

BB 101 Tutorial – 2

Assignment question.

Please write the answer on an A4 sheet and submit it at the beginning of the tutorial class. Ensure your Roll number and name are on the A4 sheet.

1. The following Lennard-Jones (LJ) potential energy function is widely used in biology as non-bonded interaction energy between two units of bio-molecules:

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

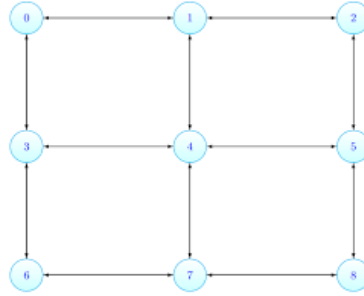
where $U(r)$ is the potential energy, σ and ϵ are the two positive constants representing the size of the unit and interaction energy strength, respectively. r is the distance between two interacting units. Make a rough sketch of the LJ potential function with $\sigma=1$ for two different epsilon values: $\epsilon=1$ and $\epsilon=2$. Both should be plotted in the same graph making it easy to compare.

2. Plot Screened coulomb potential (rough sketch) for $\lambda_D=1\text{nm}$ and $\lambda_D=10\text{nm}$. Both should be plotted in the same graph making it easy to compare.

(1+1 Marks)

(Please turn over to see tutorial questions)

Tutorial questions



1. Imagine a protein made of three connected positive charges; the bond length is fixed as $b=1\text{nm}$. This three-charge protein is lying on a 3×3 square lattice in 2D (or a 2D grid connecting 9 vertices). The Coulomb energy of the protein, in a conformation c is given by the typical formula for energy,

$$E_c = \sum_{i=1}^{i=2} \sum_{j=i+1}^3 \frac{A}{r_{ij}}$$

where r_{ij} is the distance between charges i and j . Assume $A = 1k_B T_r nm$. Note that the charges can only lie on the vertices of the lattice and the bonds on the edges, and $T_r = 300K$ unless specified otherwise. That is $A = 1k_B T_r nm \approx 4 \times 10^{-30} \text{Jm}$, a constant. Also note that the distance between any two adjacent vertices is b .

- (a) What is the energy of a protein configuration (conformation) when all the three charges on a straight line?
 - (b) What is the energy of a protein configuration that is bent (non-straight; when one bond is making 90° with the other one)
 - (c) How many straight conformations are possible on this lattice?
 - (d) How many bent conformations are possible on this lattice?
 - (e) What is the probability that you will find the protein in a straight configuration?
 - (f) What is the probability that you will find the protein in a bent configuration?
 - (g) Did you expect this? Naively one would have expected that since all 3 charges are positive, they will repel and protein will be less likely to bend. Do you appreciate the role of entropy?
2. Repeat the same when $A = 10k_B T_r nm$. Explain what is going on? (if this part could not completed in class, you could take it as a homework)