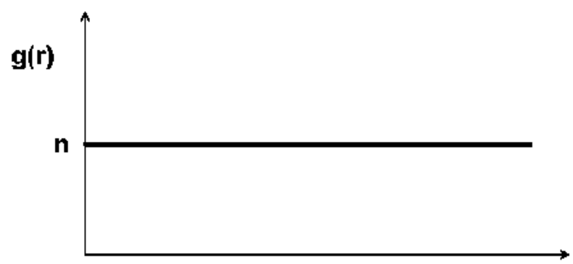
CHAPTER 2

2-1. An ideal gas consists of non-interacting, point particles that move about in rapid and incessant fashion. Sketch the form of g(r) for this ideal gas and discuss its features.

2-1. Solution:

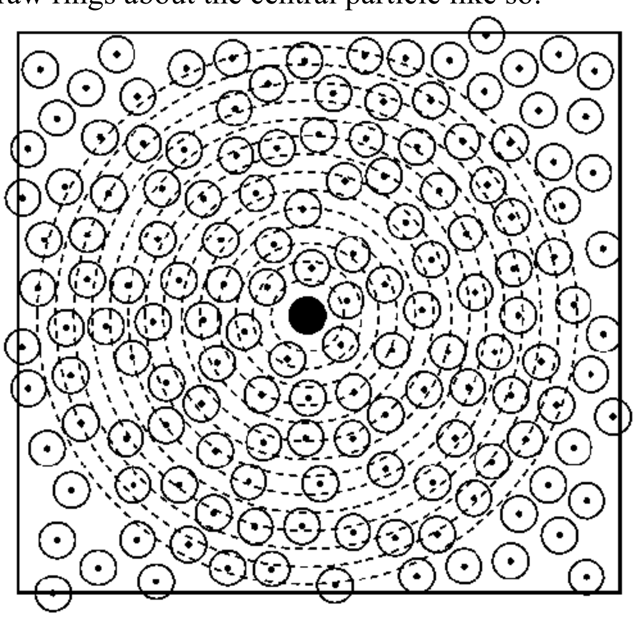
Ideal gas consists of point particles that have no attractive interaction. Probability of finding a second particle is just that of the density, n.



2-2. Make a xerox reproduction of Fig. 2-11 below that represents the atoms in a amorphous solid and, using a compass, manually calculate *g(r)* for a single ensemble using the dark particle as the central particle. Do this with a *dr* no larger than the particle radius, *b*. Plot your result and identify the first and second coordination spheres.

2-2. Solution:

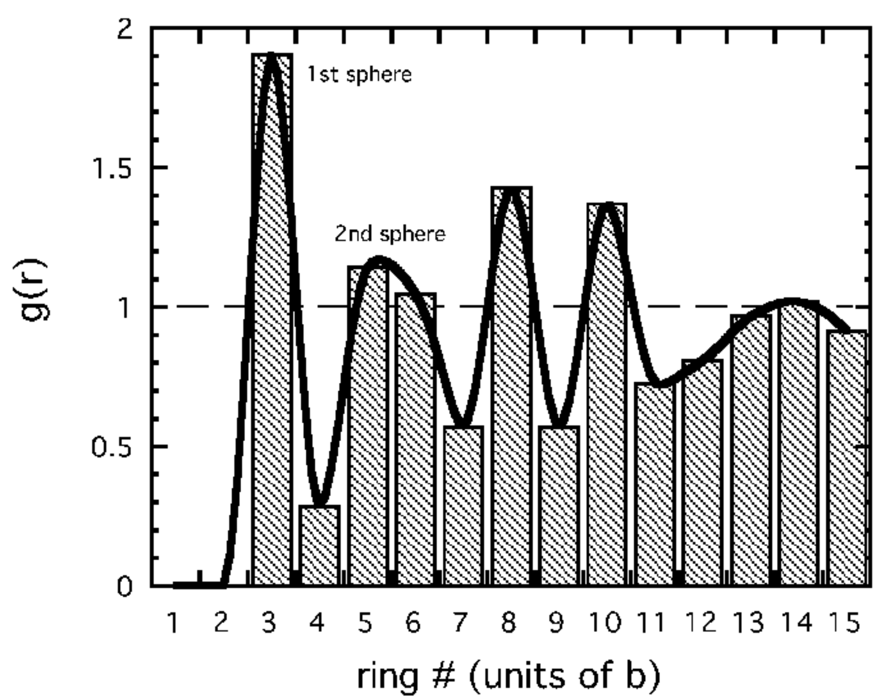
Draw rings about the central particle like so:



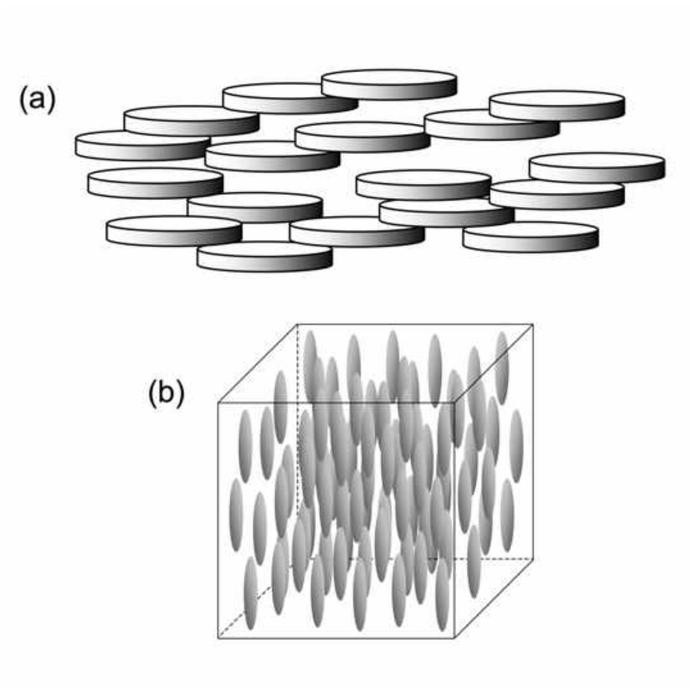
Count the number of particles centers found in each ring of size dr (here equal to b) and make a table:

	ring #	dN	g(r)
0	1.0000	0.0000	0.0000
1	2.0000	0.0000	0.0000
2	3.0000	5.0000	1.6968
3	4.0000	1.0000	0.25453
4	5.0000	5.0000	1.0181
5	6.0000	5.5000	0.93326
6	7.0000	3.5000	0.50905
7	8.0000	10.000	1.2726
8	9.0000	4.5000	0.50905
9	10.000	12.000	1.2217
10	11.000	7.0000	0.64788
11	12.000	8.5000	0.72115
12	13.000	11.000	0.86147
13	14.000	12.500	0.90902
14	15.000	12.000	0.81448

For 2D case here, $g(r) = dN/(2\pi r dr)\langle n\rangle = dN/(2\pi m b^2)\langle n\rangle$. Including the central atom, there are 98.5 centers inside the m = 15$^{\text{th}}$ ring of area $\pi(15b)^2$. A histogram of the g(r) (for only this one ensemble) looks like this:



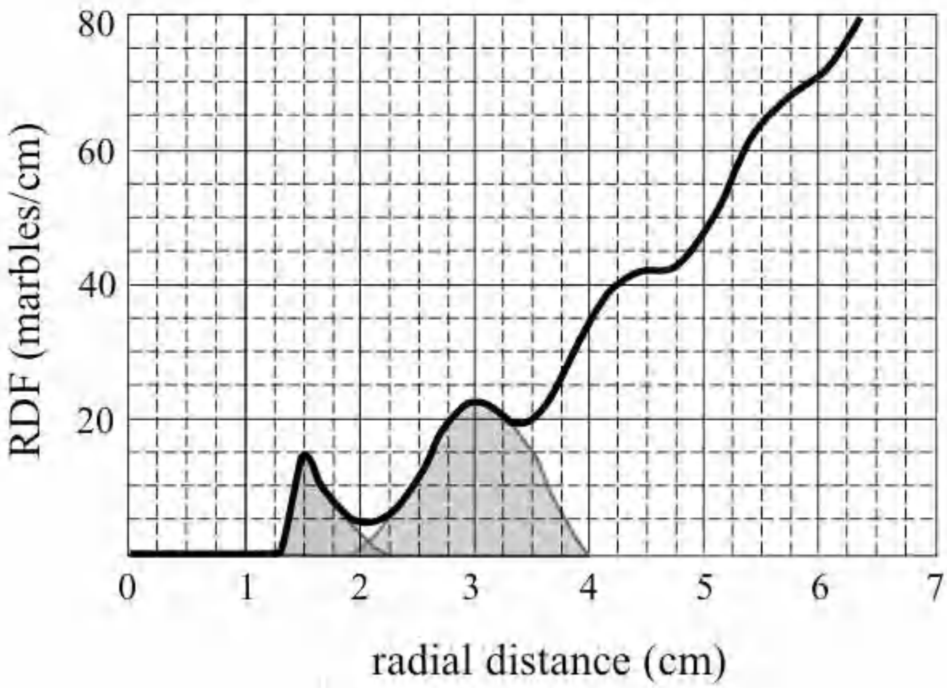
2-3. Figure 2-12 shows the nematic phases of two liquid crystals: (a) a discotic liquid crystal and (b) a lipid liquid crystal. For each of these partially amorphous systems, discuss the symmetry properties including both translational and rotational symmetries.



2-3. Solution:

(a) The discotic phase illustrated possesses a two-fold rotational symmetry about either of the two axes that are perpendicular to the common normal of the face of the discs. (b) The lipid phase illustrated possesses a two-fold rotational symmetry about either of the two axes that are perpendicular to the common direction of alignment.

2-4. The pair distribution function for a bag of marbles is shown in Fig. 2-13. From the figure, (a) determine the nearest and next-nearest separation distances corresponding to the first and second coordination shells, and (b) estimate the coordination number for the first and second coordination shells.



2-4. Solution:

Each small square in the figure is (5 marbles/cm) X (0.25 cm) = 1.25 marbles per square. The first coordination shell is approximated by the shaded region in the above figure that peaks near 1.5 cm and contains a total of roughly 4 boxes or 5 marbles. The second coordination shell peaking at 3 cm contains a total of roughly 18 boxes or 22.5 marbles.

2-5. A common chalcogenide glass is As_2Ge_3. Determine the average coordination number for this system.

2-5. Solution:

The formation of covalent bonds forces the coordination near an As to be 3 and that near Ge to be 4. Since there are two As for every 3 Ge, 40% of the atoms are As and 60% are Ge. The average coordination is the weighted value: (0.4 x 3) + (0.6 x 4) = 3.6.

2-6. Typical window glass is formed by a mixture of approximately 70% SiO_2, 20% Na_2O and 10% CaO, known as soda-lime-silicate. How does the addition of Na_2O and CaO affect the CRN of SiO_2 if the O donated by either is to end up bonded with a Si atom?

2-6. Solution:

Addition of Na_2O and CaO both lead to the formation of non-bridging oxygen bonds that serve to weaken the network structure. The O contributed by either Na_2O or CaO replaces the missing oxygen on one of two Si units when the bridging bond is broken. The pair of terminal oxygens are charge compensated by the two Na cations or the ça ion and produce a weaker ionic crosslink.