Problem 1 (20 pts): Connecting Information Theory with Thermodynamics

(a, 5). How much work does the particle do to expand the piston?

\[ W = \int_{V/2}^{V} PdV = \int_{V/2}^{V} \frac{NkT}{V} dV = kT[\ln V - \ln(V/2)] = kT \ln 2 \]  

(b, 5). What is the entropy change of the environment?

The total entropy change, \( dS_T = dS_{\text{sys}} + dS_{\text{env}} \), is \( \geq 0 \). Using the first law of thermodynamics,

\[ TdS_{\text{sys}} = TdU_{\text{sys}} + PdV_{\text{sys}} = 0 + kT \ln 2 \rightarrow dS_{\text{env}} = -k \ln 2. \]

(c, 5). What is the Shannon entropy for erasing the demon’s memory?

The memory before erasure is in one of two states with equal probability whereas after erasure, its locked in one defined state. Thus, using the definition of entropy from part a,

\[ \Delta S = S_{\text{after}} - S_{\text{before}} = (-1 \ln 1) - (2(-\frac{1}{2} \ln \frac{1}{2})) = \ln \frac{1}{2} = -\ln 2. \]

Note that the Shannon entropy is often defined using \( \log_2 \) instead of \( \ln \). This is equivalent, though, and incurs only a change in the constant in front.

(d, 5). Relate the Shannon and thermodynamics entropies.

The thermodynamic change in entropy is \( dS_{\text{demon}} = -k \ln 2 \) whereas the Shannon entropy change is \( \Delta S = -\ln 2 \). Thus, \( kS_{\text{Shannon}} = S_{\text{thermo}} \).

Problem 2 (20 pts): DNA unzipping

(a, 5) Derive the given form of the partition function.

\[ Z = \sum_{s=0}^{N} e^{-\beta s\epsilon} = \sum_{s=0}^{N} (e^{-\beta \epsilon})^{s} = \frac{1 - \exp[-(N + 1)\beta \epsilon]}{1 - \exp(-\beta \epsilon)} \]

where we use the formula for a geometric series \( \sum_{n=0}^{N} x^n = (1 - x^{N+1})/(1 - x) \).

(b, 5) Derive an expression for \( \langle s \rangle \).

\[ \langle s \rangle = \frac{1}{Z} \sum_{s=0}^{N} s e^{-\beta \epsilon} = \frac{1}{Z} \frac{-\partial}{\partial (\beta \epsilon)} \sum_{s=0}^{N} e^{-\beta \epsilon} = \frac{1}{Z} \frac{-\partial}{\partial (\beta \epsilon)} Z = -\frac{1}{\epsilon} \frac{\partial}{\partial \beta} \ln Z. \]

(c, 5) Determine \( \langle s \rangle \).
\[ \ln Z = \ln[1 - \exp(-(N + 1)\beta\epsilon)] - \ln[1 - \exp(-\beta\epsilon)] \]  
\[ \langle s \rangle = -\frac{\partial}{\partial(\beta\epsilon)} \ln Z = \frac{-(N + 1)\exp[-(N + 1)\beta\epsilon]}{1 - \exp[-(N + 1)\beta\epsilon]} + \frac{\exp(-\beta\epsilon)}{1 - \exp(-\beta\epsilon)} \]

(d, 5) What are the high-\(T\) and low-\(T\) limits of \(\langle s \rangle\)?

As \(T \to 0\), \(e^{-\beta\epsilon} \to 0\), thus making \(\langle s \rangle = 0/1 + 0/1 = 0\).

As \(T \to \infty\), \(e^{-\beta\epsilon} \approx 1 - \beta\epsilon\). Thus,

\[ \langle s \rangle \approx \frac{-(N + 1)[1 - (N + 1)\beta\epsilon]}{1 - [1 - (N + 1)\beta\epsilon]} + \frac{1 - \beta\epsilon}{1 - [1 - \beta\epsilon]} = \frac{(N + 1)\beta\epsilon - 1}{\beta\epsilon} + \frac{1 - \beta\epsilon}{\beta\epsilon} = N. \]

A lot of people got \(N/2\); I’d be curious to know if anyone can figure out why.

**Problem 3 (20 pts): Applying Jarzynski’s Equality using simulated data**

(a, 5) Plot the 10 force curves.

See Fig. 1.

(b, 5) Calculate the work, \(W(x)\).

The work curves are plotted in Fig. 2. Two of them appear to violate the Second Law for some values of \(x\), although all end above the PMF.

(c-d, 5) Plot the average work as well as the Jarzynski-averaged work along with the exact PMF.
See Fig. 3.

(e, 5) How do the curves all compare?

The first-order approximation, $\langle W \rangle$, clearly diverges significantly more from the exact PMF than the estimate from Jarzynski’s identity.