The Lecture Contains

- End-to-end displacement of fiber (contd from the last lecture)
- Chain configurations and elasticity
- Random Chain in one Dimension
- Random chain in three dimension

"Mechanics of the Cell" by David Boal, Cambridge University Press, 2002, Cambridge, UK

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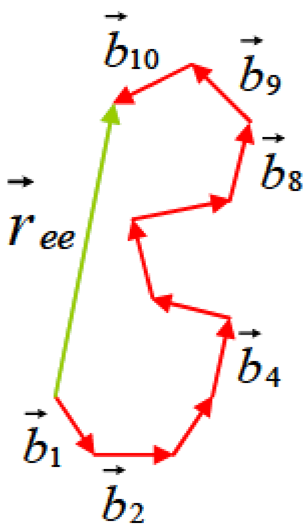
The equation simplifies in two limits. If $L_p >> L_c$, equation (34.13) is simplified by writing $\exp(x) = 1 - x + x^2/2$ reduces to $\left\langle \vec{r}_{ee}^{\,2} \right\rangle^{1/2} = L_c$. The filament rather appears like a rod with end-to-end distance close to the contour length. At the other extreme, $L_p << L_c$, equation 14.34 simplifies to

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = 2L_c L_p \qquad (35.1)$$

implying that over long distance compared to persistence length $\left\langle \vec{r}_{ee}^{\,2} \right\rangle^{1/2}$ grows like the square root of the contour length, rather than the contour length itself.



We can now repeat this calculation by discrete representation to relate the geometry of a continuous polymer to its monomeric constituents. The filament is replaced by N segments, each of which is described by a vector $\vec{b}_i$ having the same length and orientation as the segment. The end-to-end distance $\vec{r}_{ee}$ is then represented as

$$\vec{r}_{ee} = \sum_{i=1,N} \vec{b}_i \qquad (35.2)$$

Taking the ensemble average of all chains with the same number of links N, the mean squared end to end displacement is

$$\left\langle \vec{r}_{ee}^{\,2} \right\rangle = \sum_i \sum_j \left\langle \vec{b}_i \cdot \vec{b}_j \right\rangle \qquad (35.3)$$

Let's say we are concerned with the special case in which all segments of the chain has the same length b_i although their orientations differ. For a random chain, bond vector $\bar{b}_i$ can assume any orientation independent of $\bar{b}_j$, so that the result $\left\langle \bar{b}_i . \bar{b}_j \right\rangle$ vanishes. In other word only the diagonal terms remain which equals b^2. Then a chain with random orientation obeys,

$$\left\langle \bar{r}_{ee}^{2} \right\rangle = Nb^2 \tag{35.4}$$

Furthermore using $L_c = Nb$, we obtain

$$\left\langle \bar{r}_{ee}^{2} \right\rangle = L_c b \tag{35.5}$$

which is similar to equation 14.35 for $L_p << L_c$, with L_p being replaced by $b/2$.

Chain configurations and elasticity:

The tangent correlation function or the end-to-end distance does not really give the complete picture of the configuration of the chain, the probability distribution of its end-to-end distance. These distributions confirm that it is highly unlikely that a random chain will remain in a fully stretched condition, because the most likely value of r_{ee}^2 for a freely jointed chain is not far from the value of Nb^2. Basically there are far more configurations available for $r_{ee} \sim N^{1/2} b$ than available for $r_{ee} \sim Nb$. Because of this when an external load is applied to straighten a chain its entropy decreases, i.e. the chain behaves elastically because of its entropy.

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Random chain in one dimension:

Consider a one-dimensional chain with three segments, each chain starting off the origin and a link in the chain can point to the left or to the right. Since each link has two possibilities, there are $2^3 = 8$ configurations possible for the whole chain. Representing $C\left(\vec{r}_{ee}\right)$ as the number of configurations with a particular displacement $\vec{r}_{ee}$, the eight configurations are distributed as

$$C(+3b)=1,\ \ C(+1b)=3,\ \ C(-1b)=3,\ \ C(-3b)=1$$

It is easy to see that these quantities are the binomial coefficients of $(p+q)^3$. For a chain with N segments, with i vectors pointing left and N-i vectors pointing right, the number of such configurations are same as the coefficient of the binomial expansion of

$$(p+q)^N = \sum_{i=0,N} \frac{N!}{i!(N-i)!} p^i q^{N-i} \tag{35.6}$$

i.e. $\dfrac{N!}{i!(N-i)!}$. This chain with N segments can be thought of to be a random walk with each segment having probability $\frac{1}{2}$ of pointing to the left and probability $\frac{1}{2}$ of pointing to the right. Hence the probability for there to be a configuration with i segments pointing left and N-i segments pointing right is

$$P(i, N-i) = \frac{N!}{i!(N-i)!}\left(\frac{1}{2}\right)^i\left(\frac{1}{2}\right)^{N-i} \tag{35.7}$$

The probability is appropriately normalized, so that the summation of all the probabilities yield 1,

$$\sum_{i=0,N} P(i, N-i) = \sum_{i=0,N} \frac{N!}{i!(N-i)!}\left(\frac{1}{2}\right)^i\left(\frac{1}{2}\right)^{N-i} = \left(\frac{1}{2}+\frac{1}{2}\right)^N = 1 \tag{35.8}$$

As the number of links in the chain increases, the distribution looks more and more continuous, eventually the distribution converges to that of the Gaussian distribution, which is of the form,

$$P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \tag{35.9}$$

This expression is the probability density such that the probability of finding a state between x and $x+dx$ is $P(x)dx$. The mean value μ of the distribution can be found out as,

$$\mu = \langle x \rangle = \int_{-\infty}^{\infty} xP(x)dx \tag{35.10}$$

And its variance as,

$$\sigma^2 = \left\langle (x-\mu)^2 \right\rangle = \left\langle x^2 \right\rangle - \mu^2 \qquad (35.11)$$

For one Cartesian component of $\vec{r}_{ee}$ in a random chain, $\mu = 0$, because the vectors $\vec{r}_{ee}$ are isotropically distributed; furthermore, $\left\langle x^2 \right\rangle = Nb^2$, which implies $\sigma^2 = Nb^2$ in one dimension.

Random chain in three dimensions:

The configuration of a chain in three diemension can be projected onto three axes of the Cartesian system and then can be treated as three independent one dimensional systems. Thus *x* component of the end-to-end distance is the summation of the individual vectors as projected on the *x* axis:

$$r_{ee,x} = \sum_i b_{i,x} \qquad (35.12)$$

$b_{i,x}$ is the *x*-projection of monomer vector $\vec{b}_i$. For freely jointed chain, $b_{i,x}$ is independent of $b_{i+1,x}$, so the projections form a random walk in one dimension, although of variable lengths, even if all the monomenrs are of the same length. If the number of segments is large the probability distribution with variable segment lengths has the same form as that of with uniform segment length:

$$\mu = \langle x \rangle = \int_{-\infty}^{\infty} x P(x) dx \qquad (35.13)$$

with a variance $\sigma^2 = N\langle {b_x}^2 \rangle$. Here $\langle {b_x}^2 \rangle$ is the expectation of the projection of individual segments on the *x* axis. The system is however symmetric, which should ensure that the mean projections are independent of direction, so that,

$$\langle {b_x}^2 \rangle = \langle {b_y}^2 \rangle = \langle {b_z}^2 \rangle = b^2/3 \qquad (35.14)$$

because, $\langle {b_x}^2 \rangle + \langle {b_y}^2 \rangle + \langle {b_z}^2 \rangle = \langle b^2 \rangle = b^2$ for segments of constant length. Hence the variance is,

$$\sigma^2 = Nb^2/3 \qquad (35.15)$$

Now the probability of finding a three dimensional chain within the volume $dx\,dy\,dz$ centered on the position (x,y,z) is $P(x,y,z)dx\,dy\,dz$, c is the product of the probability distributions in each of the Cartesians directions,

$$P(x,y,z) = P(x)\cdot P(y)\cdot P(z) = \frac{1}{(2\pi\sigma^2)^{3/2}} \exp\left(- \frac{(x^2+y^2+z^2)}{2\sigma^2} \right) \qquad (35.16)$$

in which $\sigma^2 = Nb^2/3$ and $x \equiv r_{ee,x}$ etc. According to equation 14.49, the most probable co-ordinate for the tip of the chain is $(0,0,0)$, that does not mean that the most likely value of r_{ee} is zero. In fact the most likely value of r_{ee} can be estimated by considering that the probability for the chain to have radial end to end distance between *r* and *r*+*dr* is, $P(r)dr$. Here $P(r)$ is the probability per unit length, defined as: $P(x,y,z)dx\,dy\,dz = P_{rad}(r)\cdot dr$

so that,

(35.17)

$$P_{rad}(r) = \frac{4\pi r^2}{\left(2\pi\sigma^2\right)^{3/2}} \exp\left(-\frac{r^2}{2\sigma^2}\right)$$

Deriving $P_{rad}(r)$ with respect to *r* and equating it to zero, one obtains the most likely value of *r*,

$$\frac{dP_{rad}(r)}{dr} = \frac{8\pi r}{\left(2\pi\sigma^2\right)^{3/2}} \exp\left(-\frac{r^2}{2\sigma^2}\right) - \frac{8\pi r^3}{\left(2\pi\sigma^2\right)^{3/2} 2\sigma^2} \exp\left(-\frac{r^2}{2\sigma^2}\right) = 0 \qquad (35.18)$$
$$=> \quad r^2 = 2\sigma^2$$

Substituting the expression for 35.15 in 35.18, one obtains the expression,

$$r_{ee,\text{most likely}} = (2/3)^{1/2} N^{1/2} b \qquad (35.19)$$

The average value of r_{ee} is obtained as,

$$\langle r_{ee} \rangle = \frac{\int_{r=0}^{\infty} r P_{rad}(r) dr}{\int_{r=0}^{\infty} P_{rad}(r) dr} = \sqrt{\frac{8}{3\pi}} N^{1/2} b \qquad (35.20)$$

And the mean square end to end distance is obtained as,

$$\langle r_{ee}^2 \rangle = \frac{\int_{r=0}^{\infty} r^2 P_{rad}(r) dr}{\int_{r=0}^{\infty} P_{rad}(r) dr} = Nb^2 \qquad (35.21)$$

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