Homework 1

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Due: Thursday Sept 24 (5PM NYC)

1. (Computational) Fill in the missing pieces in the statistics computational exercise. This will demonstrate how diffusive processes converge and give you some practice with python.
   This exercise is available by logging in to https://chemga-2600-fall.rcnyu.org/ and going to the assignments tab. There you can push "Fetch" next to statistics. From here you can access the statistics exercise. When done, click validate and then submit.

   Alternatively, you can use the mybinder button on my github page or download the following notebook to run it on your local computer:
   Site: https://github.com/hockyg/chem-ga-2600
   Notebook: statistics/statistics-week1.ipynb
   When finished, download with File->Download As->ipynb so you have a copy. **If not using rcnyu, attach this notebook along with answers to the next item.**

   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 $\int_{-\infty}^{\infty} x^2 e^{-ax^2} dx$ as a function of a

ii. For a probability distribution $P(x)$, $\langle A \rangle = \int_{-\infty}^{\infty} A(x)P(x)dx$. 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. In class, an important question was raised: if X is a random variable and $f(X)$ is some function of that random variable, is $\langle f(X) \rangle \stackrel{?}{=} f(\langle X \rangle)$. *Jensen's inequality* says that if f is *convex*, then $\langle f(X) \rangle \geq f(\langle X \rangle)$. A particularly important case for statistical mechanics is the function $f(X) = e^X$.

(a) Given that $\langle X \rangle = \mu$ (where μ is a constant) and that $X = X + \mu - \mu$, show that $\langle e^X \rangle = e^{\langle X \rangle} \langle e^{X-\mu} \rangle$.

(b) Show that $e^x \geq 1 + x$ (hint, show that $e^x - x - 1$ has a global minimum at $x = 0$).

(c) Combine the previous two pieces of information to show that $\langle e^X \rangle \geq e^{\langle X \rangle}$.