Homework 1

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Due: Friday Sept 17 (5PM NYC)

1. **Normal/Gaussian distribution.** 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 science.

1.1. 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.

1.2. 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 $\langle x^2 \rangle$ for the normal distribution $\mathcal{N}(\mu,\sigma^2)$. What is $\langle x^2 \rangle$ when $\mu = 0$?

iii. Find $\langle x^4 \rangle$ for the case where $\mu = 0$ using a continuation of the trick from part i.

1.3. Use Eq. 2 to simplify the partition function for a 1-D harmonic oscillator to the final result we had in class:

$$Z = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dp e^{-\beta(\frac{1}{2}kx^2 + \frac{p^2}{2m})} \tag{3}$$

1.4. Use a result from problem 1.2. to compute the average potential and kinetic energies for a single harmonic oscillator, i.e. $\langle \frac{1}{2}kx^2 \rangle$ and $\langle \frac{p^2}{2m} \rangle$.

2. **N-independent harmonic oscillators.** We previously wrote down the partition function for one harmonic oscillator in 1-d (Eq. 3).

   (a) Write the partition function for N independent harmonic oscillators, which has the Hamiltonian
   $$H = \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \frac{1}{2}k_i x_i^2 \tag{4}$$

   (b) Solve the partition function as in the previous problem

   (c) Compute the average total energy of the system of $N-$ oscillators. How does it compare to the average energy of 1 oscillator?

3. **Harmonic oscillator with quantized energy levels..** Quantum mechanically, a single harmonic oscillator can only occupy certain discrete energy levels. These energy levels are equally spaced, and are given by the formula $E_n = \hbar\omega(n + \frac{1}{2})$, where $\omega = \sqrt{k/m}$. The partition function at constant temperature for this system is given by
   $$Z = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega(n+\frac{1}{2})} \tag{5}$$

   (a) Get a simplified formula for Z using the formula for an infinite harmonic series, $\sum_{i=0}^{\infty} ar^n = \frac{a}{1-r}$ if $r < 1$. When is $r < 1$ in this case, and do you think that makes physical sense?

   (b) Compute a formula for the average energy using the formula $\langle E \rangle = -\frac{\partial \log Z}{\partial \beta}$

   (c) Sketch a plot of this function against β from 0 to ∞

   (d) What is the value of $Z(\beta \to 0)$ and $Z(\beta \to \infty)$. Do these answers make sense?