

Solutions to **Configurations of DNA molecules**

[1] The two straight lines have length l each, the curved piece arclength s and curvature $1/r$. l and r are related to the apex angle α via $l/r = \cot(\alpha/2)$. The total length L is given by

$$L = 2l + s = 2l + (\pi + \alpha)r = 2r \cot(\alpha/2) + (\pi + \alpha)r.$$

The bending energy is given by

$$E = \frac{A}{2} \frac{s}{r^2} = \frac{A}{2} \frac{\pi + \alpha}{r} = \frac{A}{2L} (\pi + \alpha) \left(2 \cot\left(\frac{\alpha}{2}\right) + \pi + \alpha \right)$$

where A denotes the bending modulus. Minimization with respect to α leads to

$$\pi + \alpha + 2 \cot\left(\frac{\alpha}{2}\right) + (\pi + \alpha) \left(1 - \frac{1}{\sin^2(\alpha/2)} \right) = 0$$

This can be simplified to

$$-\frac{1}{\sin^2(\alpha/2)} ((\pi + \alpha) \cos \alpha - \sin \alpha) = 0.$$

This leaves us with solving the transcendental equation

$$\pi + \alpha = \tan \alpha.$$

This is solved for $\alpha = 77.5^\circ$.

[2]

$$\langle R^2 \rangle = \langle \mathbf{R}^2 \rangle = \left\langle \left(\int_0^L \mathbf{t}(s) ds \right)^2 \right\rangle = \int_0^L ds \int_0^L ds' \langle \mathbf{t}(s) \cdot \mathbf{t}(s') \rangle = \int_0^L ds \int_0^L ds' e^{-\frac{|s-s'|}{l_p}} = 2l_p^2 \left(\frac{L}{l_p} + e^{-\frac{L}{l_p}} - 1 \right)$$

[3]

$$\langle R^2 \rangle = \langle \mathbf{R}^2 \rangle = \left\langle \left(\sum_{i=1}^N \mathbf{r}_i \right)^2 \right\rangle = \sum_{i,j=1}^N \langle \mathbf{r}_i \cdot \mathbf{r}_j \rangle = \sum_{i=1}^N \langle \mathbf{r}_i \cdot \mathbf{r}_i \rangle + \sum_{i \neq j} \langle \mathbf{r}_i \cdot \mathbf{r}_j \rangle = \sum_{i=1}^N \langle \mathbf{r}_i \cdot \mathbf{r}_i \rangle = b^2 N$$

[4] The expression for $\langle R^2 \rangle$ of long wormlike chains with $L \gg l_p$ can be approximated by

$$\langle R^2 \rangle = 2l_p L.$$

This can be interpreted (up to a numerical factor) as a flexible chain of segment length l_p with a total number of segments $N = L/l_p$ which according to [3] has a mean-squared radius

$$\langle R^2 \rangle = b^2 N = l_p^2 \frac{L}{l_p} = l_p L.$$

(if you want to have the prefactor right: choose $b = 2l_p$).