The FCC packing is obtained from a cubic lattice, by inserting a ball at each of the eight extreme points of each cube and then inserting a another ball at the center of each of the six facets of each cube (Figure 1.6). The name *face-*

centered cubic comes from this construction. The edge of each cube is $\sqrt{8}$, and the diagonal of each facet is 4. The density of the packing as a whole is equal to the density within a single cube. The cube has volume $\sqrt{8}^3$ and contains a total of four balls: half a ball along each of six facets and one eighth a ball at each of eight corners. Thus, the density within one cube is

$$\frac{4(4\pi/3)}{\sqrt{8}^3} = \frac{\pi}{\sqrt{18}}.$$

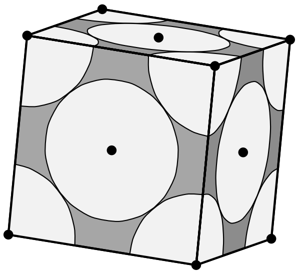

Figure 1.6 The intersection of the FCC packing with a cube of side $\sqrt{8}$. The name *face-centered cubic* comes from this depiction. The cube has volume $\sqrt{8}^3$ and contains a total of four balls (eight eighths from the corners and six halves from the facets), giving density $4(4\pi/3)/\sqrt{8}^3 = \pi/\sqrt{18}$.

The density $\pi/\sqrt{18}$ of the packing is the ratio of the volume $4\pi/3$ of a ball to the volume of a fundamental domain of the FCC lattice. The volume of the fundamental domain is therefore $4\sqrt{2}$. A fundamental domain of the FCC lattice is a parallelepiped that can be dissected into two regular tetrahedra and one regular octahedron (Figure 1.7). The FCC packing is then an alternating tiling by tetrahedra and octahedra in 2:1 ratio. A tetrahedron scaled by a factor of two consists of one tetrahedron at each extreme point and one octahedron in the center (Figure 1.8). By similarity, the total volume is $8 = 2^3$ times the volume of each smaller tetrahedron. This dissection exhibits the volume of a regular octahedron as exactly four times the volume of a regular tetrahedron of the same edge length. As a result, the volume of a regular tetrahedron of side 2 is $1/6$ the volume of the fundamental domain, or $2\sqrt{2}/3$.

The density of the FCC packing is the weighted density of the densities of the tetrahedron and octahedron. Write δ_{tet} and δ_{oct} for these densities. Explicitly, δ_{tet} is the ratio of the volume of the part within the tetrahedron of the unit balls (at the four extreme points) to the full volume of the tetrahedron. As tetrahedra fill $1/3$ of volume of the fundamental domain and an octahedron fills the

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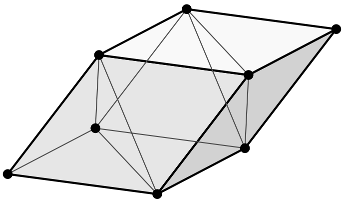

Figure 1.7 The fundamental domain of the FCC lattice can be partitioned into two regular tetrahedra and a regular octahedron. The fundamental domain tiles space. Tetrahedra and octahedra tile space in the ratio 2:1.

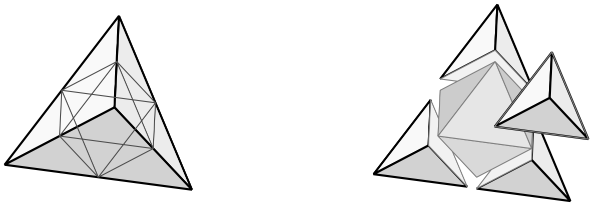

Figure 1.8 A regular tetrahedron whose edge is two units can be partitioned into four unit-edge tetrahedra and one unit-edge octahedron at its center. Similarly, a regular octahedron whose edge is two units can be partitioned into six unit-edge octahedra and eight unit-edge tetrahedra.

other 2/3,

$$\frac{\pi}{\sqrt{18}} = \frac{1}{3}\delta_{tet} + \frac{2}{3}\delta_{oct}.$$

As above, we identify a packing with the set V of centers of the balls. The *Voronoi cell* of a point v in a packing V is defined as the set of all points in $\mathbb{R}^3$ (or more generally in $\mathbb{R}^n$) that are at least as close to v as to any other point of V (Figure 1.9). Each Voronoi cell of the FCC packing is a rhombic dodecahedron (Figure 1.10), which is constructed from an inscribed cube by placing a square based pyramid (with height half as great as an edge of its square base) on each of the six facets.

Rhombic dodecahedra, being the Voronoi cells of the FCC packing, tile space. In each rhombic dodecahedron, we may color the inscribed cube black and the six square-based pyramids white. In the tiling, the black cubes fill the black spaces of an infinite three-dimensional checkerboard, and the white pyramids fill the white spaces.

A Voronoi cell contains an inscribed black cube of side $\sqrt{2}$ and a total of one white cube, for a total volume of $4\sqrt{2}$, which is again the volume of the

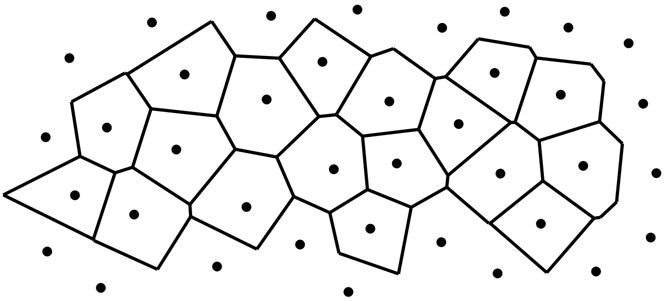

Figure 1.9 Voronoi cells of a two-dimensional sphere packing.

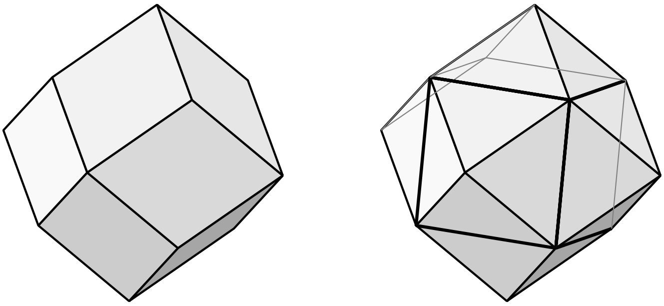

Figure 1.10 The Voronoi cell of the FCC packing is a rhombic dodecahedron. It can be constructed by placing a square-based pyramid along each facet of an inscribed cube.

fundamental domain. The density of the FCC packing is the ratio of the volume of a ball to the volume of its Voronoi cell, which gives $\pi/\sqrt{18}$ yet again.

1.3 Hexagonal-Close Packing

There is a popular and persistent misconception that the FCC packing is the only packing with density $\pi/\sqrt{18}$. The hexagonal-closed packing (HCP) has the same density.

In the FCC packing, each ball is tangent to twelve others in the same fixed arrangement. We call it the *FCC pattern*. Likewise, in the HCP, each ball is tangent to twelve others in the same arrangement (Figure 1.11). We call it the *HCP pattern*. The FCC pattern and HCP patterns are different from each other. In the FCC pattern, four different planes through the center give a regular hexagonal cross section, while the HCP pattern has only one such plane.

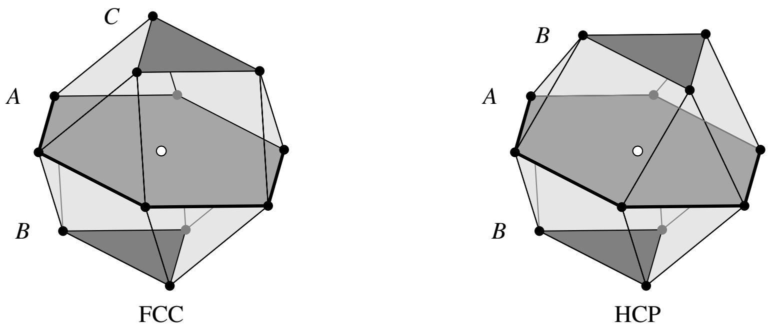

Figure 1.11 The patterns of twelve neighboring points in the FCC and HCP packings. In both cases, the convex hull of the twelve points is a polyhedron with six squares and eight triangles, but the top layer of the HCP pattern is rotated 60 degrees with respect to the FCC pattern. The FCC pattern is a cuboctahedron. In the HCP pattern, there is a uniquely determined plane of reflectional symmetry, containing six of the twelve points.

There are, in fact, uncountably many packings of density $\pi/\sqrt{18}$ in which the tangent arrangement around each ball is either the FCC pattern or the HCP pattern.

A *hexagonal layer* (Figure 1.12) is a translate of the two-dimensional hexagonal lattice (also known as the triangular lattice). That is, it is a translate of the planar lattice generated by two vectors of length 2 and angle $2\pi/3$. The FCC packing is an example of a packing built from hexagonal layers.

If L is a hexagonal layer, then a second hexagonal layer L' can be placed parallel to the first so that each lattice point of L' has distance 2 from three different points of L, which is the smallest possible distance from first layer. A choice of a unit normal vector $\mathbf{e}$ to the plane of L determines an upward direction. There are two different positions in which L' can be closely placed above L (Figure 1.12). Each successive layer (L, L', L'', and so forth) offers two further choices for the placement of that layer. Running through different sequences of choices gives uncountably many packings. In each of these packings the tangent arrangement around each ball is the FCC or HCP arrangement.

As a packing is constructed, each layer may be labeled A, B, or C depending on three possible orthogonal projections to a fixed plane with normal vector $\mathbf{e}$. Each layer carries a different label from the layers immediately above and below it. In the FCC packing, the successive layers are A, B, C, A, B, C, and so forth. In the HCP packing, the successive layers are A, B, A, B, and so forth. If the vertices of a triangle are labeled A, B, and C, then the succession of labels

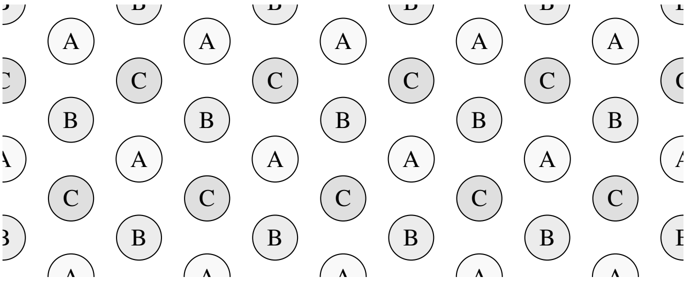

Figure 1.12 If the centers in one hexagonal layer of a close packing are placed at the sites marked A, then the hexagonal layer above it will occupy all the sites marked B, or all of the sites marked C. In general, each hexagon layer of a close packing is determined by its label A, B, or C, which must always differ from the label of the layer below. The HCP packing is $\ldots ABABAB \ldots$. The FCC packing is $\ldots ABCABCABC \ldots$. There are infinitely many other close packings, consisting of hexagonal layers, corresponding to sequences of A, B, C.

is a walk along the vertices of the triangle, and inequivalent walks through the triangle describe different packings.

The different walks through a triangle give all possible packings of infinitely many congruent balls in which each tangent arrangement is either the FCC pattern or the HCP pattern [9]. To see that there are no other possibilities, we first assume that every ball of V is surrounded by the FCC pattern. Adjacent FCC patterns interlock in a unique way that forces V itself to crystallize into the FCC packing. This completes the proof in this case.

Now we assume that a packing V contains some ball (centered at $\mathbf{u}$) in the HCP pattern. Its uniquely determined plane of reflectional symmetry contains $\mathbf{u}$ and the centers of six others arranged in a regular hexagon. If $\mathbf{v}$ is the center of one of the six other balls in the plane of symmetry, its tangent arrangement of twelve balls must include $\mathbf{u}$ and an additional four of the twelve balls around $\mathbf{u}$. These five centers around $\mathbf{v}$ are not a subset of the FCC pattern, but extend uniquely to a HCP pattern. Around $\mathbf{u}$ and $\mathbf{v}$, the HCP patterns have the same plane of symmetry. In this way, as soon as some center has the HCP pattern, the pattern propagates along the plane of symmetry to create a hexagonal layer L.

Once a packing V contains a single hexagonal layer, the condition that each ball be tangent to twelve others forces a hexagonal layer L' above L and another hexagonal layer below L. Thus, a single hexagonal layer forces an infinite sequence of close-packed hexagonal layers. The position of each layer over the