Module 4 : Nonlinear elasticity

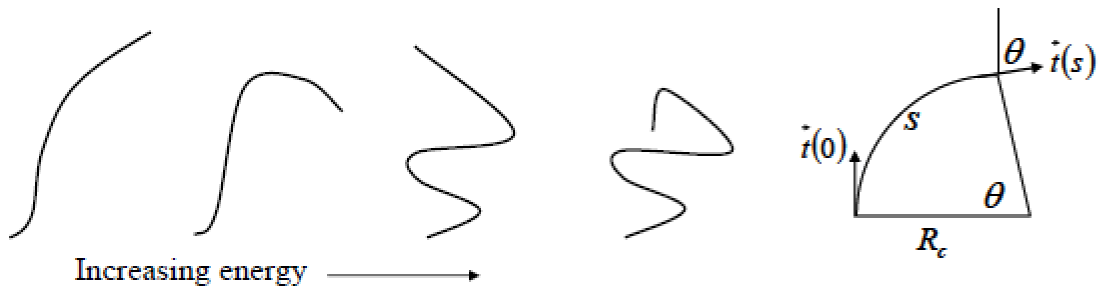
Lecture 34 : The significance of the persistence length

The Lecture Contains

- The significance of the persistence length
- End to end displacement of fiber

1. "Mechanics of the cell" by David Boal, Cambridge University Press, 2002, Cambridge, UK

The significance of the persistence length:



At zero temperature, the shape of the filament is such that its energy is minimized. In other word, it then corresponds to a straight rod. At a non-zero temperature, it exchanges energy with its surroundings, so that it fluctuates its shape. With increase in bending energy, its shape turns more contorted and the local curvature grows. Thus the shapes of filaments have increasing energy from left to right. In any case, the probability of finding a filament at a particular conformation depends upon the energy of the conformation and is determined by the Boltzman's law

$$P(\Pi) = \exp\left(-\beta\Pi\right) \quad \text{where} \quad \beta = \frac{1}{k_B T} \qquad (34.1)$$

Equation 34.1 suggests that conformations with large energy are less probable.

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The significance of the persistence length (contd...)

Let us assume that the filament adopts only gentle curves with constant curvature and it does not close on itself, so that its shape can be uniquely parameterized by the angle θ between the tangent vectors $\vec{t}(s)$ and $\vec{t}(0)$ at the two ends of the filament. For an arc of a circle, $\theta = s/R_c$, so that the bending energy is expressed as:

$$\Pi_c = EIs/2R_c^2 = EI\theta^2/2s \qquad (34.2)$$

The angle θ fluctuates back and forth and at higher temperature it has higher probability to attain larger amplitudes of oscillations. The magnitude of oscillations can be quantified by the mean value of θ^2 i.e. $\langle\theta^2\rangle$. For a filament with constant length, $\langle\theta^2\rangle$ is the weighted average over three dimensional orientation of the filament position. This implies that one end of the filament defines the co-ordinate axis z and the other end describes the three dimensional position sampled by the polar angle θ and azimuthal angle ϕ. Assuming that the shapes are all arcs of circles, the probability of each shape is equal to $P(\Pi_{arc})$, so that

$$\langle\theta^2\rangle = \frac{\int \theta^2 P(\Pi_{arc}) d\Omega}{\int P(\Pi_{arc}) d\Omega} \qquad (34.3)$$

The integration is carried out over the solid angle $d\Omega = \sin\theta\, d\theta\, d\phi$. The bending energy is independent of the azimuthal angle ϕ so that it can be integrated out, leaving

$$\langle\theta^2\rangle = \frac{\int \theta^2 \exp(-\beta\Pi_{arc}) \sin\theta\, d\theta}{\int \exp(-\beta\Pi_{arc}) \sin\theta\, d\theta} \qquad (34.4)$$

Now let us assume that the filament is sufficiently stiff, so that energy increases very rapidly with increase in θ, in other word, the filament samples only small oscillations. Then the Boltzman parameter decays rapidly with θ, implying that in equation 34.4 $\sin\theta$ can be replaced by θ.

$$\langle\theta^2\rangle = \frac{\int \theta^3 \exp(-\beta\Pi_{arc})\, d\theta}{\int \theta \exp(-\beta\Pi_{arc}) d\theta} = \frac{\int \theta^3 \exp\left(-\frac{\beta EI\theta^2}{2s}\right) d\theta}{\int \theta \exp\left(-\frac{\beta EI\theta^2}{2s}\right) d\theta} \qquad (34.5)$$

Writing $\frac{\beta EI\theta^2}{2s} = x$, equation 34.5 transforms to

$$\langle\theta^2\rangle = \frac{2s}{\beta EI} \frac{\int x^3 \exp(-x^2)\, dx}{\int x \exp(-x^2) dx} \qquad (34.6)$$

In small vibrations, the upper limit can be extended to infinity so that both integrals yield 1/2. The expression for the mean square value of θ is then obtained as,

$$\left\langle \theta^2 \right\rangle = \frac{2s}{\beta EI} = \frac{2s}{L_p}, \qquad L_p \;:\; \text{persistence length} \tag{34.4}$$

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The significance of the persistence length (contd...)

Now consider, the scaler product of the two unit tangent vectors $\hat{t}(0)\cdot\hat{t}(s)$ which has a maximum value of unity when the two vector are parallel at the ends of the filament. At non-zero temperature the filament samples variety of orientations, so that the ensemble average $\langle \hat{t}(0)\cdot\hat{t}(s)\rangle = \langle \cos\theta \rangle$ has a maximum average value of unity. The function $\langle \hat{t}(0)\cdot\hat{t}(s)\rangle$ is called the correlation function of the tangent vector, i.e. it defines the correlation of tangent vectors at different positions along the curve. At low temperature, θ is small so that $\cos\theta \sim 1-\frac{\theta^2}{2}$, yielding,

$$\langle \hat{t}(0)\cdot\hat{t}(s)\rangle = 1-\frac{\theta^2}{2} = 1-\frac{s}{L_p}, \quad \left(\frac{s}{L_p} << 1\right) \tag{34.5}$$

Similarly the mean squared difference between the tangent vectors can be obtained as

$$\left\langle \left[\hat{t}(0)-\hat{t}(s)\right]^2 \right\rangle = 2-2\langle \hat{t}(0)\cdot\hat{t}(s)\rangle \sim \frac{2s}{L_p}, \quad \left(\frac{s}{L_p} << 1\right) \tag{34.6}$$

Thus the persistence length measures the distance along the filament over which the orientation of the curves become decorreleted.

For a rigid rod, i.e. rod with contour length $L << L_p$, equation 34.5 shows that the correlation decays linearly with increase in contour length. However, if $L >> L_p$, the filament appears fluffy and $\langle \hat{t}(0)\cdot\hat{t}(s)\rangle$ should vanish as the tangent vectors at the extreme ends of the filament becomes uncorrelated. This behavior is not seen in equation 34.5. The correct expression for the tangent correlation function applicable at long and short distances is,

$$\langle \hat{t}(0)\cdot\hat{t}(s)\rangle = \exp\left(-\frac{s}{L_p}\right), \tag{34.7}$$

The proof of equation 34.7 can be found elsewhere.

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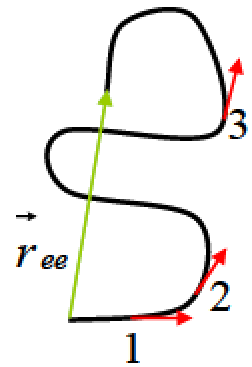
End-to-end displacement of fiber:



From different observables that characterize the size of a polymer configuration, we evaluate the end-to-end displacement vector $\vec{r}_{ee} = \vec{r}(L_c) - \vec{r}(0)$, where $\vec{r}(s)$ denotes the position of the filament at arc length s. The mean square value of $\vec{r}_{ee}$ is then

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = \left\langle \left[\vec{r}(L_c) - \vec{r}(0)\right]^2 \right\rangle, \qquad (34.8)$$

Integrating the unit tangent vector $\vec{t}(s)$

$$\vec{r}(s) = \vec{r}(0) + \int_0^s du\; \vec{t}(u), \qquad (34.9)$$

Substituting the expression for $\vec{r}(s)$ from equation 34.9 in equation 34.8,

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = \int_0^{L_c} du \int_0^{L_c} dv \left\langle t(u) \cdot t(v) \right\rangle, \qquad (34.10)$$

From equation 34.7, the correlation function $\left\langle \vec{t}(0) \cdot \vec{t}(s) \right\rangle$ decays exponentially, to yield

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = \int_0^{L_c} du \int_0^{L_c} dv \exp\left(-|u - v|/L_p\right), \qquad (34.11)$$

The condition that the argument needs to be negative can be imposed by breaking the integration into two parts,

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = 2\int_0^{L_c} du \int_0^{u} dv \exp\left(-|u - v|/L_p\right), \qquad (34.12)$$

Above integration yields the following,

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = 2\int_0^{L_c} \exp\left(-u/L_p\right) du \int_0^u dv \exp\left(v/L_p\right) = 2\int_0^{L_c} \exp\left(-u/L_p\right) du \cdot L_p \cdot \left[\exp\left(u/L_p\right) - 1\right]$$

$$= 2L_p^2 \int_0^{L_c/L_p} dw\left[1 - \exp\left(-w\right)\right] \qquad (34.13)$$

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = 2L_c L_p - 2L_p^2\left[1 - \exp\left(-L_c/L_p\right)\right]$$