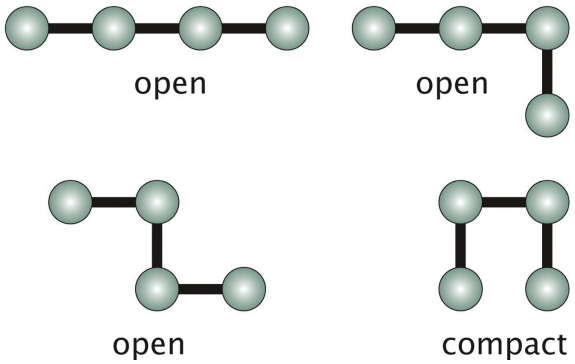
Physics 4251/6250 – Fall 2019
Problem Set 4, October 2
Due: Tuesday, October 15 by 5 PM

Problem 1: Toy model of protein folding (15 points)

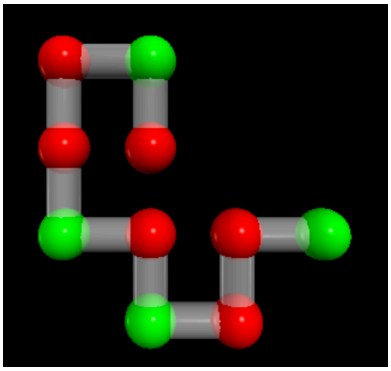
A four-residue protein can take on the four different conformations shown below. Three conformations are open and have energy ϵ ($\epsilon > 0$) and one is compact, and has energy zero.



(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?



Problem 2: Toy model of protein folding (redux) (20 points)

In this problem, you will now create your own protein and use a simple folding program to examine states it can adopt. Instead of assigning a positive energy penalty to hydrophobic-polar and

hydrophobic-solvent contacts, we will assign a favorable energy $-\epsilon$ to hydrophobic-hydrophobic contacts *that are not along the backbone*.

(a) 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.

(b) Now input your sequence into the python code `HPmodel.ipynb`, available on the course github. Note that this code must be run as vPython, meaning also that you have to restart the kernel between runs. **Run it at least five times.** What are the minimum energies for each run? (The code uses a Monte Carlo search algorithm to generate new states, so it is not guaranteed to find the lowest energy state every time.)

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

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

(a) Consider the PB equation as given in class, namely

$$\frac{\mathrm{d}^2V(x)}{\mathrm{d}x^2} = \frac{zqc_\infty}{D\epsilon_0}(e^{zqV(x)/kT} - e^{-zqV(x)/kT}) \tag{1}$$

Execute an appropriate change of variables $x \to \chi$ and $V(x) \to \nu(\chi)$ to make both χ and ν unitless. Rewrite the PB equation in terms of these new variables. We will assume a solution of NaCl and a temperature of 300 K. Hint: rescale x by the Debye length and V by an appropriate set of constants. There should be no constants (i.e., z, q, D, T, etc.) left in the final equation.
Second Hint:

$$\frac{\mathrm{d}^2V(x)}{\mathrm{d}x^2} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}V}{\mathrm{d}x}\right) = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}\nu}{\mathrm{d}\chi}\frac{\mathrm{d}V}{\mathrm{d}\nu}\frac{\mathrm{d}\chi}{\mathrm{d}x}\right) \tag{2}$$

(you will need to do this expansion a second time to take care of the second $\mathrm{d}/\mathrm{d}x$.)

(b) 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. This code uses a rather clever trick in which the PB equation is promoted to a time-dependent diffusion equation, namely $\mathrm{d}\nu/\mathrm{d}t = \nabla^2\nu - f(\nu) - \nu_0$, where $f(\nu)$ is the right-hand side of the PB equation (what you derived in (a)) and ν_0 is the potential due to the fixed charge. The steady-state solution, i.e., when $\mathrm{d}\nu/\mathrm{d}t = 0$, is then also the solution to the PB equation. (Note that there are a few other tricks, but you do not need to worry about them.)

In the code, the ∇^2 ($\mathrm{d}^2/\mathrm{d}x^2$ in 1D) is handled by a diffusion step, after which $f(\nu)$ is subtracted, and finally ν_0 is subtracted. Add in your function to the part of the code labeled "ADD YOUR FUNCTION HERE". Run the code and produce the plot at the end. If you input your function correctly, for the charge given (Q0 = -0.1), your solution (plotted in blue) and the exact solution for the linearized PB equation (plotted in red) will be identical.

(c) By testing different values of Q0, find the charge at which point the solution to the linearized PB equation diverges from the iterative solution to the exact PB equation.