Chapter 8

These are answers to the exercises in Chapter 8 of:

Understanding the Properties of Matter
by Michael de Podesta.

If you find an error in these answers, or think they could be clarified in any way, please feel free to contact me.

Thanks

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C1. Compared with the solid you should be able to note some or all of the following features

- Liquid volume is similar to (but slightly larger than) that for a solid with the same number of atoms
- The liquid should form 'a blob' which does not have the straight 'crystalline' sides of a solid
- Molecules in the liquid should occasionally change places. I have marked one molecule with a different colour so that you can follow its path over time. Alternatively switch off the 'draw circles option and switch on the 'trace' option.
- Molecules in the liquid may occasionally 'evaporate'. This also occurs for solids but *much* more rarely.

Compared with the gas you should see that the dynamics are completely different. It is interesting to compare the situation as the maximum gas density that can be achieved, with 50 molecules in the container. This is about half the density for the liquid which is simulated when 50 molecules are in the container. Comparing the liquid and gas simulations for the case when 50 molecules were simulated I was struck by how strikingly different were the dynamics. The gas (even though molecular collisions were very important) was definitely gas-like and the liquid was definitely liquid-like. These simulations are at different temperatures.

C2. There are two approaches that you could take here. The first is to say that the figures are similar to the simulations (which they are) and that this is indicative of the excellent standard of figures throughout the book. This flattery would suffice as an answer. A student with more time might like to print some screenshots and work out the radial density function! This is a lot of work and I have not done it myself but I am confident that you would obtain good results.

To obtain screen shots on a PC

Press the PRINT SCREEN button on the keyboard usually near the top right of the keyboard. This places a bitmap picture of the current screen configuration into the clipboard. Now open an application which can handle such images (WORD will do, but there are many others), and PASTE in the picture which can now be printed.

To obtain screen shots from a Mac

Use the built in help to ask for advice on 'screen shots'. There are several options about printing or saving available but roughly speaking:

- Pressing [Apple] + [shift] + [3] keys simultaneously places a picture file of your whole screen called 'picture 1' on the top level (not the desktop) of your start up disk (usually called Macintosh HD). You should hear a noise like a camera shutter. By the way, you need to press the [3] key on the main keyboard and not on the numeric keypad.
- Pressing [Apple] + [shift] + [4] keys simultaneously places a picture file of a rectangular area of screen called 'picture 1' on the top level (not the desktop) of your start up disk (usually called Macintosh HD). After pressing and releasing the keys, you need to drag the mouse to select the area to be captured. You should hear a noise like a camera shutter. By the way, you need to press the [4] key on the main keyboard and not on the numeric keypad.

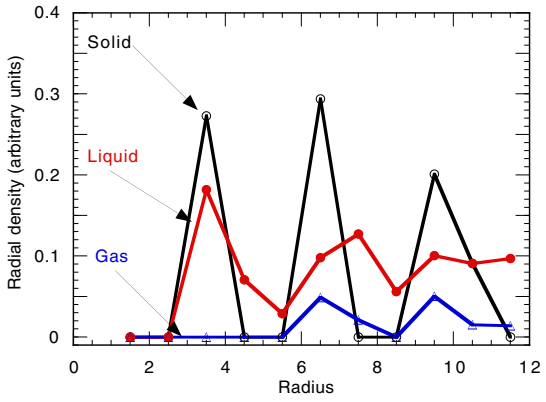
C3. Nothing for students to say here except that they have noticed that in order to allow a molecule to move within a liquid, the chance co-ordination of movements of several other molecules is required.

P4.

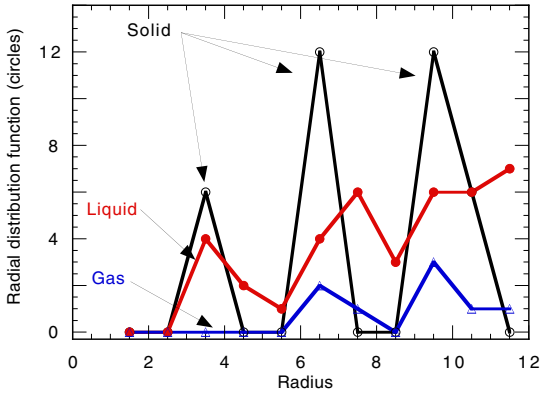
Table 8.1 Data from Example 8.1. The table shows the mean radius of each ring in Example 8.1, and summarises the data for the solid, liquid and gas examples. For each ring, it divides the number of circles (atoms) found in each ring by the approximate area of that ring, $2\pi r\Delta r$. The units are such that the width of each ring $\Delta r = 1$. This is an approximation to the radial density function for the substance. The results for the solid and liquid case are plotted in Figure 8.6.

		Solid		Liquid		Gas	
Ring	Radius	N	$n=\frac{N}{2\pi r\Delta r}$	N	$n=\frac{N}{2\pi r\Delta r}$	N	$n=\frac{N}{2\pi r\Delta r}$
1	1.5	0	0	0	0	0	0
2	2.5	0	0	0	0	0	0
3	3.5	6	0.273	4	0.182	0	0
4	4.5	0	0	2	0.071	0	0
5	5.5	0	0	1	0.029	0	0
6	6.5	12	0.294	4	0.098	2	0.049
7	7.5	0	0	6	0.127	1	0.021
8	8.5	0	0	3	0.056	0	0
9	9.5	12	0.201	6	0.101	3	0.050
10	10.5	6	0.091	6	0.091	1	0.015
11	11.5	0	0	7	0.097	1	0.014

(a) The radial density function (smoothed) for the liquid and solid is also shown in Figure 8.6



(b) the radial distribution function for the data of Table 8.1.



P5. Working out the *rdf* for a single component fluid is very similar to the procedure we have use in Example 8.1 and subsequent figures and tables. In fact its identical. For two component fluids the matter becomes much more complicated and that is really the only thing you need to realise. Not only are there 4 *rdfs* to work out, these rdfs will all change with changes in the composition of the liquid.

Amazingly, it is possible to actually measure such distribution functions for real three-dimensional liquids!

This is done using a neutron diffraction technique known as *isotope substitution*.