$16n^2 + 2$ revealed

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I show that a neat expression emerges for the number of spheres in each shell of an octahedron composed of close packed spheres, and that from this expression we can compute the value of the packing density for an infinite array of such spheres.

An obvious question that was prompted by Note 92.81 '$10n^2 + 2$ revealed' [1] (that relates to hexagonal close packed uniform spheres) is 'What is the equivalent expression for cubic close packed uniform spheres?'. Specifically, the former expression gives the number of spheres in the nth shell of spheres in a cuboctahedron that grows outwards from a central 'seed' sphere, with each sphere having a coordination number of 12. The expression is of scientific value in designing a kinetic model of the growth of aggregates from monomeric units, such as occurs with macromolecular assemblies in connective tissue [e.g. 2] and in crystal growth.

Figure 1 is an image of a pile of steel balls that are in cubic close packing; and the aim is to answer the question above in relation to such a pile of spheres.

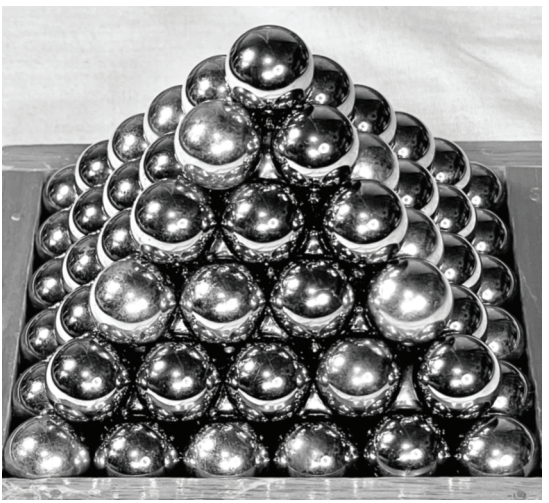


FIGURE 1: Oblique view of cubic close packed 0.5-inch (12.7 mm) diameter steel balls

The spheres in Figure 1 are constrained to line up tangentially with their immediate neighbours in the square base, in straight rows and columns, with the next layer of spheres fitting into the 'cuspate depressions' that are formed [3], while simultaneously they are tangential with their immediate neighbours.

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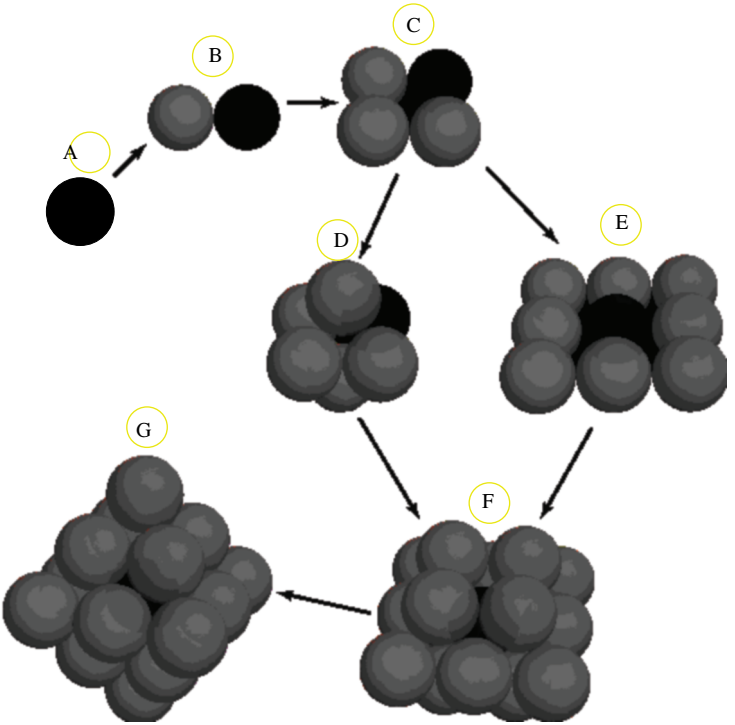


FIGURE 2: Building up the 19-sphere assembly at *G*; starting with a single 'seed' sphere (*A*, black), that forms a dimer with a grey sphere (*B*) which aggregates further to form a 4-sphere (*C*) that is capped above and below by single spheres to form a 6-sphere octahedral array (*D*), or onto a 9-sphere planar array (*E*) that is capped above and below by four spheres that fit into the cuspate depressions in the first layer (*F*); and the second two layers of four spheres is capped by a single sphere that fits into the top and bottom cuspate depressions (*G*). Alternatively, *F* can be viewed as having been built up from four overlapping sets of *D*; while *G* can be viewed as being composed of six overlapping sets of *D*. Drawn using *Mathematica* [4].

Figure 2 shows how the unit cell of cubic close packing can arise in stages from an initial sphere (identified in black). Spheres form dimers, that in turn dimerize (dimer of dimers), and these tetrads are capped on the top and bottom by spheres that fit into the cuspate depressions, making a hexamer (*D*).

Another trajectory of aggregation is achieved by extending the 2×2 array in the x, y-plane (*C*) to a 3×3 one (*E*), then capping this with four more spheres into the cuspate depressions on the top and bottom of the array (*F*); and finally adding a single sphere on the top and bottom (*G*).

The total number of spheres in the *G*-assembly is 19. To attain the array shown in Figure 1 we envisage adding shells of spheres on each face of *G*; hence our quest is to derive an expression that specifies how many spheres there are in each such successive shell.

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To start this quest, consider object G (in Figure 2) and think of it as an octahedron: we need to develop a sphere-counting strategy that avoids double counting: Thus the top-front face has $3 + 2 + 1$ spheres; the opposite (top-back) face has $3 + 2 + 1$ spheres as well, but the last one (on top) has already been counted, so the sum is $3 + 2 + 1 - 1$. The two opposite top-side faces each have one sphere that has not already been counted, making the total 1, for each of these two faces. Underneath, the front-bottom face shares the lower edge of three spheres of the top-front face; these have already been counted, leaving only $2 + 1$ spheres; while at the back the spheres number $2 + 1 - 1$, using the above reasoning. Finally, the other two sides each have one previously uncounted sphere. This gives a total (that is of course easily obtained by direct counting) of 18.

If the reasoning just given is applied to the next shell, with five spheres on each leading edge, it is seen that the total number of spheres in the shell is built up by considering each of the eight faces in turn:

Face number	Sphere count	
1	$5 + 4 + 3 + 2 + 1$	Top
2	$5 + 4 + 3 + 2 + 1 - 1$	
3	$3 + 2 + 1$	
4	$3 + 2 + 1$	

5	$4 + 3 + 2 + 1$	Bottom
6	$4 + 3 + 2 + 1 - 1$	
7	$2 + 1$	
8	$2 + 1$	(1)

Total = 66

The summations rapidly become tedious to evaluate for larger shells; and besides we seek a general expression for these successive sums. To achieve this we start by noting that the individual sums from the top and bottom shells can be rearranged so that they appear in sequential order in (2) and (3):

$$\text{Sum}[1] = 2\left(\sum_{i=1}^{3} i + \sum_{i=1}^{2} i + \sum_{i=1}^{1} i + \sum_{i=1}^{0} i\right) - 2 \tag{2}$$

$$\text{Sum}[2] = 2\left(\sum_{i=1}^{5} i + \sum_{i=1}^{4} i + \sum_{i=1}^{3} i + \sum_{i=1}^{2} i\right) - 2 \tag{3}$$

If we assign G (in Figure 2) as the *first* surface shell; namely it is of order $n = 1$ then, the first series which has a maximum value of three spheres on a leading edge takes on the value $2n + 1$. Therefore in the classical integer-sum formula (sum $= \frac{1}{2}n(n + 1)$) we replace n by $2n + 1$. Hence (4),

$$\text{Sum}[n] = 2\left(\frac{(2n+1)((2n+1)+1)}{2} + \frac{2n(2n+1)}{2} + \frac{(2n-1)2n}{2} + \frac{(2n-2)(2n-1)}{2}\right) - 2. \tag{4}$$

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Remarkably, after some algebra, (4) is seen to reduce to the elegantly simple 'neat solution' alluded to in the opening sentence, (5):

$$\text{Sum}[n] = 16n^2 + 2. \tag{5}$$

Equation (5) is akin to that for hexagonal close packing, namely $\text{Sum}[n] = 10n^2 + 2$. But does the factor of 16 in the expression not lead to a different value of the packing density, ϕ? Let's see.

The total number of spheres, T, in a sphere-array of order N is simply the sum across all orders as given in (6):

$$T = \sum_{n=1}^{N} \left(16n^2 + 2\right). \tag{6}$$

By applying the sum-of-squares formula to (6) we obtain (7):

$$T = 16\frac{N(N+1)(2N+1)}{6} + 2N. \tag{7}$$

The total volume of spheres is therefore (8):

$$V_S = \frac{4}{3}\pi R^3\left(16\,\frac{N(N+1)(2N+1)}{6} + 2N\right) \tag{8}$$

where R is the radius of each sphere.

The total volume of a regular octahedron V_O is given by (9):

$$V_O = \frac{\sqrt{2}}{3}a^3, \tag{9}$$

where a is the side length. There are $2N + 1$ spheres on each edge, and this is multiplied by the diameter of each sphere, $2R$, to give the side-length, a. Hence from (9), V_O is given by (10):

$$V_O = \frac{\sqrt{2}}{3}\left((2N+1)\,2R\right)^3. \tag{10}$$

Finally, the packing density ϕ of an array of infinite extent is given by the limit as $N \to \infty$ of the ratio of (8) and (10), yielding (11):

$$\phi = \lim_{N\to\infty}\left(\frac{\frac{4}{3}\pi R^3\left(16\,\frac{N(N+1)(2N+1)}{6} + 2N\right)}{\frac{\sqrt{2}}{3}\left((2N+1)\,2R\right)^3}\right). \tag{11}$$

This neatly 'shakes down' after some algebra to give (12):

$$\phi = \frac{\pi}{3\sqrt{2}}. \tag{12}$$

It is worth noting that the expression for ϕ can be swiftly evaluated symbolically in *Mathematica* [4]. The value of the packing density is also that of hexagonal close packing; and this is the maximum value of all possible packed arrays of uniform spheres [5, 6].

Ah but! If computing the packing density for the infinite array is all that is required, then there is a much more direct approach than that given above.

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It is this: consider Figure 1 and label the top sphere as $i = 1$, and observe that the number of spheres in successive horizontal *layers* is i^2; so for this regular square pyramid the total number of spheres T_P for which there are M spheres on an edge is given by (13):

$$T_P = \sum_{i=1}^{M} i^2 = \frac{M(M+1)(2M+1)}{6}. \tag{13}$$

The total volume of spheres V_{SP} is simply (13) multiplied by the volume of a sphere to give (14):

$$V_{SP} = \frac{4}{3}\pi R^3 \frac{M(M+1)(2M+1)}{6}. \tag{14}$$

The volume of the regular square pyramid is half that of the corresponding octahedron, specified by (9), for which the side-length is $2RM$. Hence the packing density of the infinite array (using the limit as for (11)) is (15):

$$\phi = \lim_{M \to \infty} \left(\frac{\frac{4}{3}\pi R^3 \frac{M(M+1)(2M+1)}{6}}{\frac{\sqrt{2}}{6}(2RM)^3} \right) = \frac{\pi}{3\sqrt{2}} \tag{15}$$

as given by (12).

In conclusion, we have satisfied our curiosity about the form of the expression that defines the total number of spheres on successive faces (shells) of an octahedron of spheres that grows, adhering to the constraints of cubic close packing.

The emergence of variously shaped polyhedra from packing cubes rather than spheres is similar and elicits some intriguing, related insights into the growth of polyhedra other than the cuboctahedron and octahedron mentioned here [7].

We also confirmed that the packing density of both forms of sphere stacking is the same, even considering the atypical perspective of building up the 'master polyhedron' by adding *shells of spheres*, as might occur in polymer and crystal growth.

There is also the matter of the coordination number of the spheres. The spheres in the corners of the array (E) in Figure 2 are not in contact with the seed sphere; and in (F), as with hexagonal packing, there are indeed only 12 spheres in direct contact from a top and a bottom sphere. Both forms of packing are equivalent, in the sense that if our line of sight into the array in Figure 1 is normal to a face of the octahedron the hexagonal packing of spheres can be visualised.

Finally, the difference in the value of the coefficient of the n^2 term (16 as against 10) in the Q-shell formula for hexagonal close packing [1] results from the inclusion of non-coordination spheres (not contacting the central sphere) in the 'seed' array of cubic close packing.

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