

Homework Assignment 2

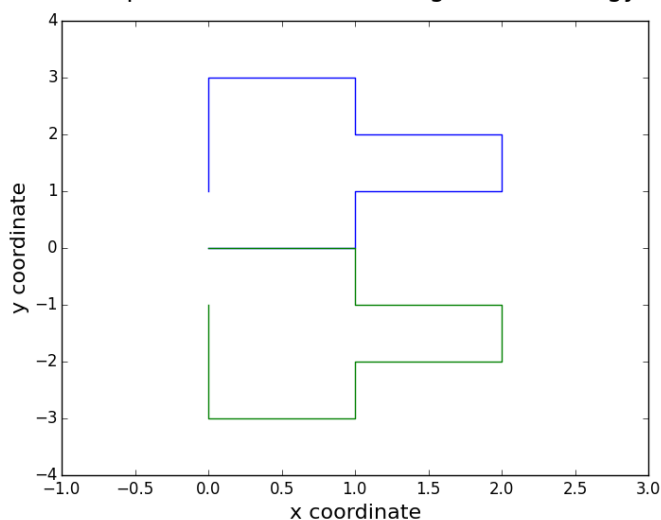
Question 1

a) Minimum energy observed is -4.0 eps kcal/mol

Row number of minimum E observed: [987 2306]

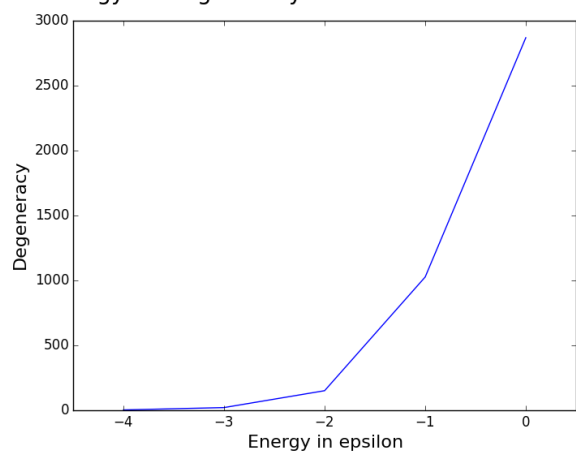
As there are two shapes of the same lowest energy observed, both shapes are plotted on the graph below.

Protein shapes of the ones showing lowest energy state



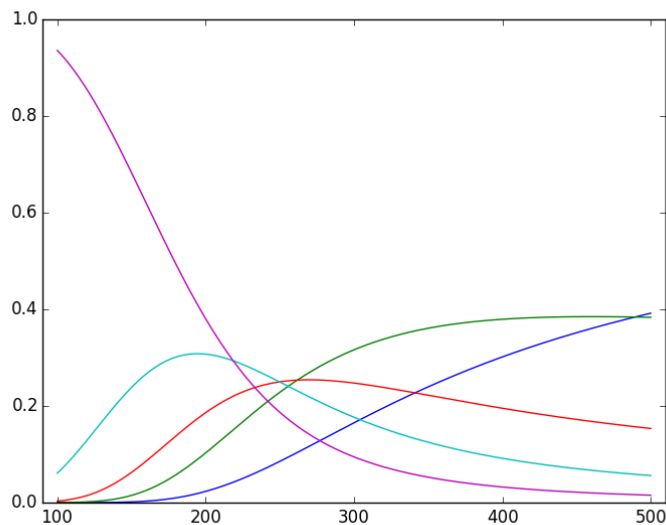
b) 2 states as shown above.

Energy Vs Degeneracy of Protein Conformations



As the energy increases, degeneracy increases exponentially.

c)



pink = ground state, energy is -4 eps
 light blue = 1st state, energy is -3 eps
 red = 2nd state, energy is -2 eps
 green = 3rd state, energy is -1 eps
 blue = 4th state, energy is 0 eps

d) $R_g^2 = 1/N^2 \sum_{i=1}^N \left(\sum_{j=1}^N (|r_i - r_j|)^2 \right)$

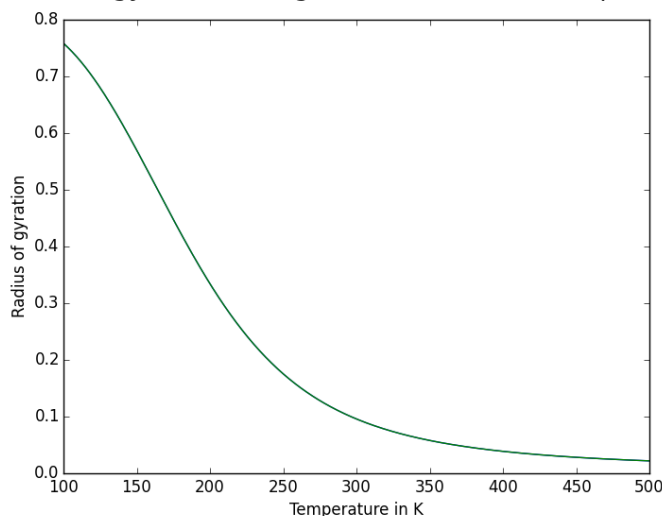
$|r_i - r_j| = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}$

$(|r_i - r_j|)^2 = (x_i - x_j)^2 + (y_i - y_j)^2$

Therefore,

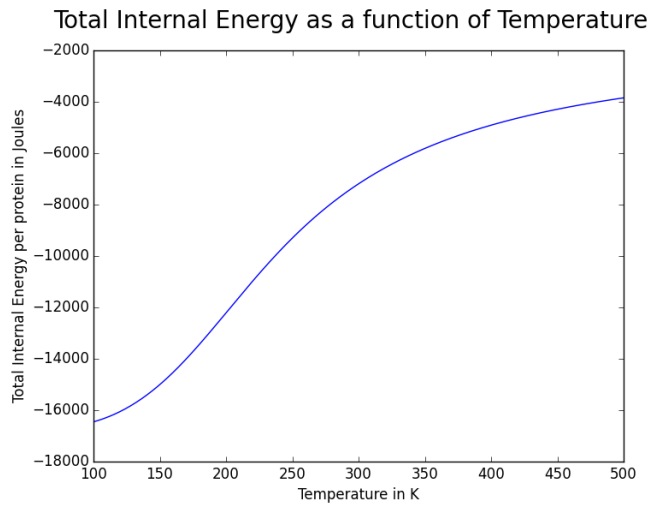
$R_g^2 = 1/N^2 * \sum_{i=1}^N \left(\sum_{j=1}^N ((x_i - x_j)^2 + (y_i - y_j)^2) \right)$

Radius of gyration change as a function of Temperature



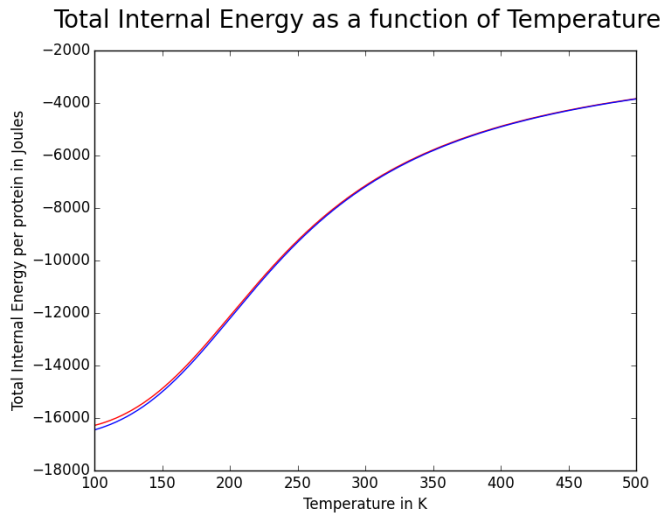
average gyration is: 3.32322350627

e) As we studied in class, the average of any identity of all constituents equals to the identity of one constituent. Therefore, instead of solving for all 10^{23} proteins, calculations were done only for 1, both to save time and also because the estimate from 1 protein is good enough to predict the value for 10^{23} proteins.

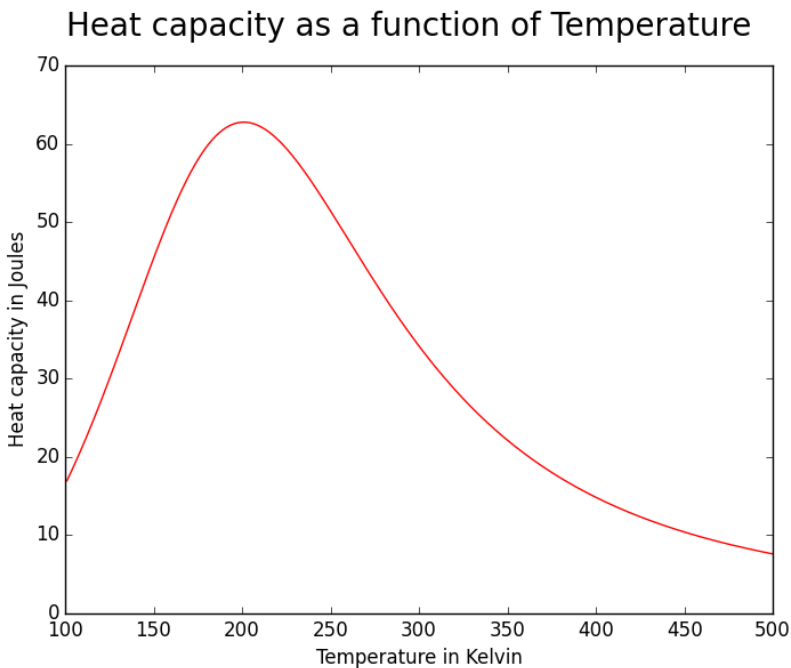


Above figure is using expectation value formula.

f)



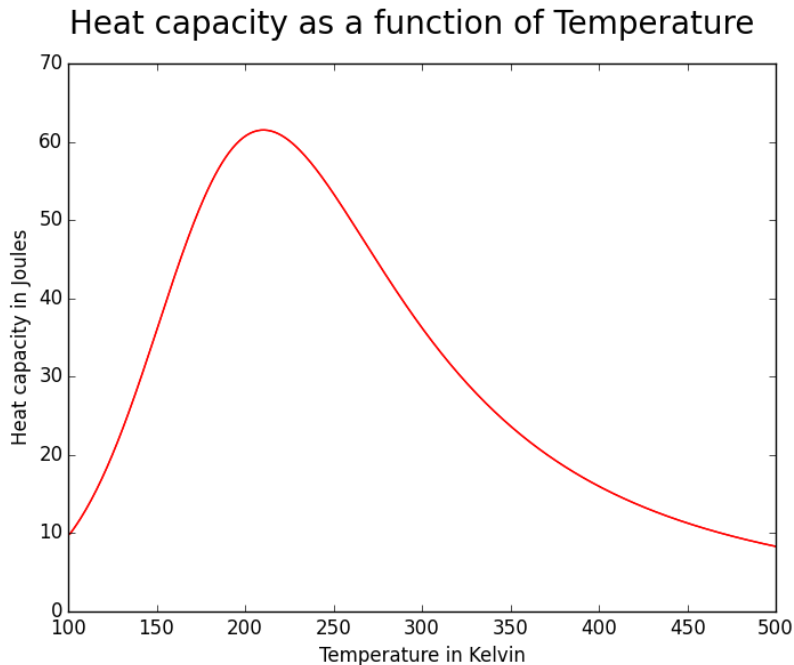
Red one is the calculation using finite difference method, and the blue one is using expectation value formula (shown in (e)). Please note that the value of dt used was 1. Both methods seem to be similar especially at higher temperatures.



g)

Melting temperature is: 200 Kelvin

for HPPHPPPHH

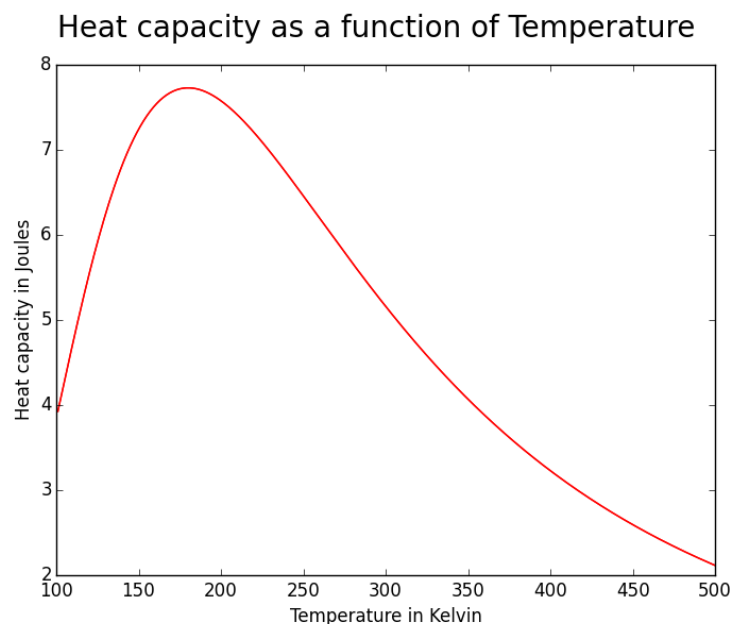


Highest energy is: 0.0 eps, and lowest energy is: -4.0 eps

Maximum value of heat capacity/Melting point is: 61.5020096224 Joules

Melting temperature is: 209 Kelvin

for HHHHHPPPPPP



Highest energy is: 0.0 eps, and lowest energy is: -1.0 eps

Maximum value of heat capacity/Melting point is: 7.72881059857 Joules

Melting temperature is: 179 Kelvin

The *first* one of all is the one that is most stable (ie. Highest melting point and highest heat capacity), whereas, the last one is the least stable (in fact, almost ten times less stable than the first one).

h) Please find attached python program that would display the x coordinates that are hydrophobic. However, it takes a looong time to process. I will leave it overnight and if it is done by morning I will

Question 2

Please find the scanned version of it attached.

Question 3

Boltzmann factor is $\exp(-E_i/kbT)$ where E_i is the energy of the state, kb is the Boltzmann factor and T is the temperature in Kelvin.

And the population of a certain state/conformation depends on:

$p_i = g_i \cdot \exp(-E_i/kbT) / Q$ (g_i is the degeneracy of a conformation i , and Q is the partition function which is the summation of all Boltzmann factors of conformations)

Therefore, the dominant conformation must have the highest p_i , as it is the conformation that is most likely to happen. However, as it can be seen, the dominant conformation depends on g_i and E_i . Perhaps, the reason why she does not see expected conformation from her theoretical calculations is because she did not account accurately the degeneracy. As proteins are made of hundreds, if not thousands, amino acids, it would consume an infinite time, is possible at all, to determine all the possible conformations of a protein. Thus, inaccuracy in the number and variety of possible conformations, causes inaccuracy in degeneracy. Inaccuracy in degeneracy, gives a mistake in population probability calculations, especially if Energy of the conformation is low (making $-E_i/kbT$ value positive).

Another problem could be that when doing theoretical calculations, she did not take into account the protein-protein interactions. That could have affected the value of Energy, thus, the population probability calculations.

To avoid all these theoretical miscalculations, one of the things she could do is lower the temperature to 0 K (or as low as possible) and redo the experimental data collection. This would “freeze” the protein so it exists in one ground/dominant conformation. She could, perhaps, also do a melting point analysis (using UV-Vis) that would help her determine the values of Energy and/or degeneracy more accurately.