

Problem Set 6
(due Monday, March 1)

1. Problem 5.1, page 152. This problem is mostly tedious arithmetic, but it's important to help give a concrete feel for these abstract quantities. Don't worry that the free energies come out to be negative.
2. Problem 5.5, pages 155–156.
3. Problem 5.8, page 158.
4. Problem 5.11, page 158.
5. Problem 5.20, page 163.
6. Use the Molecular Dynamics Applet to map out a portion of the phase boundary between the gas and liquid states for this two-dimensional Lennard-Jones fluid. To do this, let the system equilibrate to a state in which a large “droplet” of liquid is surrounded by gas. Because you have two phases in equilibrium, this system is on the phase boundary in pressure-temperature space. Let the simulation run until the temperature and pressure values have stabilized, then record these values. Then add or remove some energy and repeat. You'll get better results if, after adding or removing energy, you let the system equilibrate for a little while and then hit the “Reset stats” button to remove non-equilibrium data from the averages. Even so, you'll want to run for quite a while at each energy to make sure the averages are accurate. Take data for at least six different temperature values, then plot the phase diagram (pressure vs. temperature) either by hand (carefully!) or on a spreadsheet. Be sure to record the number of atoms in your simulation. About how many atoms were in the “droplet” at each temperature? Roughly what fraction of these atoms were on the edge of the droplet at any given time? Strictly speaking, phase diagrams with sharp boundary lines apply only to infinitely large samples in which boundary effects are negligible. In light of this fact, discuss the applicability of your data to larger systems.
7. Problem 5.28, page 171.
8. Problem 5.30, page 172.
9. Problem 5.32, page 174.
10. Problem 5.35, page 175.
11. Problem 5.36, page 175. Please use a computer to make a quantitatively accurate plot—not just a sketch. I suggest using Mathematica.

Textbook Comments

Problem Set 7

With respect to the portion of your textbook that was covered by this problem set, including the problems themselves ...

Describe at least one thing that you liked about the book. Please be as specific as you can.

Describe at least one thing that you disliked about the book, or one way in which the book could be improved. Please be as specific as you can.