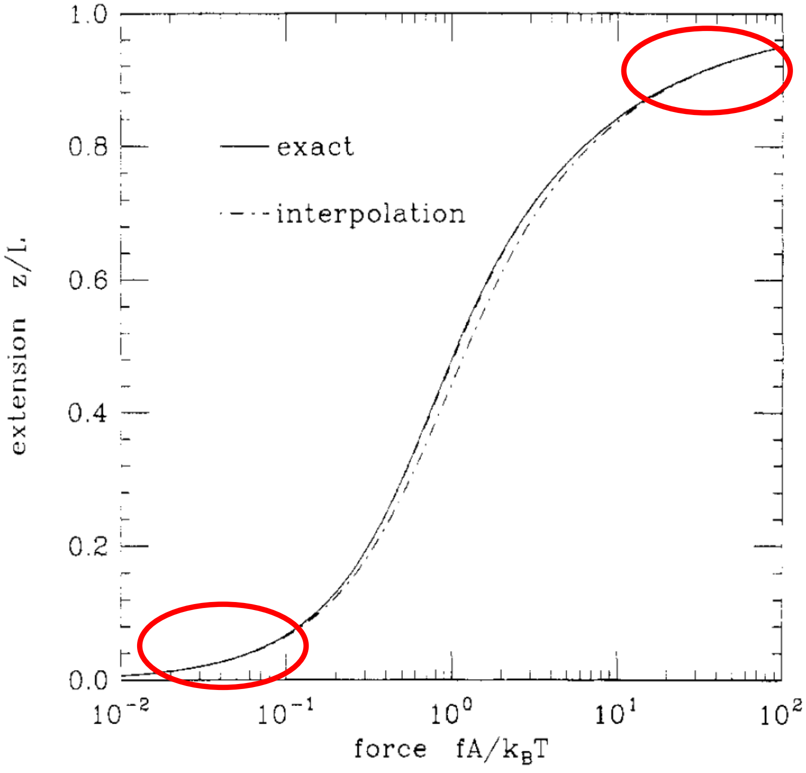
Interpolation formula for the WLC force versus extension

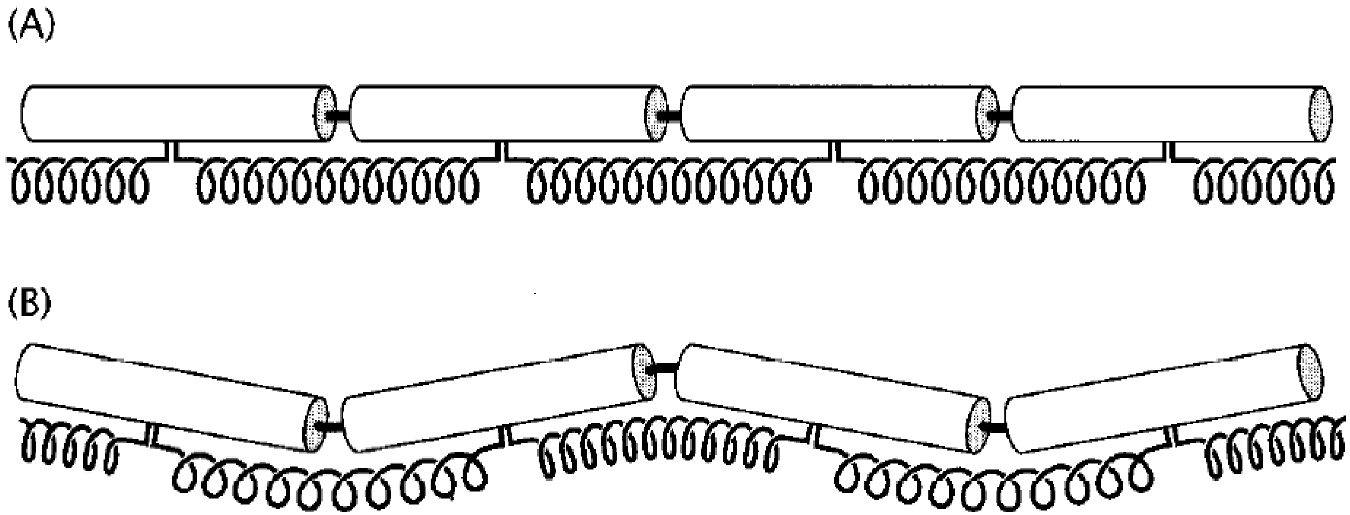
$$\frac{fA}{k_B T} = \frac{z}{L} + \frac{1}{4(1 - z/L)^2} - \frac{1}{4}$$

This is asymptotically exact in the large and small force limits



Elasticity and Entropy : the Worm-Like Chain

The Worm-Like chain Model Accounts for Both the Elastic Energy and Entropy of Polymer chain



(a) The undeformed configuration showing that the springs are unstretched, but the links are deprived of entropy because there is only one such possible arrangement of the segment

(b) A deformed configuration showing that there is an energetic cost to bend the chain, but there are more configurations of the systems

Partition function

$$Z = \int D\vec{t}(s) \exp\left(-\frac{A}{2} \int_0^L \left| \frac{d\vec{t}}{ds} \right|^2 ds \right)$$

1. Draw a curve of length L representing a possible DNA configuration

2. Evaluate its bending energy $E_{bend} = \frac{Ak_BT}{2} \int_0^L \left| \frac{d\vec{t}}{ds} \right|^2 ds$

and, the corresponding Boltzmann factor $\exp(-E_{bend} / k_BT)$

3. Repeat 1, 2 for all possible curves celebrated Feynmann path integral

All configuration is,

$$\langle z \rangle = \frac{1}{Z(f)} \int D\vec{t}(s) z \exp\left(-\frac{A}{2} \int_0^L \left| \frac{d\vec{t}}{ds} \right|^2 ds + f \int_0^L t_z ds \right)$$

$Z(f)$ is the partition function in the presence of the applied force $F = fk_B T$

Rewritten as

$$\langle z \rangle = \frac{d \ln Z(f)}{df}$$

Calculate low- , high-force limits

Low-force limit $fA << 1$

Expanded in powers of fA

$$Z(f) = \int D\vec{t}(s)\{e\mathrm{xp}\left(-\frac{A}{2}\int_0^L \left|\frac{d\vec{t}}{ds}\right|^2 ds\right)[1 + f\int_0^L t_z(s)ds$$

$$+\frac{f^2}{2}\int_0^L t_z(s)ds\int_0^L t_z(u)du + O((fA)^3)]\}$$

And retain only the first three terms in the expansion

$$Z(f) = Z(0)\left[1 + f\int_0^L < t_z(s) >_0 ds + \frac{f^2}{2}\int_0^L\int_0^L dsdu < t_z(s)t_z(u) >_0\right]$$

We obtain this equation

$$Z(f) = Z(0)\left(1 + \frac{f^2 LA}{3}\right)$$

Finally, making use of the relation given in $\langle z \rangle = \dfrac{d \ln Z(f)}{df}$ we arrive at

$$\frac{\langle z \rangle}{L} = \frac{2fA}{3}$$

high-force limit $fA >> 1$

$$\vec{t} \approx (t_x, t_y, 1 - \frac{1}{2}(t_x^2 + t_y^2))$$

This approximate expression for the tangent vector turns the formula for the Energy into a quadratic form in tx and ty given by

$$E_{tot} = \frac{Ak_BT}{2}\int_0^L ds\left[\left(\frac{dt_x}{ds}\right)^2 + \left(\frac{dt_y}{ds}\right)^2\right] + \frac{fk_BT}{2}\int_0^L ds(t_x^2 + t_y^2) - fk_BTL$$

The average extension in the high-force limit is,

$$\langle z \rangle = L - \frac{1}{2}\int_0^L ds \left\langle t_x^2 + t_y^2 \right\rangle$$

Fourier component of the tangent vector

$$t_\alpha(s) = \sum_w e^{iws} t_\alpha(w) \qquad (\alpha = x, y)$$

Where the frequencies are defined by w=2πj/L with j an integer.

In Fourier space the energy takes on the form of the potential energy of a collection
Of harmonic oscillators, two for each value of the frequency w and given by

$$E_{tot} = \frac{Lk_B T}{2} \sum_w (Aw^2 + f)(|t_x(w)|^2 + |t_y(w)|^2)$$

This observation allow us to compute the average $|t_\alpha(w)|^2$ without explicitly computing the path integral.

Which states that the average energy for every quadratic degree of freedom is

$k_B T / 2$

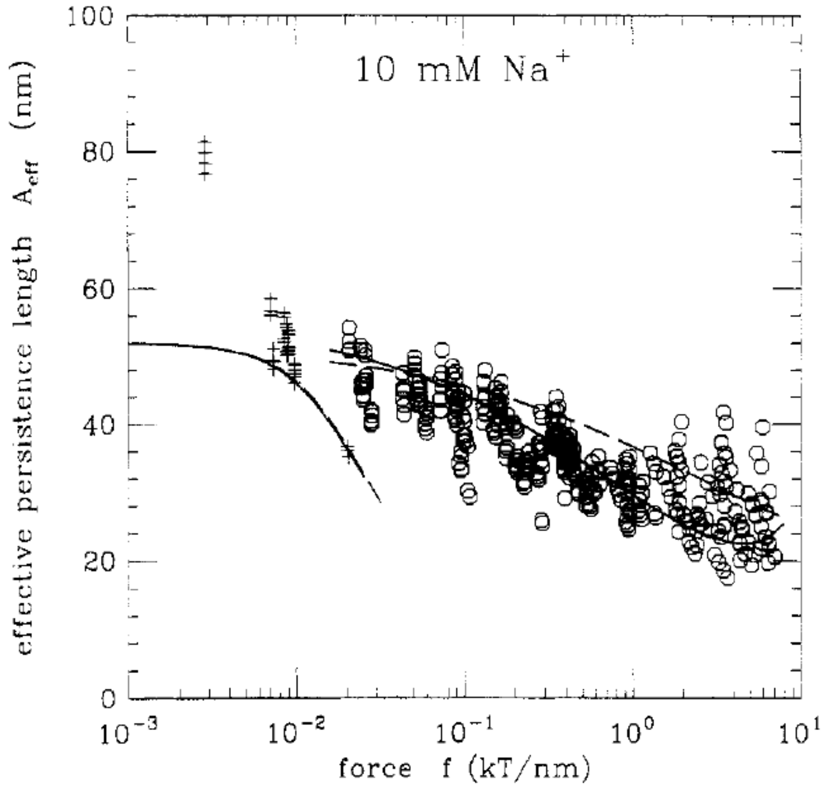
$$\left\langle \frac{Lk_B T}{2}(Aw^2 + f)|t_\alpha(w)|^2 \right\rangle = \frac{k_B T}{2} \qquad (\alpha = x, y)$$

and

$$\frac{< z >}{L} = 1 - \frac{1}{L}\sum_w \frac{1}{Aw^2 + f}$$

$$\sum_{w} \to L/2\pi\int_{-\infty}^{+\infty}$$

$$\frac{<z>}{L} = 1 - \frac{1}{2\sqrt{fA}}$$



$$A = \begin{cases} 3\langle z\rangle / 2fL & fa << 1 \\ 1/[4f(1-\langle z\rangle/L)^2 & fa >> 1 \end{cases}$$