# POLYMER PHYSICS OF DNA: ATOMIC FORCE MICROSCOPY IMAGES DELIVERS ALL THE SECRETS?

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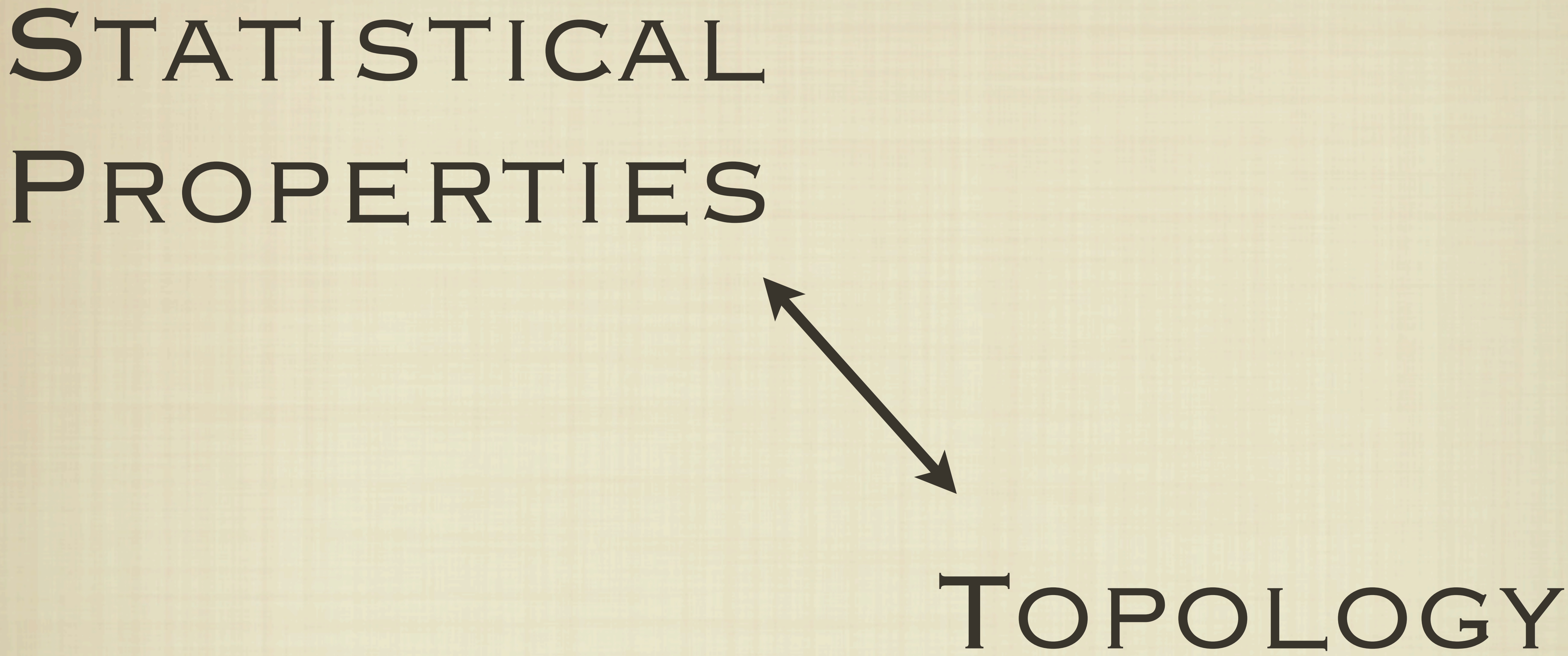
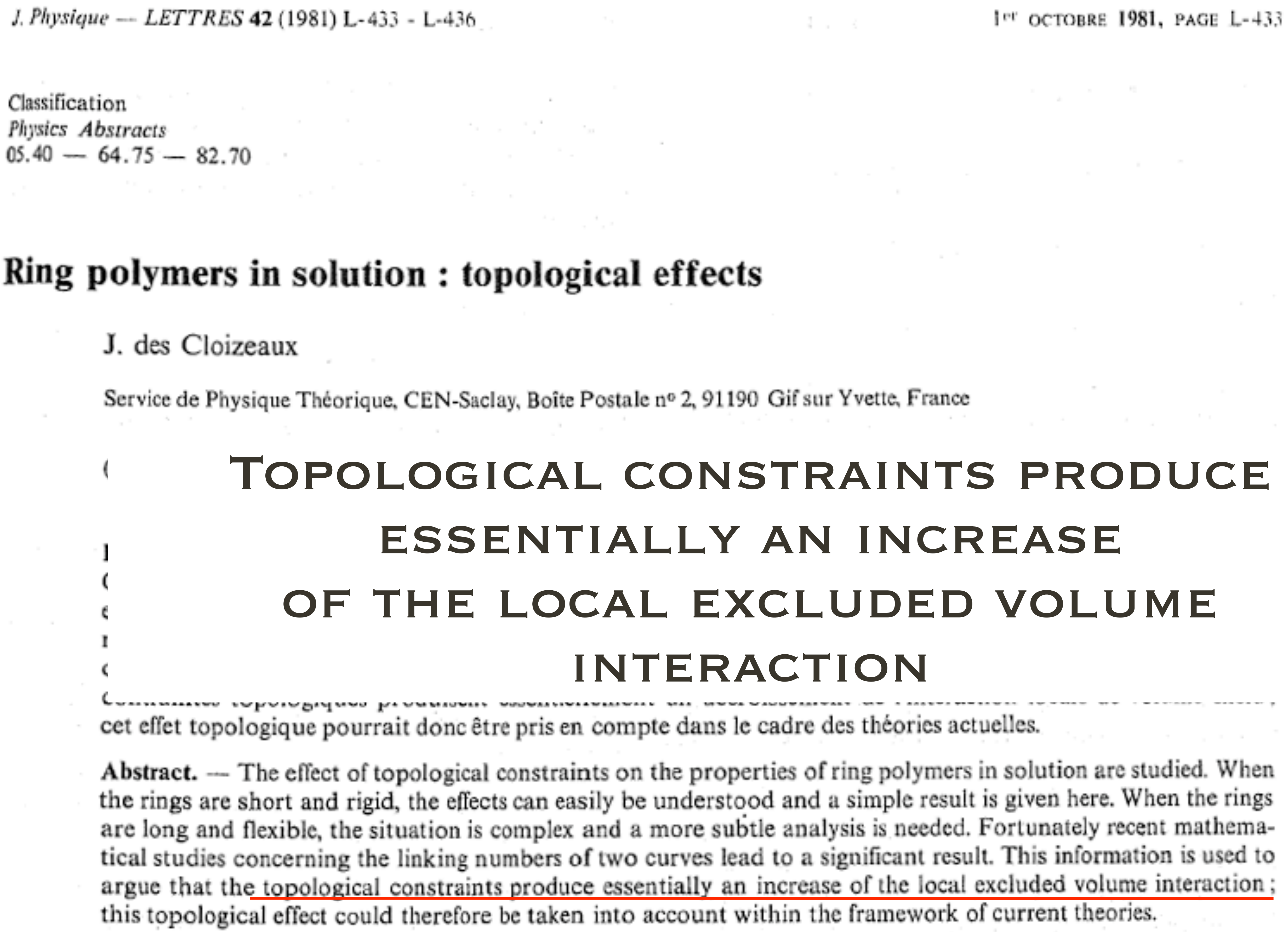
ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE



Statistical Properties

Topology


J. Physique — LETTRES **42** (1981) L-433 - L-436 1er OCTOBRE 1981, PAGE L-433

Classification
*Physics Abstracts*
05.40 — 64.75 — 82.70

# Ring polymers in solution : topological effects

J. des Cloizeaux

Service de Physique Théorique, CEN-Saclay, Boîte Postale n° 2, 91190 Gif sur Yvette, France

## Topological constraints produce essentially an increase of the local excluded volume interaction

cet effet topologique pourrait donc être pris en compte dans le cadre des théories actuelles.

**Abstract.** — The effect of topological constraints on the properties of ring polymers in solution are studied. When the rings are short and rigid, the effects can easily be understood and a simple result is given here. When the rings are long and flexible, the situation is complex and a more subtle analysis is needed. Fortunately recent mathematical studies concerning the linking numbers of two curves lead to a significant result. This information is used to argue that the topological constraints produce essentially an increase of the local excluded volume interaction ; this topological effect could therefore be taken into account within the framework of current theories.

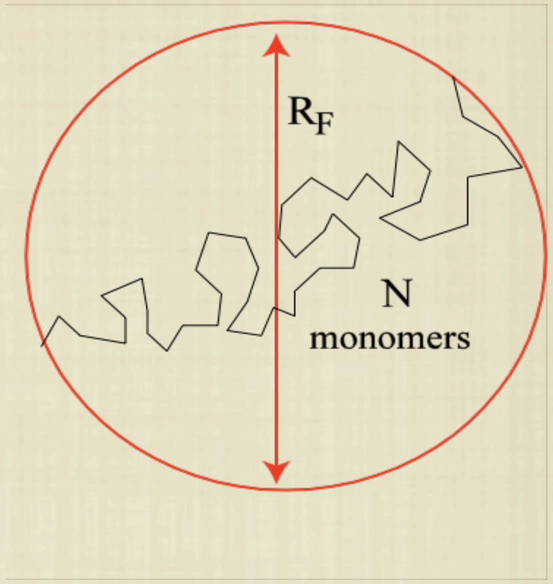
| Universality Class | | Theoretical Model | Physical System | Order Parameter |
|---|---|---|---|---|
| d=2 | n=1 | Ising Model in two dimen. | Adsorbed Films | Surface Density |
| | n=2 | XY Model in two dimen. | Helium-4 films | Amplitude of superfluid phase |
| | n=3 | Heisenberg Model in two dimen. | | Magnetization |
| d>2 | n=∞ | "Spherical" Model | None | |
| d=3 | n=0 | Self-Avoiding random walk | Conformation of long polymers | Density of chain ends |
| | n=1 | Ising Model in 3 dimen. | Uniaxial ferromagnet | Magnetization |
| | | | Fluid near a critical point | Density difference between phases |
| | | | Mixture of fluids near a consolute point | Concentration difference |
| | | | Alloys near a order-disorder transition | Concentration difference |
| | n=2 | XY Model in 3 dimen. | Planar ferromagnet | Magnetization |
| | | | Helium-4 near superfluid transition | Amplitude of the superfluid phase |
| | n=3 | Heisenberg model in 3 dimen. | Isotropic ferromagnet | Magnetization |
| d>=4 | n=-2 | | none | |
| | n=32 | Quantum chromodynamics | Quarks bound in protons, etc | |

# Universality and Universality Classes: behavior depends only from d and n

$$d=1;\ \nu=1.00;\quad \xi=\xi_o L$$

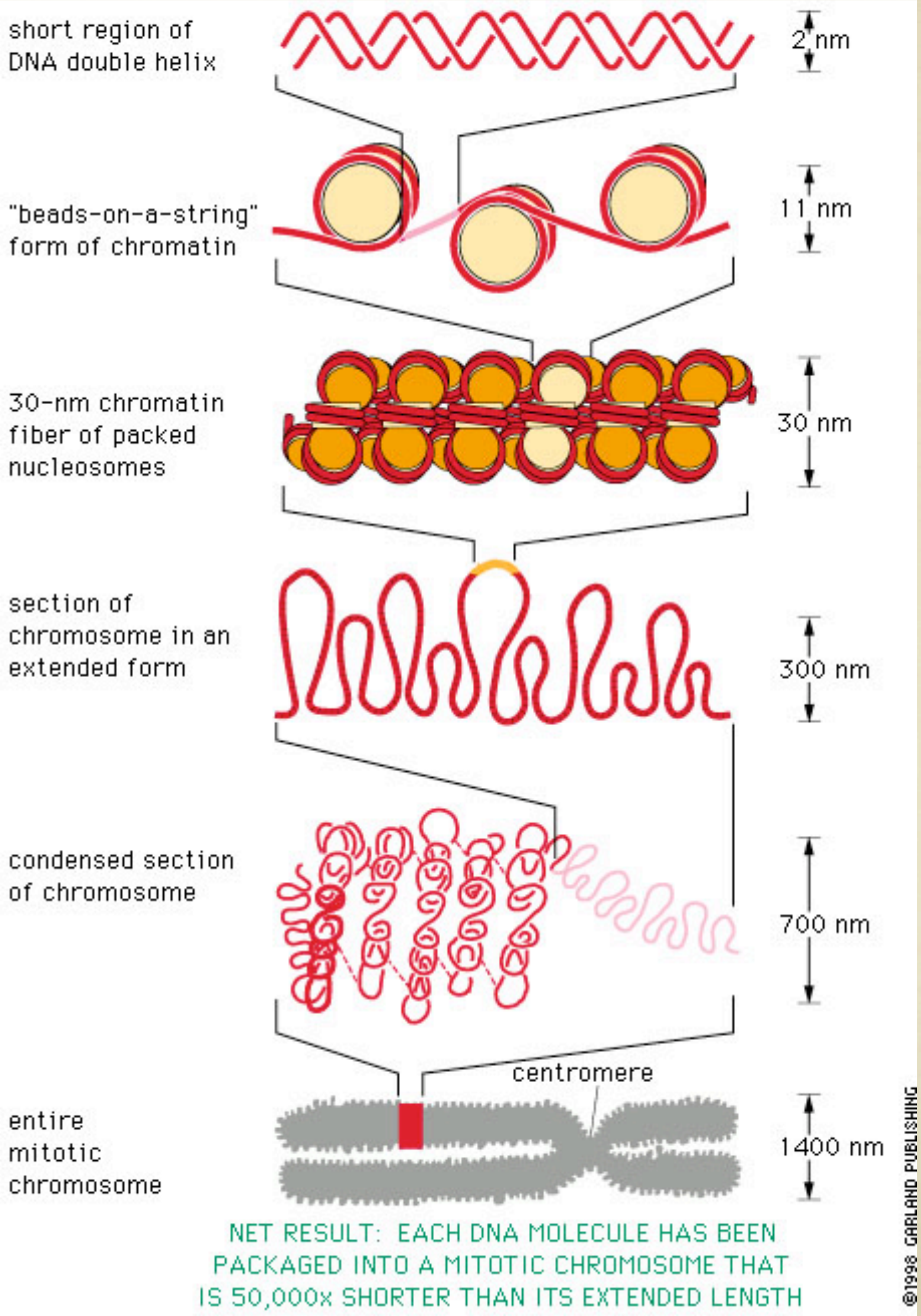
$$d=2;\ \nu=0.75;\quad \xi=\xi_o L^{0.750}$$

$$d=3;\ \nu=0.588;\ \xi=\xi_o L^{0.588}$$



from K. Wilson, 1974

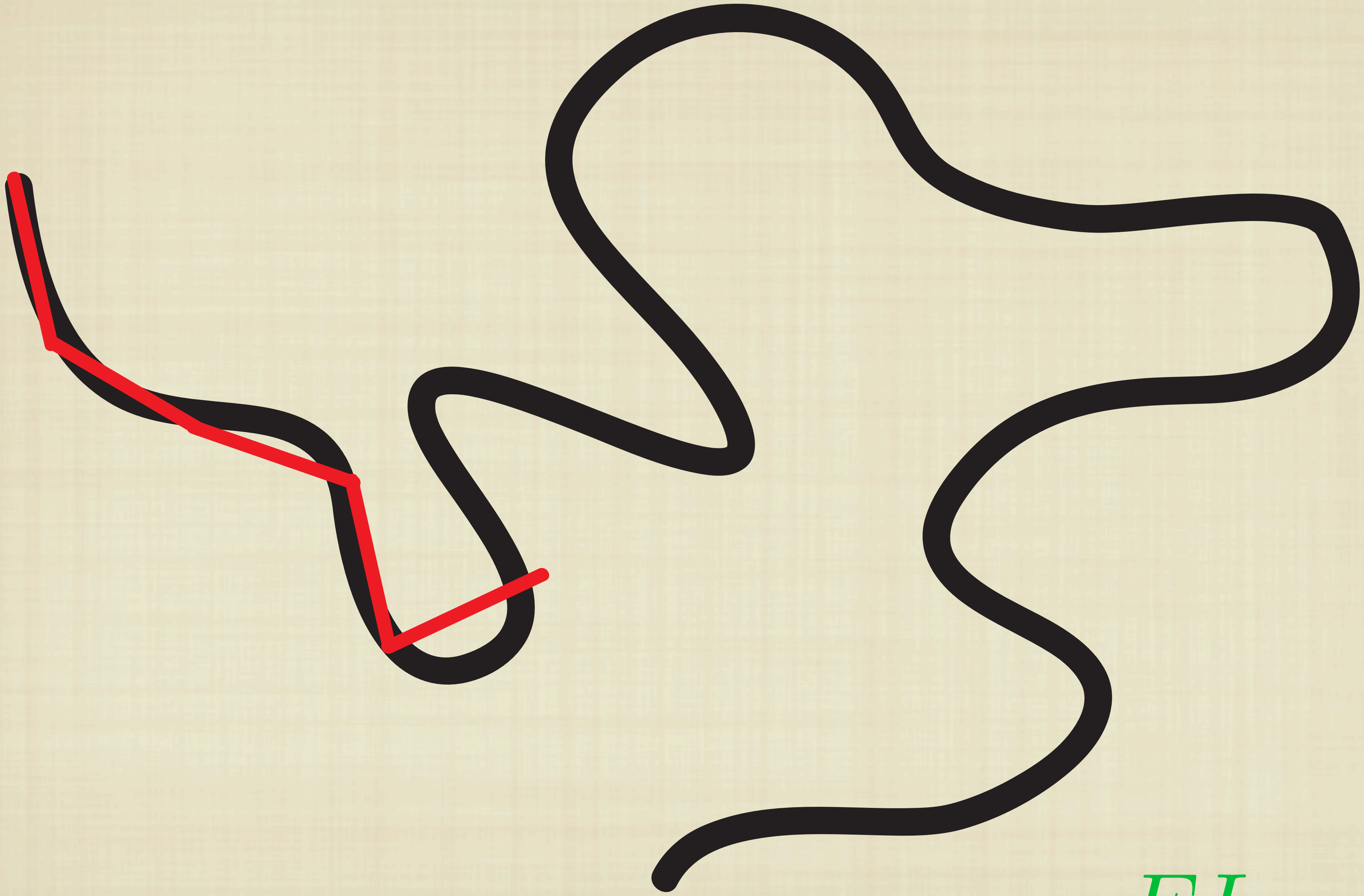
# ORGANIZATION OF THE DNA



NET RESULT: EACH DNA MOLECULE HAS BEEN PACKAGED INTO A MITOTIC CHROMOSOME THAT IS 50,000x SHORTER THAN ITS EXTENDED LENGTH

# DNA Model

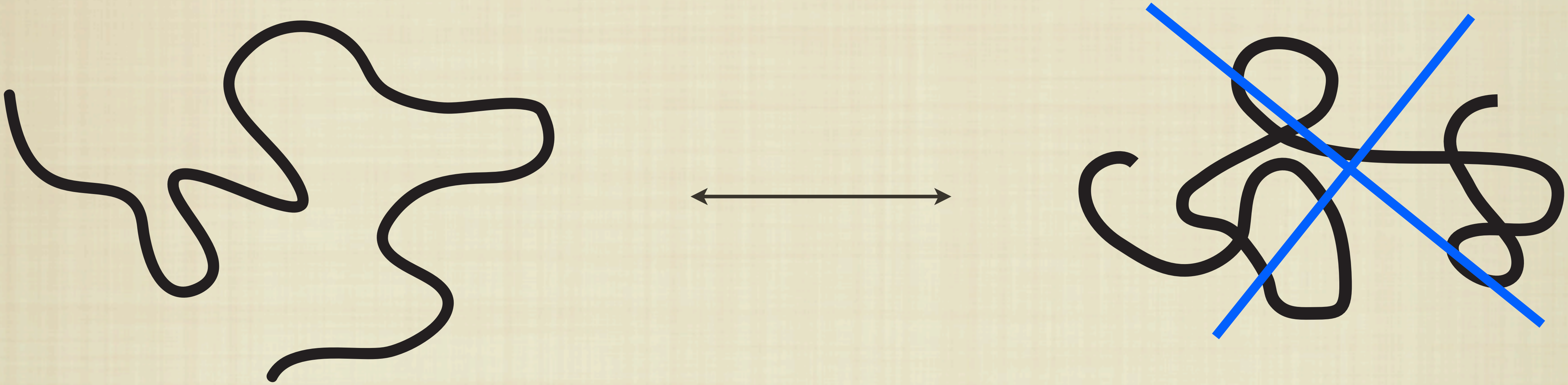
# DNA in a Thermal Bath



— Persistence Length $\boldsymbol{\ell_p} = \dfrac{EI}{k_B T}$

# DNA IS A SELF-AVOIDING WALK (SAW)

## GOOD SOLVENT CONDITIONS

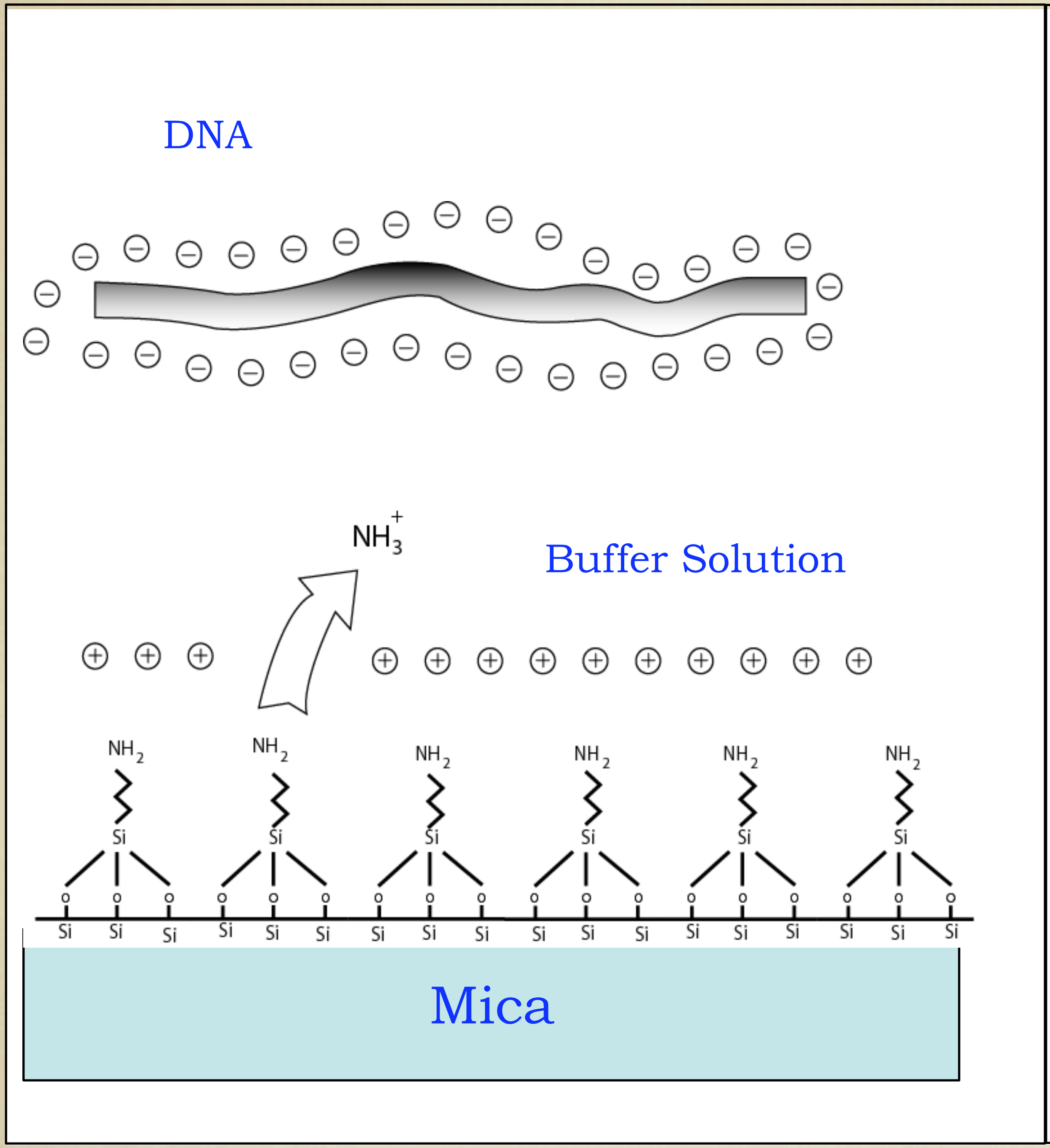


**SAW**

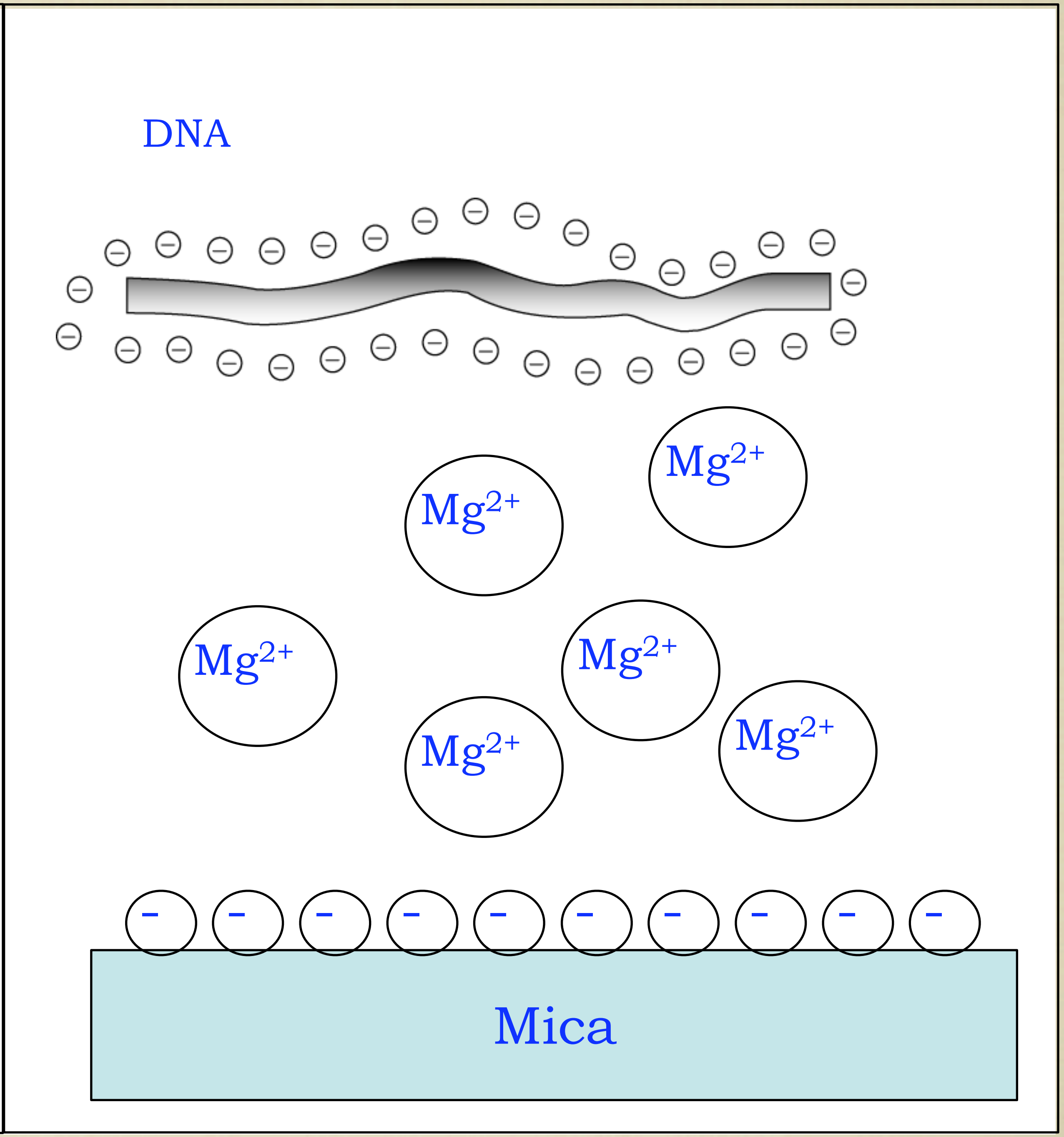
**RANDOM WALK (RW)**

# Deposition of linear and knotted DNA

…on APTES-mica

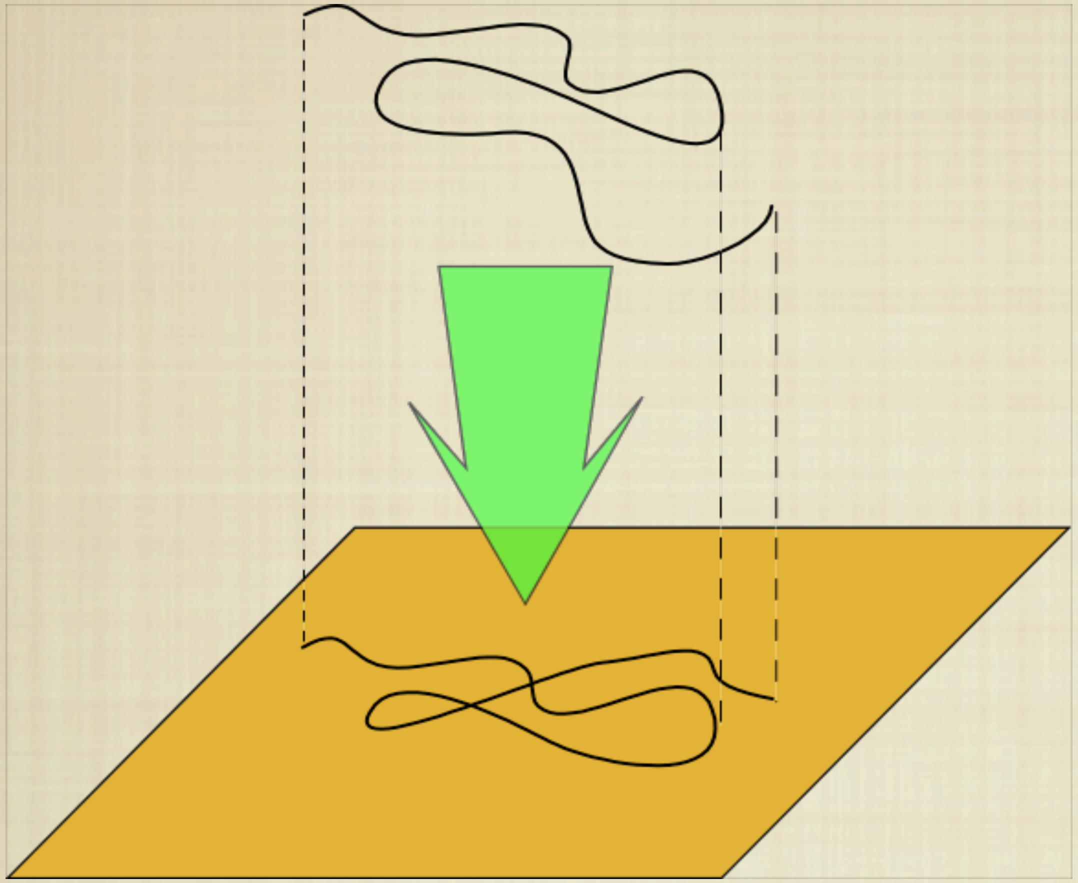


…from a solution containing $Mg^{2+}$ ions



# Deposition

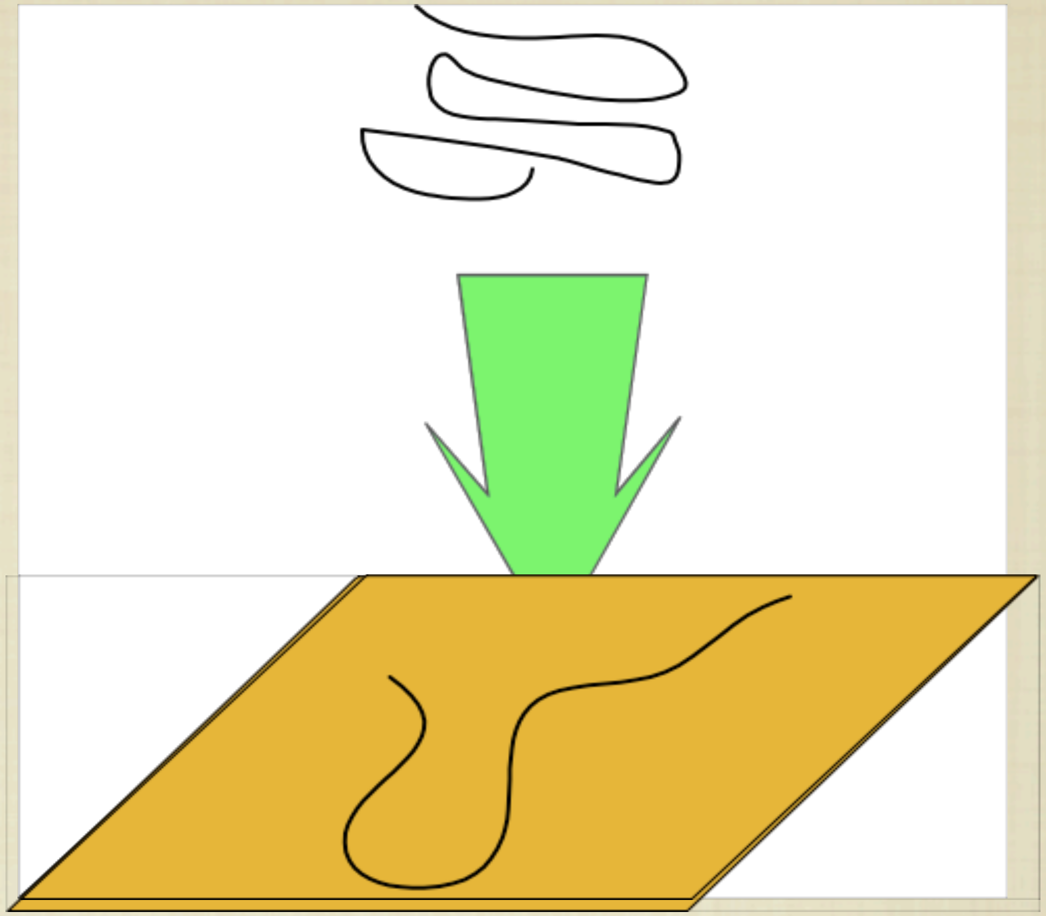
## APTES



Trapping

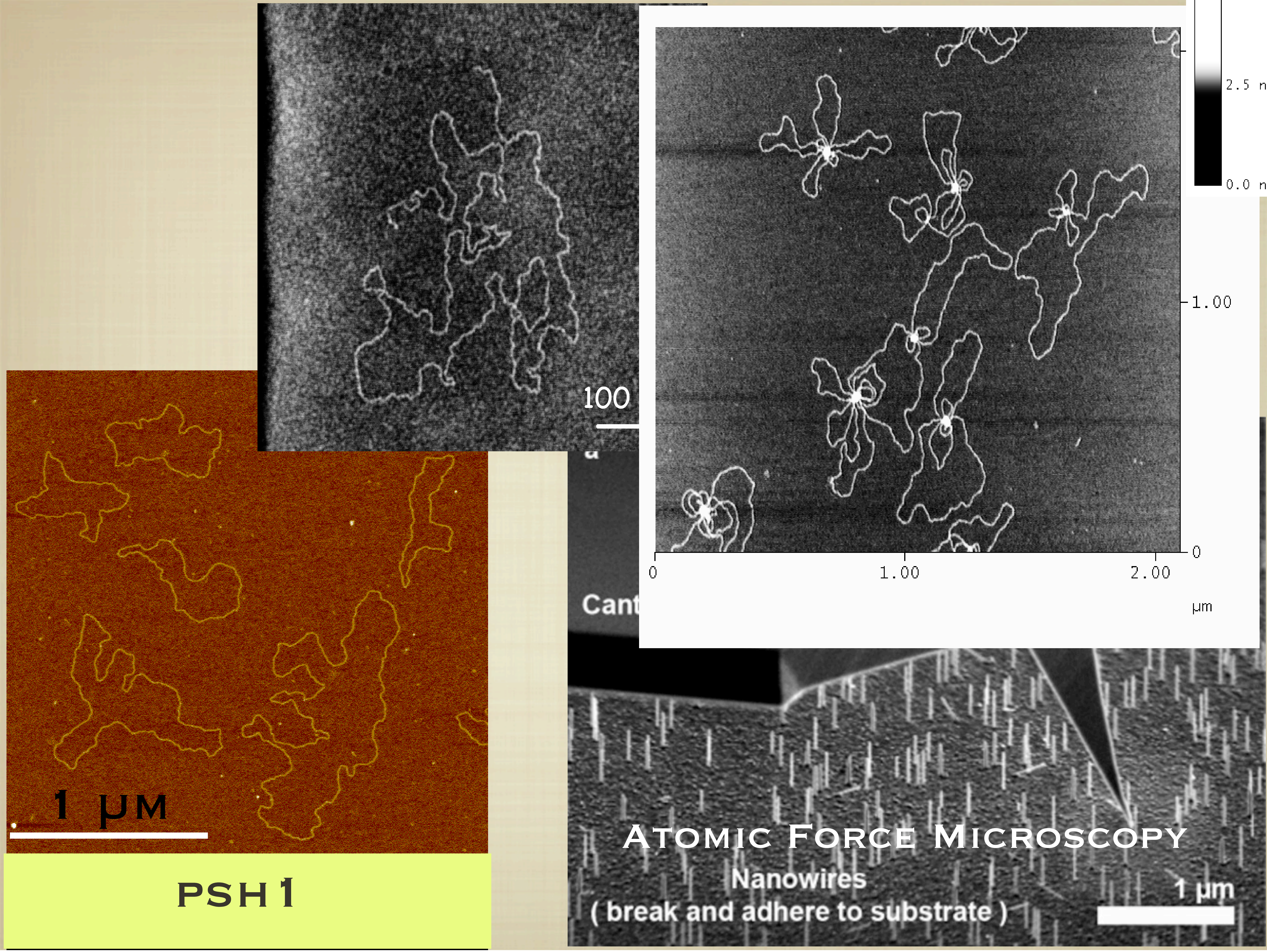
Strong interaction
DNA-surface
$U_{int} >> k_B T$

## Mg$^{2+}$



Equilibration

Weak interaction DNA-surface
$U_{int} \leq k_B T$

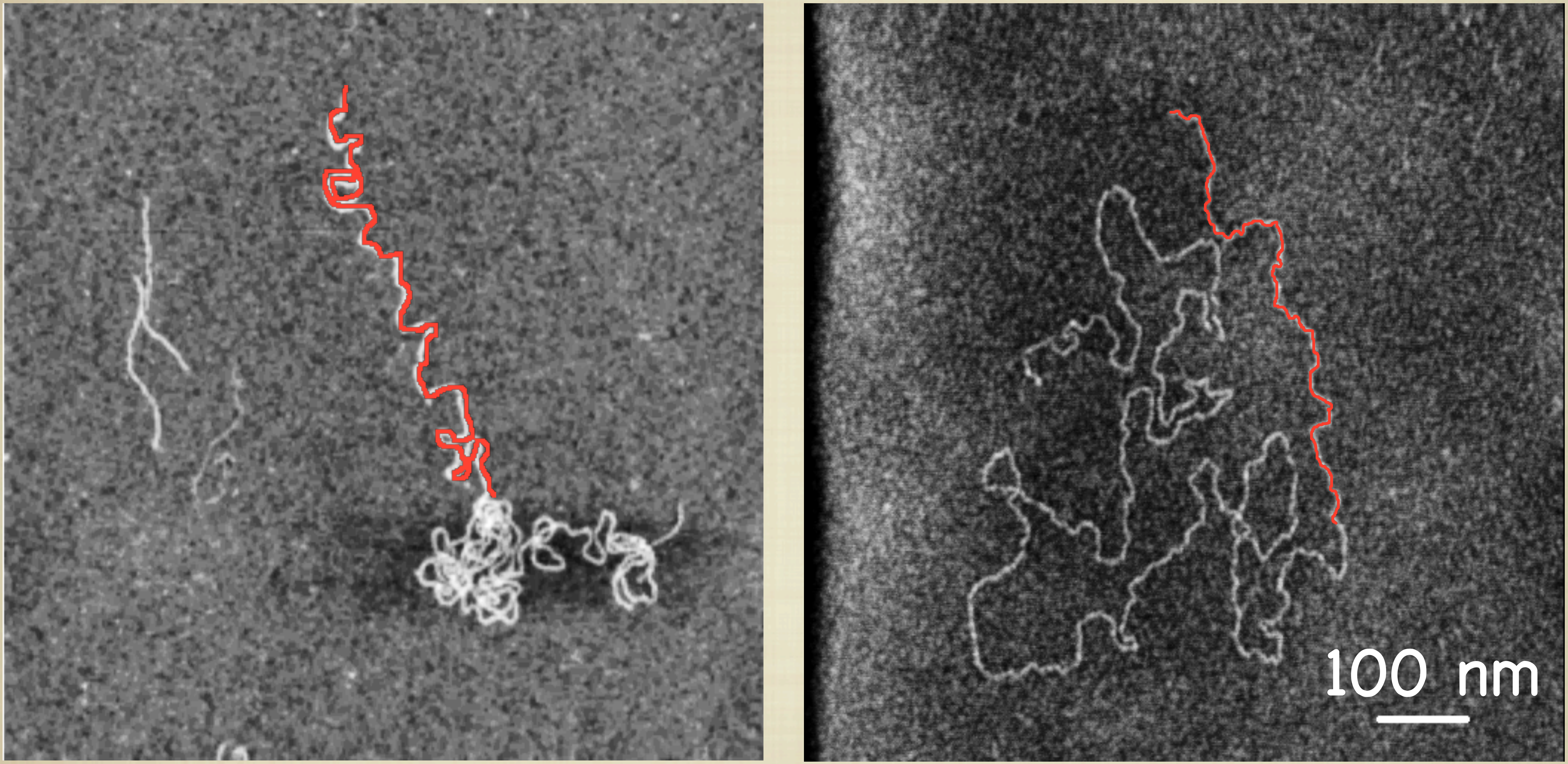


# ATOMIC FORCE MICROSCOPY

Nanowires
( break and adhere to substrate )

**PSH1**

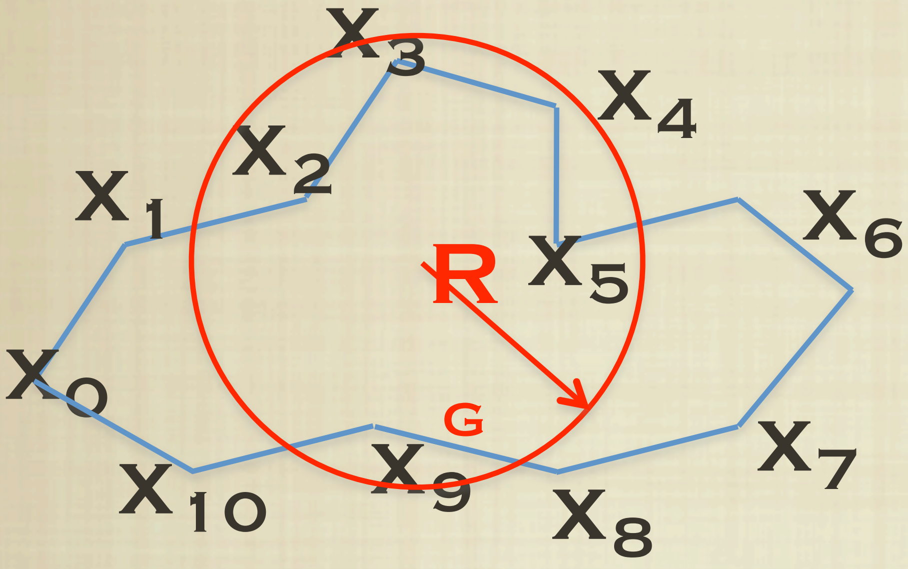
# ANALYZING DNA



# STATISTICAL PROPERTIES OF DNA

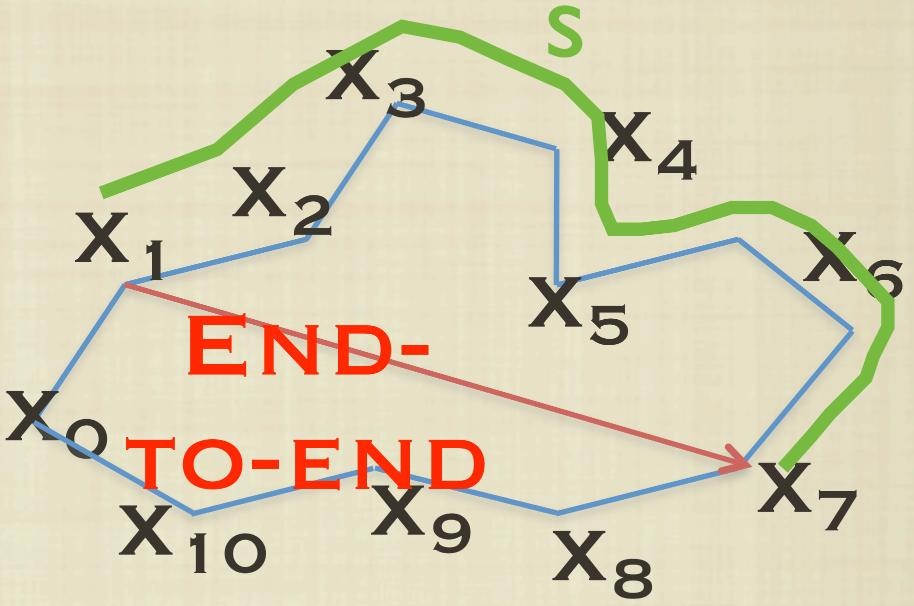
## Scaling of the radius of gyration

$$\langle R_G^2 \rangle = \frac{1}{N}\sum_{i=1}^{N}(r_i - r_{cm})^2 \sim L^{2\nu}$$



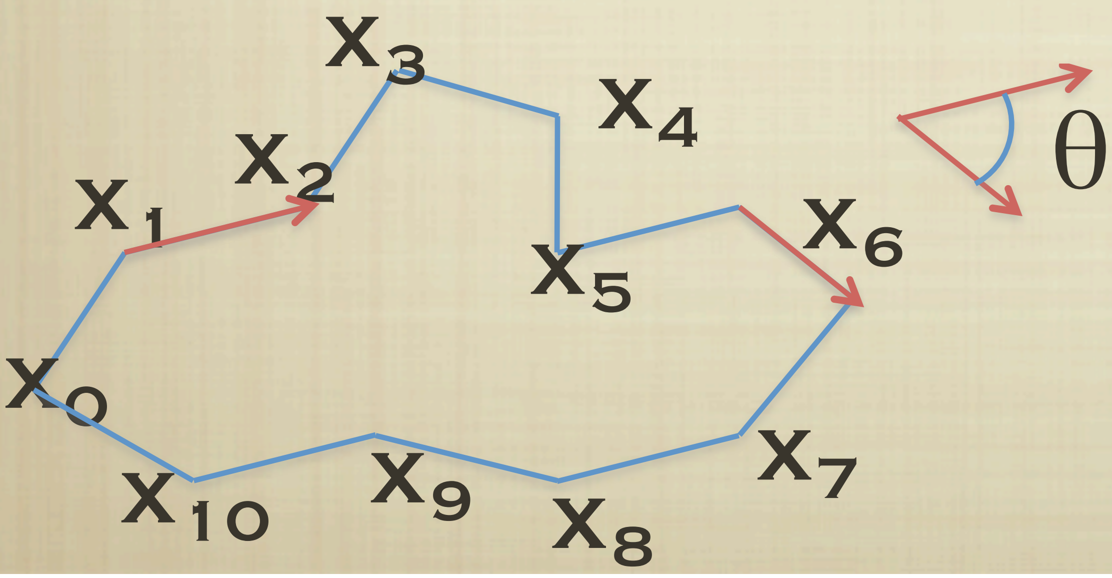
## Scaling of the internal End-to-end distance

$$\langle \xi(s) \rangle = s^{\nu}$$



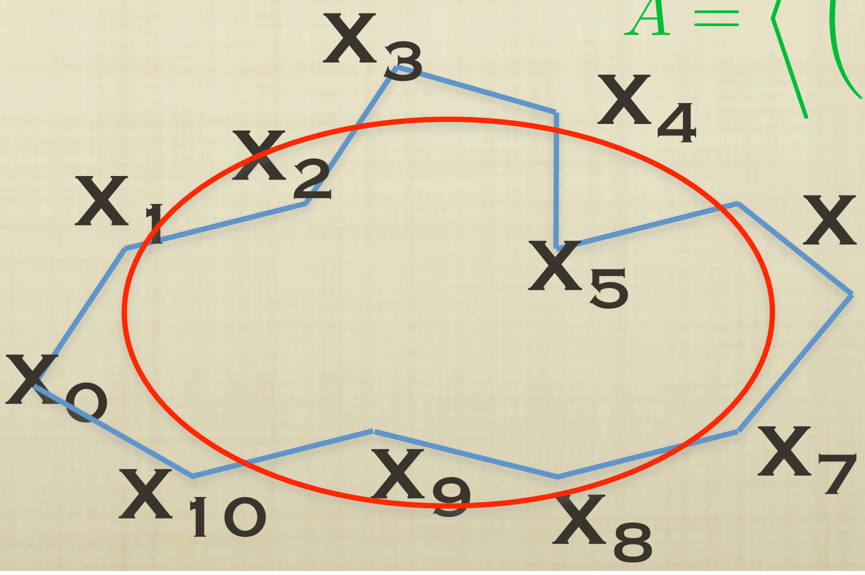
## Directional correlation

$$\langle \cos\theta(s) \rangle = e^{(-s/2\ell_p)}$$



## Shape properties: asphericity

$$A = \left\langle \left( \frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} \right)^2 \right\rangle$$



# Statistical properties of DNA

## Scaling of the radius of gyration

$$\langle R_G^2 \rangle = \frac{1}{N}\sum_{i=1}^{N}(r_i - r_{cm})^2 \sim L^{2\nu}$$

$$\langle \xi(s) \rangle = s^{\nu}$$

## Scaling of the internal End-to-end distance

**SAW**

$$\nu = 1 \quad \text{in 1D}$$

$$\nu = 0.75 \quad \text{in 2D}$$

$$\nu = 0.588 \quad \text{in 3D}$$

**RW**

$$\nu = 0.5$$

## Directional correlation

$$\langle \cos\theta(s) \rangle = e^{(-s/2\ell_p)}$$

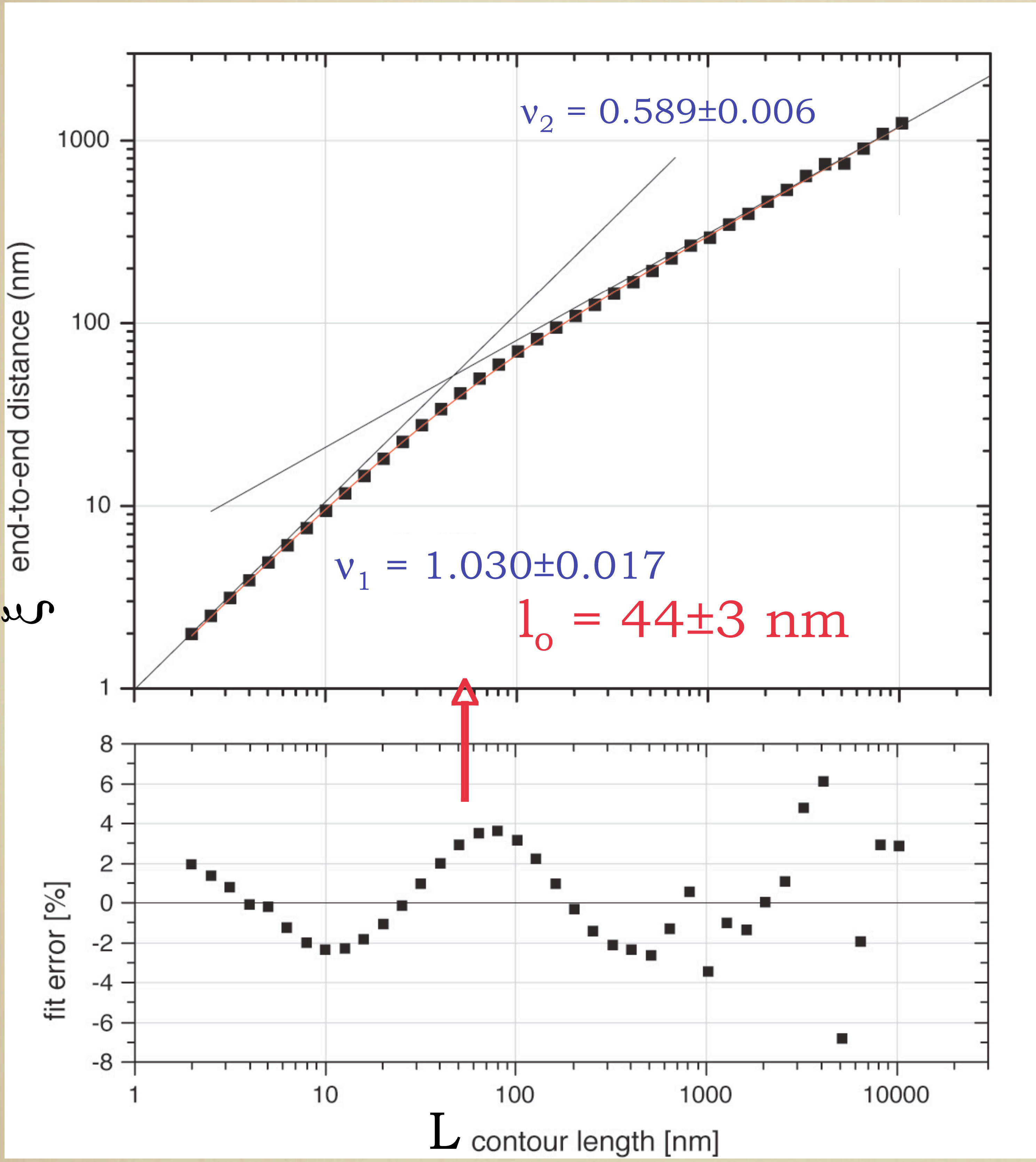
$$\ell_p = 50\ nm$$

## Shape properties: asphericity

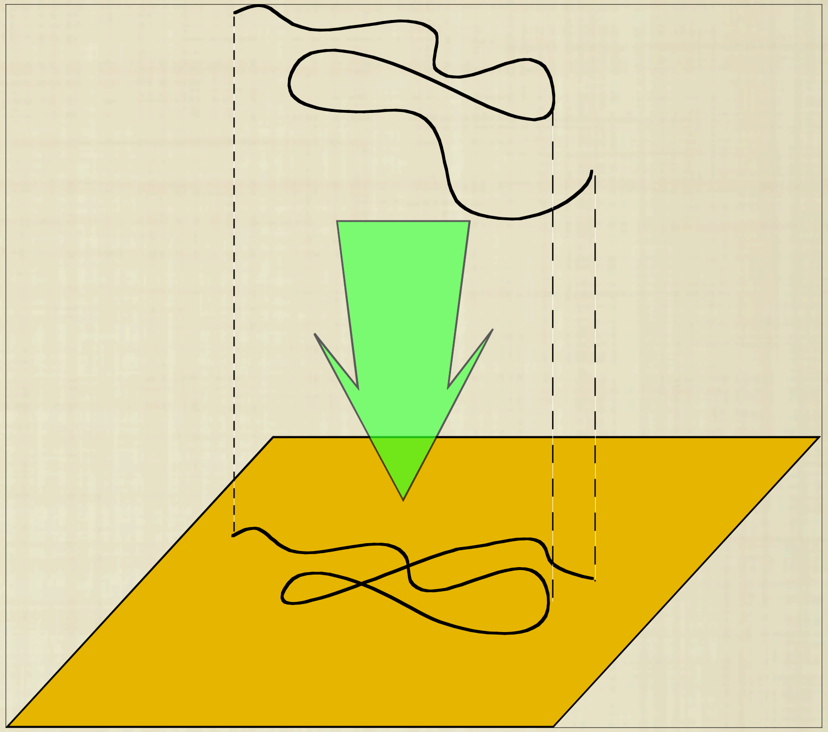
$$A = \left\langle \left( \frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} \right)^2 \right\rangle$$

| | |
|---|---|
| Circle | A=0 |
| Rod | A=1 |
| | |

# PREVIOUS RESULTS ON LINEAR DNA

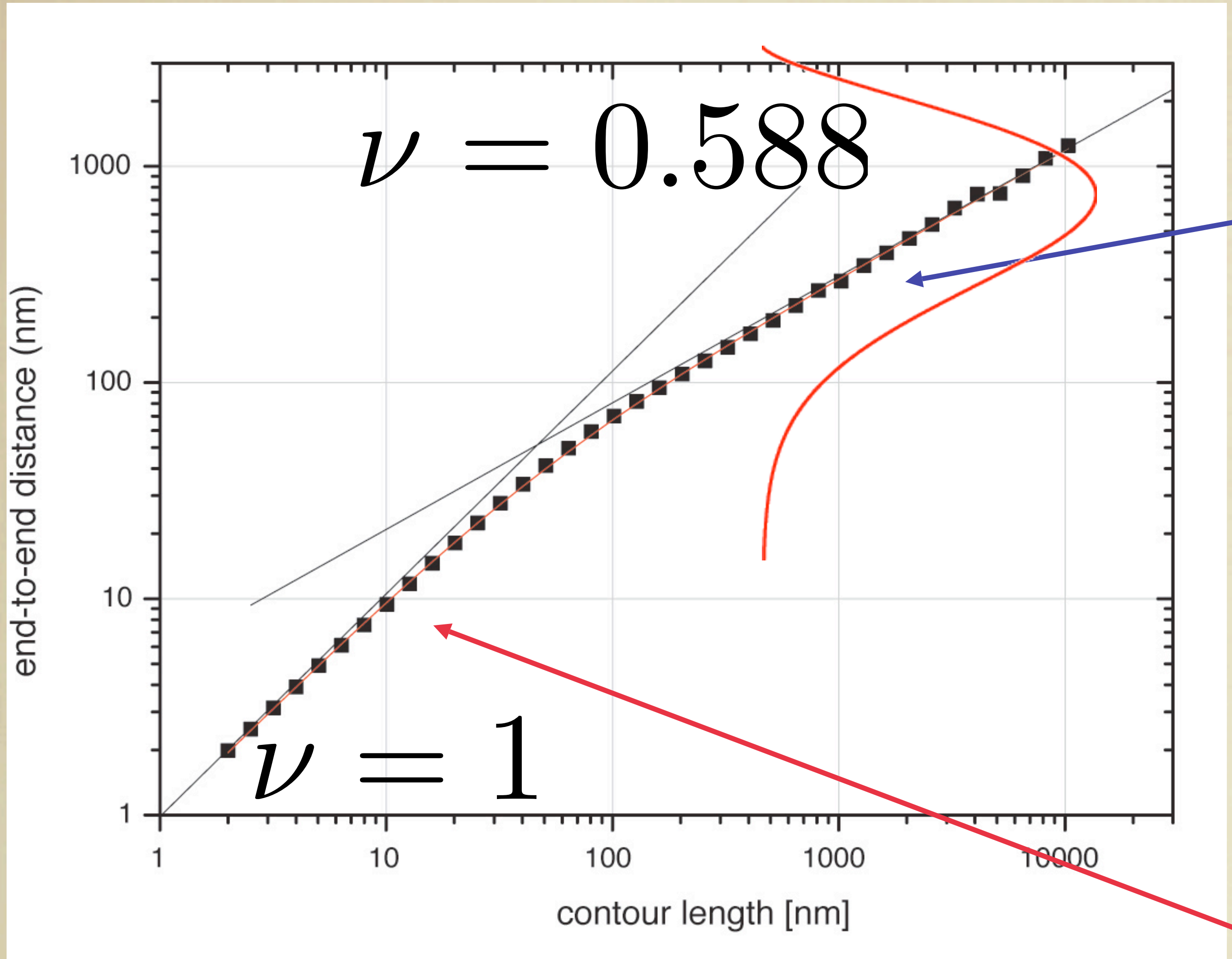


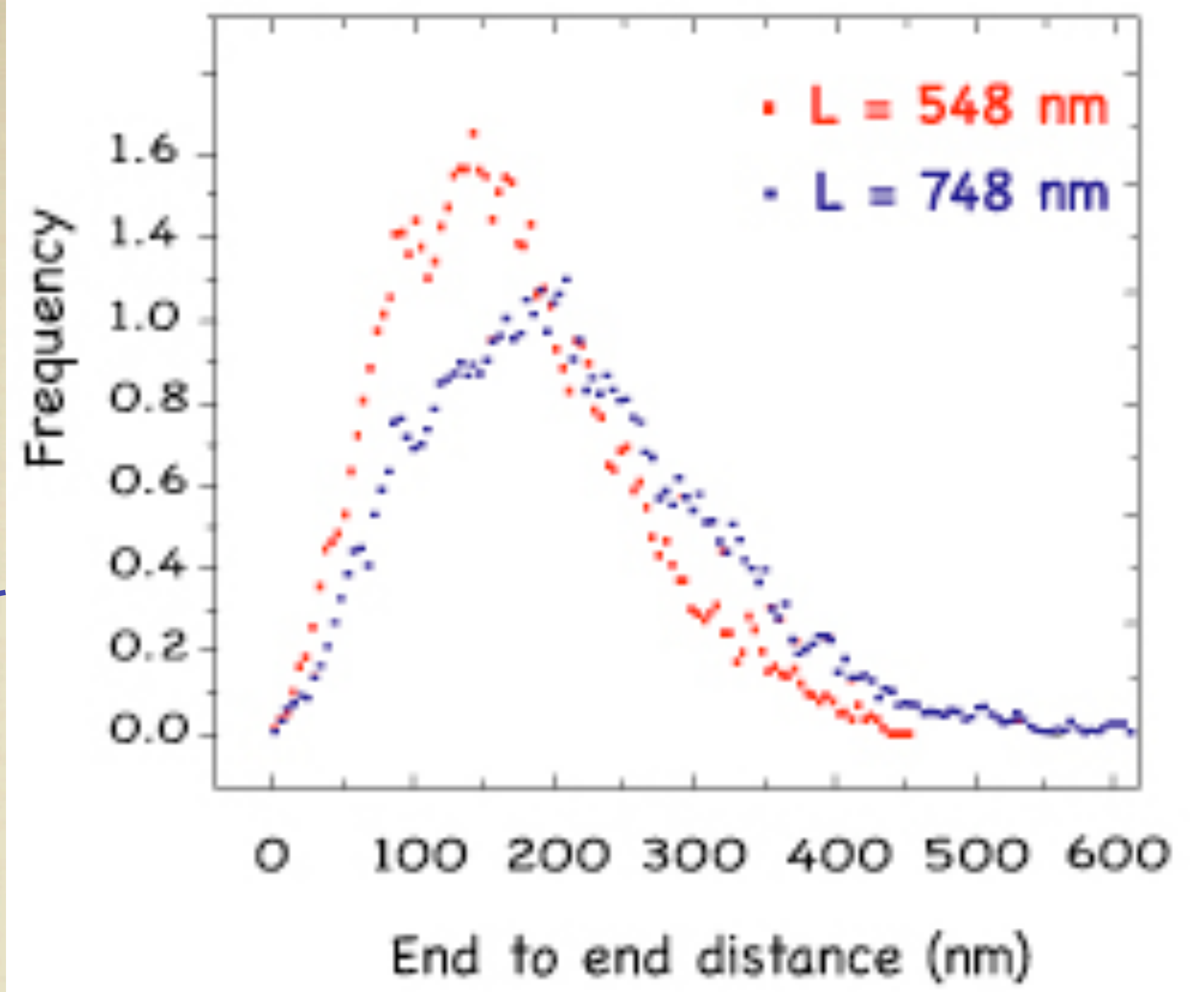
$$\xi = \xi_o \left(\frac{L}{l_o}\right)^{\nu_1}\left(1+\frac{L}{l_o}\right)^{\nu_2-\nu_1}$$

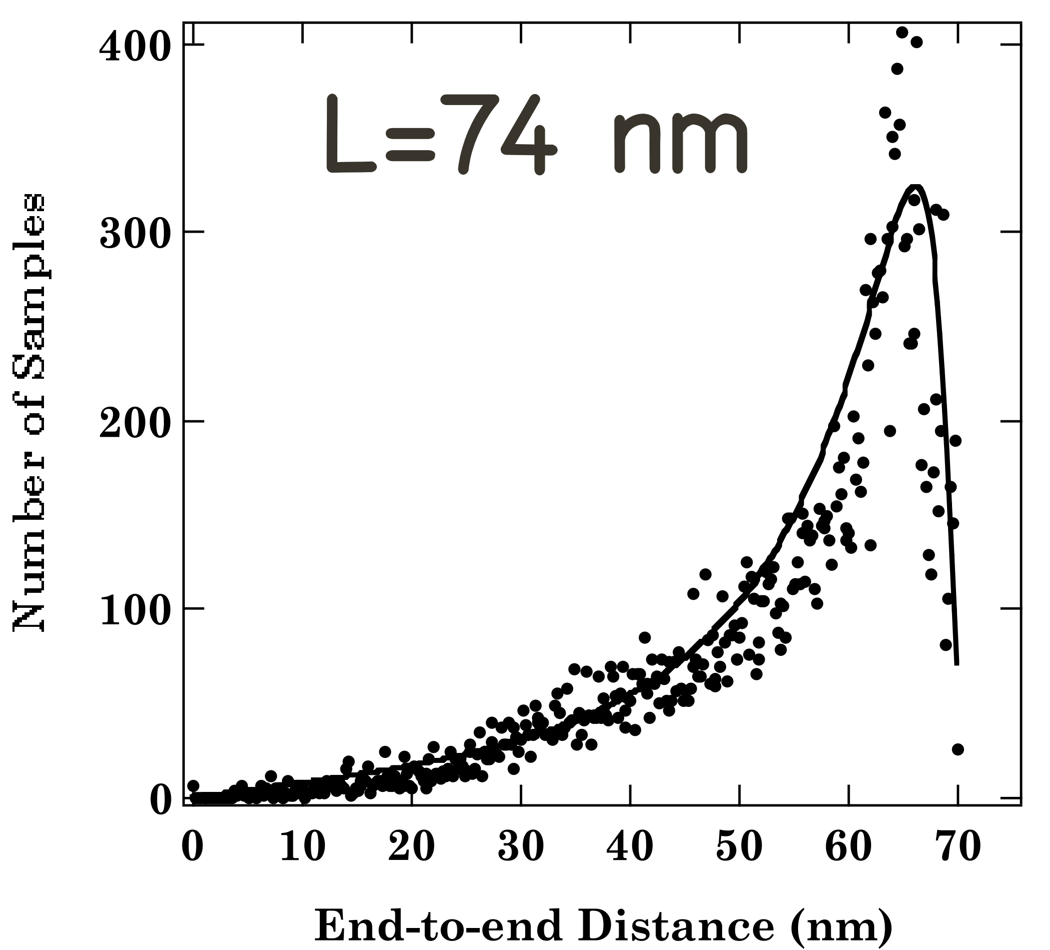


Trapping
Strong interaction DNA-surface
$U_{int} >> k_B T$

[Valle, Favre, De Los Rios, Rosa and Dietler, PRL, **95** 158105 (2005)]


$\nu = 0.588$
$\nu = 1$
1000
100
10
1
end-to-end distance (nm)
1
10
100
1000
10000
contour length [nm]

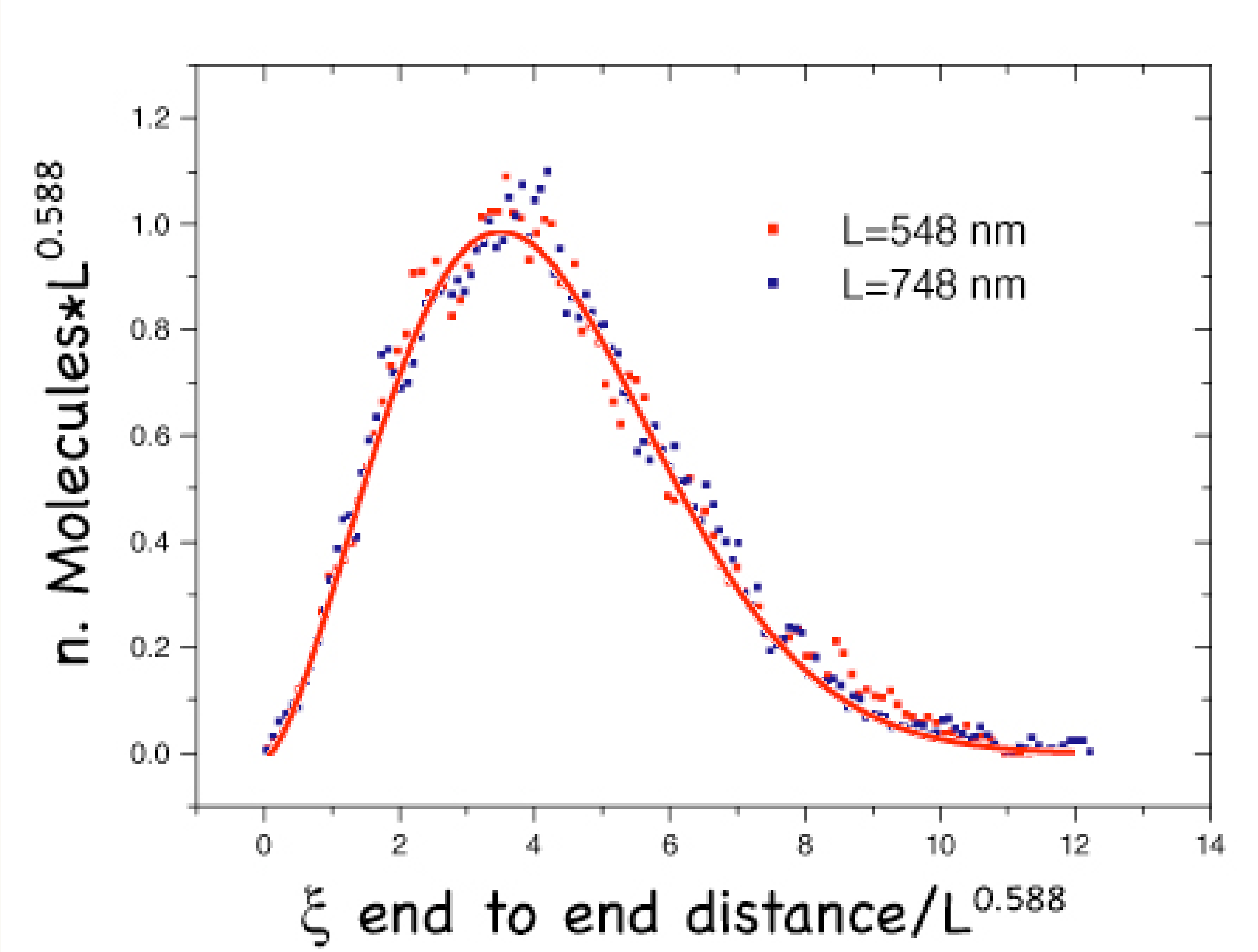

L = 548 nm
L = 748 nm
Frequency
1.6
1.4
1.0
0.8
0.6
0.4
0.2
0.0
0
100
200
300
400
500
600
End to end distance (nm)


L=74 nm
Number of Samples
400
300
200
100
0
0
10
20
30
40
50
60
70
End-to-end Distance (nm)

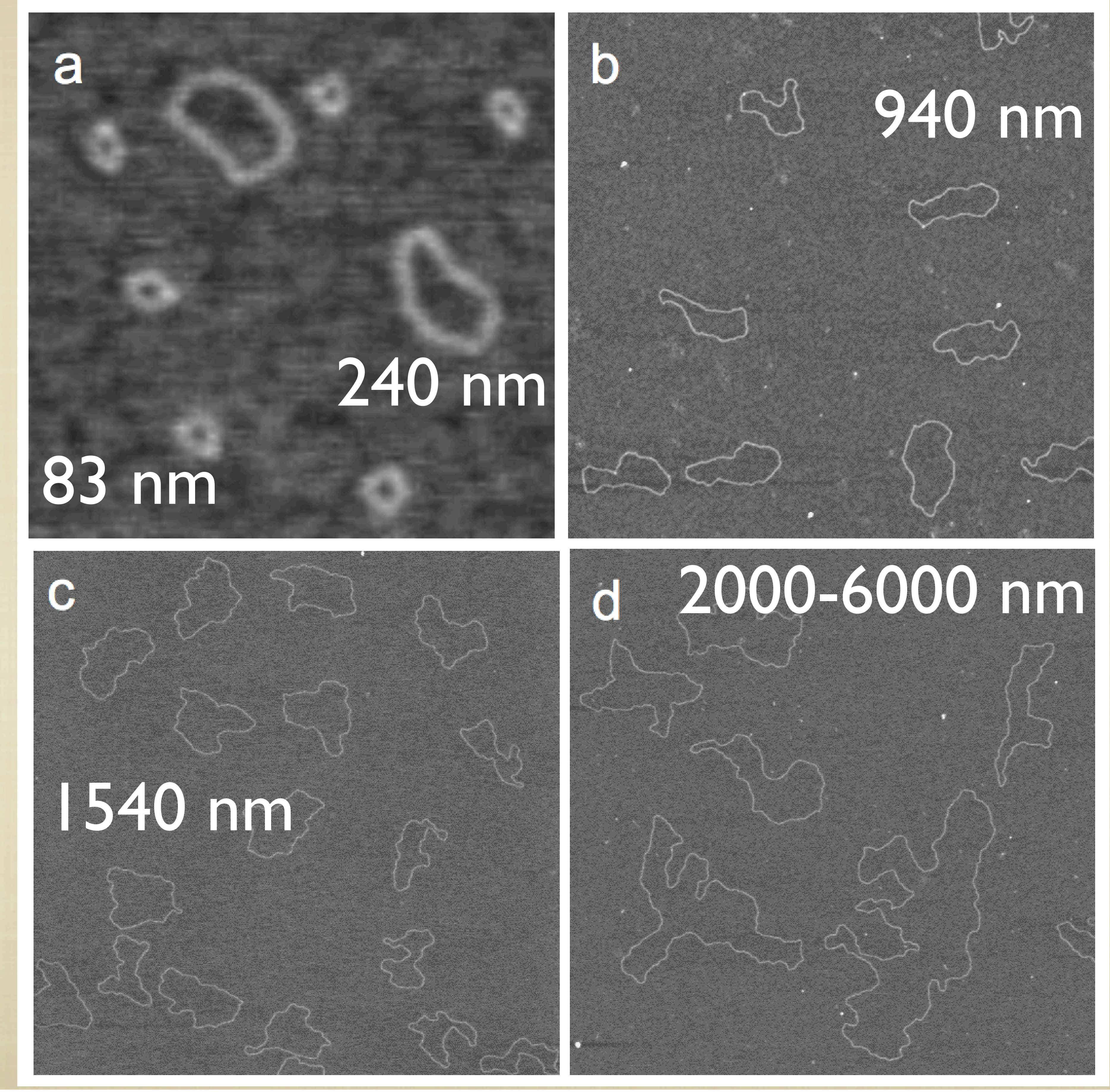
# DISTRIBUTION FOR A SAW LINEAR DNA

$$f(\xi) = \xi^{d-1+\sigma} e^{-b\xi^{\delta}} \qquad \delta = \frac{1}{1-\nu} = 2.42$$

$$\delta_{fit} = 2.56 \pm 0.72$$



# Circular DNA in 2D



# DNA Model

# STATISTICAL PROPERTIES OF DNA

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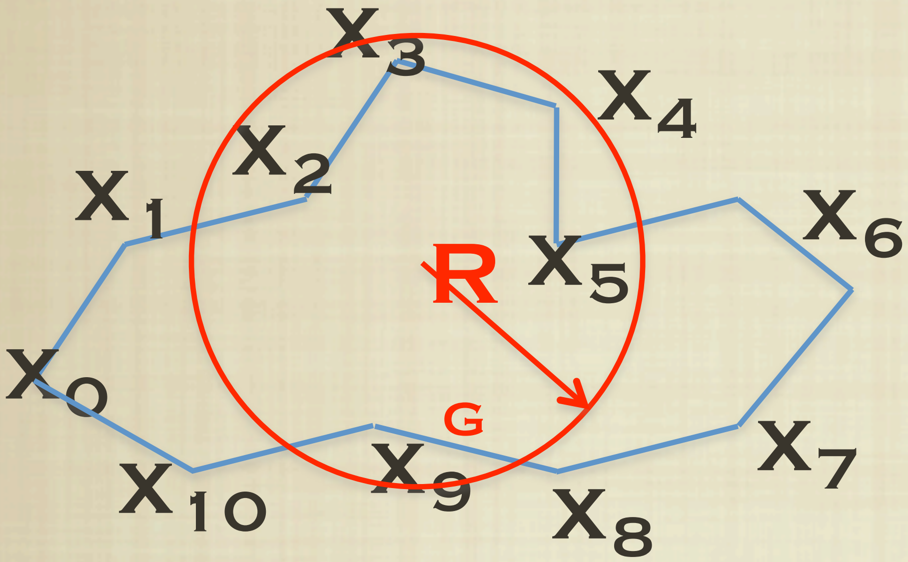
$$\langle R_G^2 \rangle = \frac{1}{N}\sum_{i=1}^{N}(r_i - r_{cm})^2 \sim L^{2\nu}$$



**SAW**

$$\nu = 1 \quad \text{in 1D}$$

$$\nu = 0.75 \quad \text{in 2D}$$

$$\nu = 0.588 \quad \text{in 3D}$$

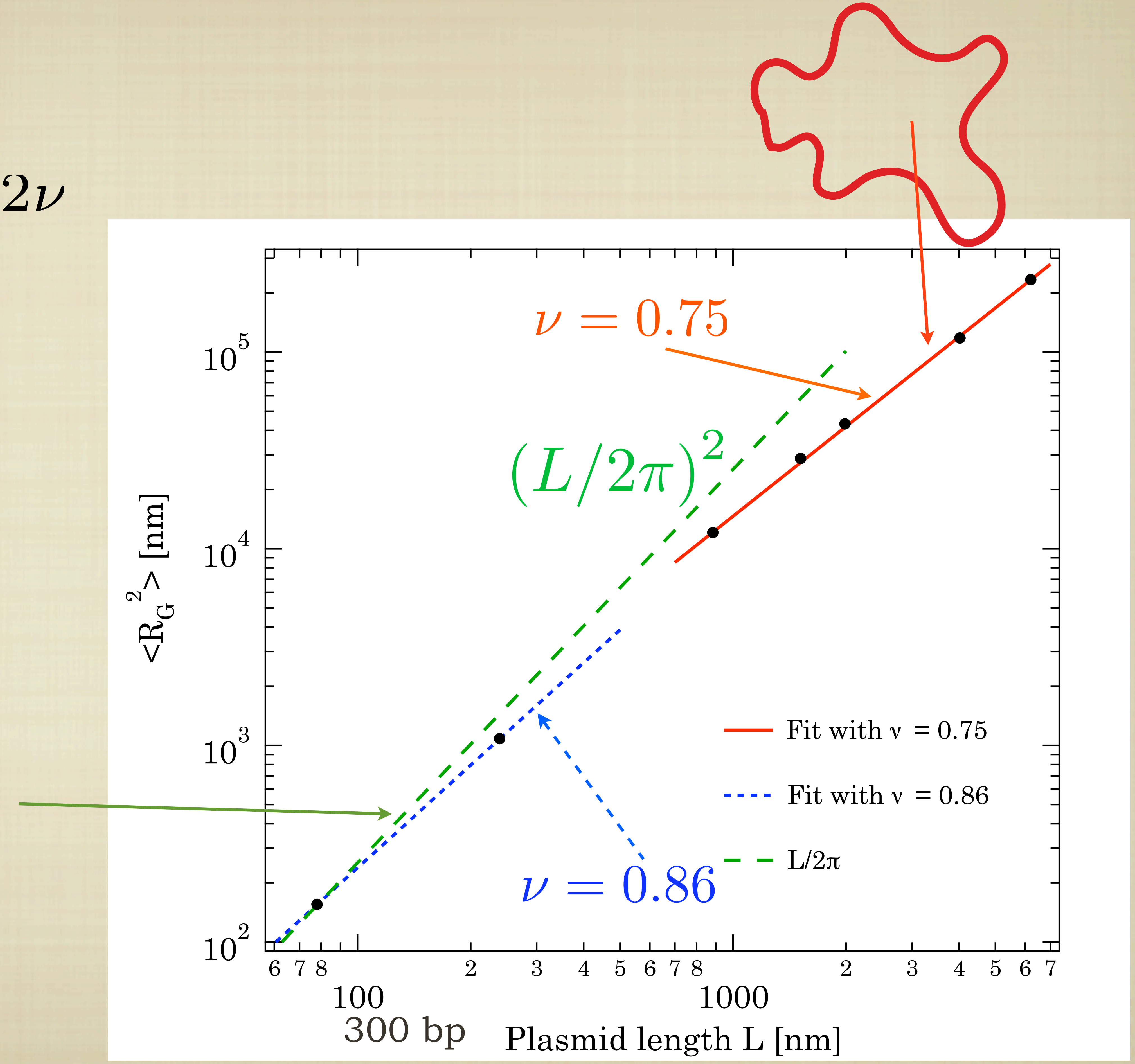
**RW**

$$\nu = 0.5$$

# RADIUS OF GYRATION FOR CIRCULAR DNA IN 2D

PREDICTION

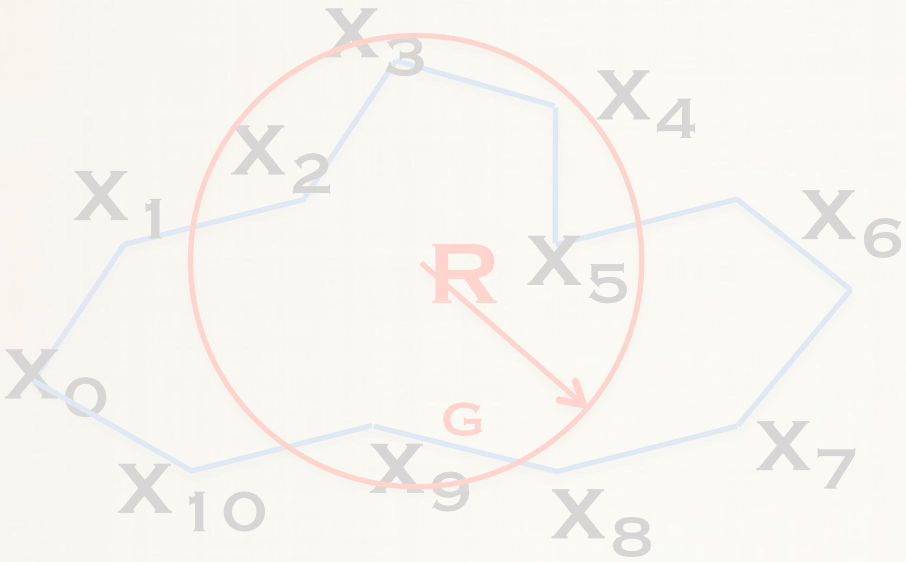
$$\langle R_g^2 \rangle \sim L^{2\nu}$$



# STATISTICAL PROPERTIES OF DNA

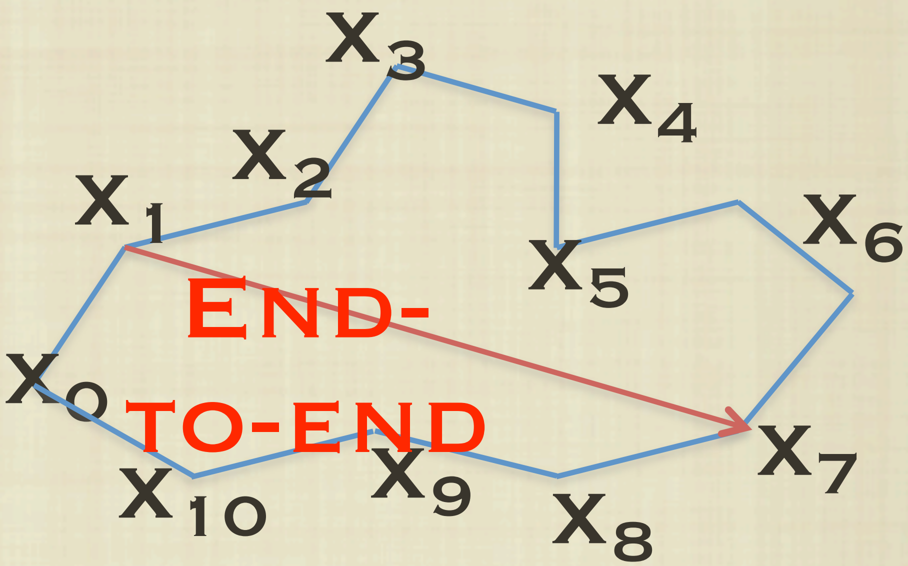
## Scaling of the radius of gyration

$$\langle R_G^2\rangle = \frac{1}{N}\sum_{i=1}^{N}(r_i - r_{cm})^2 \sim L^{2\nu}$$



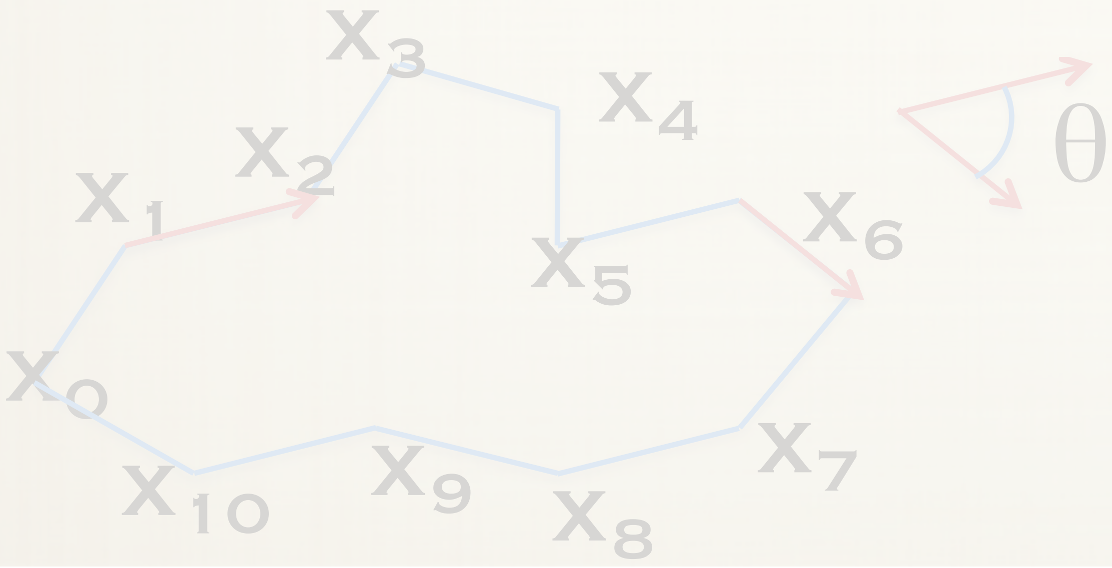
## Scaling of the internal End-to-end distance

$$\langle \xi \rangle \sim L^{\nu}$$



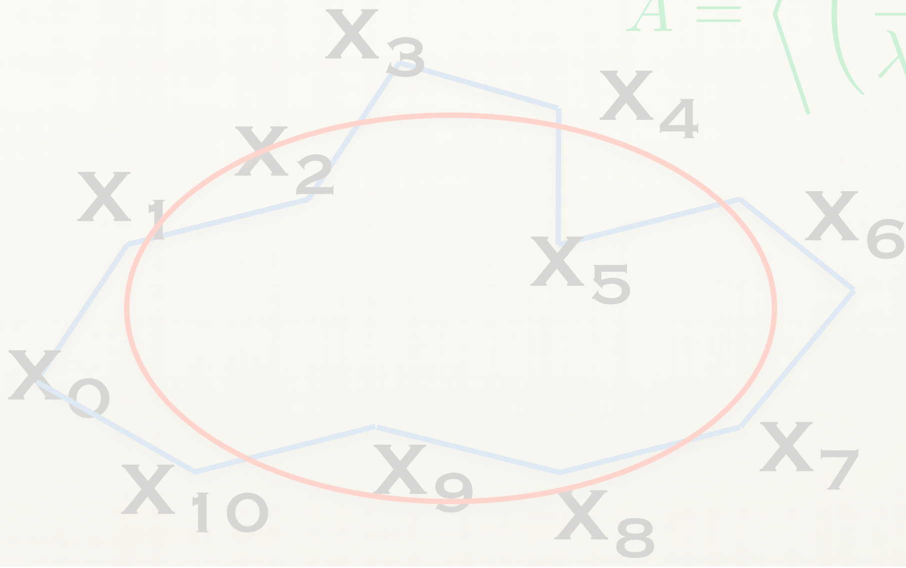
## Directional correlation

$$\langle \cos\theta(s)\rangle = e^{(-s/2\ell_p)}$$



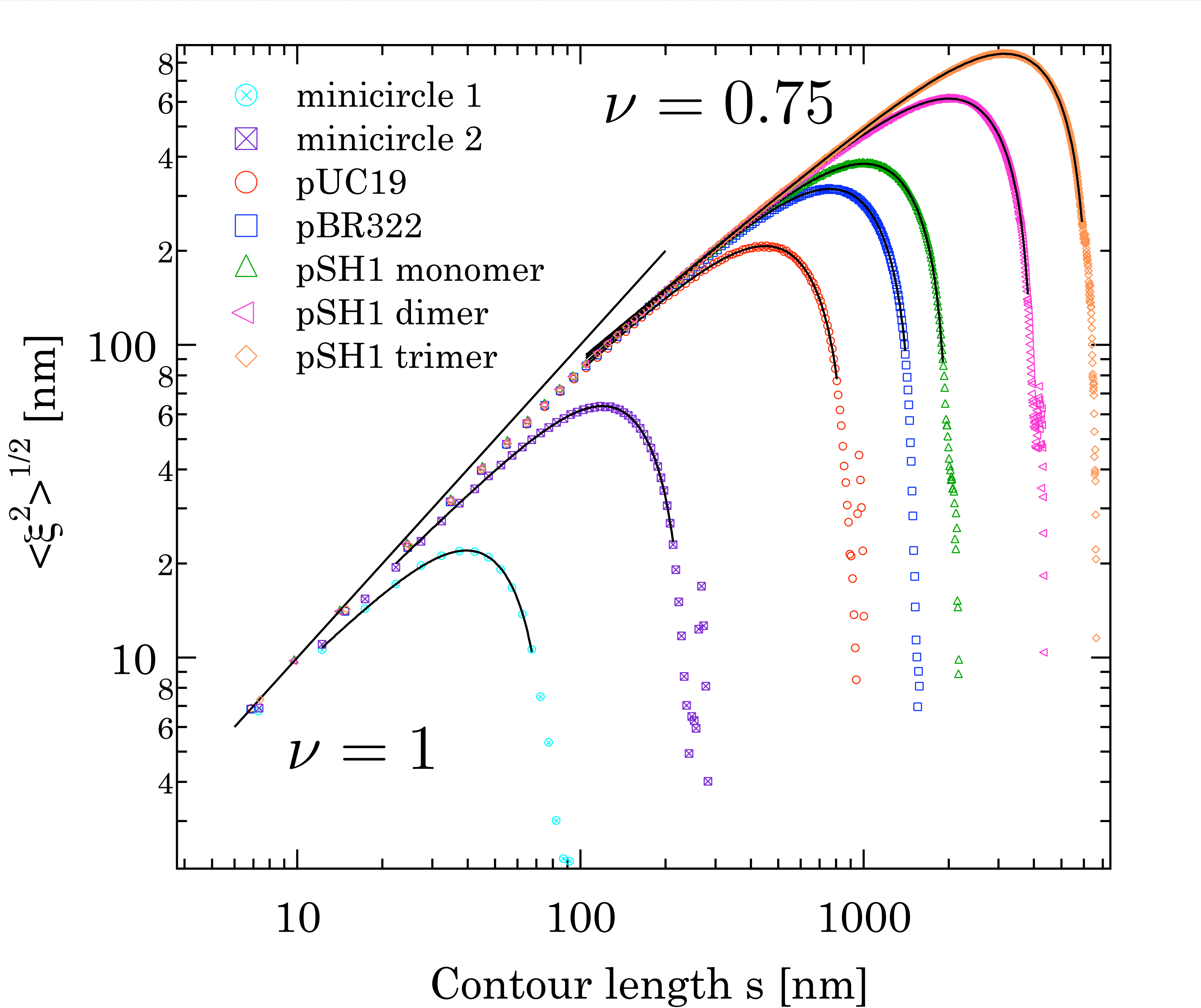
## Shape properties: asphericity

$$A = \left\langle \left(\frac{\lambda_1-\lambda_2}{\lambda_1+\lambda_2}\right)^2 \right\rangle$$



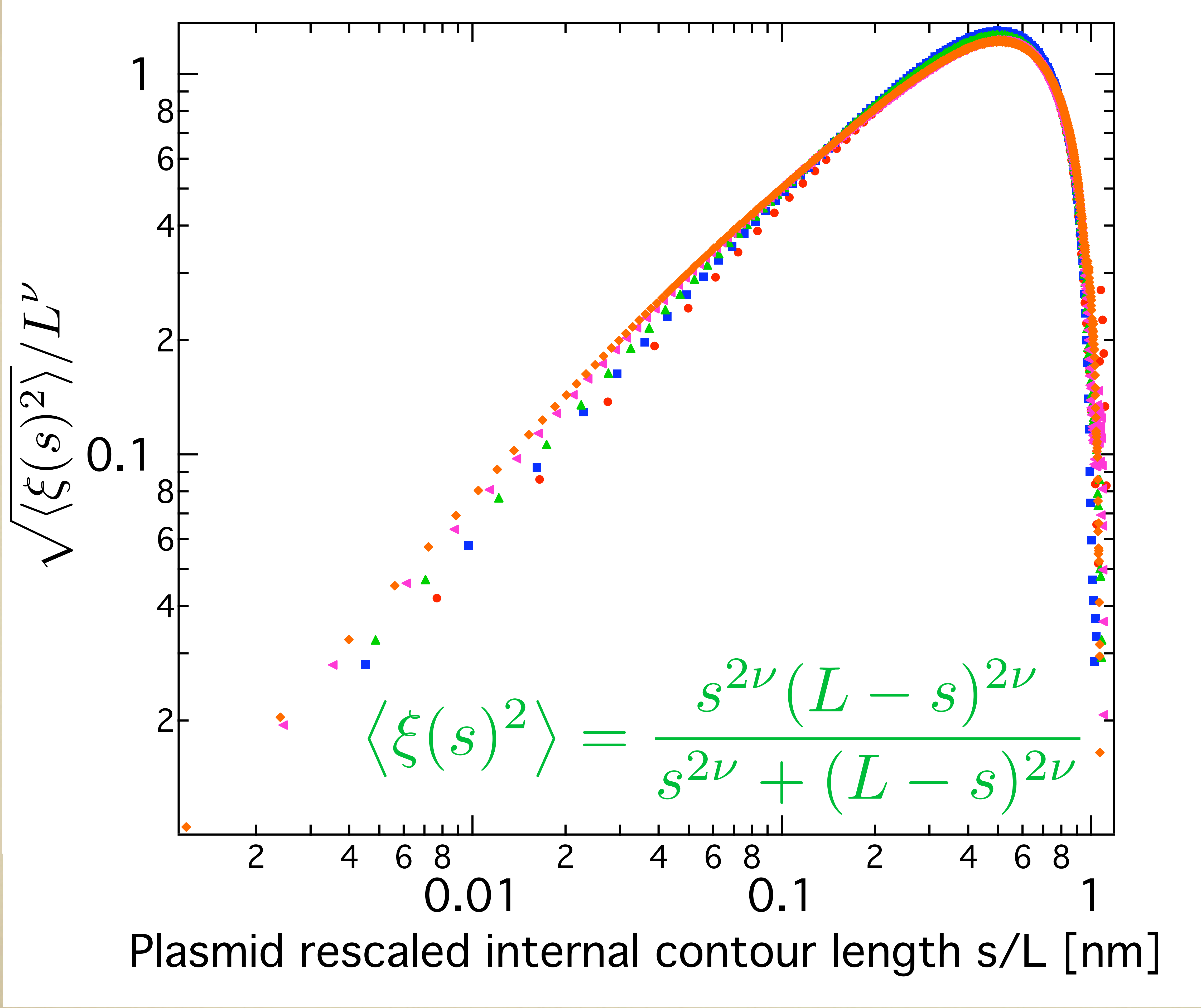
# INTERNAL END-TO-END DISTANCE FOR CIRCULAR DNA

$$\langle r^2(s) \rangle \sim \frac{s^{2\nu}(L_o - s)^{2\nu}}{s^{2\nu} + (L_o - s)^{2\nu}}$$



V. Bloomfield & B.H. Zimm,
J. Chem. Phys. 44, 315(1966).

# RESCALED DATA

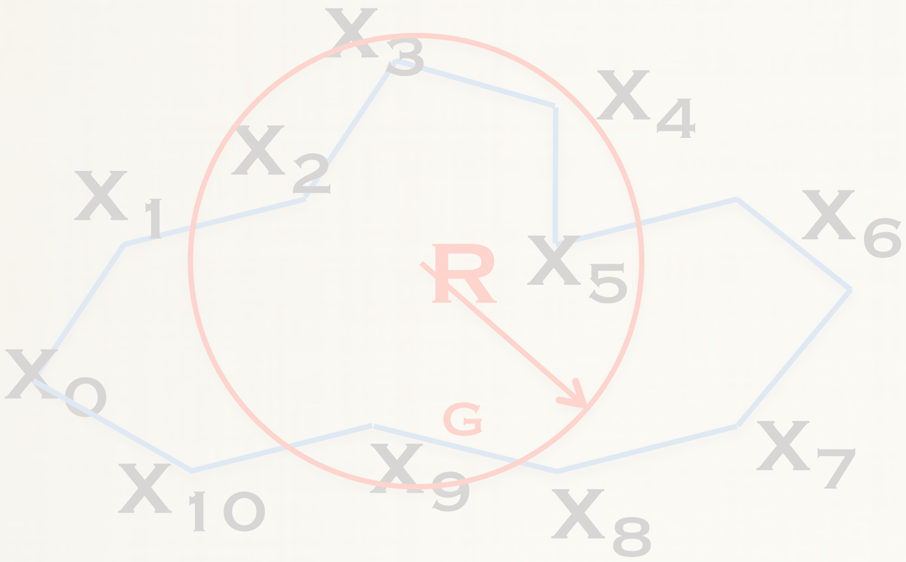


$$\langle \xi(s)^2 \rangle = \frac{s^{2\nu}(L-s)^{2\nu}}{s^{2\nu}+(L-s)^{2\nu}}$$

# STATISTICAL PROPERTIES OF DNA

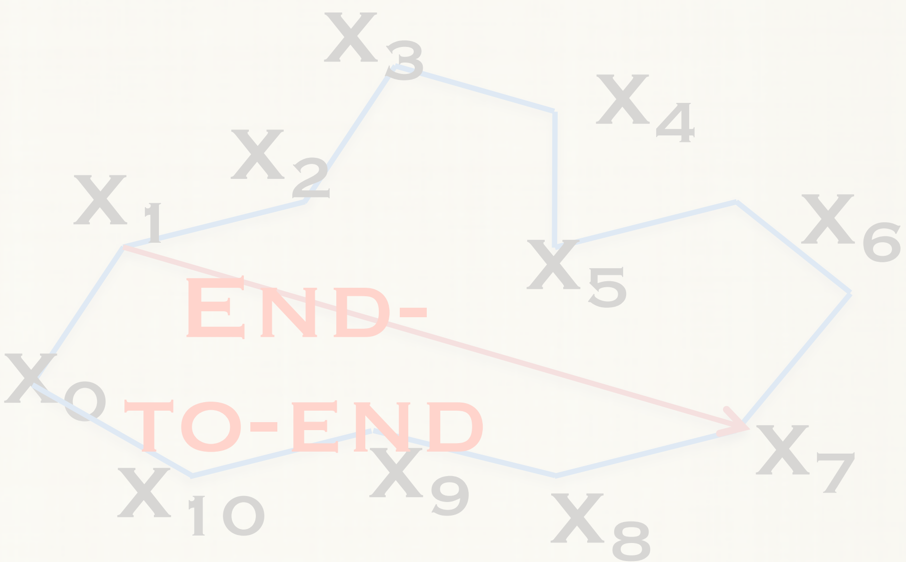
## Scaling of the radius of gyration

$$\langle R_G^2 \rangle = \frac{1}{N} \sum_{i=1}^{N} (r_i - r_{cm})^2 \sim L^{2\nu}$$



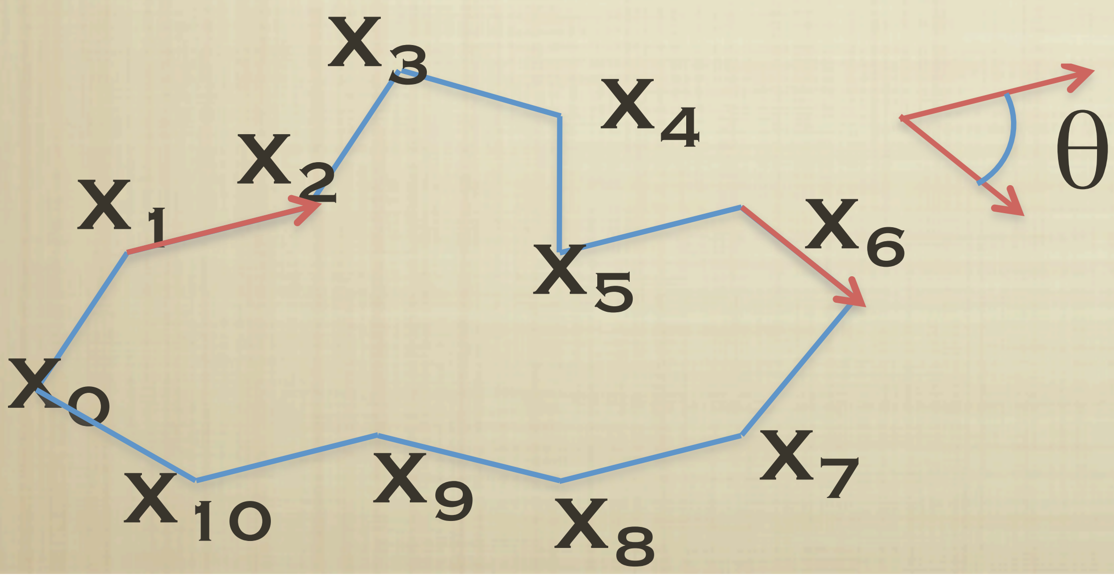
## Scaling of the internal End-to-end distance

$$\langle \xi \rangle \sim L^{\nu}$$



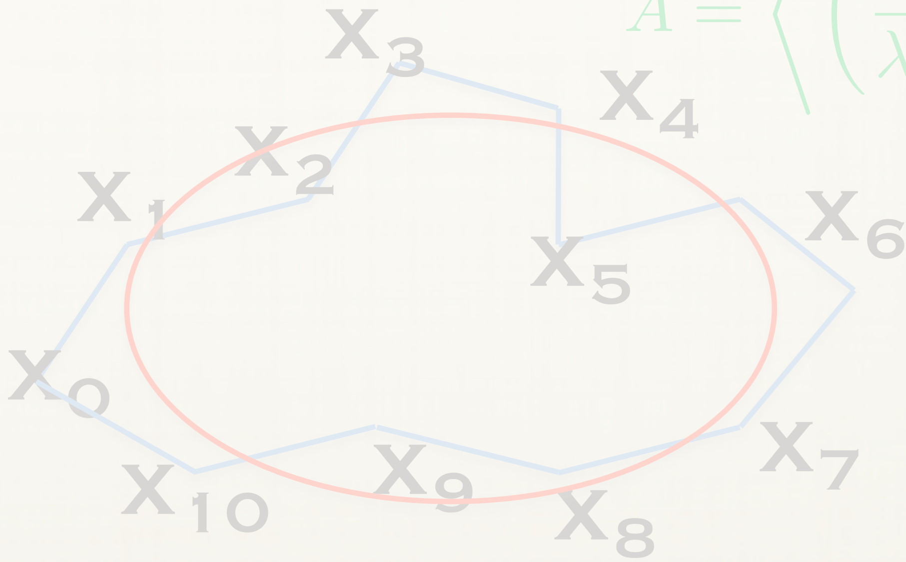
## Directional correlation

$$\langle \cos \theta(s) \rangle = e^{(-s/2\ell_p)}$$

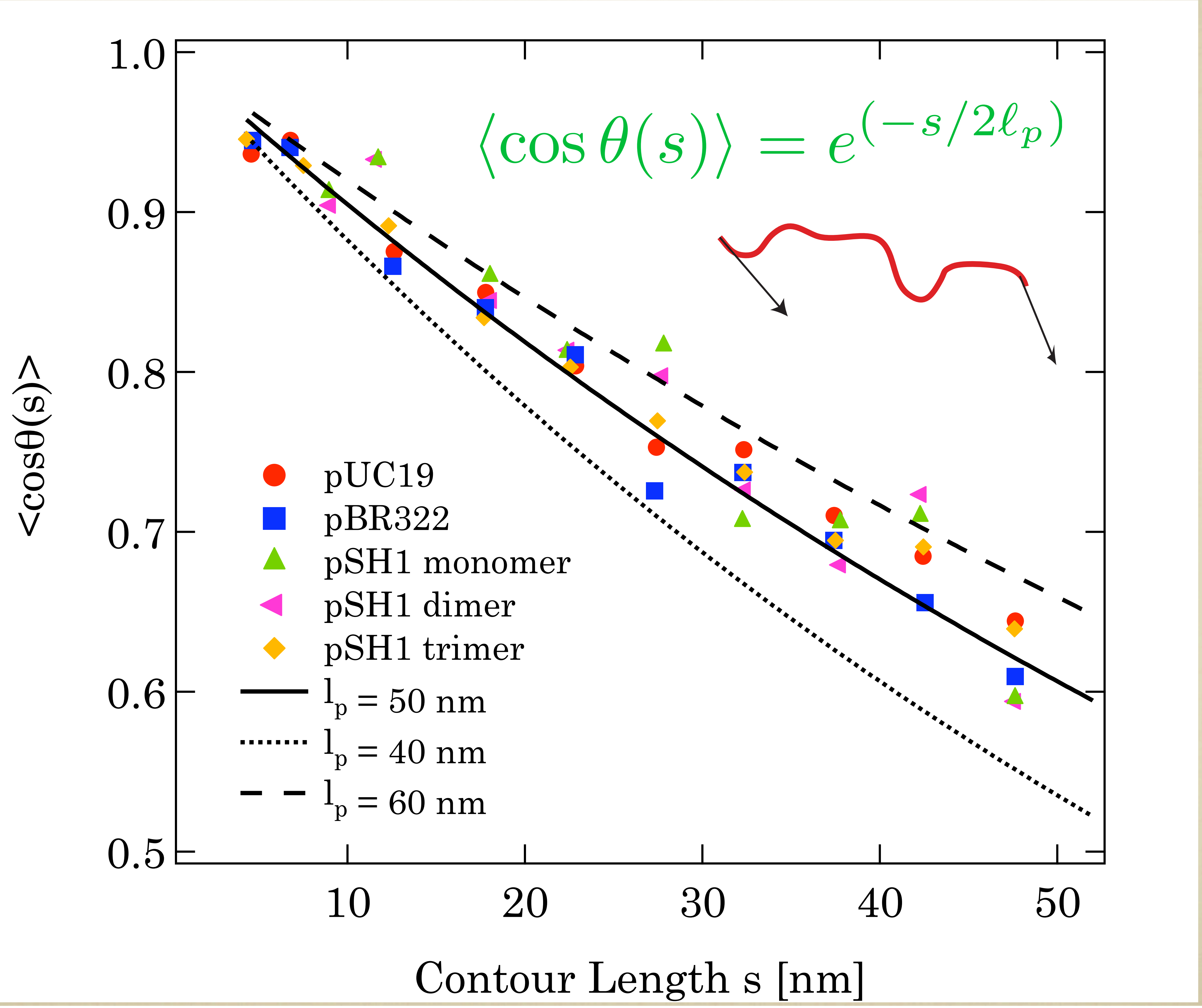


## Shape properties: asphericity

$$A = \left\langle \left( \frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} \right)^2 \right\rangle$$



# Bond Correlation Function



# STATISTICAL PROPERTIES OF DNA

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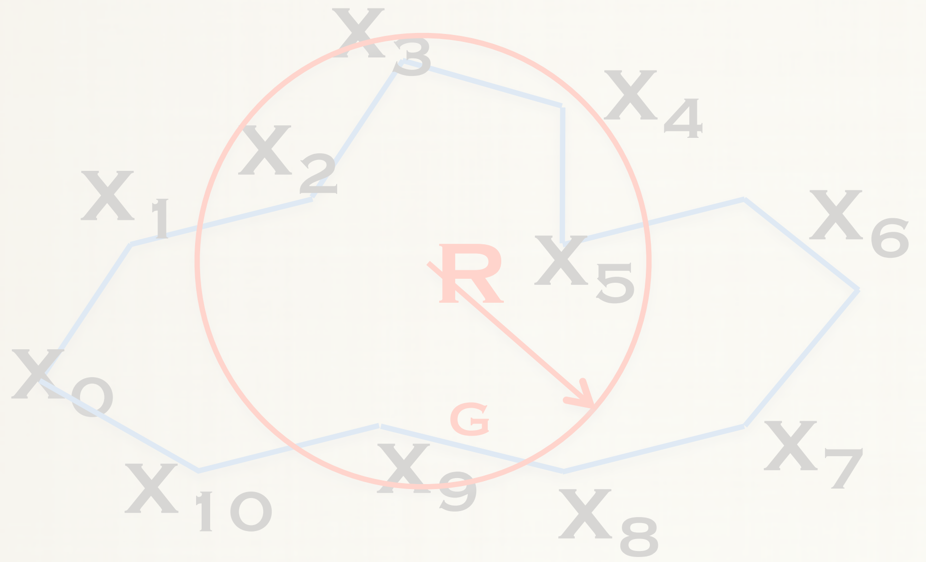
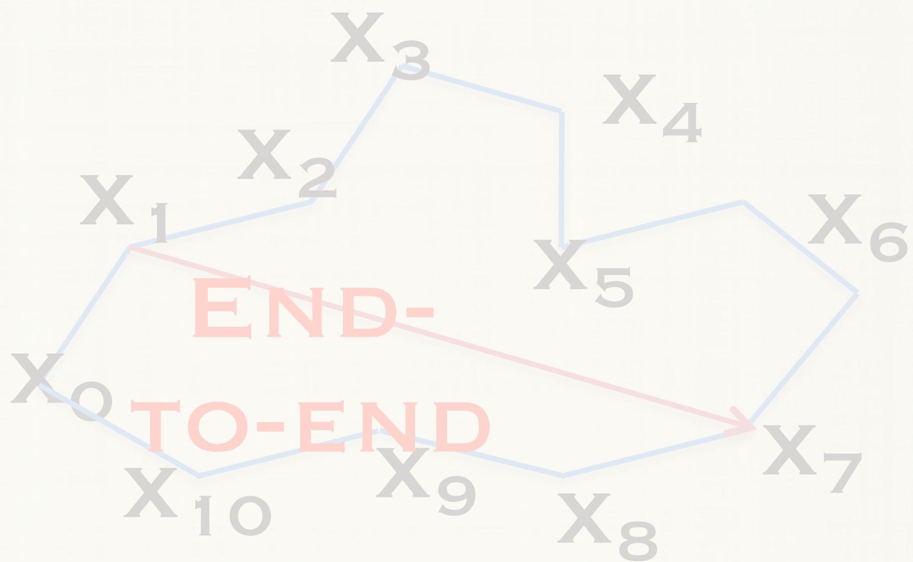


## Scaling of the internal End-to-end distance

$$\langle \xi \rangle \sim L^{\nu}$$



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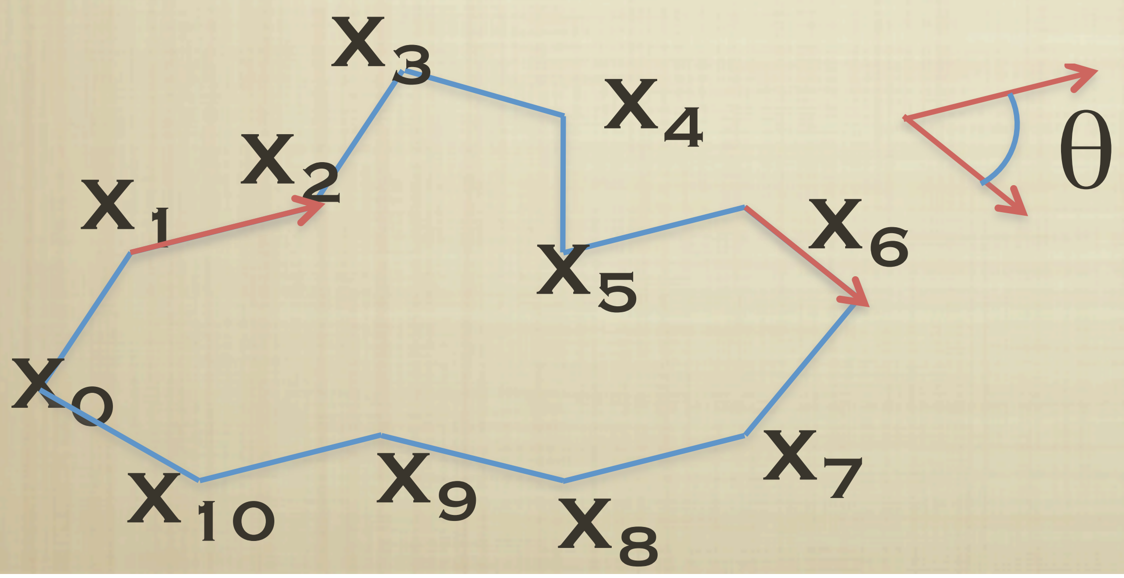

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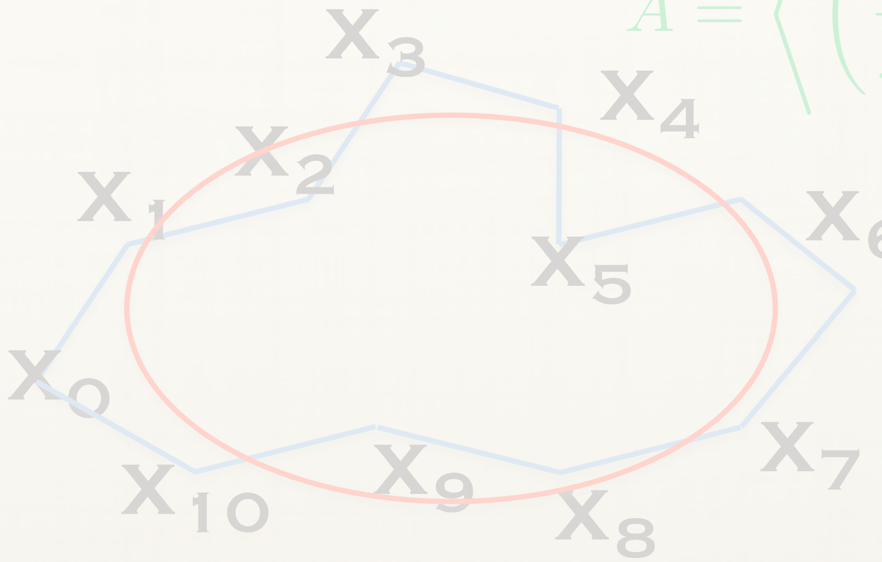
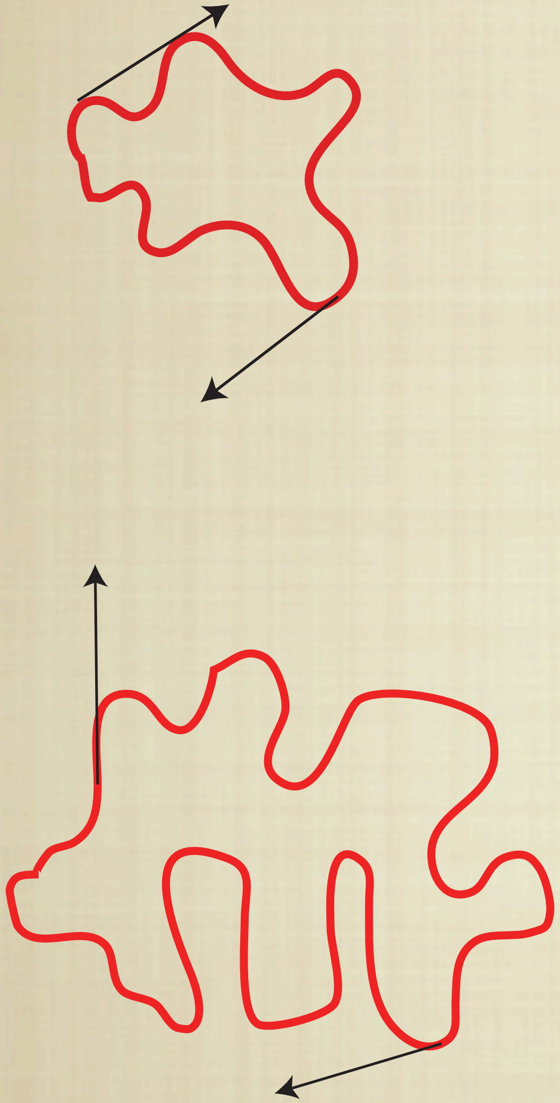
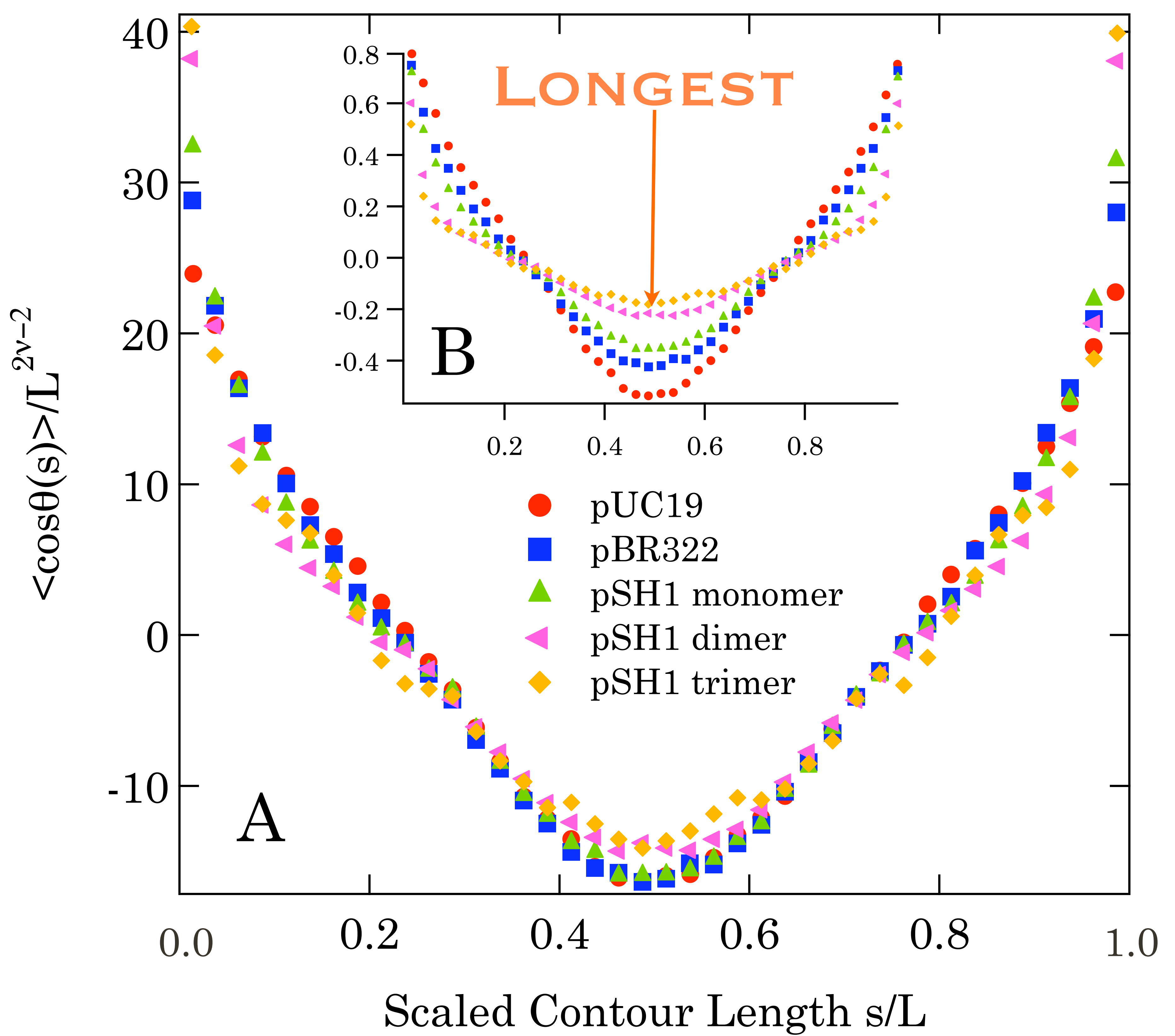


# BOND CORRELATION FUNCTION OF DNA

$$\langle \cos\theta(s)\rangle = \phi\left(\frac{s}{L_o}, v\right) L_o^{2\nu-2}$$

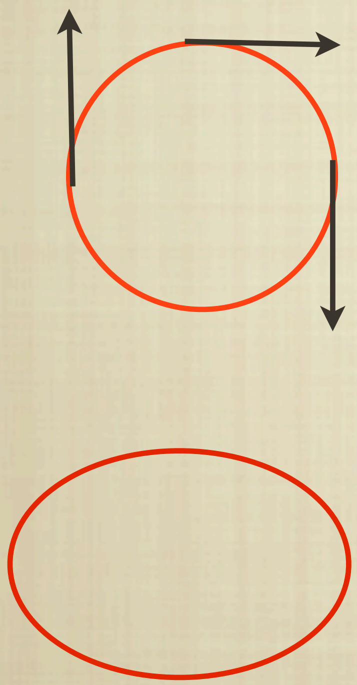


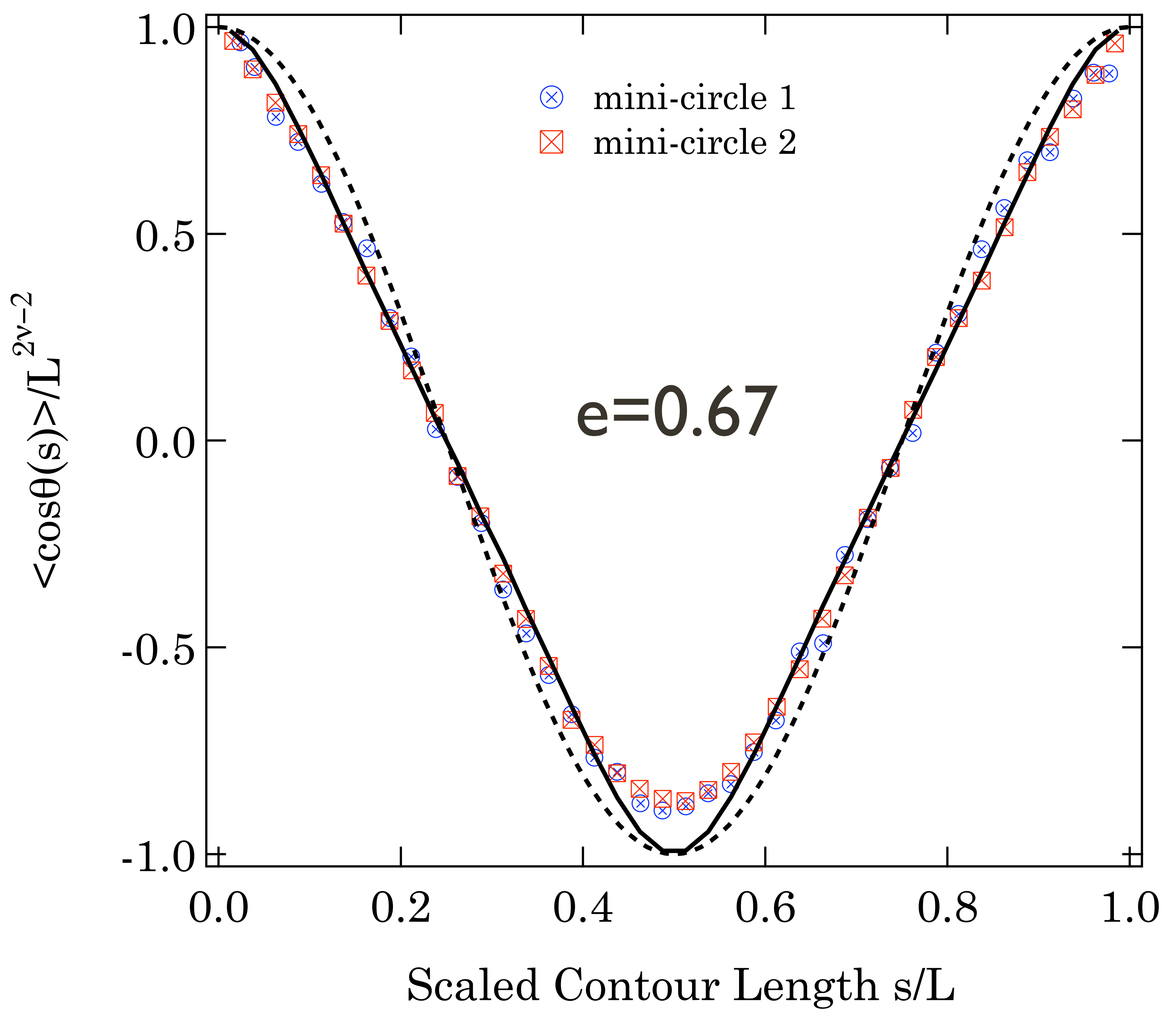


A. Baumgärtner,
J. Chem. Phys., **76**,
4275 (1982).

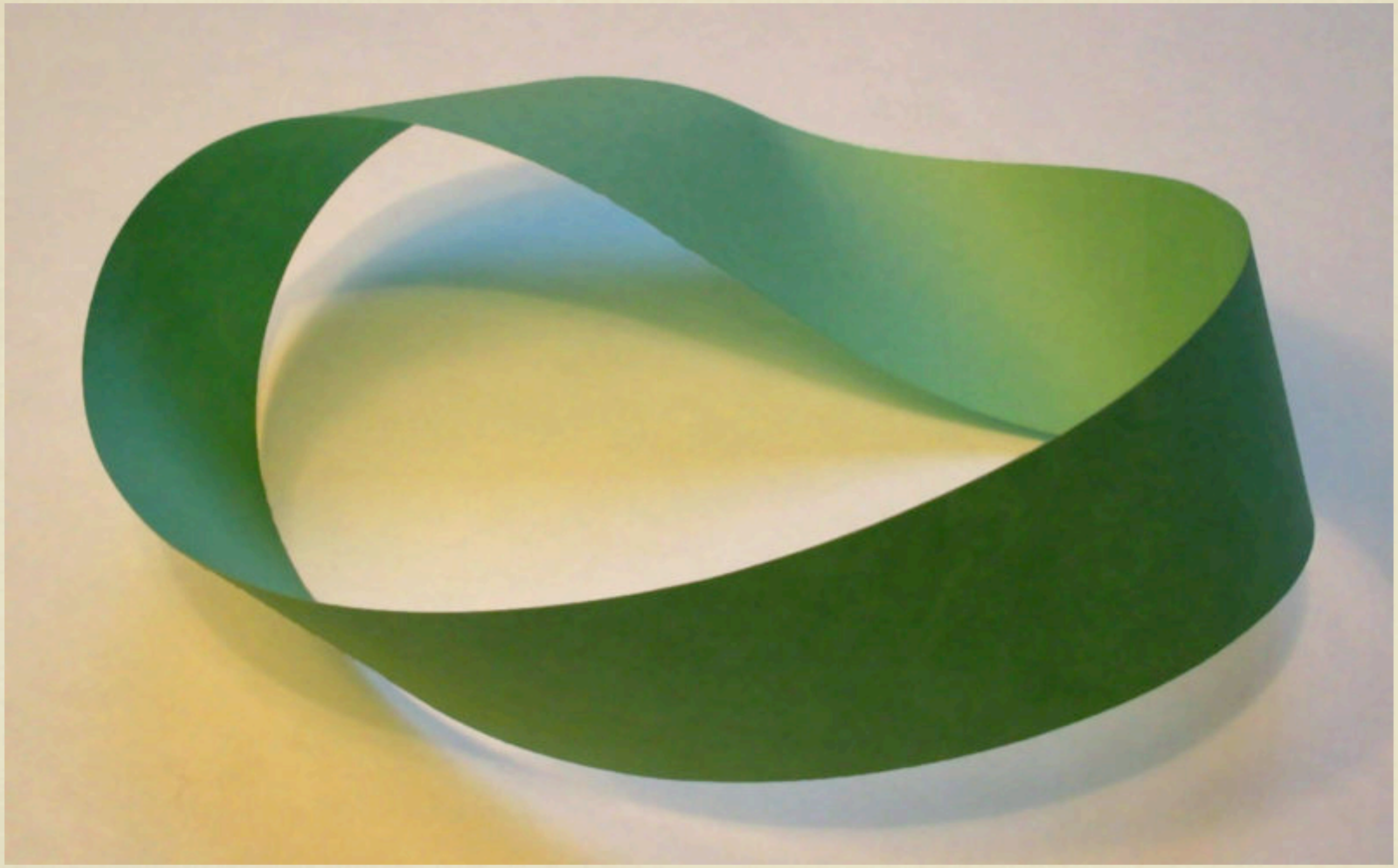
# Bond Correlation Function
# Circular DNA

241 bp
676 bp





# THE DOUBLE HELIX DETERMINES THE SHAPE OF SMALL DNA CIRCLES



# ASPHERICITY

## GYRATION TENSOR

$$T_{ij} = \frac{1}{N}\sum_{\ell=1}^{N}(x_{\ell i} - < x_i >)(x_{\ell j} - < x_j >)$$

$$R_G^2 = Tr(\mathbf{T}) = \sum_{i=0}^{d} \lambda_i$$

$$A_d = \frac{1}{d-1}\frac{\sum_{i>j}^{d}(\lambda_i - \lambda_j)^2}{(\sum_{i=1}^{d} \lambda_i)^2}$$

$$A_2 = \frac{(\lambda_2 - \lambda_1)^2}{(\lambda_1 + \lambda_2)^2} \qquad A_2 = \left\langle \frac{(\lambda_2 - \lambda_1)^2}{(\lambda_1 + \lambda_2)^2} \right\rangle$$

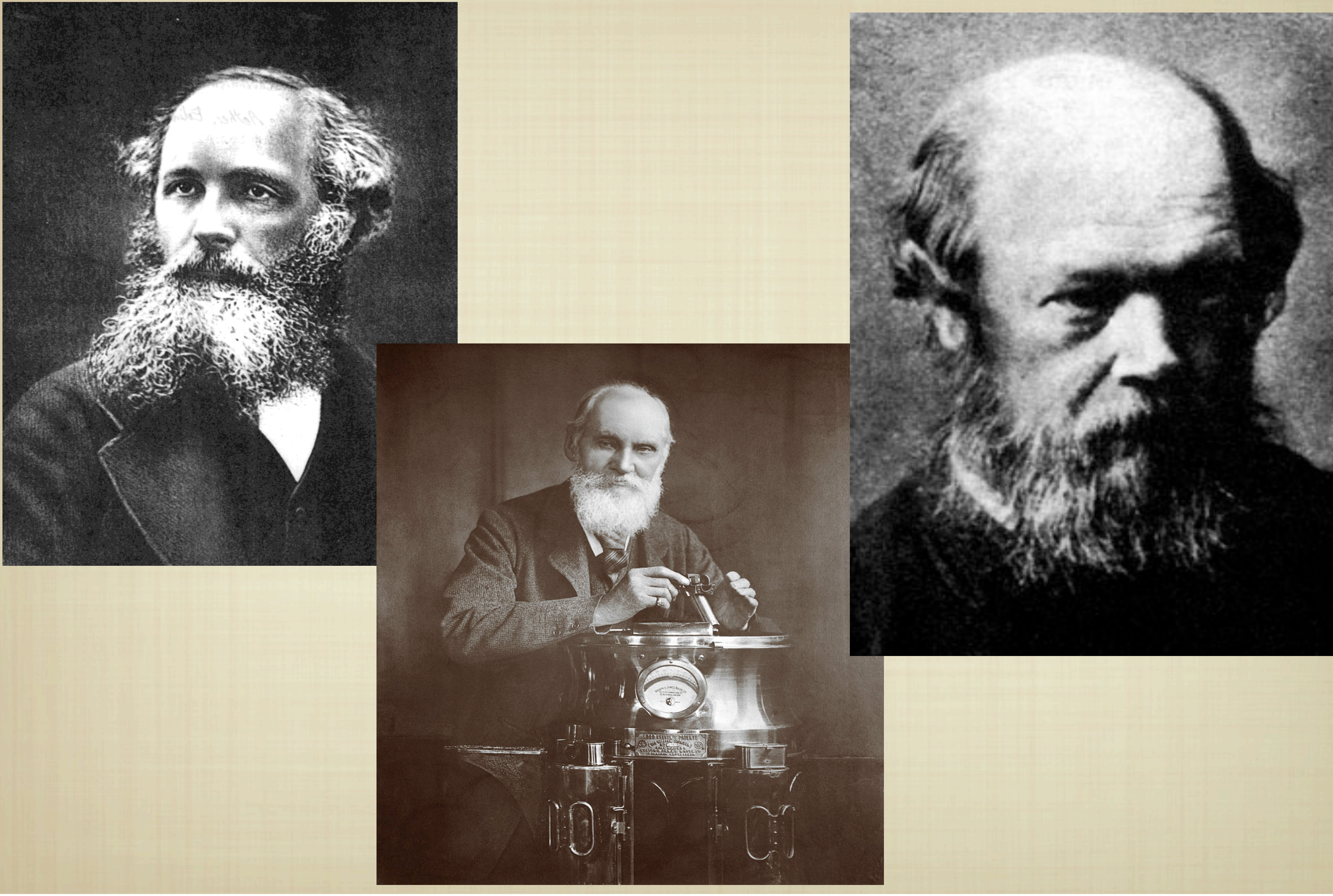
# RESULTS FOR CIRCULAR DNA

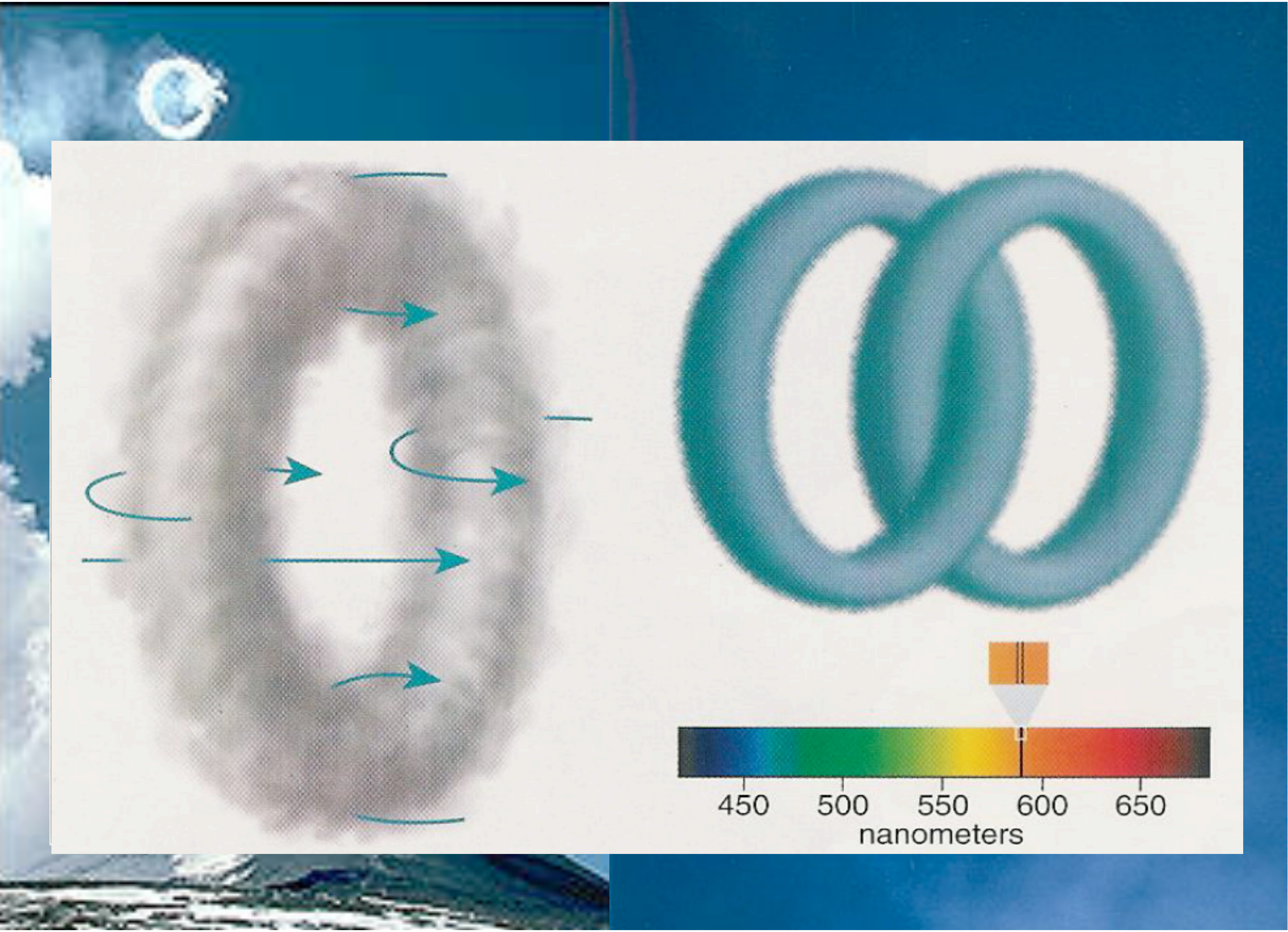
| | | | |
|---|---|---|---|
| Theoretical Values | Ring SAW<br>0.206 | Ring RW<br>0.279 | Bishop 1988 |

## EXPERIMENTAL VALUES

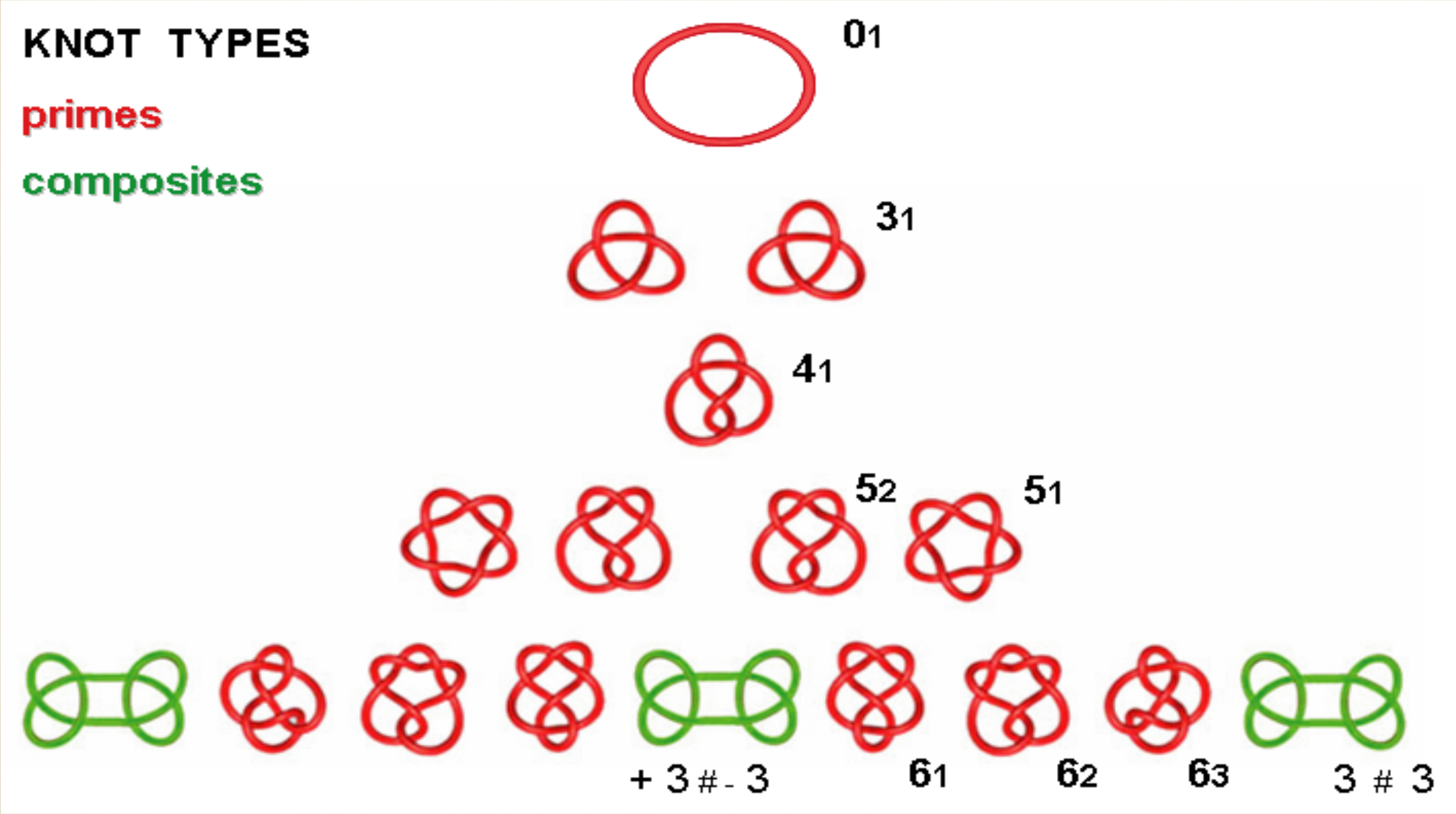
| Plasmid | mini 1 | mini 2 | pUC19 | pSH1 | pBR322 |
|---|---|---|---|---|---|
| A-value | 0.083 | 0.13 | 0.28 | 0.299 | 0.265 |
| Length (L/l_p) | 1.6 | 4.5 | 18 | 40-120 | 30 |

# J.C. Maxwell, W. Thomson (Kelvin) & G. Tait



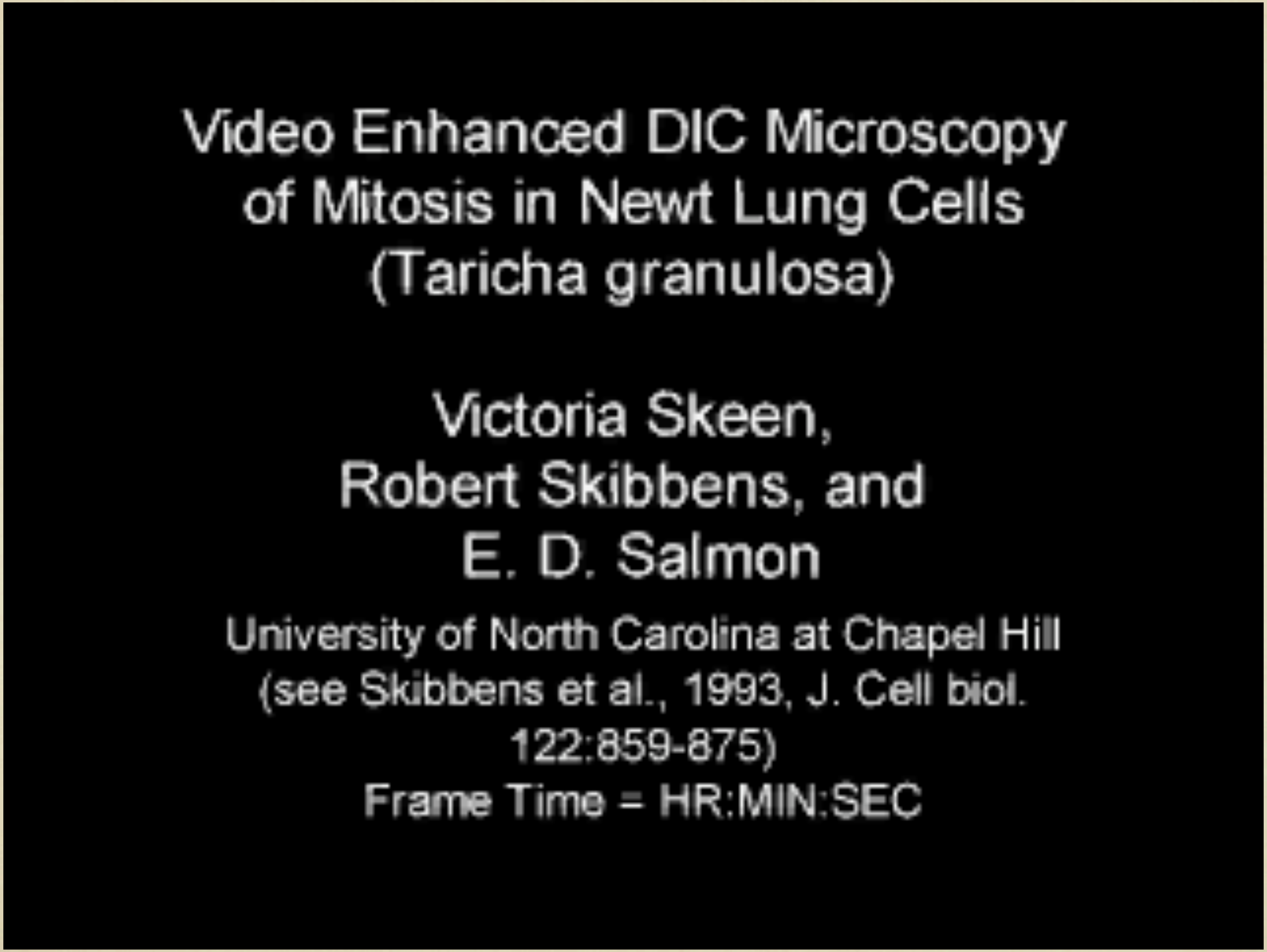

450
500
550
600
650
nanometers

# Knots



Knots are classified according to the minimal number of crossings

# Cell division



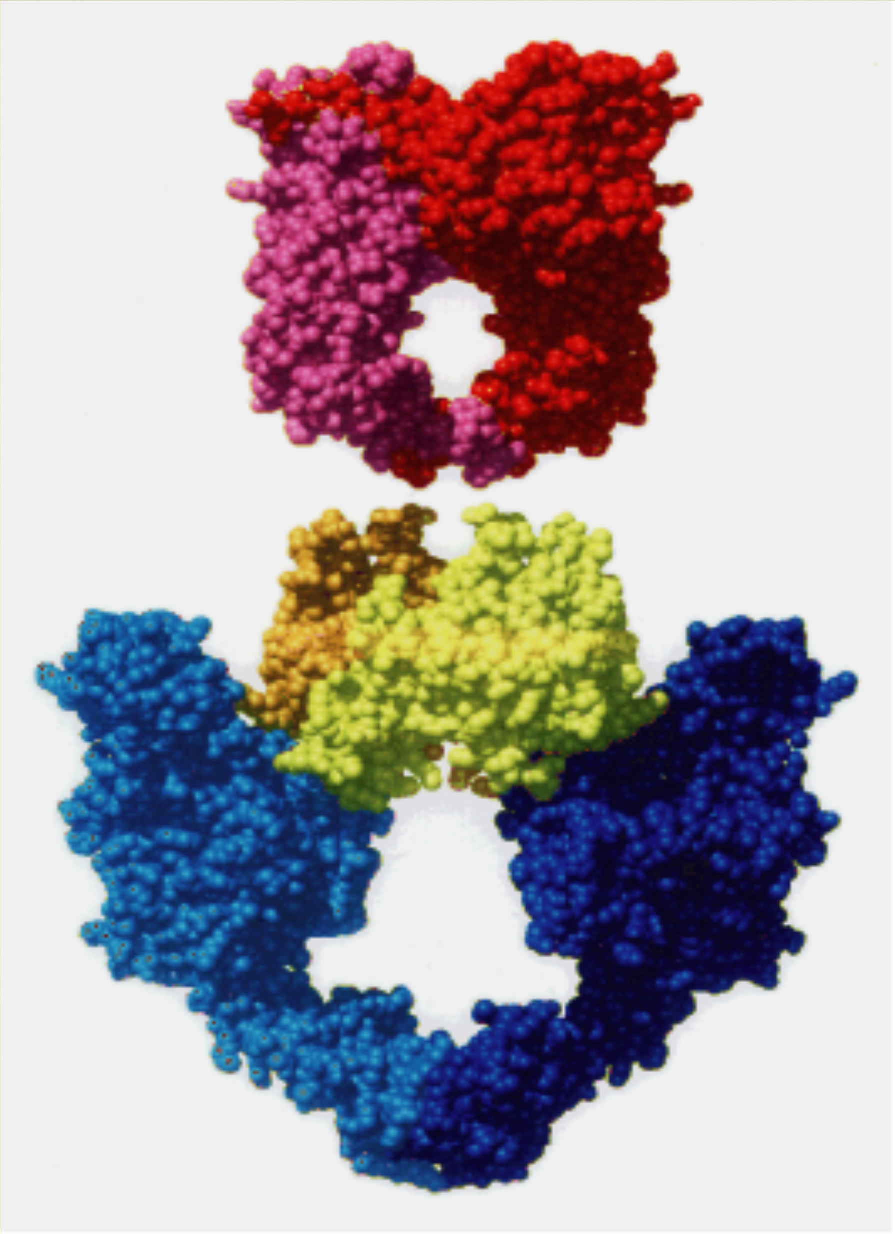
Video Enhanced DIC Microscopy
of Mitosis in Newt Lung Cells
(Taricha granulosa)

Victoria Skeen,
Robert Skibbens, and
E. D. Salmon

University of North Carolina at Chapel Hill
(see Skibbens et al., 1993, J. Cell biol.
122:859-875)
Frame Time = HR:MIN:SEC

# How does the cell proceed to disentangle the DNA strands?

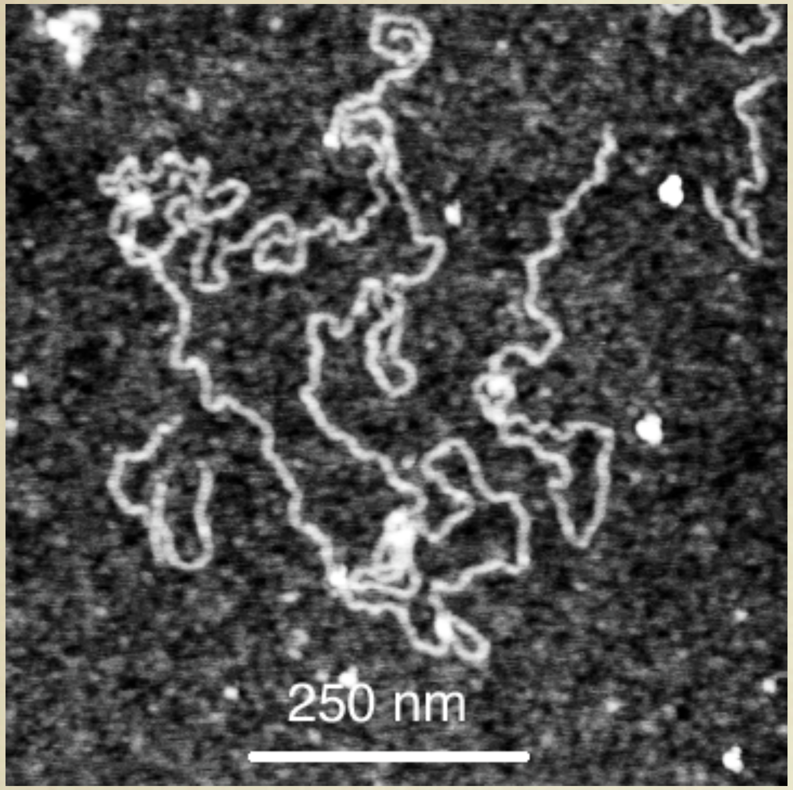
La Topoisomerase II



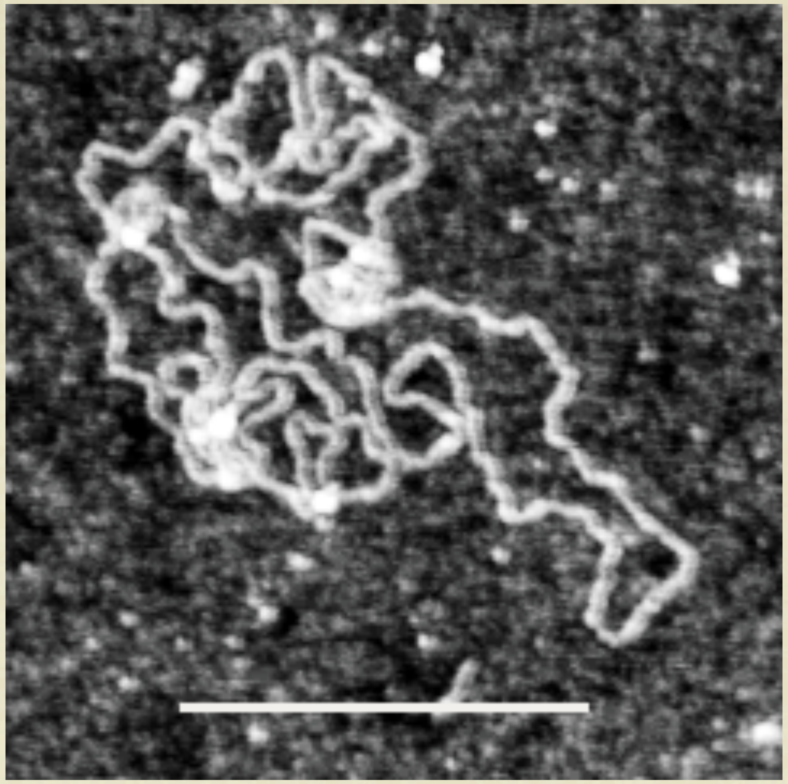
Topoisomerases
The tailor
of the cell

Wang’s lab 1996

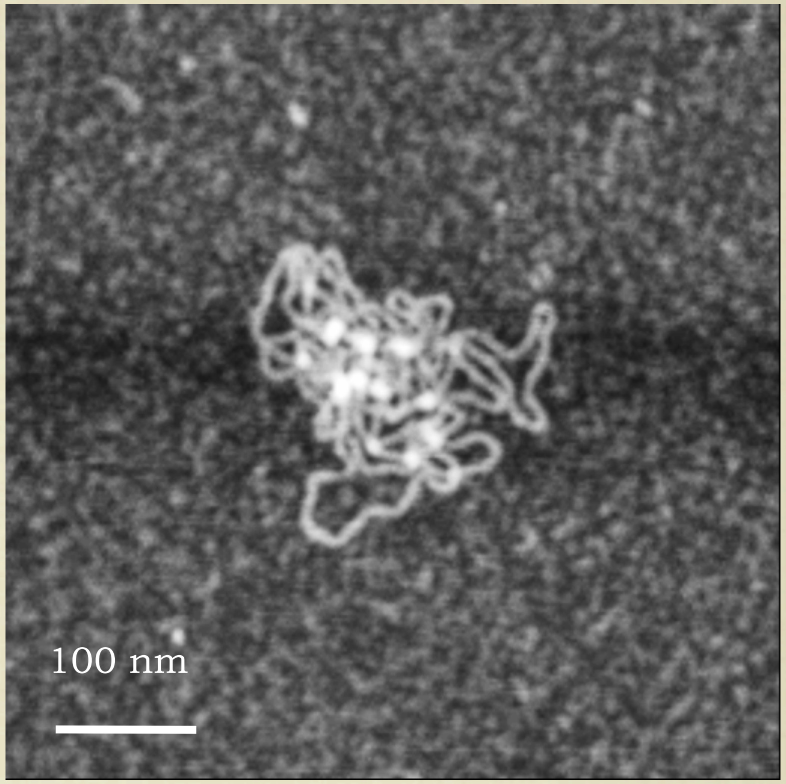
# KNOTTED DNA: STRONG ADSORPTION



Unknot



Simple



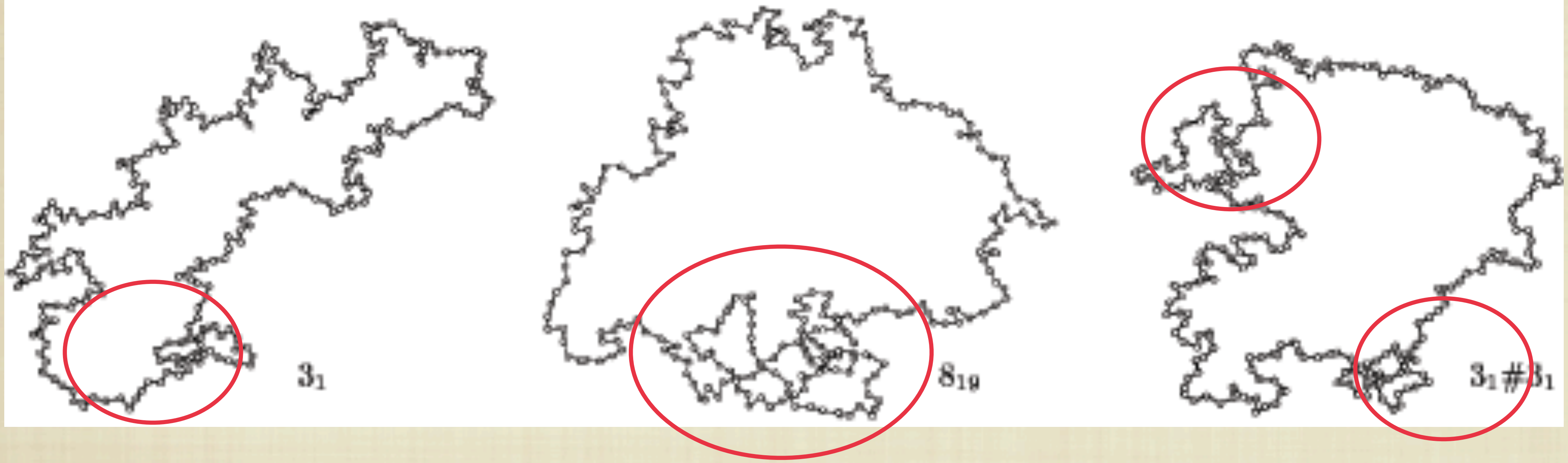
Complex

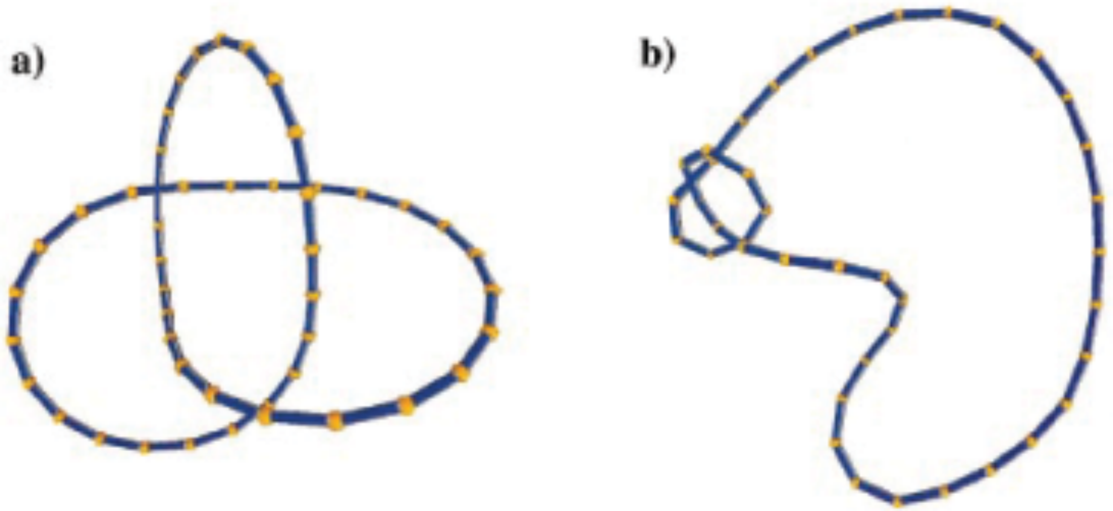
| Strong adsorption | | |
|---|---|---|
| | $d_f$ | $\nu = 1/d_f$ |
| Unknots | $1.711 \pm 0.042$ | $0.585 \pm 0.014$ |
| Simple knots | $1.685 \pm 0.055$ | $0.594 \pm 0.019$ |
| Complex knots | $1.835 \pm 0.076$ | $0.545 \pm 0.024$ |

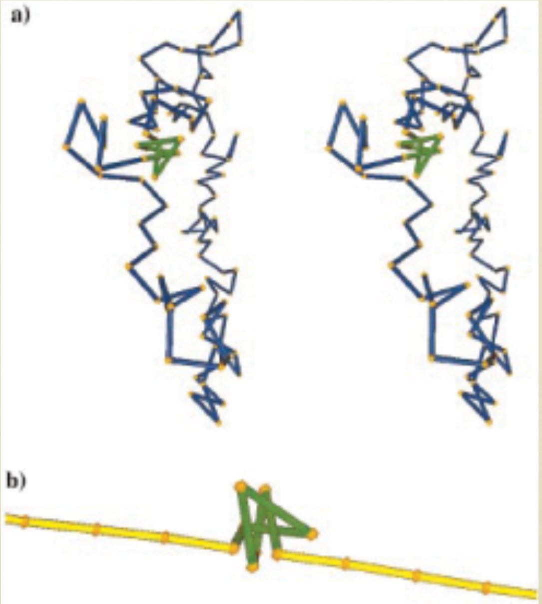
Ercolini et al., PRL, **98**, 058102 (2007)

# WEAK ADSORPTION OF DNA KNOTS

Metzler et al. ‘Equilibrium shape of flat knots’,
*PRL* (2002) **88**, p188101

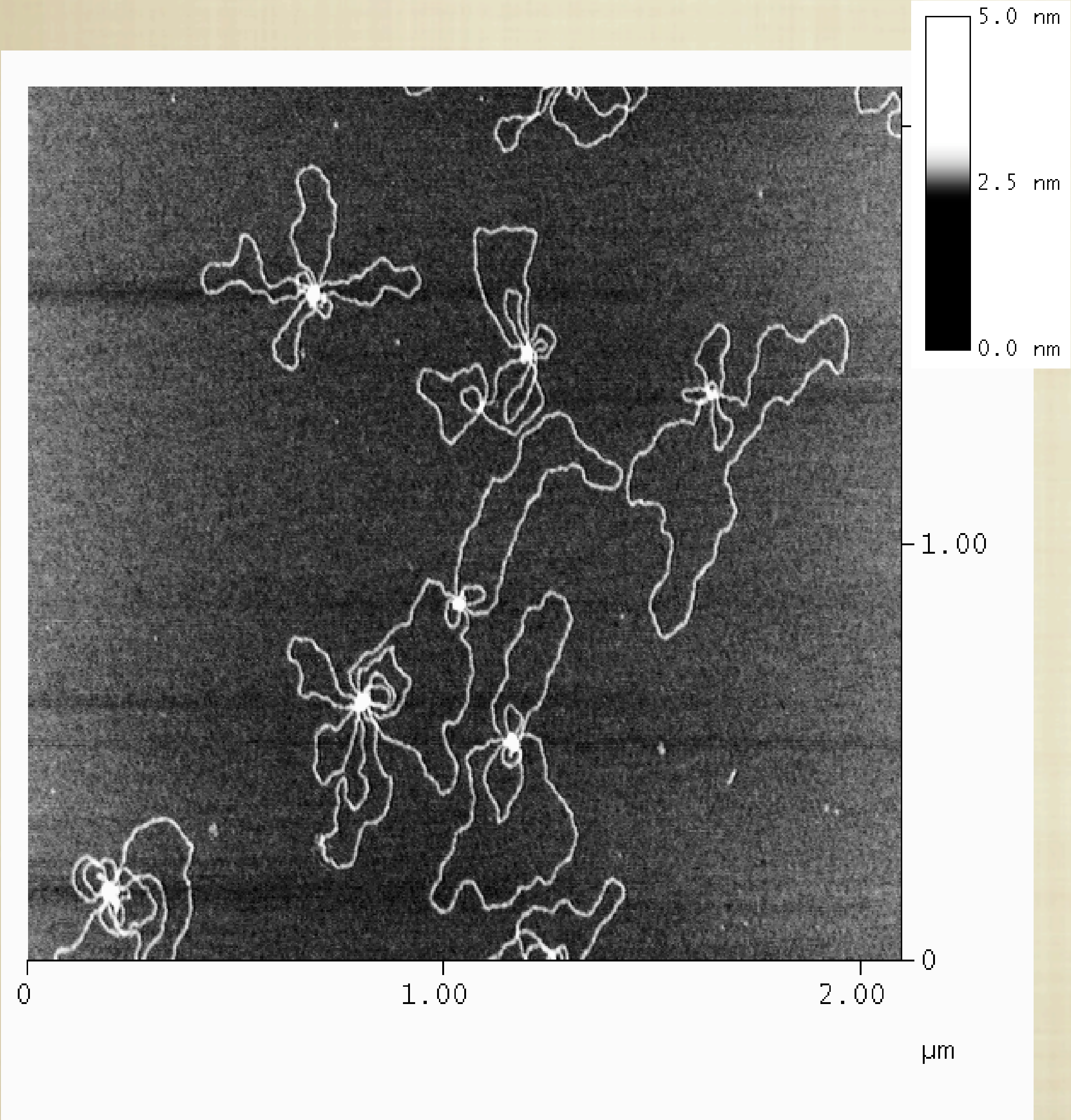


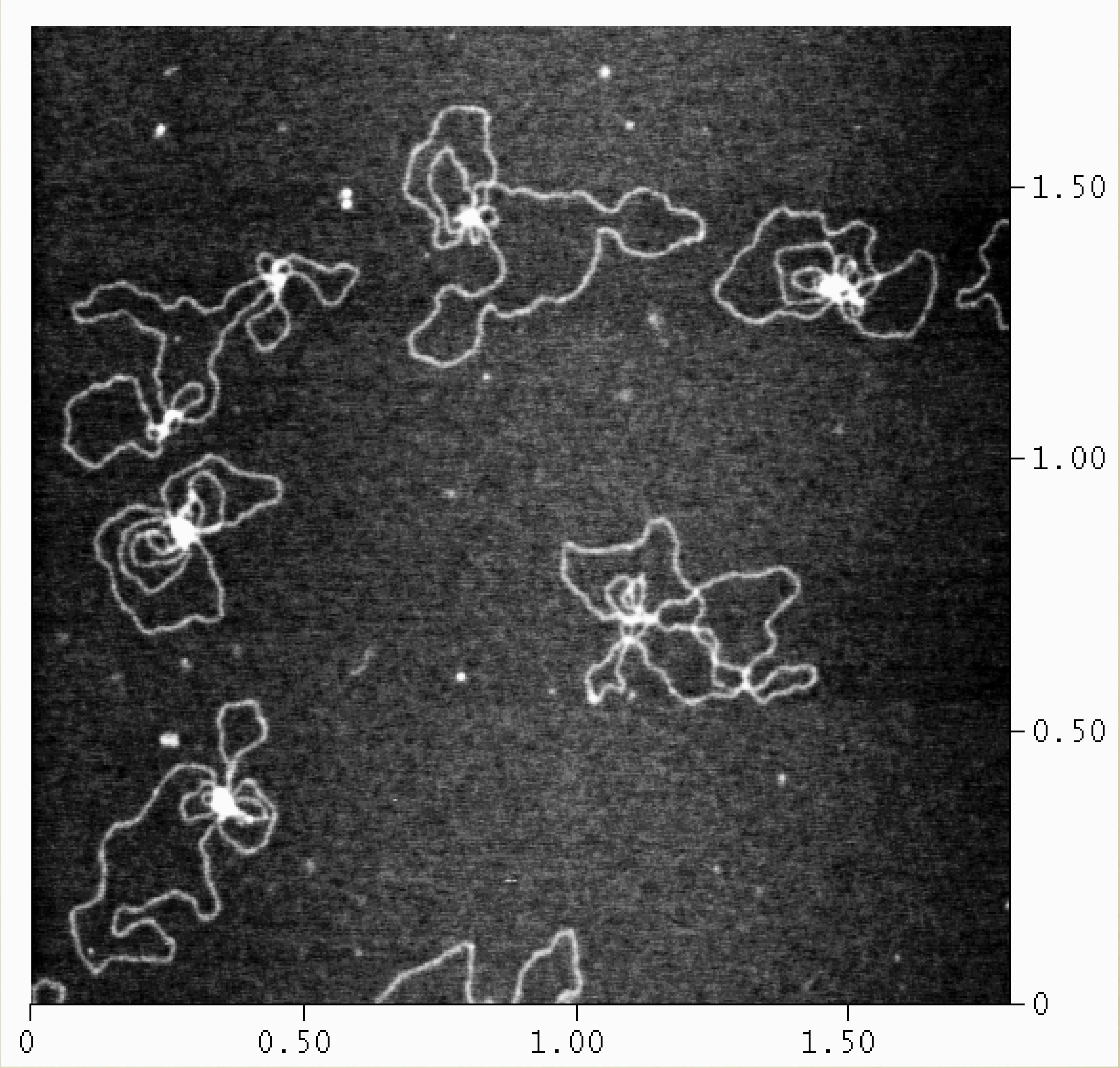




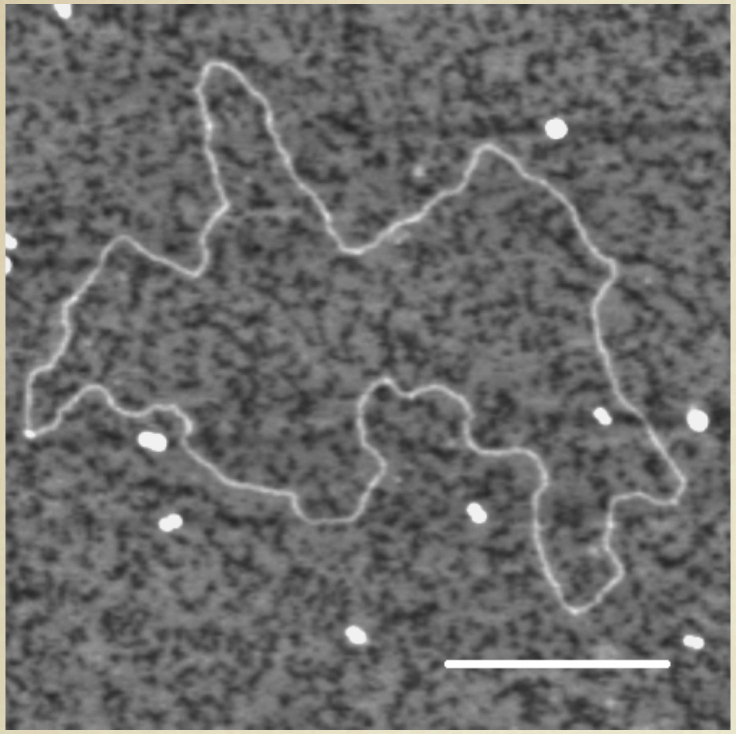
Katritch et al. ‘Tightness of random knotting’,
PRE (2000) **61**,p 5545

# COMPLEX KNOTS ARE COMPOSITE?

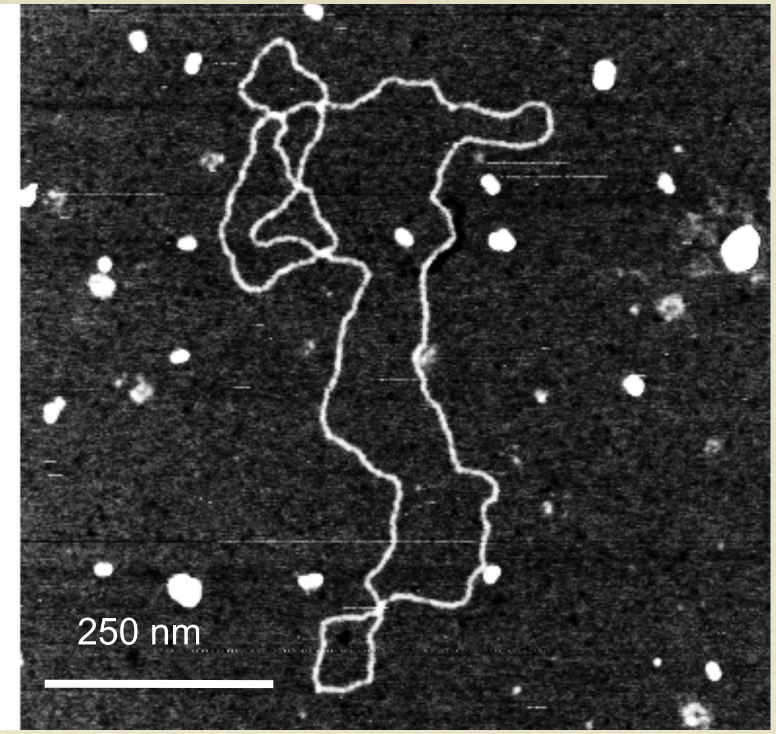




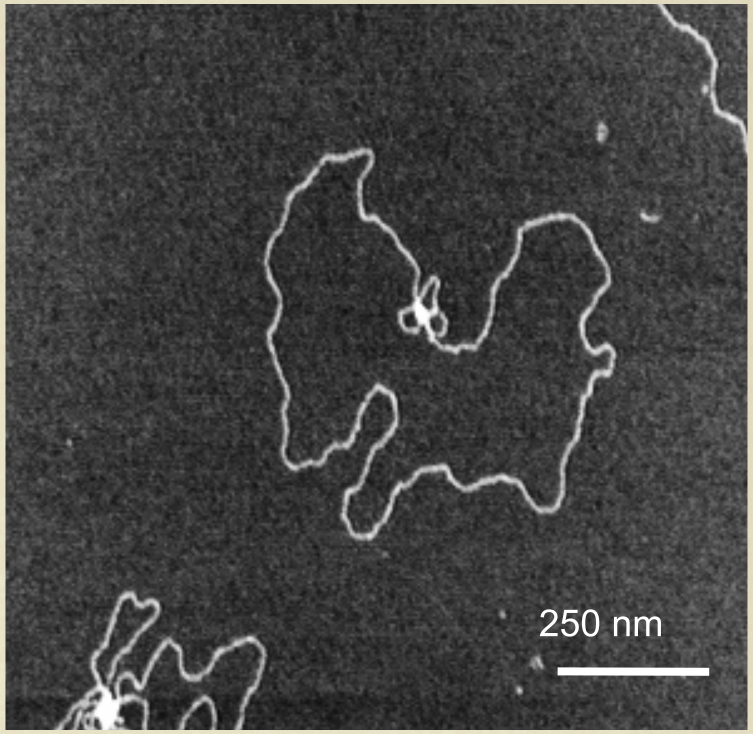
# WEAK ADSORPTION



Unknot



Simple



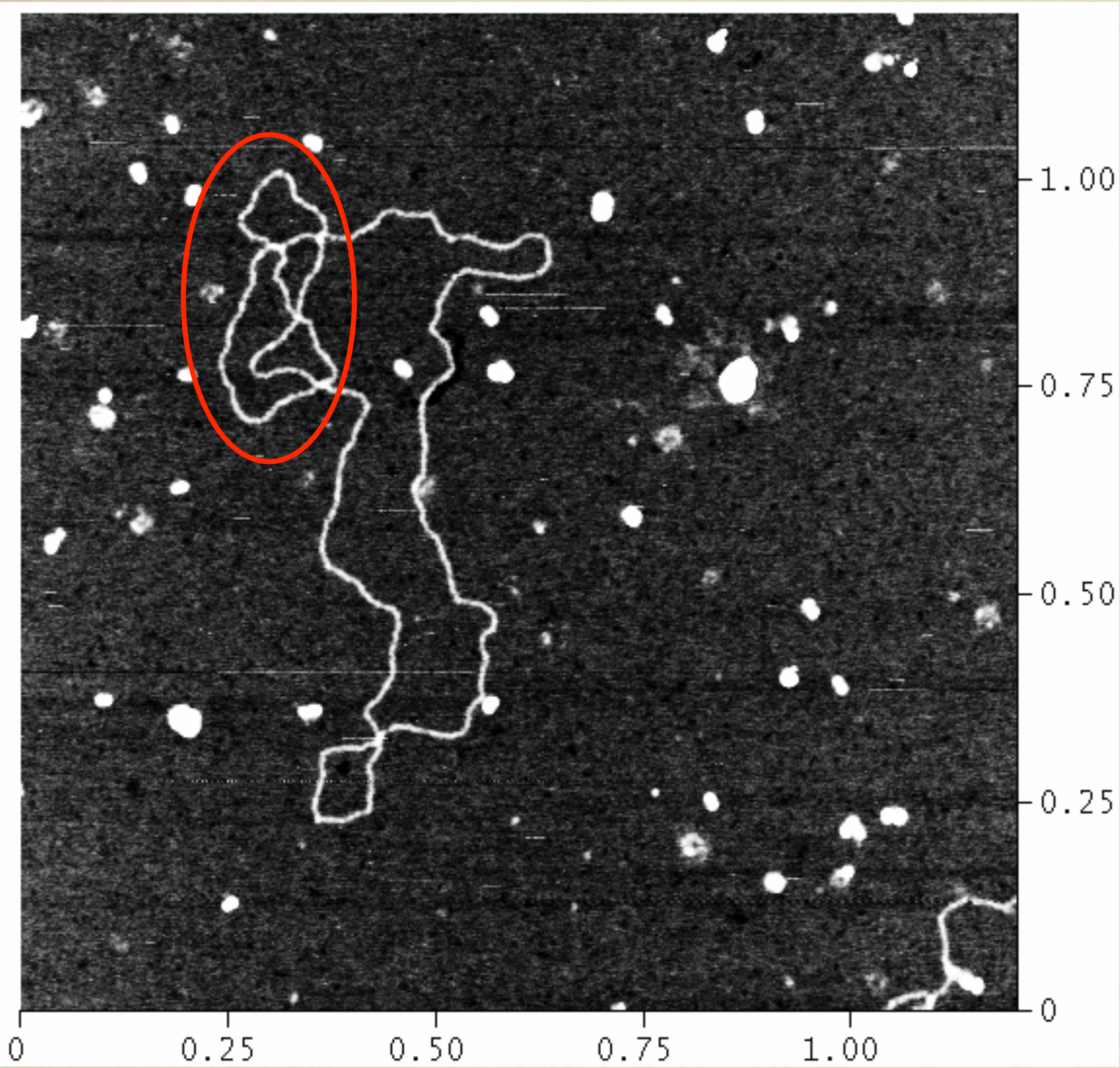
Complex

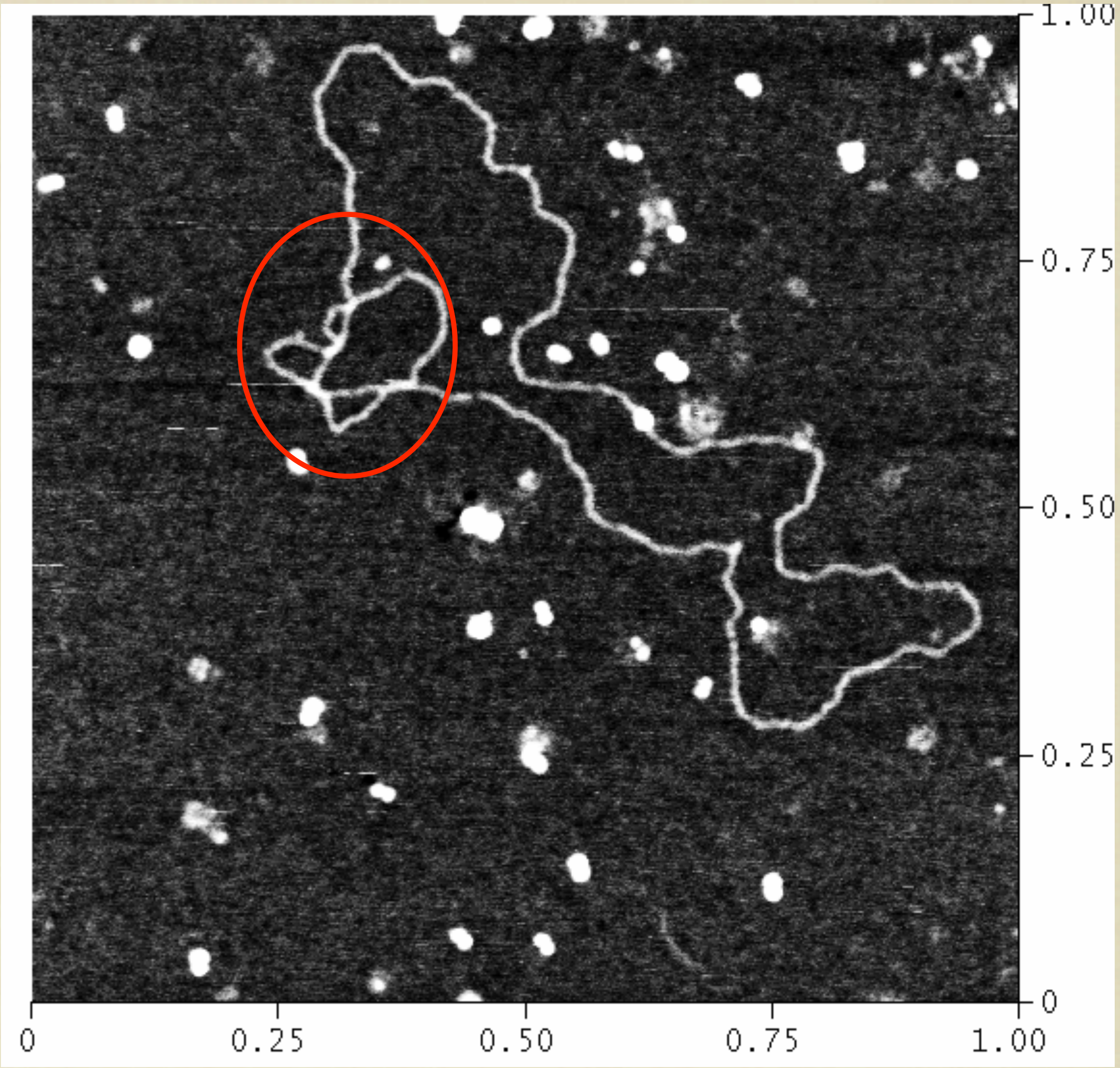
Weak adsorption

| | $d_f$ | $\nu = 1/d_f$ |
|---|---|---|
| Unknots | $1.491 \pm 0.037$ | $0.670 \pm 0.017$ |
| Simple knots | $1.530 \pm 0.065$ | $0.654 \pm 0.028$ |
| Complex knots | $1.541 \pm 0.086$ | $0.650 \pm 0.036$ |

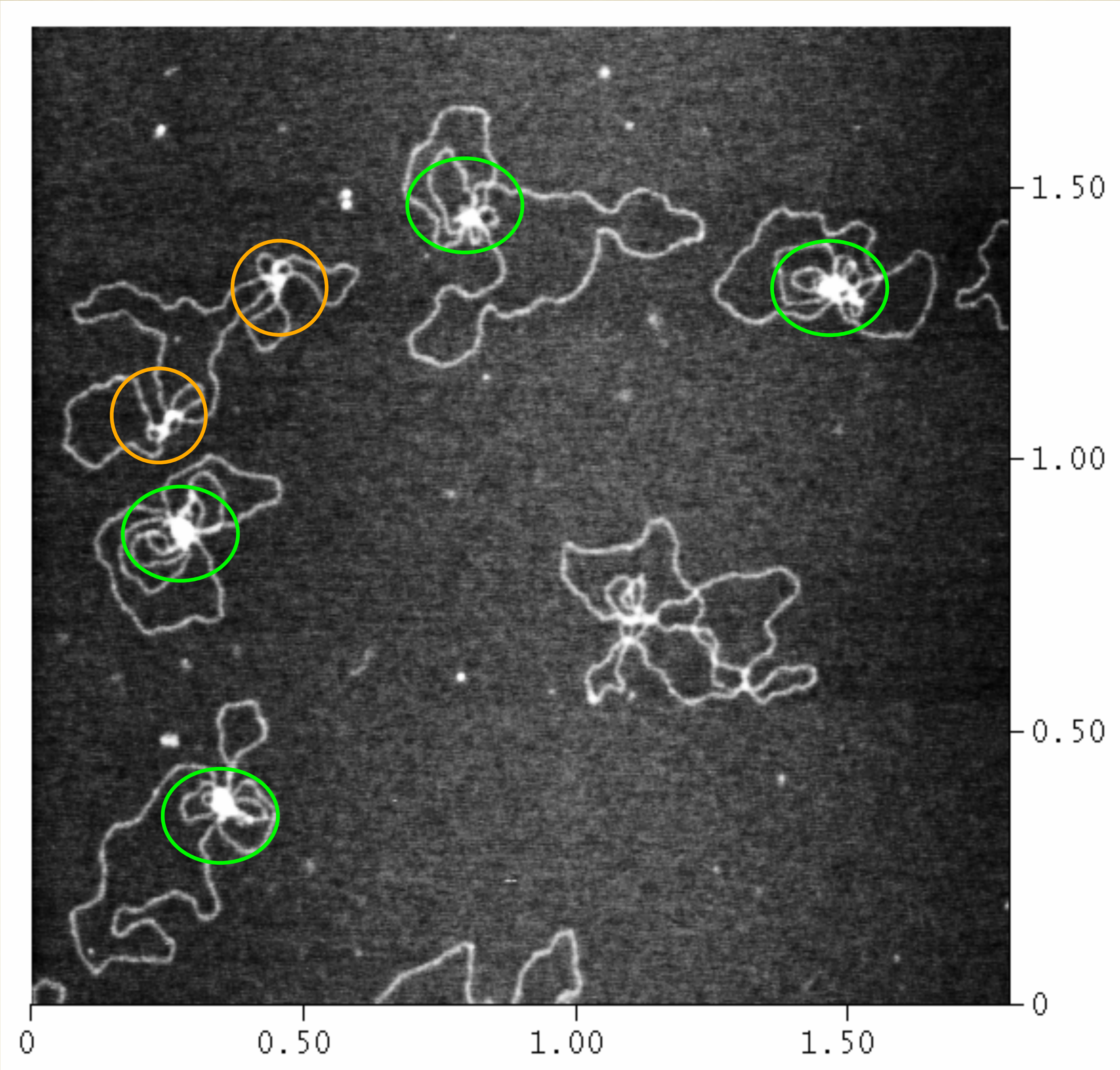
Ercolini et al., PRL, **98**, 058102 (2007)

# LOCALIZATION:
# WEAK ADSORPTION ---> 2D



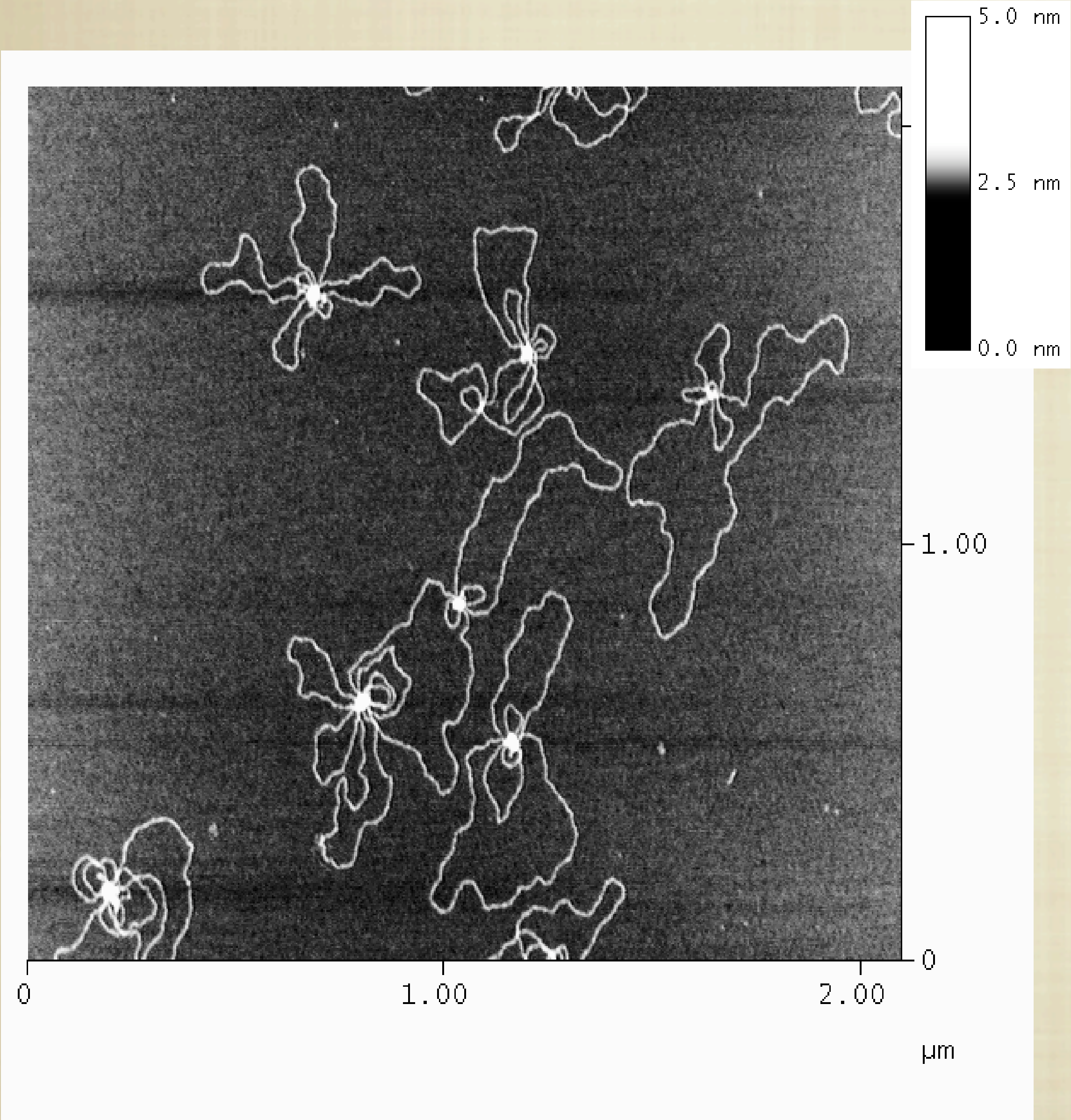


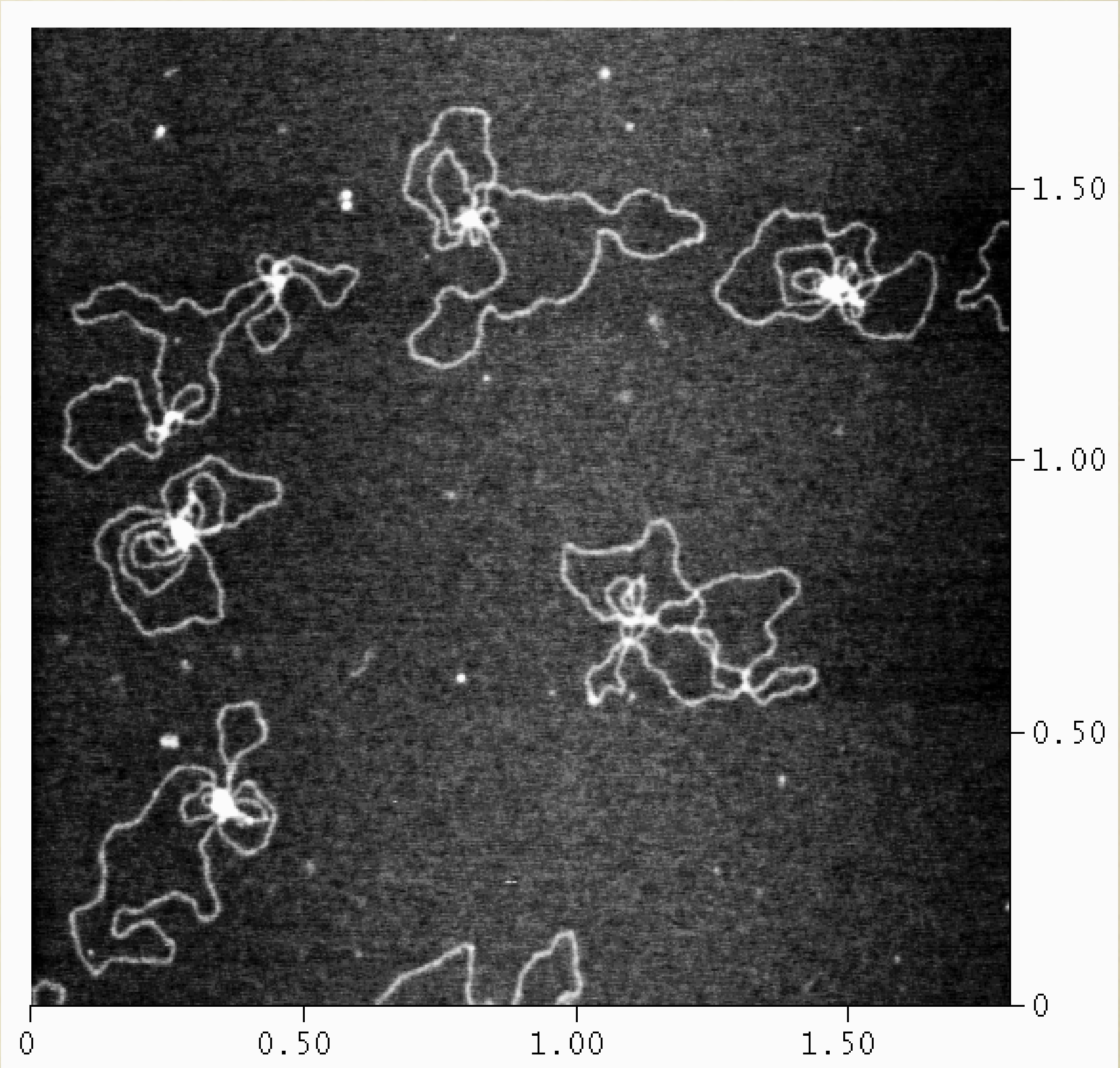
## SIMPLE KNOTS



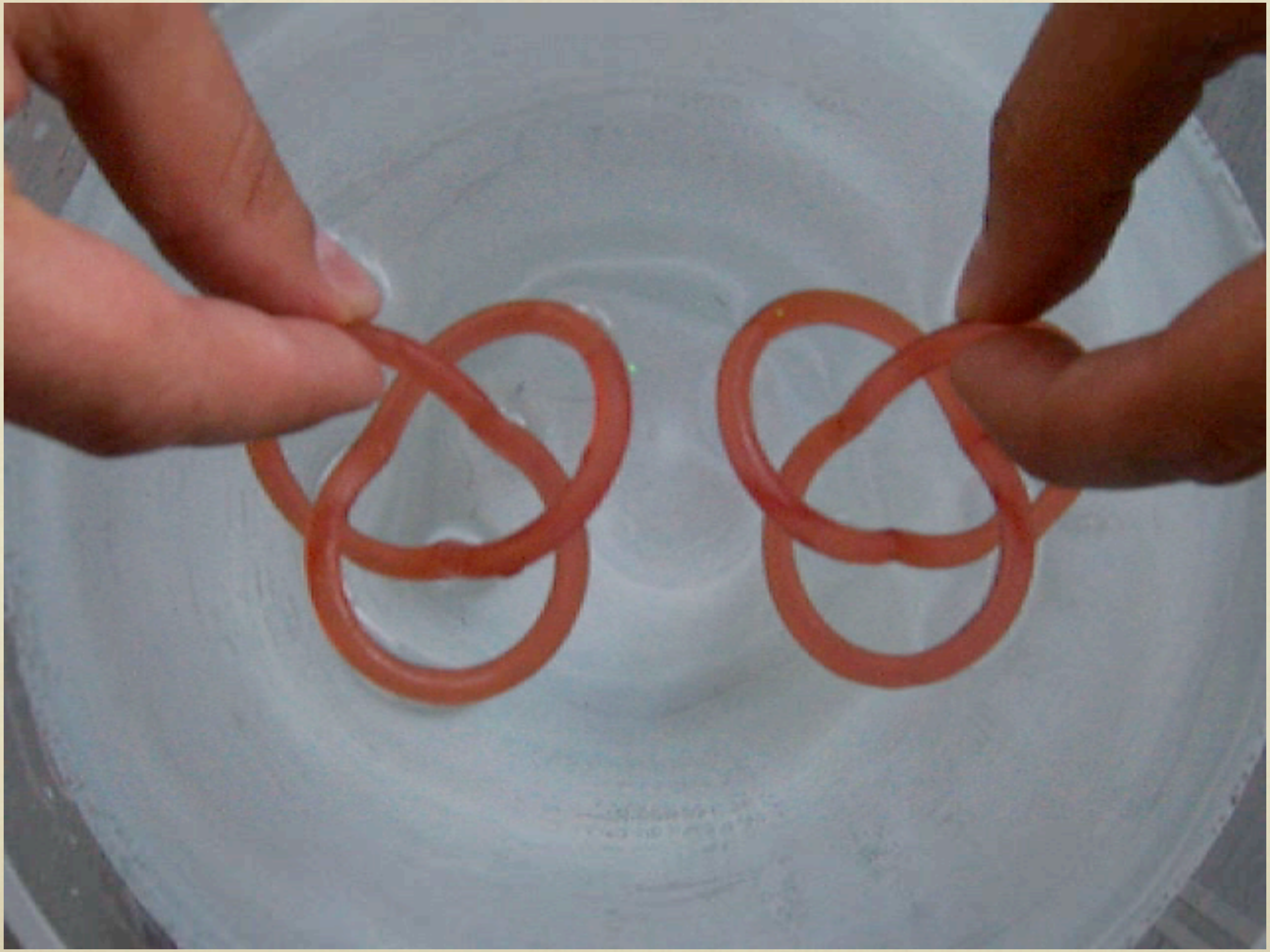
# COMPLEX KNOTS

# COMPLEX KNOTS ARE COMPOSITE?





# CHIRALITY OF KNOTS




SUB-SS
27MHz
SUB-SS

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