

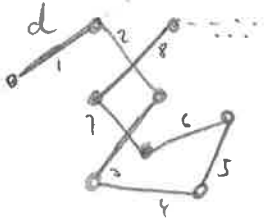
# Polymers in Biology

①

- DNA, RNA: information storage
- actin, microtubules: structure & transport
- polypeptides: folded proteins, unstructured proteins

## Observations

- polymers are floppy
  - conformation is random
- simplest possible model: hinged stiff segments



$$\vec{R}_N = d \sum_{i=1}^N \vec{e}_i$$

↑ direction vector of unit length

→ the average end to end distance

$$\langle \vec{R}_N \rangle = d \sum_{i=1}^N \langle \vec{e}_i \rangle = 0$$

→ the average squared end-to-end distance

$$\langle \vec{R}_N^2 \rangle = d^2 \sum_{i,j} \langle \vec{e}_i \cdot \vec{e}_j \rangle$$



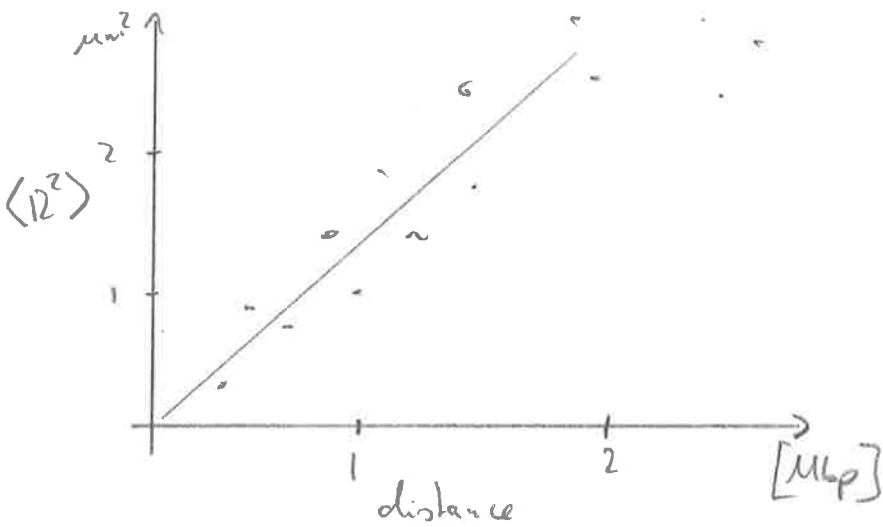
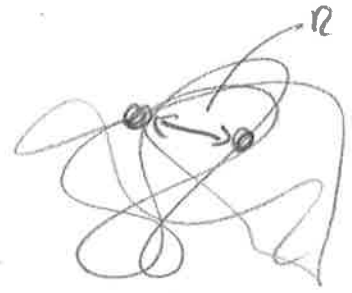
$$= d^2 \left[ \sum_{i \neq j} \langle \vec{e}_i \cdot \vec{e}_j \rangle + \sum_{i=1}^N \langle \vec{e}_i^2 \rangle \right] = d^2 N$$

$= 0 \qquad = 1$

# Polymer properties of Chromatin

(2)

- van den Engh probed avg sq distance at different genomic distance



$$\langle R^2 \rangle \approx 1.5 \frac{\mu\text{m}^2}{\text{Mbp}} S$$

$$S = Nd$$

$$\langle R^2 \rangle = Nd^2$$

$$\Rightarrow d = \frac{\langle R^2 \rangle}{S} = 1.5 \frac{\mu\text{m}^2}{\text{Mbp}} = 5 \text{ nm}$$

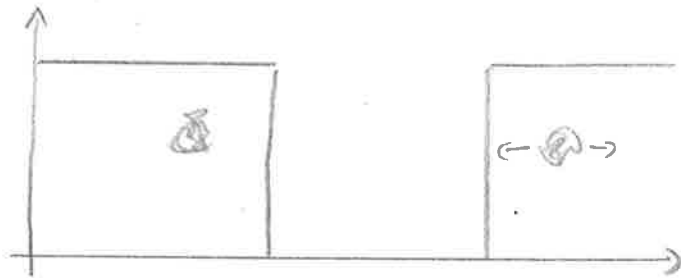
$\approx$  histone diameters (10 nm)



# Single Stranded DNA

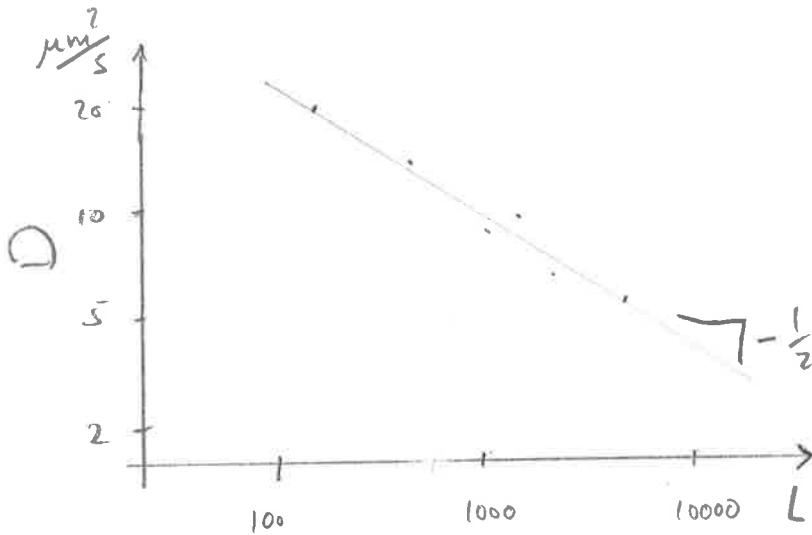
(3)

- Tinland, 1997
- via diffusion measurements by FRAP
- ss DNA + dye
- different length fragments



$$D = \frac{4T}{6\bar{a}r^2}$$

$r$  = radius of gyration



$$D \approx 20 \frac{\mu\text{m}^2}{\text{s}} \cdot \left(\frac{100\text{bp}}{L}\right)^{1/2}$$

$$\approx \frac{\mu\text{m}^3}{15\text{s}} \frac{1}{r}$$

$$\Rightarrow r^2 = \frac{\mu\text{m}^2}{300} \frac{L}{100\text{bp}}$$

$$= Nd^2$$

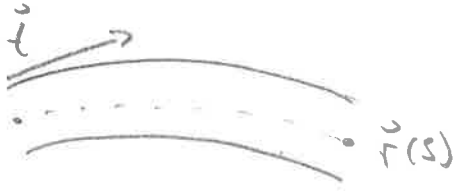
$$\frac{\mu\text{m}^2}{300} \frac{Nd}{100\text{bp}} = Nd^2$$

$$\Rightarrow d = \frac{\mu\text{m}}{300} \approx 1\text{nm}$$

$\Rightarrow$  order of magnitude one base

# Worm-like chain

- continuous polymer that resists bending



$$\vec{r}(s) = \int_0^s ds' \vec{t}(s')$$

- bending requires energy

$$E_b = \frac{\kappa}{2} \int_0^L ds \left( \frac{d\vec{r}(s)}{ds} \right)^2$$

$\uparrow$  curvature

$\kappa$  = stiffness

- bending modes are activated by thermal fluctuations

- direction decorrelates

$$\langle \vec{t}(0) \vec{t}(s) \rangle = e^{-s/l_p} \quad l_p \text{ persistence length}$$

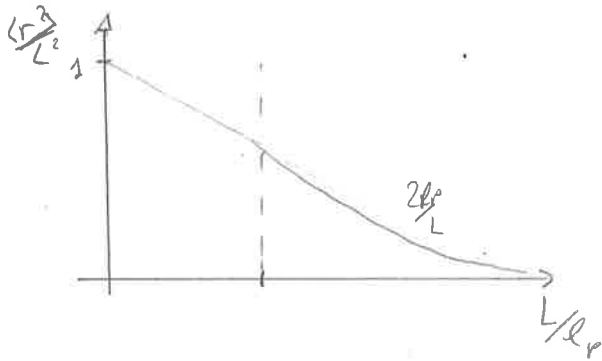
$$l_p = \frac{\kappa}{kT}$$

Does this change the basic properties?

$$\begin{aligned} \langle \vec{r}^2(s) \rangle &= \int_0^s du \int_0^s dv \langle \vec{t}(u) \vec{t}(v) \rangle = \int_0^s du \int_0^s dv e^{-|u-v|/l_p} \\ &= \int_0^s du \left[ \int_0^u dx e^{-x/l_p} + \int_0^{s-u} dx e^{-x/l_p} \right] \\ &= \int_0^s du l_p \left[ 1 - e^{-u/l_p} + 1 - e^{-(s-u)/l_p} \right] \\ &= 2l_p \left[ L - l_p (1 - e^{-s/l_p}) \right] \end{aligned}$$

• for a polymer of length  $L$ , the end-to-end distance is

$$\langle \vec{r}^2(L) \rangle = 2l_p \left[ L - l_p (1 - e^{-L/l_p}) \right] = \begin{cases} 2l_p L & \text{if } L \gg l_p \\ L^2 (1 - L/3l_p) & L \ll l_p \end{cases}$$



• the persistence length of dsDNA is  $l_p \approx 50 \text{ nm} \approx 150 \text{ bp}$

• bacterial genome:  $30,000 l_p \Rightarrow \langle r^2 \rangle \approx 2l_p L = 6 \times 10^4 l_p^2 = 6 \times 25 \mu\text{m}^2$

$$\sqrt{\langle r^2 \rangle} = 12 \mu\text{m}$$

• mammalian:  $1000 \times$  genome  $\Rightarrow 30 \times$  radius

### Microtubules

• very stiff,  $l_p \approx 1 \text{ mm}$

• cargo highways, dynein & kinesin



-  $\alpha, \beta$  tubulin heterodimers

- large diameter makes them stiff

— 20 nm

# Phase behavior

- so far we assumed ideal chain
- depends on solvent, specific solvent with ideal conditions =  $\Theta$  solvent
- charge leads to swelling
- self-interaction (base-pairing, hydrophobic) to collapse
- polymer melts
  - entangled chains
  - often behave ideally (they make each other solvent)