Homework 2: Microcanonical ensemble

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Due: Oct 1, 2021 at 5pm

1. *The Gamma (Γ) function as a generalized factorial.* The Γ function has an important property that we will use to derive the microcanonical partition function for an ideal gas, which is that it acts as a factorial operator for integers. The gamma function is defined as

$$\Gamma(z) = \int_0^\infty x^{z-1} e^{-x} dx \tag{1}$$

Show that $\Gamma(N+1) = N! = N(N-1)(N-2)...(2)(1)$ by the following steps:

   (a) Show that $\Gamma(1) = 1$

   (b) Using integration by parts, show that $\Gamma(z+1) = z\Gamma(z)$ for z as a real number

   (c) Using the above two properties, show that $\Gamma(N+1) = N!$ for N integers greater or equal to 1.

2. *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,

$$V_d = \int_0^1 dr S_{d-1} r^{d-1} = S_{d-1} \frac{1}{d} r^d \bigg|_0^1 = \frac{S_{d-1}}{d} \tag{2}$$

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 to derive certain things. We saw that if the function we want to integrate only depends on distance from the origin, and $r^2 = \sum_{i=1}^{d} x_i^2$, then

$$\int dx_1 dx_2 ... dx_d f(r) = \int_0^\infty dr S_{d-1} f(r) r^{d-1} = S_{d-1} \int_0^\infty dr f(r) r^{d-1}, \tag{3}$$

(do you see how this is true for spherical and polar coordinates?). If $f(r) = 1$ then we get back Eq. 2 (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. 3.

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 the final result for surface areas, (book equation 3.5.14, with $n = d - 1$)

$$S_{d-1} = 2 \frac{\pi^{d/2}}{\Gamma(d/2)} \tag{4}$$

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.

3. *Microcanonical ideal gas, finishing the derivation.* In class, we worked out that the

microcanonical partition function has the form

$$\Omega(N, V, E) = \frac{E_0 V^N}{h^{3N} N!} \int_{-\infty}^{\infty} dp_1 dp_2 ... dp_{3N} \delta \left(\sum_{i=1}^{3N} \frac{p_i^2}{2m} - E \right) \tag{5}$$

If we substitute $p_i = \sqrt{2m} y_i$ here, we get

$$\Omega(N, V, E) = \frac{E_0 V^N (2m)^{3N/2}}{h^{3N} N!} \int_{-\infty}^{\infty} dy_1 dy_2 ... dy_{3N} \delta \left(\sum_{i=1}^{3N} y_i^2 - E \right) \tag{6}$$

(a) Use Eq. 3 and Eq. 4 to rewrite this as

$$\Omega(N, V, E) = \frac{E_0 V^N (2m)^{3N/2}}{h^{3N} N!} \frac{2\pi^{3N/2}}{\Gamma(3N/2)} \int_0^{\infty} dr \delta(r^2 - E) r^{3N-1} \tag{7}$$

(b) Use the formula from class to split this delta function into two delta functions, then perform the integral to show that

$$\Omega(N, V, E) = \frac{E_0 V^N (2m)^{3N/2}}{h^{3N} N!} \frac{\pi^{3N/2}}{\Gamma(3N/2)} \frac{E^{3N/2}}{E} \int_0^{\infty} dr \delta(r^2 - E) r^{3N-1} \tag{8}$$

$$= \frac{E_0}{E} \frac{1}{N!} \frac{1}{\Gamma(3N/2)} \left[V \left(\frac{2\pi m E}{h^2} \right)^{3/2} \right]^N \tag{9}$$

(c) *Stirling's approximation* says that $\log(N!) \approx N \log N - N$ or equivalently $N! \approx N^N e^{-N}$ for large N. Substituting $\Gamma(X - 1) = X!$, using the approximation $N - 1 \approx N$ for very large N, and using Sterling's approximation for this term, show that

$$\Omega(N, V, E) = \frac{E_0}{N!} \left[V \left(\frac{4\pi m E e}{3N h^2} \right)^{3/2} \right]^N \tag{10}$$

(d) Using our formula for entropy, $S = k_B \log(\Omega(N, V, E))$, substituting the formula we derived $E = \frac{3}{2} N k_B T$, and neglecting $k_B \log(E_0)$ both because it is an arbitrary constant and because it is not proportional to N,

i. Show that the entropy of a monatomic ideal gas is:

$$S(N, V, E) = N k_B \log \left[V \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \right] + \frac{3 N k_B}{2} - k_B \log(N!) \tag{11}$$

ii. And using Stirling's approximation, derive the *Sackur-Tetrode* equation:

$$S(N, V, E) \approx N k_B \log \left[\frac{V}{N} \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2} \right] + \frac{5}{2} N k_B \tag{12}$$

4. *Gibbs Paradox*. Show using the entropy formula from above (Eq. 11), 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).