Physics 319 W2020 Assignment 3

Due: Saturday Feb 22, 2020 by 11:59 PM online submission on MyCourses
No extensions on this assignment as solutions will be posted on Sunday (ahead of test)

1. Entropy versus energetics in a lattice model of ligand receptor binding

Consider a simple lattice model with 25 solvent lattice sites and 7 ligands. Assume one ligand binds to a receptor and is removed from the solvent lattice (the receptor is not part of the solvent lattice while ligands in solution occupy lattice cells).

i) Sketch two possible microstates one each for before and after ligand binding. Calculate the entropy S for the two cases.
ii) Calculate the change in entropy ΔS upon ligand binding
iii)Is the entropy change after ligand binding favorable? Explain.

iv) What would the difference between the solution and ligand binding energies have to be a multiple of k_bT to exactly counter (match) this entropy change? Use the partition function weights for the two cases to solve this.

2. Book question 7.4 State probabilities in the MWC model

Plot the p_0, p_1, and p_2, the probabilities of different states of occupancy for both the T and R states for the MWC model of the hypothetical dimoglobin (the subscripts refer to 0, 1 and 2 ligand molecules bound for both T and R states). Use the same parameters to generate your plot that were use used to generate Figure 7.21 (see below).

Hint: for each ligand occupancy state, consider both the T and R states together not separately.
Also since there is only one ligand; so instead of having two concentration variables x and y, it makes more sense to have one concentration variable x and a parameter De equal to the difference in binding energies between the R and T states.

The values of these parameters dictated by Fig. 7.21 are $\varepsilon = 2k_BT$ and $\Delta\varepsilon =$ $-4\ k_BT$;$-2\ k_BT$; and 0. Use Matlab to plot your derived equations.

3. Book question 7.6

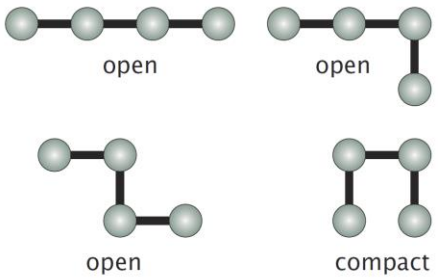

Figure 7.26: Toy model of protein folding showing four different conformations.

A four-residue protein can take on the four different conformations shown in Figure 7.26 (see above). Three conformations are open and have energy ε ($\varepsilon > 0$) and one is compact, and has energy zero.
(a) 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?
(b) What happens to the probability p_c, calculated in (a), in the limit of very large and very low temperatures?
(c) What is the average energy of the molecule at temperature T?

4. Matlab Question

3-D random walks:

a) Write a function that generates a 3-D random walk of a particle diffusing on a cubic lattice with a given number of steps N. Each step is taken in either the +x, -x, +y, -y, +z, or -z direction, each with an equal probability of 1/6. The step size is 1 pixel. The time between each step is 1 unit. Test your function with N = 1000 steps and display the trajectory on a 3-D plot (you can use the function plot3).
b) Calculate the mean squared displacement. Plot it, fit a line, and calculate the diffusion coefficient of the walk from the fit (express it in terms of pixels^2/units time).
c) Now, let's say you only measure the particle's position once every 50 time units. Show a 3-D plot of the trajectory you observe. Calculate the diffusion coefficient from the observed positions. How does it compare to your answer in b)?
d) We can also use 3-D random walks to model a polymer chain, where each step is a monomer in the chain. One interesting value from this model is the distance between the ends of the polymer. Simulate 100 random walks each after 100 different numbers of steps (N). Plot the mean of the squared displacement between the start and the end of the walk for each step size.

Hints:

1. Be careful about how many steps your random walk has. The start position of (0,0,0) does not count as a step. If your walk has N steps, the step-by step position vector of the walk has N+1 points in total including the starting point.
2. Each step of the random walk is taken in one of the +x, -x, +y, -y, +z, or -z directions with $1/6$ probability for each, not simultaneously in one of +x or -x with probability $1/2$, one of +y or -y with probability $1/2$, and one of +z or -z with probability $1/2$.
3. In part b, the squared displacement for a given time lag is given by:

$$mean\ squared\ displacement(\tau) = \sum_{i=\tau}^{N(frames)} \frac{[(x_i - x_{i-\tau})^2 + (y_i - y_{i-\tau})^2 + (z_i - z_{i-\tau})^2]}{N - \tau}$$

You need to calculate this for all timelags (1 to N-1).
4. Don't forget to hand in your full code for this question.