5163, Homework Assignment 8
due on Monday (!!!), 04/18/2022, at 6pm (to be uploaded to Canvas)

This homework set consists of four problems.

Problem 1:
This is a quantum statistical mechanics problem.
Consider N identical bosons, each of which is treated as an isotropic three-dimensional harmonic oscillator.
Using the recursion relation from P. Borrmann and G. Franke, J. Chem. Phys. **98**, 2484 (1993) [you can access this paper through the OU library] for the partition function in the canonical ensemble, write a little code that plots (or allows you to plot) the internal energy per particle as a function of the temperature for $N = 10$.
WARNING 1: I suggest that you test your code with $N = 2, 3, \cdots$ to get results quickly. For large N, the calculations may take hours (please do not run this for $N = 1,000$).
WARNING 2: If you set your loops up incorrectly, you might end up writing a code that runs infinitely long or eats up tremendous amounts of memory. Please carefully test your code to ensure that this is not happening.
Hint: How to approach this problem?

- Step 1: Find a compact analytical expression for $S(k)$ defined in Eq. (2) of the paper [you can get rid of the infinite sum(s)—note that the subscript j is hiding three infinite sums and note that k is an integer and not Boltzmann's constant...].

- Step 2: Implement the finite sum for $Z(N)$ given in Eq. (1) of the paper. Note that Z is used to denote the canonical partition function; in class, we used Q or Q_N. It can be recognized that $Z(N)$ is defined recursively—this is where you might encounter problems if your code is not set up correctly... To give you a sense, my Mathematica notebook is seven lines long/short.

Problem 2:
In class we discussed configuration integrals. For three particles, e.g., there exist four different configuration integrals, three with two "connections" (two of the "circled" 1, 2, and 3 are connected) and one with three "connections" (the three "circled" 1, 2, and 3 are connected). We can refer to this loosely as two "topologically distinct" classes, containing respectively three graphs and one graph.
For four particles, work out the number of topologically distinct classes as well as the number of graphs per class. Do not just write down your answers—please also explain how you arrived at your answers.

Problem 3:
This problem considers the cluster expansion using classical statistical mechanics.
(a) Calculate a_2 for the hard sphere potential, which is given by $v(r) = \infty$ for $r < \sigma$ and $v(r) = 0$ otherwise.
(b) Calculate a_2 for the square well potential, which is given $v(r) = \infty$ for $r < \sigma$, $v(r) = -\epsilon$ for $\sigma \leq r \leq \alpha\sigma$ ($\epsilon > 0$ and $\alpha > 1$), and $v(r) = 0$ otherwise.
(c) What are realistic parameters for σ, ϵ, and α? And how do you know? What is the temperature regime in which you might expect the description to work reasonably well.

Problem 4:
In looking at the virial equation of state, we faced the following mathematical problem. Given the expansions

$$x = t + a_2 t^2 + a_3 t^3 + \cdots \tag{1}$$

and

$$y = t + b_2 t^2 + b_3 t^3 + \cdots, \tag{2}$$

where $a_2, a_3, \cdots$ and $b_2, b_3, \cdots$ are assumed to be known, one needs the expansion coefficients A_n that appear in the expansion

$$y = x + A_2 x^2 + A_3 x^3 + \cdots \tag{3}$$

Task of this problem: Obtain explicit expressions for A_2, A_3, and A_4.
Note: Obtaining expressions for all A_n is, in general, non-trivial.