Fys2160 – 2013 – Oblig 4

Rotation of diatomic molecules

In this project we will address the rotation of diatomic molecules using the canonical ensemble and the partition function approach.

For a diatomic molecule, the rotational energies are quantized into energy levels described by j:

$$\epsilon_j = j(j+1)\theta_r k \quad j = 0, 1, 2, \ldots \tag{14}$$

where

$$\theta_r k = \frac{\hbar^2}{2I} \, , \tag{15}$$

where I is the moment of inertia for the molecule. The values of θ_r for some molecules are listed below:

	H_2	HCl	HI	N_2	Cl_2	I_2
θ_r(K)	85.4	15.2	9.0	2.86	0.346	0.054

The energy states are degenerate, and the degeneration of each energy given by j is $g(j) = 2j + 1$.

(a) Write down the partition function $Z_R(T)$.

(b) Make a script to plot the terms in the partition function for various values of T/θ_r. Include examples where $T \ll \theta_r$ and where $T \gg \theta_r$.

(c) Find Z_r in the limit of $T \gg \theta_r$. (Convert the sum to an integral).

(d) Find Z_r in the limit of $T \ll \theta_r$. (Only include a few terms of the sum).

(e) Find the energy $E(T)$ for high and low T.

(f) Find the heat capacity $C_V(T)$ for high and log T.

We will now calculate the partition function, the energy and the heat capacity numerically to get the full behavior of the curve $U(T)$ and $C_V(T)$.

(g) Write a program that calculates the partition function $Z(T, V, N)$ for a particular value of T/θ_r. (Subject for class discussion: How to ensure that you include a reasonable number of terms in the sum.)

(h) Use the program to calculate $Z(T)$ for T ranging from $T \ll \theta_r$ to $T \gg \theta_r$. Plot the result as a function of T/θ_r.

(i) Show that your estimate for the high temperature limit above was a bit too low and estimate by how much. Can you explain this by referring to the plots of the terms in teh partition function?

(j) How can you calculate the energy and heat capacity when you know $Z(N, V, T)$? Find expressions you may use to find $U(T)$ and $C_V(T)$ numerically from $Z(N, V, T_i)$ calculated at discrete values of T_i.

(k) Calculate $U(T)$ and $C_V(T)$ numerically for T/θ_r from 0 to 3 by only including terms up to $j = 6$. Have you now kept enough terms to make the results accurate within this temperature range?

(l) Include as many terms as you deem necessary and plot $U(T)$ and $C_V(T)$. Compare with your analytical results in the low and high temperature limit. Comment on the results.

DNA zipper

In this project we will address the splitting of the double helix of the DNA molecule by approximating it a zipper. The zipper has N elements. Each element has two possible states: closed with energy 0 or open with energy ϵ. We will assume that the zipper can only be opened from one size, and that an element n can be open only if all the preceeding elements $(1, 2, \dots, n-1)$ are open – just as for an ordinary zipper.

(a) Show that the partition function for the zipper can be written as:

$$Z = \frac{1 - \exp(-(N+1)\beta\epsilon)}{1 - \exp(-\beta\epsilon)} \ . \qquad (16)$$

(b) Find the average number of open elements as a function of temperature and study the limits

- $\epsilon \gg kT$
- $\epsilon \ll kT$ and $\epsilon(N+1) \gg kT$, $(N \gg 1)$
- $\epsilon(N+1) \ll kT$

(c) How will you interpret the zipper pressure?

End of Oblig 4