Homework 2: Microcanonical ensemble and Canonical Ensemble (intro)

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1. *Surface area of an N-dimensional sphere.* In order to derive the partition function for an ideal gas of particles, we needed to know the formula for the surface area of a sphere in 3N-dimensions. Let's actually derive this formula so we can see where it comes from. It takes advantage of knowledge and similar techniques you learned from Homework 1.

   First, a quick definition, the way mathematicians write things. The volume of a sphere-like object of radius 1 (every point is distance $r <= 1$ from the origin) in d dimensions is called V_d. Confusingly, the surface area of that same object is called S_{d-1} (since it is an object which is 1-dimension "flatter"). The volume of d-sphere of radius R is $V_d R^d$ and the surface area is $S_{d-1} R^{d-1}$. So, e.g. $V_3 = \frac{4}{3}\pi R^3$ and $S_2 = 4\pi R^2$.

   (a) A d-sphere can be built by adding up a bunch of shells of smaller radius (Think, make up a disk ($d = 2$) by drawing a bunch of concentric circles). The volume is the addition of all of the surface areas of the shells. So,

   $$V_d = \int_0^1 dr S_{d-1} r^{d-1} = S_{d-1}\frac{1}{d}r^d \Big|_0^1 = \frac{S_{d-1}}{d} \qquad (1)$$

   Show that this formula is correct for $d = 2$ and $d = 3$ using your knowledge of circles and spheres.

   (b) We already used polar and spherical coordinates in class to derive certain things. We saw that if the function we want to integrate only depends on distance from the origin, then

   $$\int dx_1 dx_2 ... dx_d f(r) = \int_0^\infty dr S_{d-1} f(r) r^{d-1} = S_{d-1} \int_0^\infty dr f(r) r^{d-1}, \qquad (2)$$

   where $r^2 = \sum_{i=1}^d x_i^2$ (do you see how this is true for spherical and polar coordinates?). If $f(r) = 1$ then we get back Eq. 1 (with different integration limits).

If we can solve both sides of this integral for any $f(r)$, then we will have a general formula for S_{d-1}.

Do the following steps:

i. Similar to last week, define $I = \int_{-\infty}^{\infty} e^{-x^2} dx$. Write I^d as a product of integrals over different coordinate variables and get an integral over a function of r that looks like the left hand size of Eq. 2.

ii. Now that you an $f(r)$, show that the right-hand side can be rewritten as something proportional to $\Gamma(d/2)$. You will have to do a substitution.

iii. Since we know the value of I from last time, we also know the value of I^d. Equate this value with the formula from the proceeding step to get our answer from class, $S_{d-1} = 2\frac{\pi^{d/2}}{\Gamma(d/2)}$ (book equation 3.5.14, with $n = d - 1$).

iv. Given this result, what is the formula for the Volume of a $d-$sphere of radius 1, V_d? Use the fact that $\frac{d}{2}\Gamma(\frac{d}{2}) = \Gamma(\frac{d}{2} + 1)$ to simplify the equation.

(c) i. Use the definition of the gamma function to show $\Gamma(1/2) = \sqrt{\pi}$. Hint: The right hand side should look familiar here. Reverse your substitution from earlier to get a familiar integral.

ii. Use this result and the formula for V_d above to show that V_3 has the value you expect for a sphere.

2. *Gibbs Paradox*. Show that the entropy of mixing of two boxes of identical particles is non-zero unless the $1/N!$ factor is included in the microcanonical partition function (follow Tuckerman book Section 3.5.1).

3. *Two-level system*. Two level systems are a very common way to model systems in chemistry and physics. For example, the nuclear spin state of a proton might be considered to have two states (up and down). We will study the thermodynamic properties of this kind of system at constant temperature.

(a) Write the partition function for a single spin at constant temperature in the canonical ensemble (remember this is a discrete system). The energies of the two states are $E_0 = 0$ and $E_1 = \epsilon$. We can call this partition function $q(T)$ since there is only one particle and there isn't really a volume.

(b) Now consider N isolated and distinguishable two level systems. Isolated means that the state of one doesn't effect the state of the other. Show that in this case, the total partition function $Q(N, T) = q^N$.

(c) Compute the average number of independent two level systems that are in the excited state (out of N systems at temperature T). This number is equals $\langle \sum_{i=1}^{N} n_i \rangle$, with n_i is either 0 or 1. Sketch $N_{excited}$ as $\epsilon/k_B T$ goes from 0 to ∞.

(d) Use the results from class/the book to calculate the thermodynamic quantities A, E, S, and C_V (heat capacity) for the system with N two level systems. Sketch the result for E as a function of ϵ.