Statistical Mechanics Assignment 2

Due: January 26, 11:00 a.m.

Marks: 32

1. Consider the unnormalized probability density function

$$f(x) = xe^{-ax}$$

defined on the interval $x \in [0, \infty)$. In this function, a is a positive constant.

   (a) Determine the normalization constant for this distribution. [1 mark]

   Note: You can do the necessary integral by hand or using a table of integrals, or you can use Maple. The integration function in Maple is called `int()`. You can use the help system in Maple to see how it's used. The Maple keyword `infinity` has the obvious meaning, and can be used as a limit of integration. You will need to tell Maple the sign of a before you carry out this integral. This is done using the command `assume(a>0)`. After issuing this command, Maple will attach a tilde to the variable to indicate that it carries an assumption. If you use Maple, you can simply attach your worksheet to the assignment rather than reproducing all your work by hand. If you put some comments into your worksheet to explain what you're doing (which you can do using the button with a 'T' logo), you can even submit your Maple worksheet as your entire solution.

   (b) Calculate $\langle x \rangle$ for this probability density function. [1 mark]

   (c) Calculate the standard deviation of x. [2 marks]

2. One tool which is often used in statistical mechanics is coarse graining, where we take some space and divide it into imaginary boxes so that we can calculate some statistics for the contents of the boxes. In this problem, we will apply a very simple version of coarse graining to the gas molecules in a room.

   (a) Suppose that we have a $4\,\mathrm{m} \times 4\,\mathrm{m} \times 3\,\mathrm{m}$ room at $20°\mathrm{C}$ and an altitude of $1000\,\mathrm{m}$ above sea level (roughly the altitude in Lethbridge). Roughly how many oxygen and nitrogen molecules (N_{O_2} and N_{N_2}) does this room contain? In the rest of this question, we will assume that air is made up entirely of oxygen and nitrogen. [4 marks]

   Hint: Look at problem 13.7 from the textbook.

   (b) Now imagine dividing the room into two $2\,\mathrm{m} \times 4\,\mathrm{m} \times 3\,\mathrm{m}$ rectangular volumes. Denote the number of oxygen molecules in each of these two boxes by $N_{\mathrm{O}_2}^{(1)}$ and $N_{\mathrm{O}_2}^{(2)}$, and use a similar notation for the nitrogen molecules. What is the weight of a configuration for particular (given) values of $N_{\mathrm{O}_2}^{(1)}$ and $N_{\mathrm{N}_2}^{(1)}$ at fixed N_{O_2} and N_{N_2}? [2 marks]

   Hint: This is a bit like flipping a coin for each molecule to decide whether it will go into the box 1 or box 2, and then asking how many ways there are to end up with $N_{\mathrm{O}_2}^{(1)}$ molecules in box 1 out of N_{O_2} trials (flips), and similarly for the N_2 molecules.

   (c) If the number of gas molecules is very different in the two boxes, there will be a pressure difference which will result in an observable air current. Suppose that we exclude this possibility, i.e. that we only consider the case of rooms containing still air. Thus, define the total number of molecules in each box $N_i = N_{\mathrm{O_2}}^{(i)} + N_{\mathrm{N_2}}^{(i)}$ and only consider configurations for which $N_1 = N_2$. Then specifying, e.g., $N_{\mathrm{O_2}}^{(1)}$ will completely determine the system since we have three relationships (total number of oxygen molecules, total number of nitrogen molecules, and total number of molecules in each box). What is the weight of a configuration for a given value of $N_{\mathrm{O_2}}^{(1)}$ with this added constraint? [2 marks]

(d) Estimate $\ln W$ for the room described in part 2a if each of the boxes contains the same number of oxygen and of nitrogen molecules. [3 marks]

(e) Now suppose that box 1 is contains only 49% of the oxygen molecules, but that each box contains the same total number of gas molecules. What is $\ln W$ for this configuration? Also calculate the ratio of the weight calculated in the previous question to that calculated in this question. What does this calculation tell you? [4 marks]

3. A molecule has energy levels at 0, 0.03 eV and 1 eV.

(a) Calculate the partition function for this molecule at 25°C. Are all the energy levels relevant to this calculation? [3 marks]

(b) If we have 100 of these molecules, how many would we expect to be in the ground state? How many in the first excited state? [2 marks]

(c) Plot the probabilities that the molecule is in each of the three states vs temperature. What happens at very high temperatures? Discuss any other features of your graph(s) (you may need more than one to see all the relevant details) that you think are interesting. [5 marks]

(d) Obtain an expression for the average energy as a function of temperature, and plot this quantity. [3 marks]