Physics 4251 / Fall 2017
Problem Set 2, September 1
Due: Tuesday, September 12 before class

Policy on emailed homework: If you want to move into an all-digital age, you may email your homework to me (`gumbart@physics.gatech.edu`) provided that you do it **BEFORE** class on the due date. Begin the subject with [**PHYS 4251**] for easy identification.

Problem 1: Connecting Information Theory with Thermodynamics

We swept the problem of Second Law violations by a Maxwell's Demon under-the-rug by claiming that the demon must be part of the system and therefore its entropy will increase to cancel out that lost by the gas. However, what does it mean physically for the demon?

An extension of Maxwell's Demon is the so-called "Szilard engine", in which an agent creates useful work from a single temperature bath. In the setup, a Maxwell demon sits on top of a box containing a single particle in contact with a thermal bath. The demon then inserts a partition in the center of the box and measures which half of the box the particle is in. From there, the demon inserts a piston into the empty side of the box and allows the particle to isothermally expand the piston until it reaches the edge. If this piston is attached to a weight, the system has now extracted useful work from a thermal bath, in apparent violation of the Second Law.

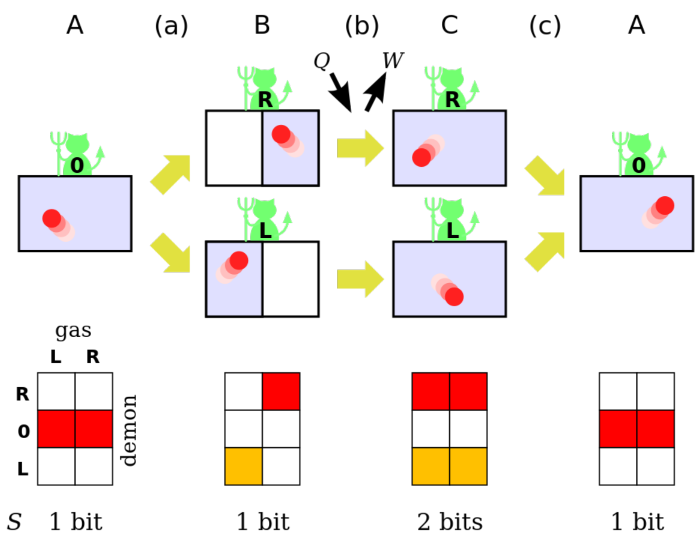

Figure 1: Szilard engine. In (a), the demon inserts the partition and measures the state of the particle, placing a piston on the opposite side. In (b) the particle then expands against the piston, exchanging heat from the bath to do work. The engine/demon go through states A, B, and C, finally resetting to A when the demon erases the added bit of information.

(a) How much work does the particle do in expanding the piston? Assume it's an ideal gas ($PV = kNT$).

(b) Because we assume all aspects of the demon's operation can be done such that $\delta Q = 0$, what must be the corresponding **minimum** entropy increase of the demon in order to recover the Second Law?

(c) In order to perfectly reset to its original state, the demon must erase its memory of which half of the box the particle was in. What is the Shannon entropy ($S = -\sum_{i=1}^{N} p_i \ln p_i$) associated to this process? (Hint: Its memory is essentially a two-state system.)

(d) Finally, using the results of parts b and c, derive an expression connecting the Shannon entropy with the thermodynamic entropy.

Rather than being purely abstract, the connection between information and energy has been experimentally demonstrated! See the paper Toyabe et al. "Experimental demonstration of information-to-energy conversion and validation of the generalized Jarzynski equality". (2010) *Nature Physics*. 6:988–992.

Problem 2: 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 $\langle \epsilon \rangle = -\frac{\mathrm{d}(\ln Z)}{\mathrm{d}\beta}$).

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

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

Problem 3: Applying Jarzynski's Equality using simulated data

For this problem, we are going to analyze the unfolding of a deca-alanine helix using real simulation data. On the course website are 10 files, `FvD1.dat - FvD10.dat`, that contain the force (units of kcal/mol·Å) as a function of extension (units of Å) for 10 constant-velocity steered MD simulations. The unfolding speed was 10 Å/ns and the temperature was 300 K. You will provide three plots, one for (a), one for (b), and one for (c)-(d), in addition to your short answers. 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) Plot the 10 force curves on top of one another. They should appear quite noisy.

(b) 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`? Do any violate the Second Law of Thermodynamics, i.e., is the work done ever less than the free energy?

(c) Calculate $\langle W(x) \rangle$ and plot it.

(d) 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 (c) and the exact PMF from `PMFexact.dat`.

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

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