Stretching DNA

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ABSTRACT: A statistical mechanical treatment of the wormlike chain model (WLC) is used to analyze experiments in which double-stranded DNA, tethered at one end, is stretched by a force applied directly to the free end, by an electric field, or by hydrodynamic flow. All experiments display a strong-stretching regime where the end-to-end distance approaches the DNA contour length as $1/(\text{force})^{1/2}$, which is a clear signature of WLC elasticity. The elastic properties of DNA become scale dependent in the presence of electrostatic interactions; the effective electric charge and the intrinsic bending elastic constant are determined from experiments at low salt concentration. We also consider the effects of spontaneous bends and the distortion of the double helix by strong forces.

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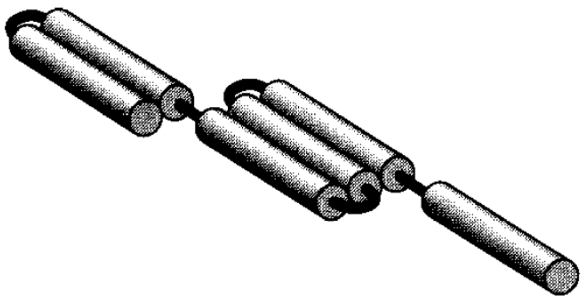
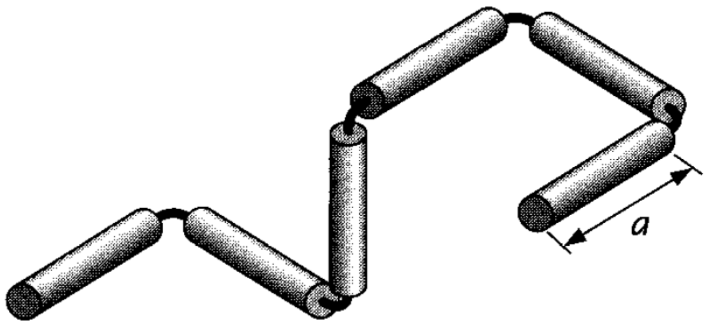
Random Walk models of polymer(ideal chain)



1-D case



3-D case

Physical biology of the cell, Rob phillips, 283p

a three dimensional random walk as an arrangement of linked segments of length a

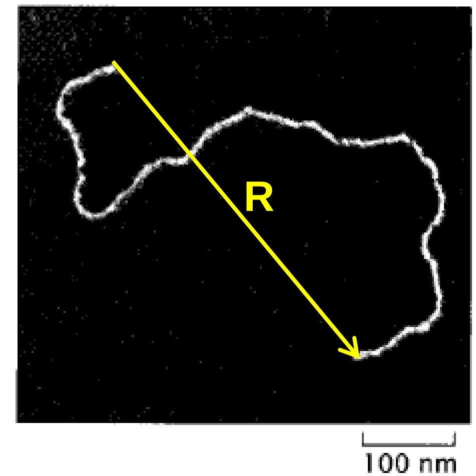
All bond lengths are the same

no correlation between the directions of bond angles

no treatment of torsional angles.

no interactions between monomers

average end-to-end distance of the polymer



Expected value of the walker's distance form the origin, R, after N step

$$\langle R \rangle = \left\langle \sum_{i=1}^{N} x_i \right\rangle$$

Variance of the probability distribution of R

$$\langle R^2 \rangle = \left\langle \sum_{i=1}^{N} \sum_{j=1}^{N} x_i x_j \right\rangle \quad \Rightarrow \quad \langle R^2 \rangle = \left\langle \sum_{i=1}^{N} \langle x_i{}^2 \rangle + \cancel{\sum_{i \neq j=1}^{N} \langle x_i x_j \rangle} \right\rangle$$

Each and every step is independent of all steps that precede and follow it.

In addition $x_i = \pm a$ $\langle x_i{}^2 \rangle = a^2$

Result that

$$\langle R^2 \rangle = N a^2 \qquad \sqrt{\langle R^2 \rangle} = a\sqrt{N}$$

The distance from the origin grows as the square root of the number of segments in the chain

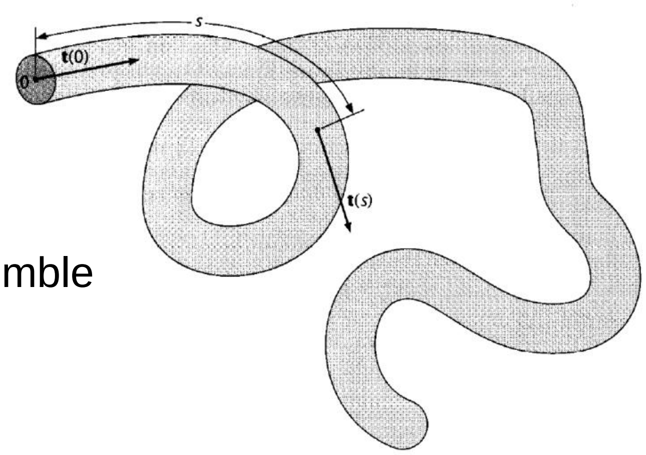
persistence length, worm-like chain model

Worm like chain model

particularly suited for describing stiffer polymers

all pointing in roughly the same direction

At room temperature, the polymer adopts a conformational ensemble that is smoothly curved



Polymer of length L

path of the polymer s ∈ (0, l)

$$\hat{t}(s) = \frac{\partial \vec{r}(s)}{\partial s}$$

$\hat{t}(s)$ is unit tangent vector to the chain at s

$\vec{r}\,(s)$ is position vector along the chain

$$\vec{R}(s) = \int_0^L \hat{t}(s)ds$$

end-to-end distance

Persistence length in worm like chain model

$$\left\langle \vec{t}(s)\cdot\vec{t}(0)\right\rangle = <\cos\theta(s)> = e^{-s/A}$$

A is polymer's characteristic persistence length.

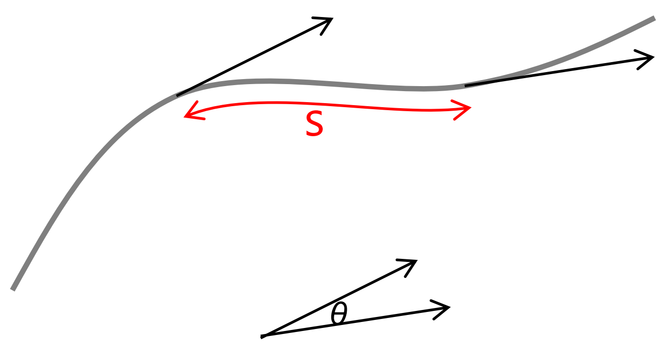
s is tangent vector at a distance

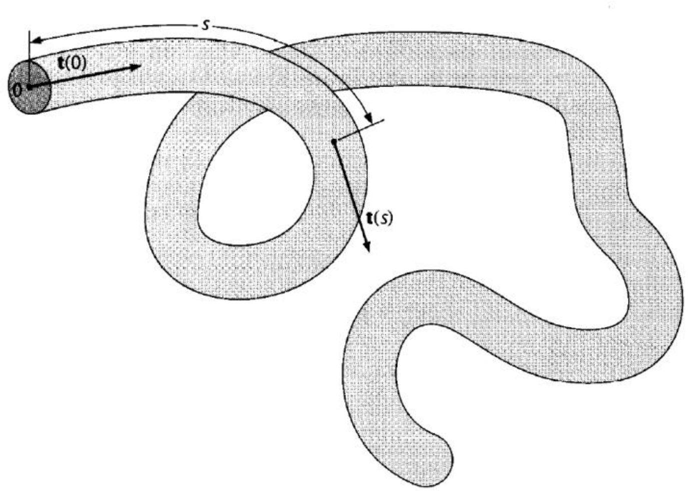
θ is between a vector that is tangent to the polymer

Persistence length

basic mechanical property quantifying the stiffness of a polymer.

Persistence length of DNA in vivo(150mM Na+, other ions)= 50nm, 150bp





mean square end-to-end distance of the polymer

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

$$= \left\langle \int_0^L \hat{t}(s) ds \cdot \int_0^L \hat{t}(s') ds' \right\rangle$$

$$= \int_0^L ds \int_0^L \langle \hat{t}(s) \cdot \hat{t}(s') \rangle ds'$$

$$= \int_0^l ds \int_0^l e^{-|s-s'|/p} ds'$$

$$\langle R^2 \rangle = 2AL\,[1 - \frac{A}{L}(1 - e^{-L/A})]$$

If L >> A $\langle R^2 \rangle = 2AL$ $\qquad \langle R^2 \rangle = Na^2 = (Na)a = aL$ $\qquad 2A = a$

WLC model $\qquad$ In ideal chain

Entropic Elasticity of the Worm like Chain

Bending costs an energy per length

$$E_{bend} = \frac{k_B T A}{2} k^2$$

$\hat{t} = \left| \partial_s \vec{r} \right|$ Tangent vector (unit vector)

$k = \left| \partial_s{}^2 \vec{r} \right|$ Curvature(the reciprocal of the bending radius)

$k_B T A$ Flexural rigidity

Effective energy of a stretched WLC

$$\frac{E}{k_B T} = \int_0^L \frac{A k^2}{2} ds - fz$$

compute the equilibrium extension
using the Boltzmann distribution

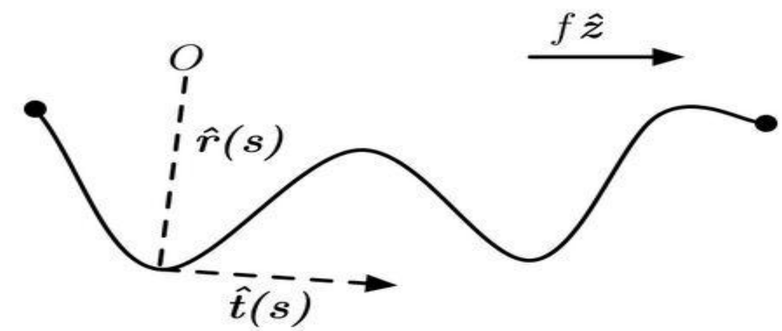
$$z \equiv \hat{z} \cdot [\vec{r}(L) - \vec{r}(0)]$$

$$e^{-E_{bend}/k_B T}$$

Simple Calculation of WLC strong-stretching behavior

Large forces are applied to a WLC

Extension approaches the total length L



Tangent vector fluctuates only slightly around $\hat{z}$

From the constraint $\left|\hat{t}\right| = 1$

Independent components $t_x \quad t_y$

t_z Fluctuations are quadratic in the two-vector $\vec{t}_\perp \equiv [t_x, t_y]$

$$t_z = 1 - t_\perp{}^2 / 2 + \vartheta(t_\perp{}^4)$$

The quadratic order $k^2 = \left(\partial_s \vec{t}_\perp\right)^2$

Obtain Gaussian approximation

$$\frac{E}{k_B T} = \frac{1}{2}\int_0^L ds[A(\partial_s \vec{t}_\perp)^2 + f\vec{t}_\perp{}^2] - fL$$

Fourier transforms decouple the energy into normal modes

$$\tilde{t}_\perp(q) \equiv \int ds\, e^{iqs}\vec{t}_\perp(s)$$

$$\frac{E}{k_B T} = \frac{1}{2}\int \frac{dq}{2\pi}[Aq^2 + f]\left|\tilde{t}_\perp\right|^2 - fL$$

Average of $t_\perp{}^2$ **at any point s is simply given by**

$$\left\langle t_\perp{}^2 \right\rangle = \int \frac{dq}{2\pi}\left\langle \left|\tilde{t}_\perp(q)\right|^2 \right\rangle = 2\int \frac{dq}{2\pi}\frac{1}{Aq^2 + f} = \frac{1}{(fA)^{1/2}}$$

$$\left\langle t_\perp{}^2 \right\rangle = \int \frac{dq}{2\pi} \left\langle \left| \tilde{t}_\perp(q) \right|^2 \right\rangle = 2\int \frac{dq}{2\pi} \frac{1}{Aq^2 + f} = \frac{1}{(fA)^{1/2}}$$

The leading factor of 2 in equation counts the two components of $\vec{t}_\perp$

The extension is

$$\frac{z}{L} = \hat{t}\cdot\hat{z} = 1 - \left\langle \vec{t}_\perp{}^2 \right\rangle / 2 = 1 - \frac{1}{(4fA)^{1/2}}$$

In large forces, $\frac{1}{f^{1/2}}$

z approaches L

Side to side excursions of the chain over arc length s

$$R_\perp{}^2 = \frac{2}{f}\left(s - \frac{1 - \exp[-s(f/A)^{1/2}}{(f/A)^{1/2}} \right)$$

Interpolation formula for the WLC force versus extension

$$\frac{fA}{k_B T} = \frac{z}{L} + \frac{1}{4(1 - z/L)^2} - \frac{1}{4}$$

This is asymptotically exact in the large and small force limits