

BB 101: Module II

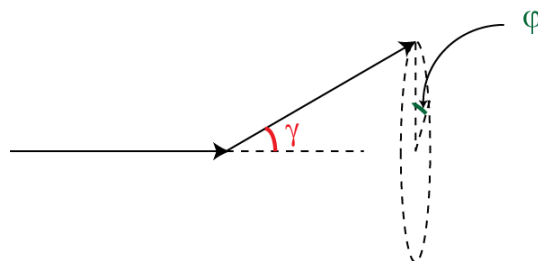
TUTORIAL 3

1. The probability that a polymer chain of N monomers has a particular end-to-end distance is given by $P(\vec{r}, N) = \left(\frac{3}{2\pi N b^2}\right)^{3/2} e^{-\frac{3r^2}{2N b^2}}$

Polymer cyclization can happen when two ends of a polymer chain come close enough together for them to react with each other i.e. separation between two ends become less than or equal to length of a monomer b . Calculate cyclization probability using above given probability distribution. (Hint: You can use the approximation that $\frac{r^2}{N b^2} \ll 1$)

2. In chromosomes, DNA molecules are wrapped tightly around protein molecules called histones, whose radius is 45 \AA . Given bending stiffness $k_b = 300 \text{ \AA kcal mol}^{-1}$, Calculate the energy required to bend the DNA molecule in a circle?

3. Freely-jointed chain is the simplest model of a polymer. In this model, fixed length monomers are connected such that all bond and torsion angles are equally likely. Freely-rotating chain improves the freely-jointed chain model by taking into account that monomers make a fixed bond angle with neighboring monomer units because of specific chemical bonding. Under this fixed angle, the monomers are still free to rotate and all torsion angles are equally likely. Calculate radius of gyration R_g for a freely rotating chain? $R_g = \sqrt{\langle R^2 \rangle}$, where \vec{R} is end-to-end vector. For simplicity assume $\varphi = 0$ for all bonds.



4. Suppose that drug molecules diffuse out of a tablet (which is modelled as a thin plane wall) into a solution. The drug undergoes a chemical reaction which causes drug to deplete in proportion to its present concentration. The rate of the chemical reaction which depletes the drug molecules is k and D is the diffusion constant of the drug. Find out the concentration profile for the drug as a function of distance x away from the tablet wall in the solution. Show that drug will be drawn out of the tablet rapidly if it has high diffusion constant or has a high reaction rate in solution.

5. Suppose a drug is encapsulated between two planes at $x=0$ and $x=h$. The drug diffuses out of both planes at a constant rate R

(i) Write down the corresponding diffusion equation

(ii) Solve for $c(x)$ inside the tablet, subject to boundary condition $c(0)=c(h)=0$, that is, the drug is used up the instant it is released

(iii) Compute the flux of the drug out of the tablet