

WLC Model in 2D

1. Bending angle statistics:

$$p(\varphi) = \frac{1}{Z} e^{-\frac{U(\varphi)}{k_B T}} = \frac{1}{Z} e^{-\frac{\rho}{2\alpha L} \varphi^2} \quad \text{with} \quad \rho = \frac{EI}{k_B T}$$

$$\text{with standardization} \quad \int_{-\infty}^{+\infty} p(\varphi) d\varphi \stackrel{!}{=} 1 \rightarrow Z = \sqrt{\frac{2\pi\alpha L}{\rho}}$$

initially assuming DL < L for integration to $\pm\infty$, but not necessarily restricting (see below)

$$\langle \cos \varphi \rangle_{2D} = \langle \vec{t}(0) \cdot \vec{t}(DL) \rangle$$

$$\begin{aligned} &= \int_{-\infty}^{+\infty} \cos \varphi \, p(\varphi) d\varphi = \frac{1}{Z} \left[\int_{-\infty}^{+\infty} e^{i\varphi} e^{-\frac{\rho}{2\alpha L} \varphi^2} d\varphi + \int_{-\infty}^{+\infty} e^{-i\varphi} e^{-\frac{\rho}{2\alpha L} \varphi^2} d\varphi \right] \\ &\quad \underbrace{\frac{1}{2}(e^{i\varphi} + e^{-i\varphi})}_{\cos \varphi} \\ &= \frac{1}{Z} \int_{-\infty}^{+\infty} e^{-\frac{\rho}{2\alpha L} \left[\varphi^2 - \frac{2i\alpha L}{\rho} \varphi + \left(\frac{i\alpha L}{\rho}\right)^2 - \left(\frac{i\alpha L}{\rho}\right)^2 \right]} d\varphi \\ &= \frac{1}{Z} \int_{-\infty}^{+\infty} e^{-\frac{\rho}{2\alpha L} \left(\varphi - \frac{i\alpha L}{\rho} \right)^2} d\varphi \cdot \underbrace{e^{-\frac{\alpha L}{2\rho}}}_{\text{completing the square}} = e^{-\frac{\alpha L}{2\rho}} \\ &= 1 \quad (\text{standardization, with } \tilde{\varphi} = \varphi - \frac{i\alpha L}{\rho}) \end{aligned}$$

Note: Is $\langle \cos \varphi \rangle = \dots$ only valid for $DL < L$?

No, because one can show (s. Landau-Lifshitz)



$$\begin{aligned} \langle \cos \varphi_{ac} \rangle &= \langle \cos \varphi_{ab} \cdot \cos \varphi_{bc} \rangle \\ &= \langle \cos \varphi_{ab} \rangle \cdot \langle \cos \varphi_{bc} \rangle \end{aligned}$$

$$\begin{aligned} \text{since } \cos \varphi_{ab} &= \cos \varphi_{ab} \cdot \cos \varphi_{bc} \\ &\quad - \sin \varphi_{ab} \cdot \sin \varphi_{bc} \cdot \cos \varphi \end{aligned}$$

2. End-to-end distance:

$$\begin{aligned} \langle R^2 \rangle_{20} &= \langle \vec{R} \cdot \vec{R} \rangle = \left\langle \int_0^L \vec{t}(l) dl \cdot \int_0^L \vec{t}(l') dl' \right\rangle \\ &= \int_0^L \int_0^L \underbrace{\langle \vec{t}(l) \cdot \vec{t}(l') \rangle}_{e^{-\frac{|l-l'|}{2P}}} dl dl' \end{aligned}$$


$$\begin{aligned} &= \int_0^L \int_0^L e^{-\frac{|l-l'|}{2P}} dl dl' \\ &\quad \underbrace{\int_0^{l'} e^{-\frac{l'-l}{2P}} dl + \int_{l'}^L e^{-\frac{l-l'}{2P}} dl}_{\text{Separation:}} \\ &\quad |l-l'| = \begin{cases} l'-l & \text{for } l \leq l' \\ l-l' & \text{for } l \geq l' \end{cases} \\ &= 2P \left(2 - e^{-\frac{l'}{2P}} - e^{-\frac{L-l'}{2P}} \right) \\ &= 2P \left[\underbrace{\int_0^{l'} 2 dl'}_{2l'} - \underbrace{\int_0^{l'} e^{-\frac{l'}{2P}} dl'}_{-2P(e^{-\frac{l'}{2P}} - 1)} - \underbrace{\int_{l'}^L e^{-\frac{l-l'}{2P}} dl'}_{2P(1 - e^{-\frac{L-l'}{2P}})} \right] \\ &= 4PL \left[1 + \frac{2P}{L} (e^{-\frac{L}{2P}} - 1) \right] \end{aligned}$$

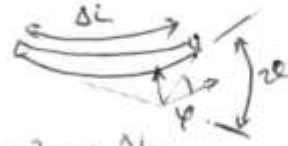
WLC Model in 3D

since $U(r)$ is independent of φ ,

Boltzmann statistics is also independent

$$p(r, \varphi) = \frac{1}{Z} e^{-\frac{P}{2\Delta L} r^2}$$

but $\sigma_r^2 = 2 \frac{\Delta L}{P}$ (so 2x larger than for 2D)



with standardization $\int p(r, \varphi) d\Omega = 1$

$$\frac{1}{Z} (e^{i\varphi} + e^{-i\varphi}) \quad \hookrightarrow \quad Z = 2\pi \frac{\Delta L}{P}$$

$$\langle \cos \varphi \rangle_{3D} = \int \cos \varphi \, w(r, \varphi) \, d\Omega$$

$$= \frac{1}{2Z} \underbrace{\int_0^{2\pi} d\varphi}_{2\pi} \int_0^\infty (e^{i\varphi} + e^{-i\varphi}) e^{-\frac{P}{2\Delta L} r^2} r \, dr$$

$$\text{with } \int_0^\infty e^{i\varphi} e^{-\frac{P}{2\Delta L} r^2} r \, dr$$

$$= \dots = e^{-\frac{\Delta L}{P}}$$

analogue to 2D

$$\langle R^2 \rangle_{3D} = \dots = 2PL \left[1 + \frac{P}{L} \left(e^{-\frac{L}{P}} - 1 \right) \right]$$