Homework 1: Statistics and phase space distributions

Glen Hocky

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1. (Computational) Fill in the missing pieces in this exercise: https://github.com/hockyg/chem-ga-2600/blob/master/statistics/statistics-week1.ipynb. This will demonstrate how diffusive processes converge and give you some practice with python.

   When finished, download with File->Download As->ipynb so you have a copy. You can either email this to me or print it out and attach to the other homework.

   If you want to do this on your local computer, you can install the anaconda python 3.6 distribution for your local computer from this link: https://www.anaconda.com/download Then from anaconda you will have to install at least jupyter, numpy, matplotlib, and scipy. Afterwards, type 'jupyter notebook' on your command prompt or terminal.

2. The normal distribution,

$$\mathcal{N}(\mu,\sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-(x-\mu)^2}{2\sigma^2}}, \tag{1}$$

   is extremely important for statistical mechanics, and generally in physics. We looked in exercise 1 at the central limit theorem, where the sum of random numbers converges to a normal distribution, and how this is important for showing that our measurements of averages of an observable will converge to the true mean of that observable.

   2.1. Often this function comes up without normalization. An equivalent function is $f(x) = \exp(-ax^2)$, $a > 0$. Show that

$$\int_{-\infty}^{\infty} \exp(-ax^2)dx = \sqrt{\pi/a} \tag{2}$$

Hint: this is done by setting $I = \int_{-\infty}^{\infty} \exp(-ax^2)dx$ and showing that $I^2 = \pi/a$. You will find this solution many many places on the internet, but I'm asking you to write it all out so you know where it comes from.

2.2. An important "trick" in statistical mechanics is to look at constants inside of a function or an integral and pretend they are variables that you might change. For example, you can think of I as I(a).

i. Show that you can take the derivative of both sides of Eq. 2 with respect to a to find $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx$, and find out what the result is as a function of a

ii. For a probability distribution, $\langle A \rangle = \int_{-\infty}^{\infty} A(X)P(X)$. Use this trick and proceeding result to find $\langle x^2 \rangle$ and $\langle x^4 \rangle$ for the normal distribution $\mathcal{N}(\mu, \sigma^2)$.

3. I asserted in class that, at equilibrium, $\{f, H\} = 0$ means that the phase space distribution f must be a direct function of H (and it also doesn't depend on time any more), i.e. we can write something like $f(\vec{x}, t) = \mathcal{F}(H)$. Under these conditions, $\frac{dH}{dt} = 0$.

   Let's show that $\frac{df}{dt} = 0$ if $\mathcal{F}$ can be written in the following form, which covers most functions, including $\mathcal{F}(H) = \exp(-H(x)/k_B T)$.

$$\mathcal{F}(H) = \sum_{n=-\infty}^{n=\infty} c_n H^n \tag{3}$$

   (a) First, show that $\frac{dH^n}{dt} = 0$. Hint: remember the chain rule, $\frac{dx^n}{dy} = nx^{n-1}\frac{dx}{dy}$.

   (b) Show for Poisson brackets that $\{A(a+b), c\} = A\{a, c\} + A\{b, c\}$ where A is a constant that doesn't depend on any of $\{q_i\}$ or $\{p_i\}$.

   (c) Show $\frac{d\mathcal{F}}{dt} = \{\mathcal{F}, H\} = 0$ for $\mathcal{F}$ in the form of Eq. 3.