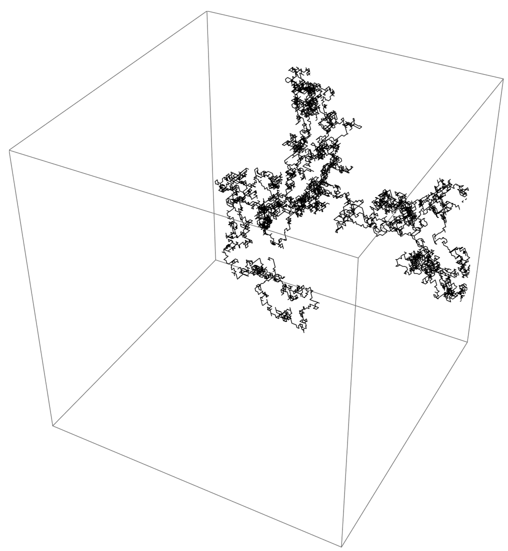
CBP Summer School

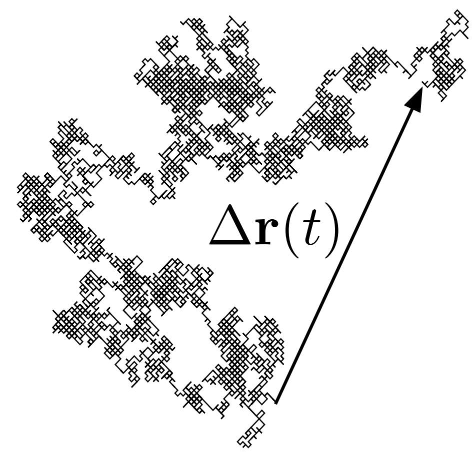
5 - 16 August, 2024

Physics Department, ASU

Lecture 7
Brownian motion and statistics of chains

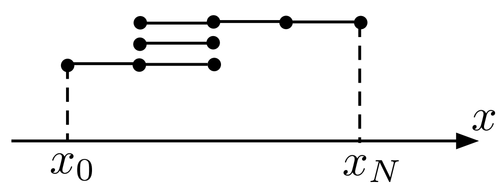
Conformations of a polymer chain can be viewed as random walks





A simplest way to characterize a given conformation is in terms of the end-to-end distance

1D random walk



mean displacement

$$\langle x_N \rangle = a(\langle m \rangle - \langle n \rangle) = 0.$$

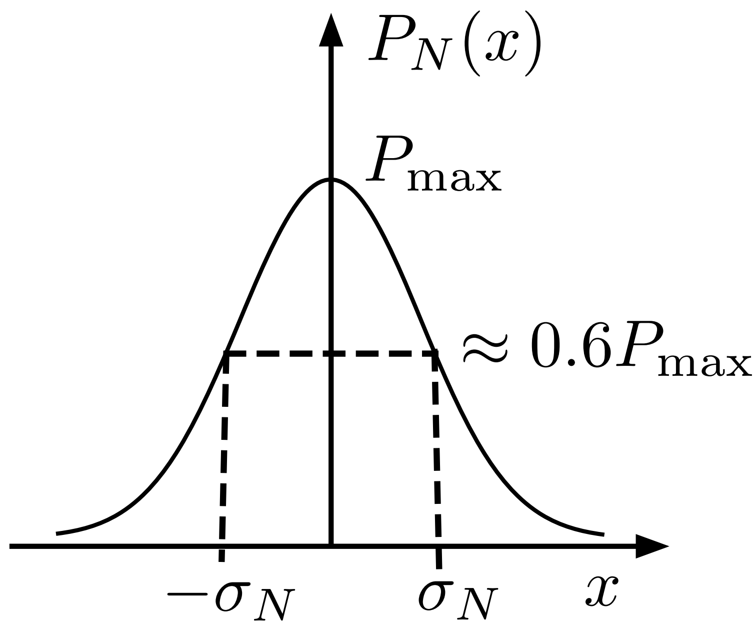
Variance

$$\langle x_N^2 \rangle = a^2 \langle (\delta m - \delta n)^2 \rangle$$

$$\sigma_N^2 = \langle x_N^2 \rangle = a^2 N$$

Gaussian distribution of end-to-end distances

$$P_N(x_N) = \frac{1}{\sqrt{2\pi\sigma_N^2}} \exp\left[-\frac{x_N^2}{2\sigma_N^2}\right]$$



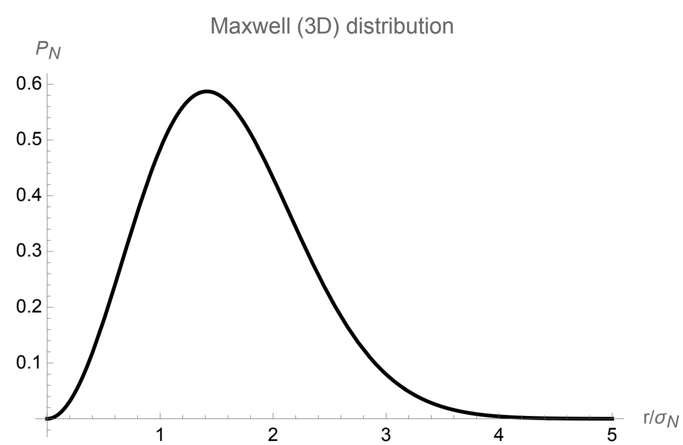
3D random walk

$$\langle \mathbf{r}_N^2 \rangle = \langle (x_N^2 + y_N^2 + z_N^2) \rangle = 3\sigma_N^2.$$

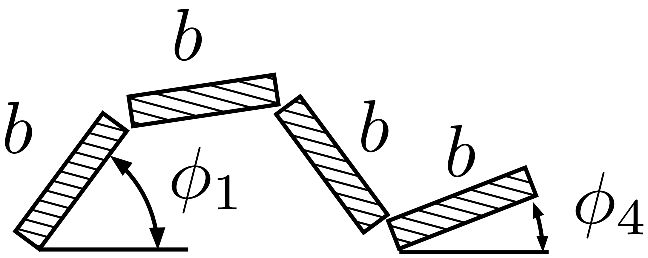
$$\boxed{\langle \mathbf{r}^2 \rangle_t = 2dDt,} \qquad D = a^2/(2\tau)$$

Maxwell distribution

$$P_N(r) = 4\pi r^2 \frac{1}{(2\pi\sigma_N^2)^{3/2}} \exp\left[-\frac{r^2}{2\sigma_N^2}\right]$$



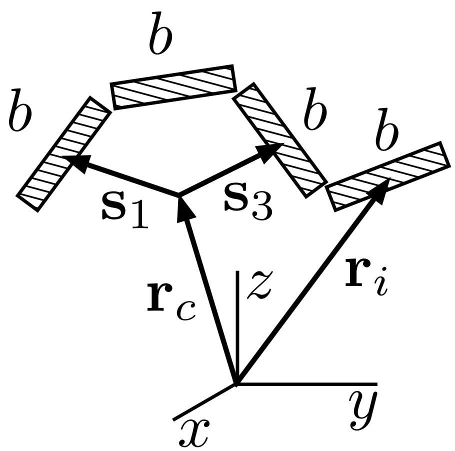
Freely jointed chain



random angles taken at each step

$$R_{\mathrm{rms}} = \sqrt{\langle \mathbf{R}^2 \rangle} = b\sqrt{N}$$

Radius of gyration



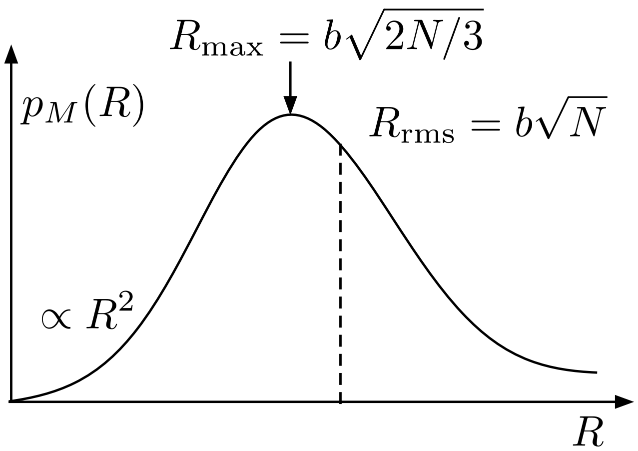
$$\mathbf{r}_c = \frac{1}{N}\sum_{i=1}^{N} \mathbf{r}_i$$

$$R_g^2 = \frac{1}{N}\sum_{i=1}^{N} s_i^2$$

Freely jointed chain:

$$\boxed{R_g^2 = \langle \mathbf{R}^2 \rangle / 6, \quad R_g = R_{\mathrm{rms}}/\sqrt{6}.}$$

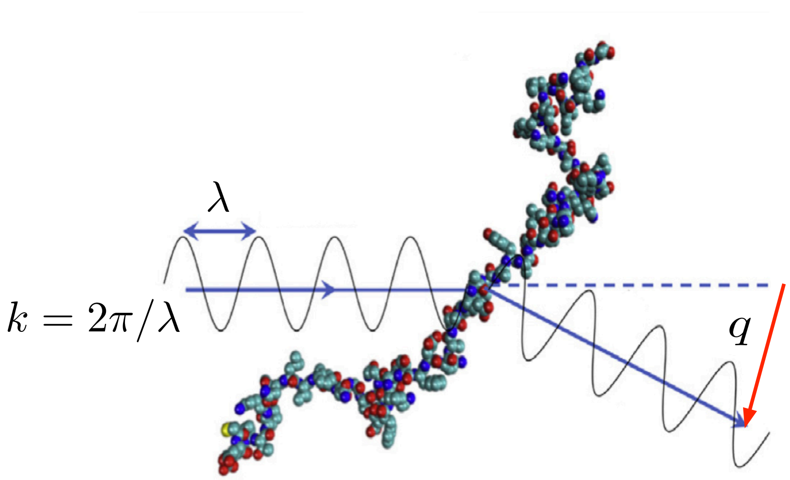
Distribution of end-to-end distances



Maxwell probability density:

$$\boxed{p_M(R) = 4\pi R^2 \left(\frac{3}{2\pi N b^2}\right)^{3/2} \exp\left[-\frac{3\mathbf{R}^2}{2Nb^2}\right].}$$

Scattering of light and radius of gyration



Structure factor:

$$S(q) = \frac{I_s(\theta)}{I_s(0)}$$

$$S(q) \simeq 1 - \frac{q^2}{3} R_g^2$$

Radius of gyration and FRET

FRET=Foerster resonant energy transfer

$$E(R) = \left[1 + (R/R_0)^6\right]^{-1}$$

FRET efficiency