

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 $r \leq 1$ from the origin) in d dimensions is called V_n . 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,

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

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

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

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. 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 side of Eq. 2.
 - ii. Now that you have $f(r)$, 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 preceding 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 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 .