The canonical ensemble

- What thermodynamic potential can be calculated from the canonical partition function? How is this done and how is this result derived?

- Give an expression that allows one to calculate the ensemble average, $\langle A \rangle$, for the observable A. You may assume that this quantity can be calculated based on the positions, $\mathbf{x}$, and momenta, $\mathbf{p}$, of the atoms using a function $A(\mathbf{x}, \mathbf{p})$.

- Explain why $1 = \sum_j e^{-\beta H(\mathbf{x}_j, \mathbf{p}_j) - \Psi}$

- Now calculate the first derivative of $1 = \sum_j e^{-\beta H(\mathbf{x}_j, \mathbf{p}_j) - \Psi}$ with respect to β and hence show that $\langle E \rangle = -\frac{\partial \Psi}{\partial \beta}$

The canonical ensemble

- Calculate the second derivative of $1 = \sum_j e^{-\beta H(\mathbf{x}_j, \mathbf{p}_j) - \Psi}$ with respect to β and hence show that $\langle (H - \langle E \rangle)^2 \rangle = \frac{\partial^2 \Psi}{\partial \beta^2}$

- Explain (in your own words) why $\langle (H - \langle E \rangle)^2 \rangle = -\frac{\partial \langle E \rangle}{\partial \beta}$.

- Use the chain rule to show that: $\frac{\partial \langle E \rangle}{\partial \beta} = k_B T^2 \frac{\partial \langle E \rangle}{\partial T}$

- Use the result you have just arrived at to write an expression that tells you how the heat capacity can be calculated from the fluctutations in the total energy $\langle (H - \langle E \rangle)^2 \rangle$