BB 101: Module II

TUTORIAL 3: Solutions

1. Given $P(\vec{r}, N) = \left(\frac{3}{2\pi N b^2}\right)^{3/2} e^{-\frac{3r^2}{2Nb^2}}$

To calculate the cyclization probability above probability should be integrated over a volume element dV. The volume dV is enclosed between the circle of radius r and $r + dr$ and hence limits of integration would be from 0 to b

Therefore, $Cyclization\ probability = \int_0^b 4\pi \left(\frac{3}{2\pi N b^2}\right)^{3/2} e^{-\frac{3r^2}{2Nb^2}} r^2 dr$

Since $\frac{r^2}{Nb^2}$ << 1

$$Cyclization\ probability = \int_0^b 4\pi \left(\frac{3}{2\pi N b^2}\right)^{3/2} r^2 dr$$

$$= 4\pi \left(\frac{3}{2\pi N b^2}\right)^{3/2} \int_0^b r^2 dr$$

$$= 4\pi \left(\frac{3}{2\pi N b^2}\right)^{3/2} \left[\frac{r^3}{3}\right]_0^b$$

$$= 4\pi \left(\frac{3}{2\pi N b^2}\right)^{3/2} \frac{b^3}{3}$$

Therefore, $$Cyclization\ probability = \sqrt{\frac{6}{\pi}} N^{-3/2}$$

2. Energy required to bend DNA in a circle of radius R is given by

$$E = \frac{k_b \pi}{R}$$

$$= \frac{300\text{ÅKcal } mol^{-1} \times 3.14}{45\text{Å}}$$

$$= 20.93 \text{ Kcal } mol^{-1}$$

$$\approx 21 \text{ Kcal } mol^{-1}$$

3. We have calculate R_g for a freely-rotating chain

$$R_g = \sqrt{\langle R^2 \rangle}$$

Let's first calculate $\langle R^2 \rangle$

$$\langle R^2 \rangle = \langle \vec{R} \bullet \vec{R} \rangle$$

Now $\vec{R}$ is the sum of all segment vectors

Therefore,

$$\langle R^2 \rangle = \langle \left(\sum_{i=1}^{N} \vec{t}_i \right) \bullet \left(\sum_{j=1}^{N} \vec{t}_j \right) \rangle$$

$$= \sum_{i=1}^{N} \langle \vec{t}_i^{\,2} \rangle + \sum_{i,j=1, i \neq j}^{N} \langle \vec{t}_i \bullet \vec{t}_j \rangle$$

$$= Nb^2 + b^2 \sum_{i,j=1, i \neq j}^{N} \langle \cos \theta_{i,j} \rangle$$

Where $\theta_{i,j}$ is the angle between i^{th} and j^{th} segment

$$\langle \cos \theta_{i,j} \rangle = \cos^{j-i} \gamma$$

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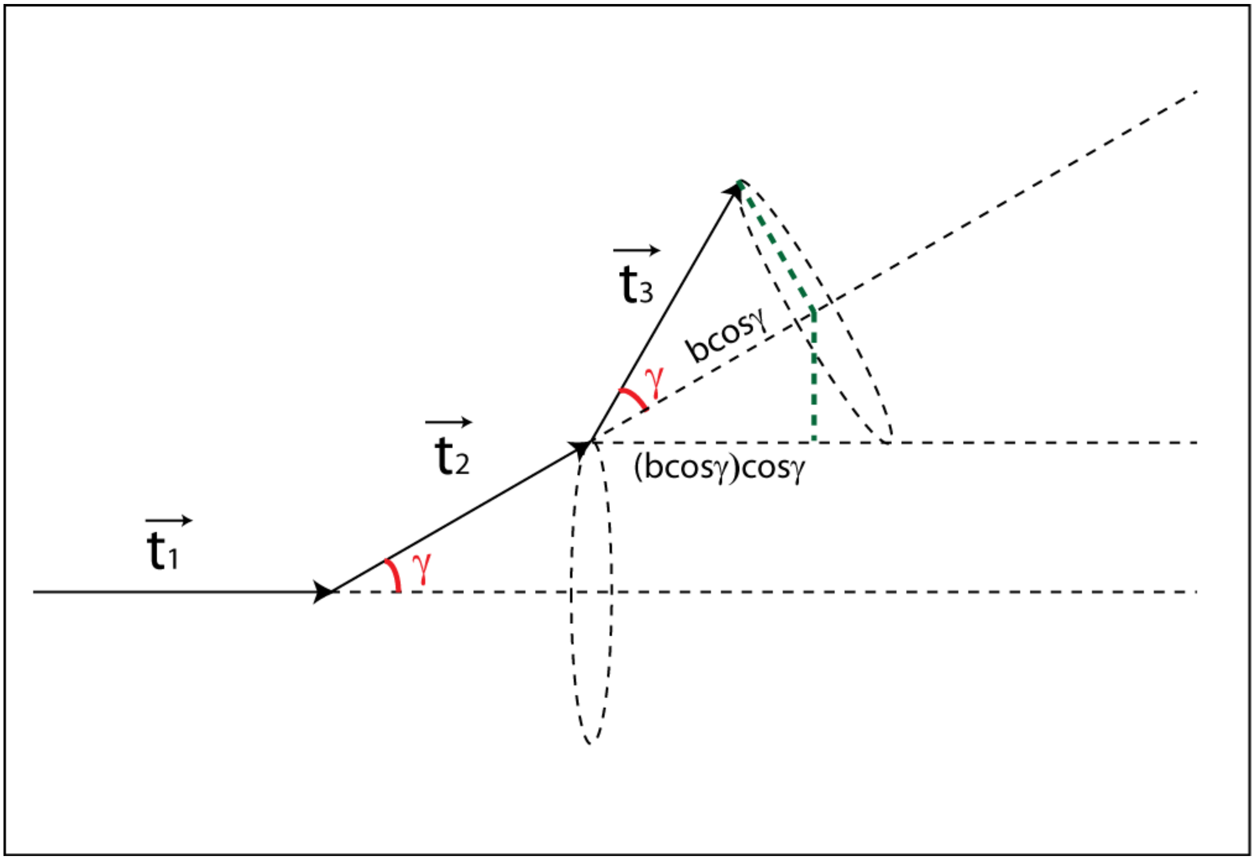
$$\boldsymbol{Proof} \ \langle \boldsymbol{\cos \theta_{i,j}} \rangle = \boldsymbol{\cos^{j-i} \gamma}$$

Let's choose $i = 1$ and $j = 3$ as shown in figure below and let's calculate $\vec{t}_1 \bullet \vec{t}_3$



Now, $\vec{t}_1 \bullet \vec{t}_3 = magnitude\ of\ \vec{t}_1\ \times projection\ of\ \vec{t}_3\ along\ the\ direction\ of\ \vec{t}_1$

Caution: Projection of $\vec{t}_3$ along direction of $\vec{t}_1$ should not taken as $|\vec{t}_3|\ cos2\gamma$ as this would give wrong projection of vector $\vec{t}_3$ along direction of $\vec{t}_1$ for a freely rotating chain. We are interested in projection of $\vec{t}_3$ along direction of $\vec{t}_1$, which result from rotation of $\vec{t}_3$ at an angle γ with respect to direction of $\vec{t}_2$and rotation of $\vec{t}_2$ at an angle γ with respect to direction of $\vec{t}_1$. Taking projection as $|\vec{t}_3|\ cos2\gamma$ means that we are taking projection of $\vec{t}_3$ along $\vec{t}_1$ happening due to rotation of $\vec{t}_3$ around $\vec{t}_1$ with a constant angle 2γ. This is obviously not the case here as discussed above. The correct way of calculating projection of $\vec{t}_3$ along $\vec{t}_1$, due to rotation of $\vec{t}_3$ at angle γ with respect to direction of $\vec{t}_2$ and rotation of $\vec{t}_2$ at an angle γ with respect to direction of $\vec{t}_1$, is to first calculate projection of $\vec{t}_3$ along $\vec{t}_2$ (say X, $X = bcos\gamma$) and then to calculate projection of this projection along $\vec{t}_1$ i.e. $Xcos\gamma$ ($Xcos\gamma = (bcos\gamma)cos\gamma$)

Therefore

$$\vec{t}_1 \bullet \vec{t}_3 = b\ \times b(bcos\gamma)cos\gamma =\ b^2 \cos^2\gamma$$

Now $\langle \vec{t}_1 \bullet \vec{t}_3 \rangle = b^2 \langle \cos\theta_{1,3} \rangle = \langle b^2 \cos^2\gamma \rangle$

This implies, $\langle \cos\theta_{1,3} \rangle = \cos^2\gamma$

Continuing the same way we can get

$$\langle \cos\theta_{i,k} \rangle = \cos^k\gamma$$

Therefore, $\langle R^2 \rangle = Nb^2 + b^2 \sum_{i,j=1,i\neq j}^{N} \langle \cos\theta_{i,j} \rangle$

Since

$$\langle R^2 \rangle = Nb^2 + 2b^2 \sum_{i=1}^{N} \sum_{k=1}^{N-i} \langle \cos\theta_{i,i+k} \rangle$$

Here, $k = j - i$

$$\langle R^2 \rangle = Nb^2 + 2b^2 \sum_{i=1}^{N} \sum_{k=1}^{N-i} \cos^k\gamma$$

$$\approx Nb^2 + 2Nb^2 \frac{\cos\gamma}{1 - cos\gamma} \ For\ large\ N$$

Or,

$$\langle R^2 \rangle = Nb^2 \frac{1 + \cos\gamma}{1 - cos\gamma}$$

Therefore,

$$R_g = \sqrt{\langle R^2 \rangle} = N^{1/2} b \sqrt{\frac{1 + \cos\gamma}{1 - cos\gamma}}$$

4. Let the concentration of the drug in the tablet be C_0. In this case there are two processes that are happening, diffusion of the drug and reaction of the drug

Therefore, equation capturing both reaction and diffusion is given by

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - kC$$

We shall solve this equation under steady state condition i.e. $\frac{\partial C}{\partial t} = 0$

Therefore, equation to solve is

$$0 = D\frac{\partial^2 C}{\partial x^2} - kC$$

Or,

$$\frac{\partial^2 C}{\partial x^2} = \frac{k}{D}C \qquad (1)$$

The general solution of this second order differential equation is given by

$$C(x) = A_1 e^{-B_1 x} + A_2 e^{+B_2 x}$$

Let use the boundary condition $C(x) = 0$ at $x = \infty$ and $C(x) = C_0$ at $x = 0$

Let us the first boundary condition $(x) = 0$ at $x = \infty$

$$\Rightarrow A_2 = 0$$

Therefore,

$$C(x) = A_1 e^{-B_1 x}$$

Now let's use the second boundary condition $C(x) = C_0$ at $x = 0$

$$\Rightarrow A_1 = C_0$$

Therefore,

$$C(x) = C_0 e^{-B_1 x} \qquad (2)$$

To determineB_1, substitute (2) in (1)

$$\Rightarrow B_1^2 = \frac{k}{D}$$

$$\Rightarrow B_1 = \sqrt{\frac{k}{D}}$$

Therefore, $$C(x) = C_0 e^{-\sqrt{\frac{k}{D}}x}$$

To compute the rate at which the drug is being drawn out, we have to calculate flux at $x = 0$

Therefore, $$J(x) = -D\frac{\partial C}{\partial x} = \sqrt{kD}C_0 e^{-\sqrt{\frac{k}{D}}x}$$

$$J(x = 0) = -D\frac{\partial C}{\partial x} = \sqrt{kD}C_0$$

This suggests that flux at $x = 0$ is proportional to both k and D i.e. drug will be drawn out rapidly if either diffusion rate or reaction rate is higher

5. (i) In this case we have to solve the diffusion equation with condition $\frac{\partial C}{\partial t} = R$

Therefore,

$$D\frac{\partial^2 C}{\partial x^2} = \frac{\partial C}{\partial t} = -R$$

Or, $$D\frac{\partial^2 C}{\partial x^2} = -R$$

$$\frac{\partial^2 C}{\partial x^2} = -\frac{R}{D}$$

(ii) Integrating w.r.t. x twice we get

$$C(x) = -\frac{R}{2D}x^2 + A_1 x + A_2$$

Where A_1 and A_2 are arbitrary constants

Using condition $C(0) = 0$ gives $A_2 = 0$

Therefore,

$$C(x) = -\frac{R}{2D}x^2 + A_1 x$$

Using condition $C(h) = 0$ gives $A_1 = \frac{R}{2D}h$

Therefore,

$$C(x) = -\frac{R}{2D}x^2 + \frac{Rh}{2D}x$$

$$C(x) = \frac{R}{2D}x(h - x)$$

(iii) Flux out of the tablet is given by

$$J = -D\frac{\partial c}{\partial x} = Rx - \frac{R}{2}h$$

Therefore,

$$J|_{x=0} = -\frac{Rh}{2}$$

$$J|_{x=\frac{h}{2}} = +\frac{Rh}{2}$$