Problem 1 (15 points): Toy model of protein folding
(a, 5) At temperature $T$, what is the probability, $p_o$, of finding the molecule in an open conformation? What is the probability, $p_c$, that it is compact?

\[
p_o = \frac{\sum_{\text{open states}} e^{-E_o/kT}}{\sum_{\text{open states}} e^{-E_o/kT} + \sum_{\text{closed states}} e^{-E_o/kT}} = \frac{3 e^{-\epsilon/kT}}{3 e^{-\epsilon/kT} + 1}
\]

\[
p_c = \frac{\sum_{\text{closed states}} e^{-E_c/kT}}{\sum_{\text{open states}} e^{-E_o/kT} + \sum_{\text{closed states}} e^{-E_c/kT}} = \frac{1}{3 e^{-\epsilon/kT} + 1}
\]

Note that the two probabilities sum to 1.

(b, 5) What happens to the probability $p_c$, calculated in (a), in the limit of very large and very low temperatures?

At high temperatures, $e^{-\epsilon/kT} \to 1$ and $p_c \to 1/4$. This makes sense, as at high temperatures, all states become equally likely. (If you’re confused because of the DNA zipper problem, that one was interpreted a bit differently.)

(c, 5) What is the average energy of the molecule at temperature $T$?

From the class notes, we know that $\langle E \rangle = -\partial / \partial \beta \ln Z$.

\[
\langle E \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \ln \left(3 e^{-\beta \epsilon} + 1\right) = \frac{3 \epsilon e^{-\beta \epsilon} + 1}{3 e^{-\beta \epsilon} + 1} = \frac{3 \epsilon}{3 + e^{\beta \epsilon}}.
\]

Problem 2 (20 points): Toy model of protein folding (redux)
(a, 10) Create your own 10-residue protein sequence. Draw three possible folds on a 2D lattice, at least one of which is compact and one of which is open. Label each of them with its energy.

I will use the sequence HPHPPHRHP. See Fig. 1 on the next page for the example folds.
Figure 1: Three folds of the selected sequence.

(b, 5) Now input your sequence into the python code `HPmodel.ipynb`. **Run it at least five times.** What are the minimum energies for each run?

For my five runs, I got $E_{\text{min}} = -2, -2, -2, -3, -2$. The fact that only 1/5 runs produced the lowest energy demonstrates why we run it multiple times.

(c, 5) Paste a picture of the chain with the lowest energy found in part (b).

Figure 2: Lowest-energy conformation of the HP protein with energy $E_{\text{min}} = -3\epsilon$.

**Problem 3 (20 points): The Poisson-Boltzmann equation**

(a, 10) Consider the PB equation and carry through a change of variables that eliminates dependence on units.

$$
\frac{d^2 V(x)}{dx^2} = \frac{zq_c}{D\epsilon_0} \left( e^{zqV(x)/kT} - e^{-zqV(x)/kT} \right)
$$

(4)
To eliminate units, we let \( \chi = x/\lambda_D = \sqrt{2z^2q^2c_\infty/D\epsilon_0kT} \) and \( \nu(\chi) = zqV(\chi)/kT \). The right hand side of Eq. 4 is simple to replace \( V \) and \( x \), giving \( zqc_\infty/D(\epsilon_0(\nu(x) - e^{-\nu(x)}) \) but the derivative on the left requires more care, namely
\[
\frac{d^2V(x)}{dx^2} = d\frac{dV}{dx} \left( \frac{d\nu}{dx} \frac{dV}{d\chi} \right) = \frac{d}{dx} \left( \frac{d\nu}{d\chi} \frac{kT}{zq} \sqrt{2z^2q^2c_\infty/D\epsilon_0kT} \right).
\]
where the second \( d/dx \) proceeds in a similar fashion. Thus, you should find that a number of constants cancel out, leaving
\[
\frac{d^2\nu(\chi)}{d\chi^2} = \frac{1}{2} \left( e^{\nu(\chi)} - e^{-\nu(\chi)} \right).
\]

(b, 5) Now we will use a simple python code, given in PBsolver.ipynb, to iteratively solve the PB equation for the potential around a fixed charge in a solution. Add your function at the noted location and produce the plot at the end showing the two curves are identical.

The function is \( v -= c_l*DT*0.5*(exp(v)-exp(-v)) \). The resulting plot is given in Fig. 4.

(c, 5) By testing different values of \( Q_0 \), find the charge at which point the solution to the linearized PB equation diverges from the iterative solution to the exact PB equation.

Based on the plot below, I would say the linearized solution diverges around \( Q_0 = -4 \).