Chemistry 430/530a Practice Midterm 1

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Problem 1.1.

$k_BT =$ ____________________
(any unit system)

$Q(N, V, T) =$ ____________________

$Q(N, V, E) =$ ____________________

$S(p_j) =$ ____________________

$\binom{N}{n} =$ ____________________
(how many ways to order N distinguishable particles in n slots)

Problem 1.2.

In class we derived, $\langle E \rangle$ *and* $\left\langle E^2 \right\rangle$. *Please derive an expression for the ensemble average energy to the nth power,* $\langle E^n \rangle$ *using your Q(N,V,T) from Problem 1.1.*

Problem 1.3.

Please draw, roughly to scale, the phase space plot for a classical particle in a 1D box of length L *with energies* E_0, $2E_0$ *and* $4E_0$. *Please label the axes. How does the distance between contours depend on energy?*

Problem 1.4.

Given

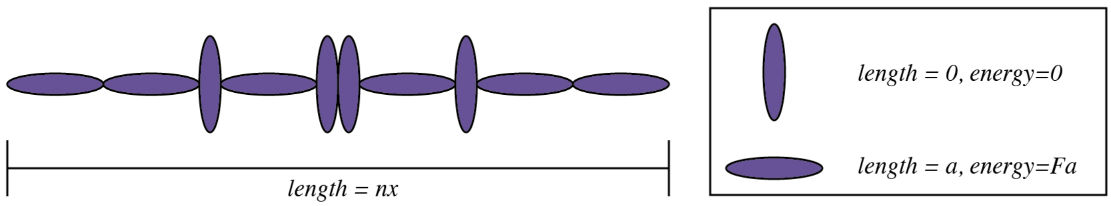
$$Q = \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega}},$$

please evaluate

$$\begin{aligned} A &= -\frac{1}{\beta} lnQ \\ \langle E \rangle &= -\frac{\partial}{\partial\beta} lnQ \\ S &= klnQ + \frac{\langle E \rangle}{T} \\ C_V &= \frac{\partial \langle E \rangle}{\partial T}, \end{aligned}$$

and show that $C_V = k_B$ *when* $k_B T \gg \hbar\omega$ *using the approximation valid at high temperatures,* $e^{\hbar\omega/k_B T} \approx 1 + \frac{\hbar\omega}{k_B T}$.

Problem 1.5. *Here we consider a one-dimensional chain of n segments, as illustrated below. Each segment can exist in two states- length $x = a$ or length $x = 0$. When tension F is applied, the energy of a segment is $F \cdot x$, or $a \cdot F = aF$ for extended or $0 \cdot F = 0$ for contracted segments, respectively. Thus by changing F, we can change the energy difference between the two states.*



What is the partition function, Q, for one segment at temperature T and tension F?

Using this result, calculate the average length, $\langle x \rangle$ of one segment as a function of T.

For n segments, the length will be $n \langle x \rangle$. Verify that this result leads to Hooke's Law, $n \langle x \rangle = c_0 + c_1 F$, at high temperatures where the limit $e^{-Fa/k_BT} \approx 1 - \frac{Fa}{k_BT}$ is applicable.

Problem 1.6. *Recall the 1D Ising model with N spins, each situated at a lattice site, and each spin may be up or down.*

$$\boxed{\uparrow}\boxed{\downarrow}\boxed{\uparrow}\boxed{\uparrow}\boxed{\downarrow}\boxed{\uparrow}\cdots\boxed{\downarrow}$$

We will treat four spins with no nearest neighbor coupling. If we represent an $\boxed{\uparrow}$ *with* $s_i = +1$ *and* $\boxed{\downarrow}$ *with* $s_i = -1$*, then the energy function for the system, the Hamiltonian, is*

$$H = -J \sum_{i=1}^{4} s_i. \tag{1}$$

For ***four spins****, please write out all possible energy levels and the degeneracy for each energy level.*

Sketch a plot of how the entropy S changes as a function of the energy of the system. Recall that we define the temperature $\frac{1}{T} = \frac{dS}{dE}$. Show that the temperature is negative as $E \to E_{max}$. Does negative temperature mean the system is "colder"?