Physics 4251/6250 – Fall 2019
Problem Set 2, September 4
Due: Friday, September 13 by 5 PM

Problem 1: DNA unzipping

A zipper has N links; each link has a state in which it is closed with energy 0 and a state in which it is open with energy ϵ. We require, however, that the zipper can only unzip from the left end, and that the link number s can only open if all links to the left (1,2,....,s-1) are already open. This is a simplified model of two-stranded DNA unwinding (credit goes to C. Kittel, Amer. J. Physics 37, 917 (1969).)

(a) Show that the partition function can be written in the form

$$Z = \frac{1 - \exp[-(N+1)\beta\epsilon]}{1 - \exp(-\beta\epsilon)}. \tag{1}$$

(b) Derive an expression for the average number of open links, $\langle s \rangle$, in terms of the partition function Z. (Hint: recall that $\langle \epsilon \rangle = -\mathrm{d}(\ln Z)/\mathrm{d}\beta$).

(c) Determine $\langle s \rangle$.

(d) What are the high-T and low-T limits of $\langle s \rangle$?

Problem 2: Applying Jarzynski's Equality using simulated data

For this problem, we are going to generate and analyze the unfolding of a deca-alanine helix. On the course website is `HW2-files.zip`, which contains the files needed to run a 1-ns `namd2` simulation stretching deca-alanine in vacuum at 20 Å/ns (note: this is VERY fast!) and T=300 K. Use the commands in the Jupyter notebook provided in the HW2 folder on the course's Github as a starting point. You will have to fill in some parts, clearly indicated.

(a) Download the molecular dynamics simulation program NAMD from
http://www.ks.uiuc.edu/Research/namd/ (see "Download NAMD" on the left side of the page). Choose the version appropriate for your computer, likely `Win64`, `MacOSX-x86_64`, or `Linux-x86_64-multicore`. There is no installation needed; the executable `namd2` or `namd2.exe` can be run directly at the command prompt.

(b) Run the simulation `smd.namd` by typing at the command prompt `namd2 smd.namd > smd.log`. Among the various output files will be `da_smd_tcl.out`, which contains the time (in ps), the position (in Å), and the force (in kcal/mol·Å). Rename this file to `da_smd_tcl.1.out` and then run the simulation again. Do this at least five times. NOTE: if you have any problems running the simulations, let me know.

(c) Load `da.psf` in VMD, followed by `da_smd.dcd` (the trajectory from your most recent run). Make a figure of the starting and ending states of deca-alanine in a "nice" representation of your choosing, i.e., not the default lines, that clearly indicates the stretching process.

(d) **Using the provided python code as a starting point**, plot the force curves on top of one another. They should appear quite noisy. **Include the image in your submitted homework**.

(e) Calculate the work,

$$W(x) = \int_{x_0}^{x} F(x')dx' \tag{2}$$

for each force curve and plot them. How do they compare to the exact free-energy curve (a potential of mean force, PMF) provided in `PMFexact.dat`? **Include the image in your submitted homework**.

(f) Do any of the work curves plotted in (e) violate the Second Law of Thermodynamics, i.e., is the work done ever less than the free energy?

(g) Calculate $\langle W(x) \rangle$ and plot it. **Include the image in your submitted homework**.

(h) Now use Jarzynski's equality

$$e^{-F/kT} = \langle e^{-W/kT} \rangle \tag{3}$$

to calculate the free energy, F, as a function of x. Make sure to use appropriate units for k. Plot this along with the curve from (g) and the exact PMF from `PMFexact.dat`. **Include the image in your submitted homework**.

(i) How does the first-order approximation to the free energy in (g) compare to the exact PMF? How does the estimate from Jarzynski's equality in (h) compare?

Note that the simulation for this problem comes from the tutorial "Stretching Deca-alanine", available at `www.ks.uiuc.edu/Training/Tutorials/`.