The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

2038-13

Conference: From DNA-Inspired Physics to Physics-Inspired Biology

1 - 5 June 2009

Physics Point of View. Topology and Dimensionality Effects

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DNA from the Polymer Physics Point of View: Topology and Dimensionality Effects

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Ecole Polytechnique Fédérale de Lausanne (EPFL),
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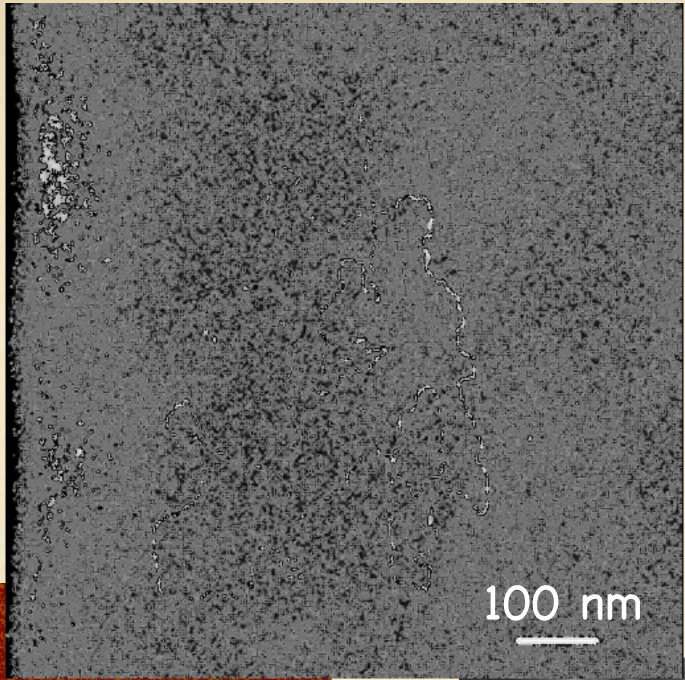
Summary of the following publications

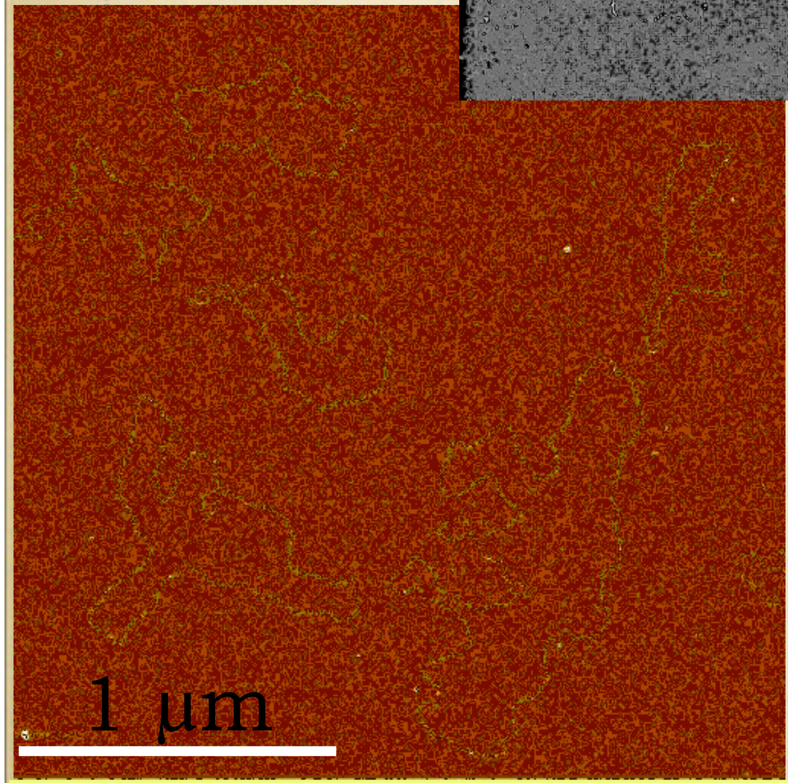
- Valle, Favre, De Los Rios, Rosa, Dietler, PRL, **88** (2005) 158105.
- Adamcik, Klinov, Witz, Sekatskii, Dietler, FEBS Lett., **580** (2006) 5671.
- Ercolini, Valle, Adamcik, Witz, Metzler, De Los Rios, Roca, Dietler, PRL, **98** (2007) 058102.
- Witz, Rechendorff, Adamcik, Dietler, PRL, **101** (2008) 148103.
- Witz, Rechendorff, Adamcik, Dietler, J. Chem. Phys., submitted

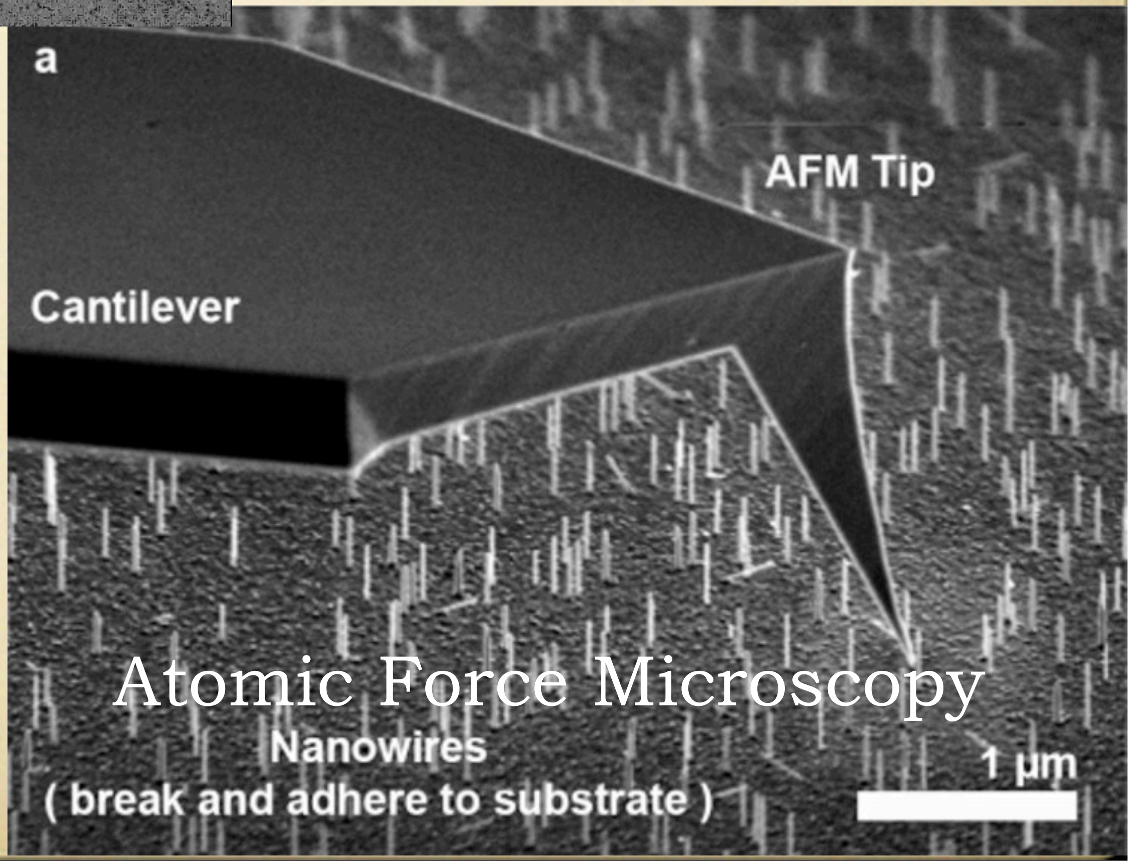
- Statistical Properties of 2D double-stranded circular DNA
- Statistical Properties of 2D single-stranded circular DNA

Methods :

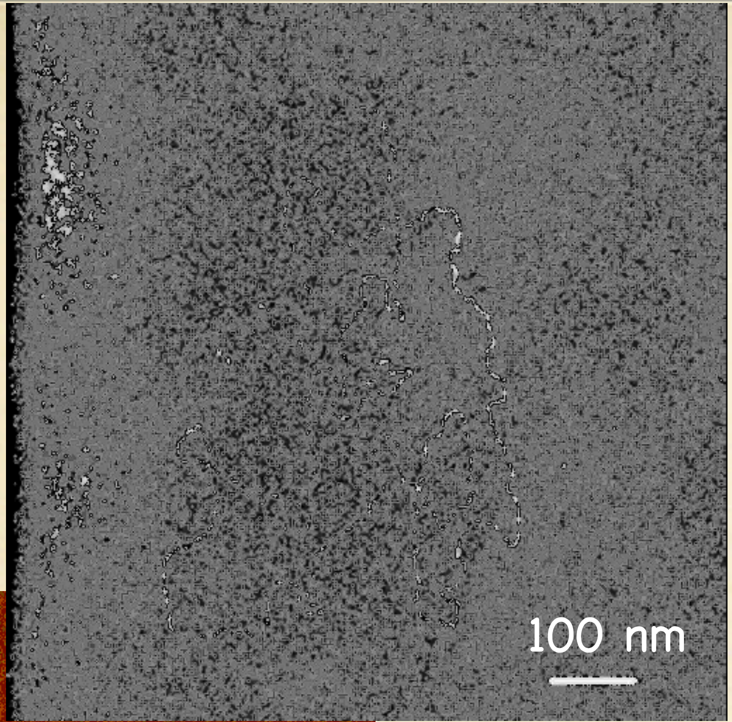
- Imaging of DNA by Atomic Force Microscopy
- Tracing the DNA molecules
- Statistical Properties in 2 D:
  - End-to-End Distance
  - Correlation Function
  - Distributions

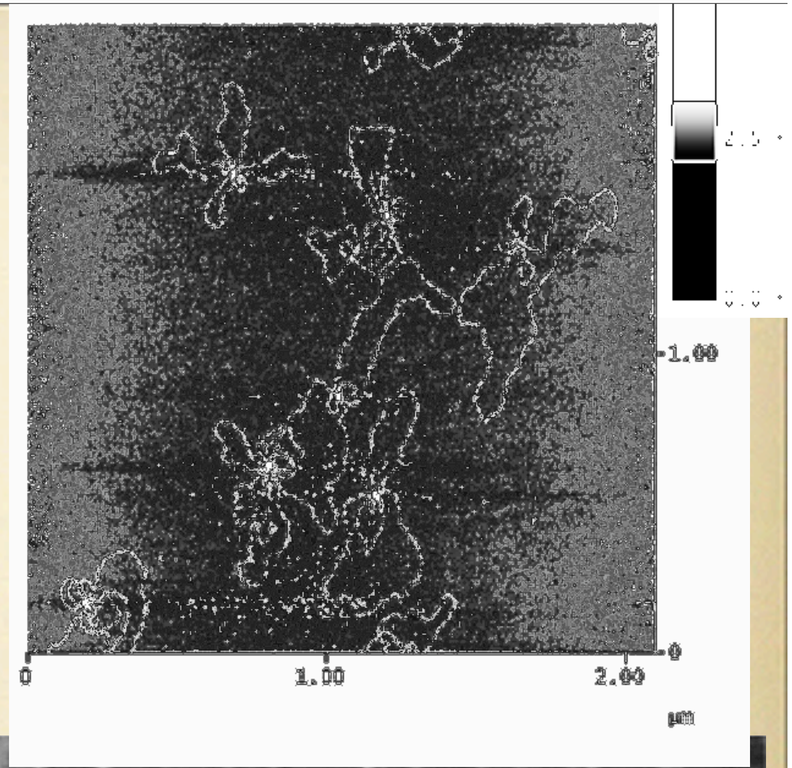

100 nm

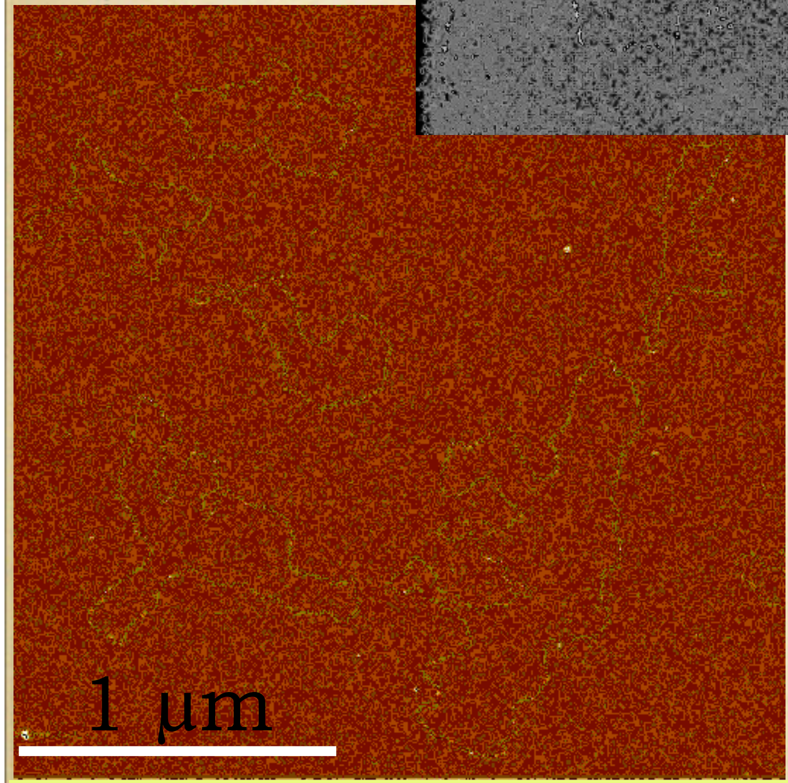

1 μm

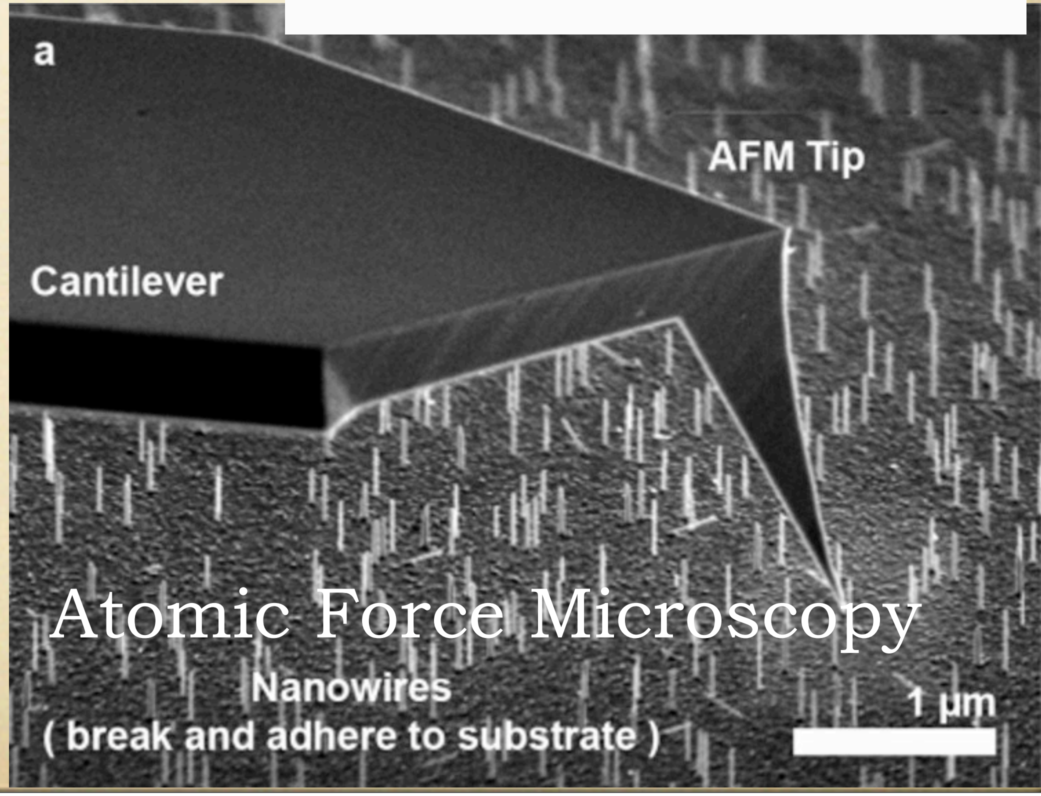

a
AFM Tip
Cantilever
Atomic Force Microscopy
Nanowires
(break and adhere to substrate)
1 μm

Atomic Force Microscopy

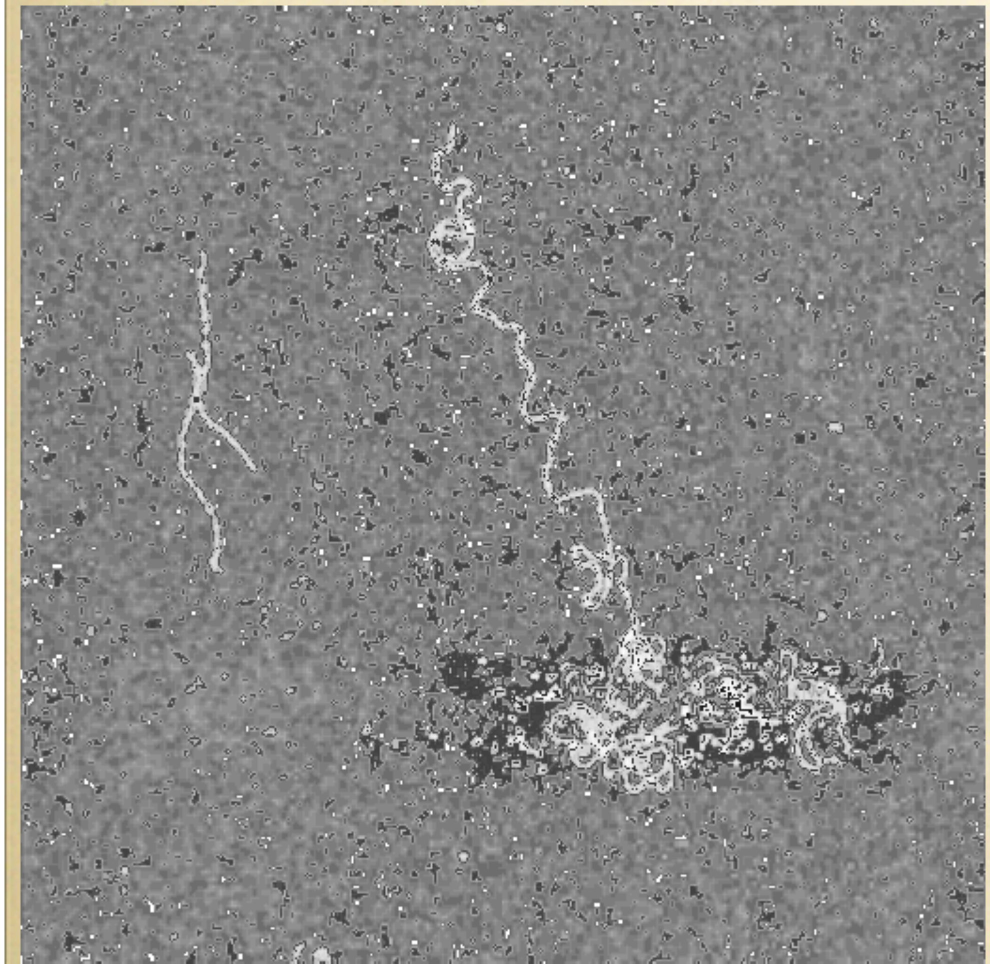


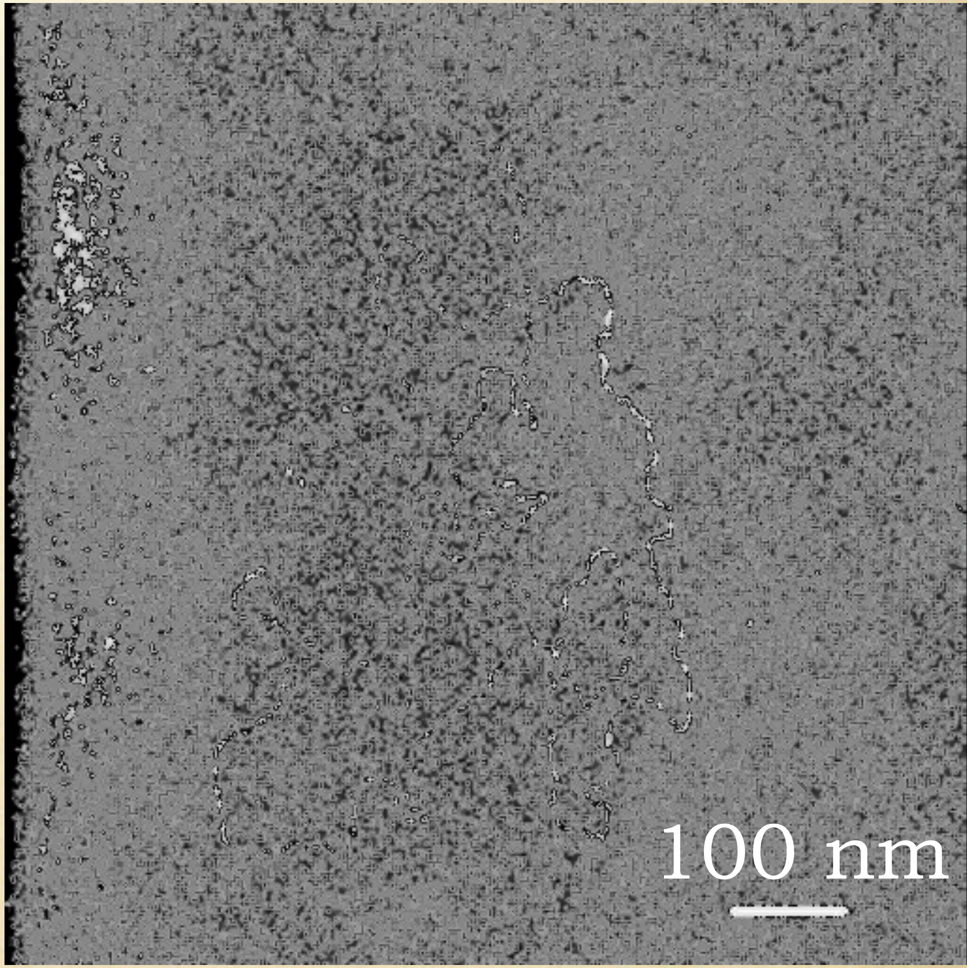






Analyzing DNA

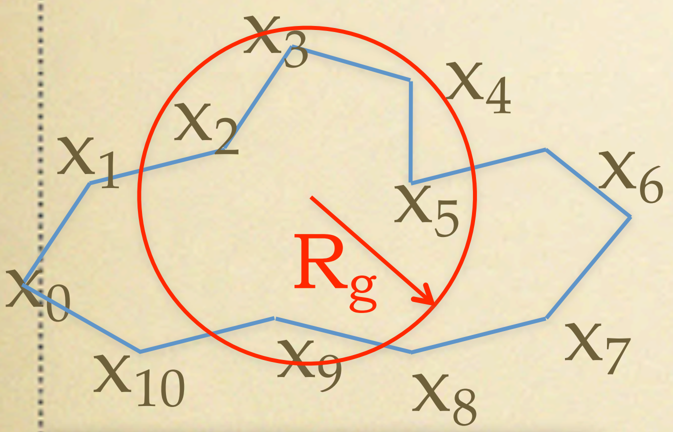




Statistical properties of DNA

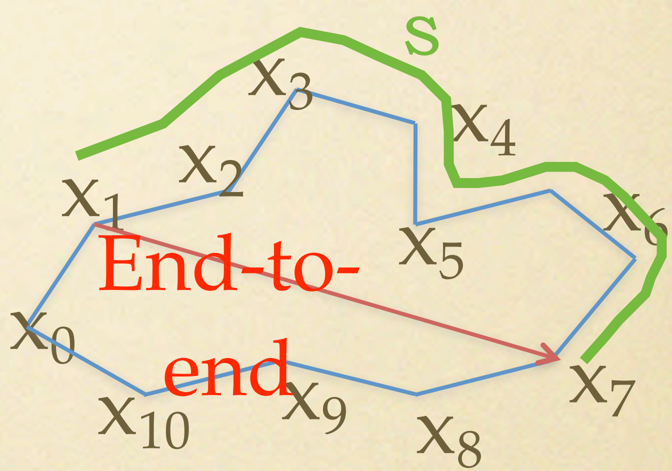
Scaling of the radius of

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



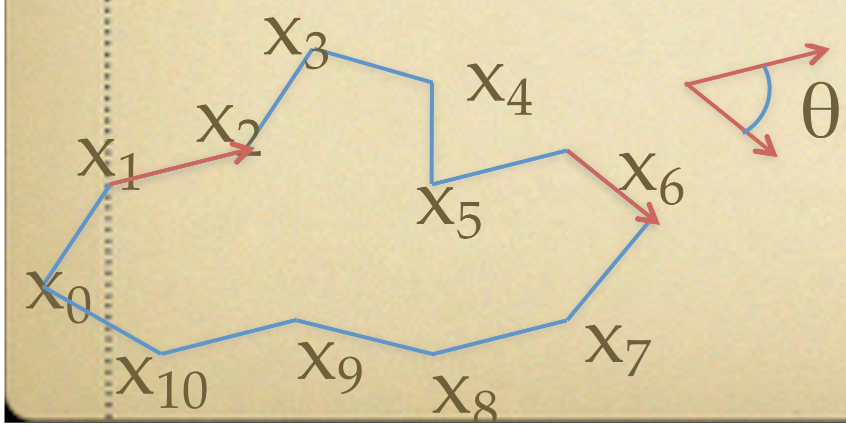
Scaling of the internal End-to-end distance

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



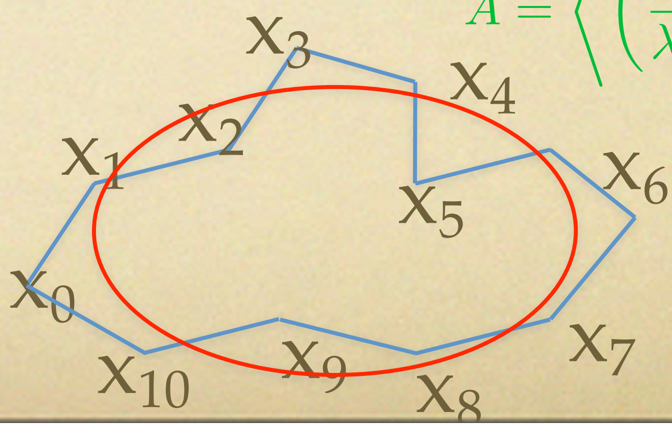
Directional correlation

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



Shape properties: asphericity

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



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

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

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

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

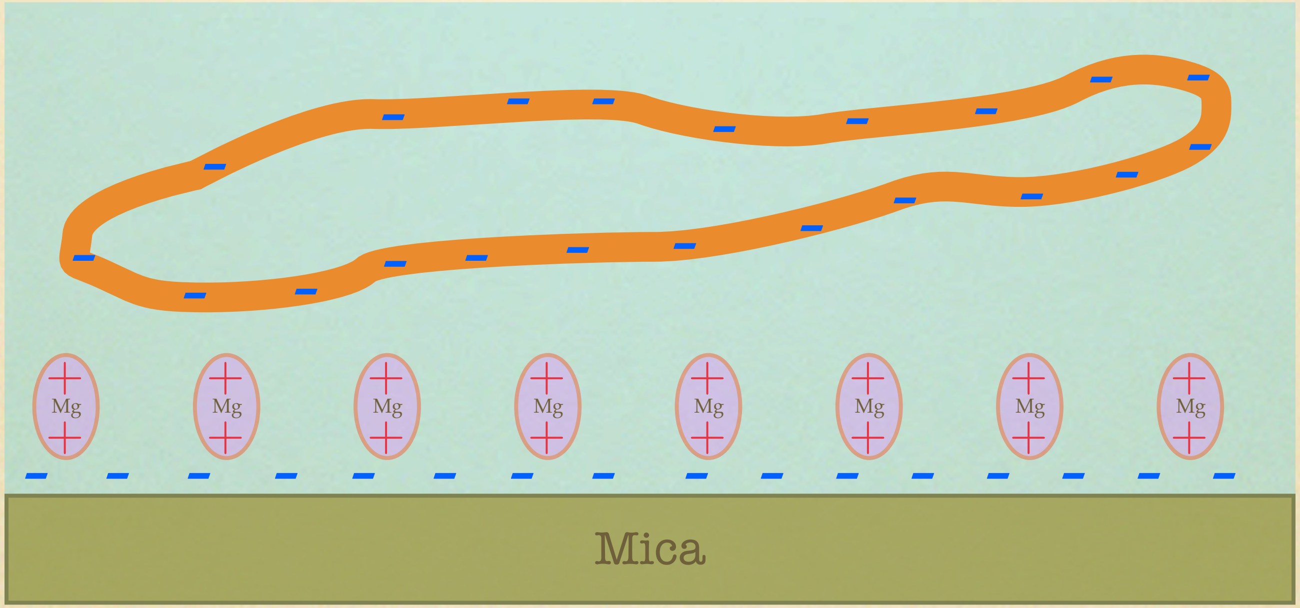
$$\ell_p = 50\ nm$$

Shape properties: asphericity

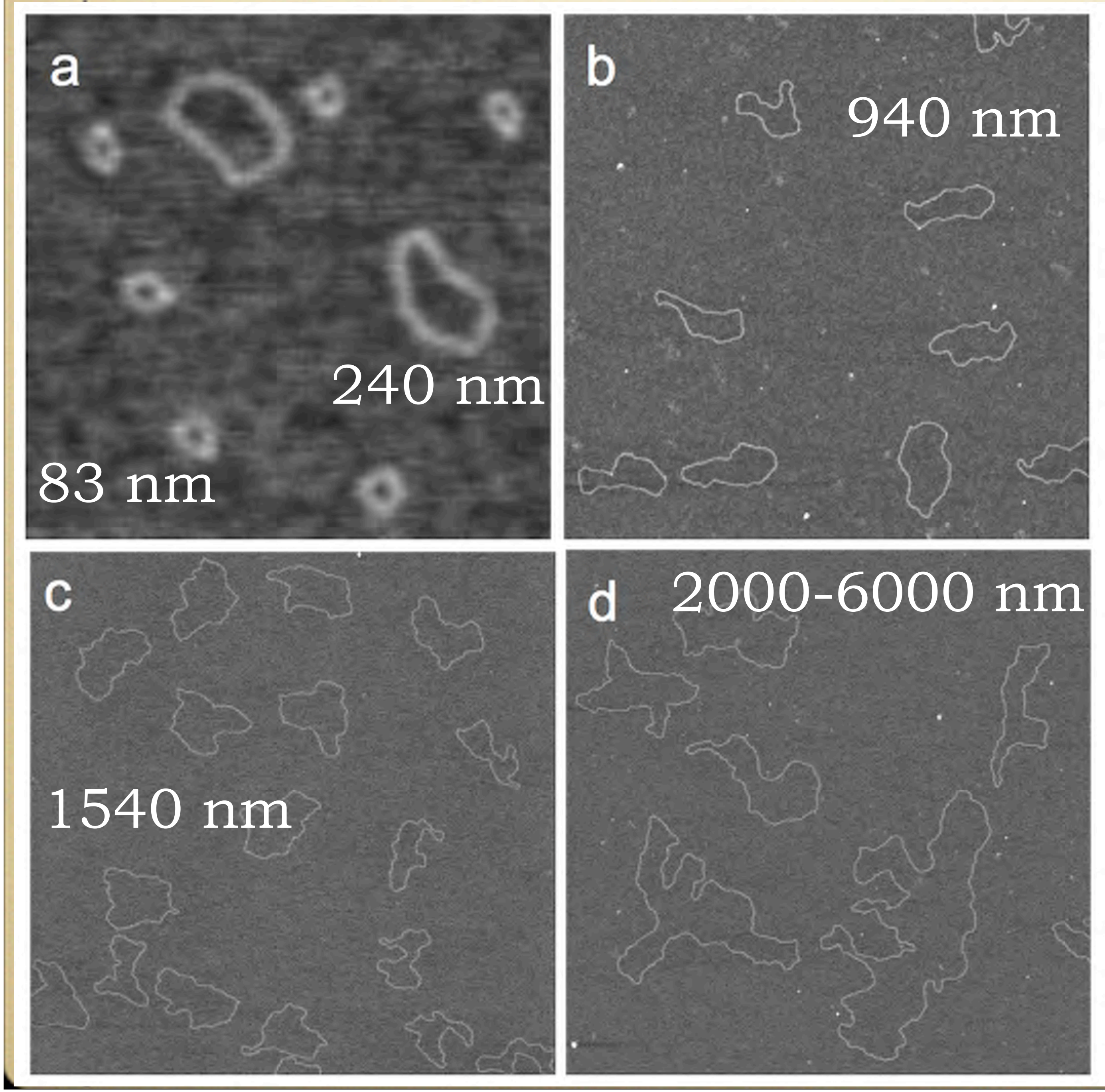
$$A = \left\langle \left(\frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} \right)^2 \right\rangle$$

Circle	A=0
Rod	A=1

2 D deposition of nicked dsDNA



Circular dsDNA in 2D

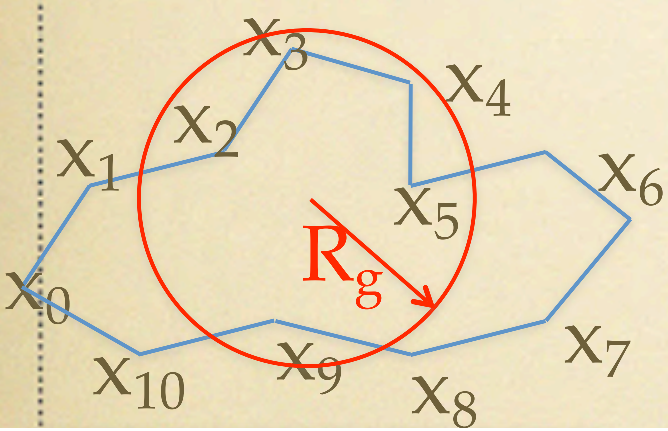


*Witz et al., PRL, **101**, (2008) 148103.*

Statistical properties of DNA

Scaling of the radius of gyration

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



SAW

$$\nu = 1 \quad \text{in 1D}$$
$$\nu = 0.75 \quad \text{in 2D}$$
$$\nu = 0.588 \quad \text{in 3D}$$

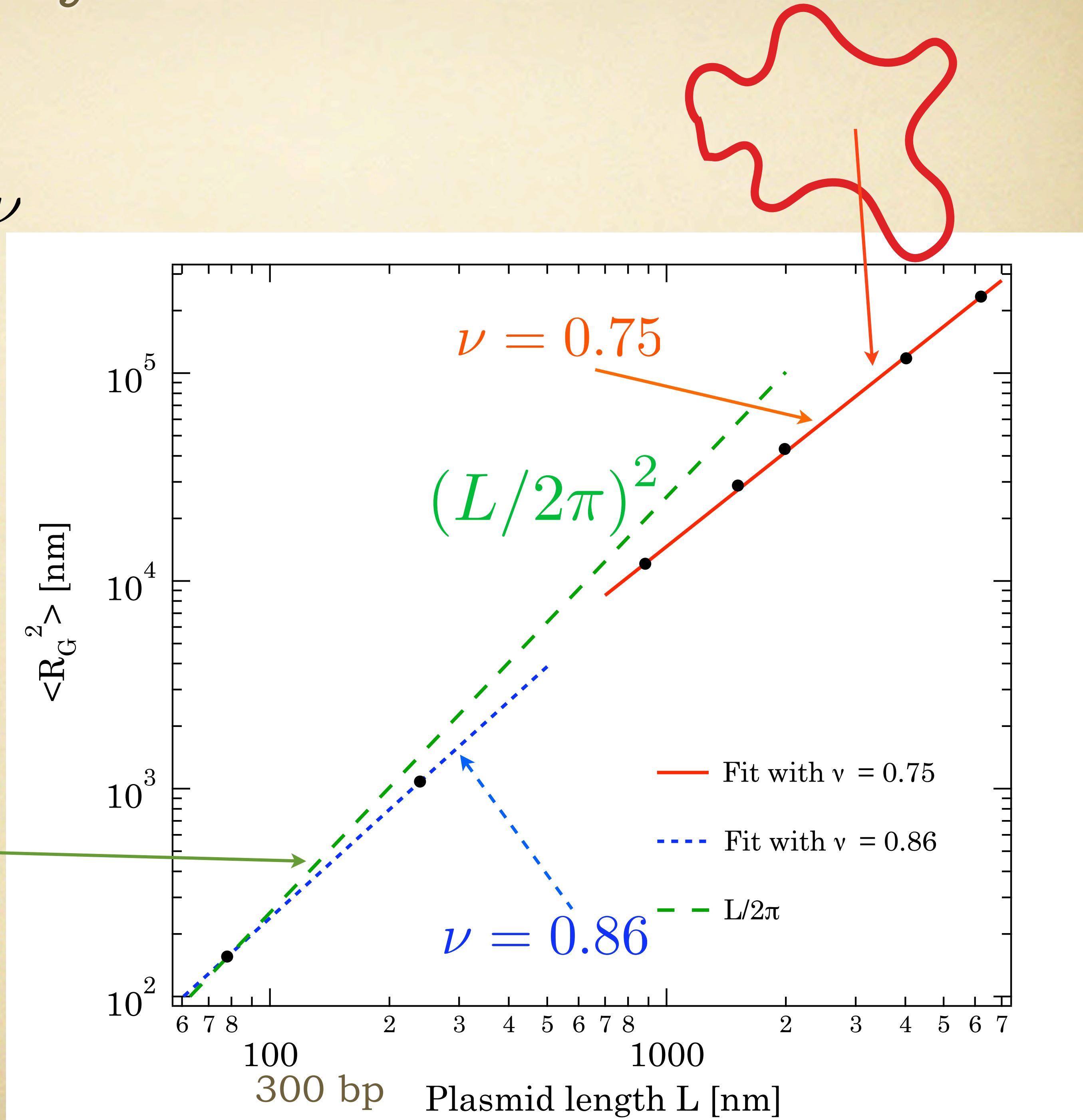
RW

$$\nu = 0.5$$

Radius Of Gyration for Circular DNA in 2D

Prediction

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



Statistical properties of DNA

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

Scaling of the internal End-to-end distance

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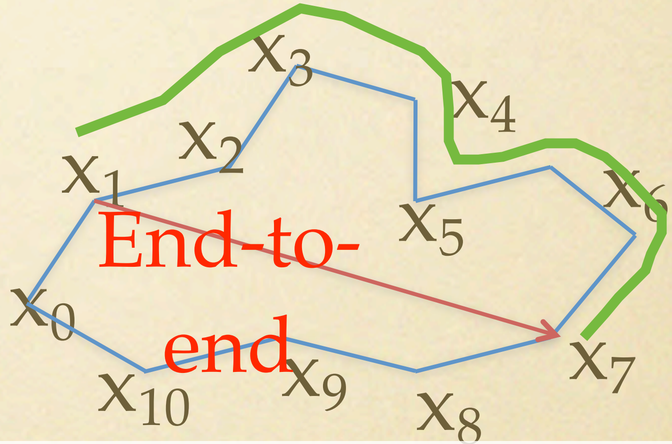


Directional correlation

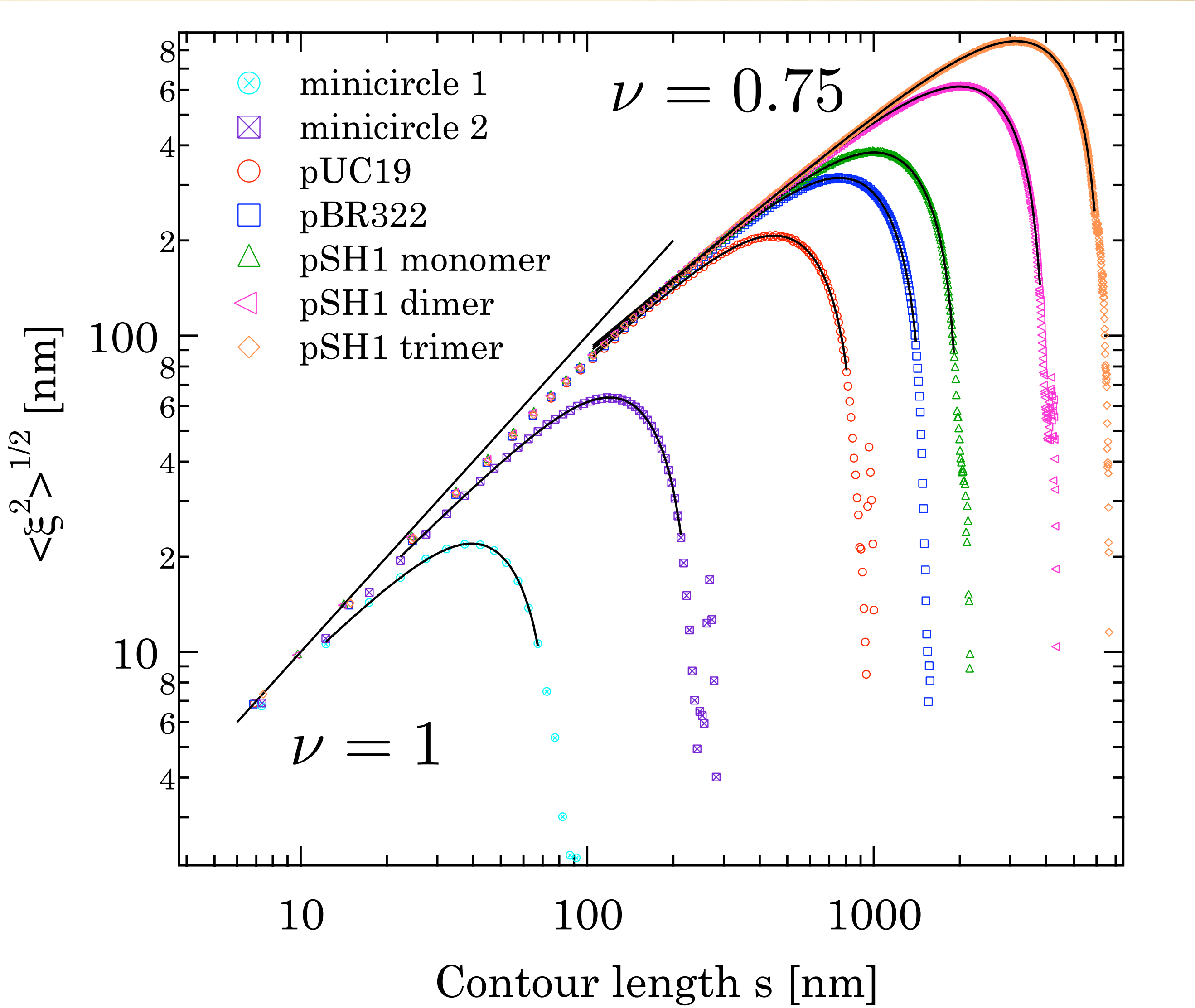
$$\langle \cos\theta(s) \rangle = e^{(-s/2\ell_p)}$$

Shape properties: asphericity

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

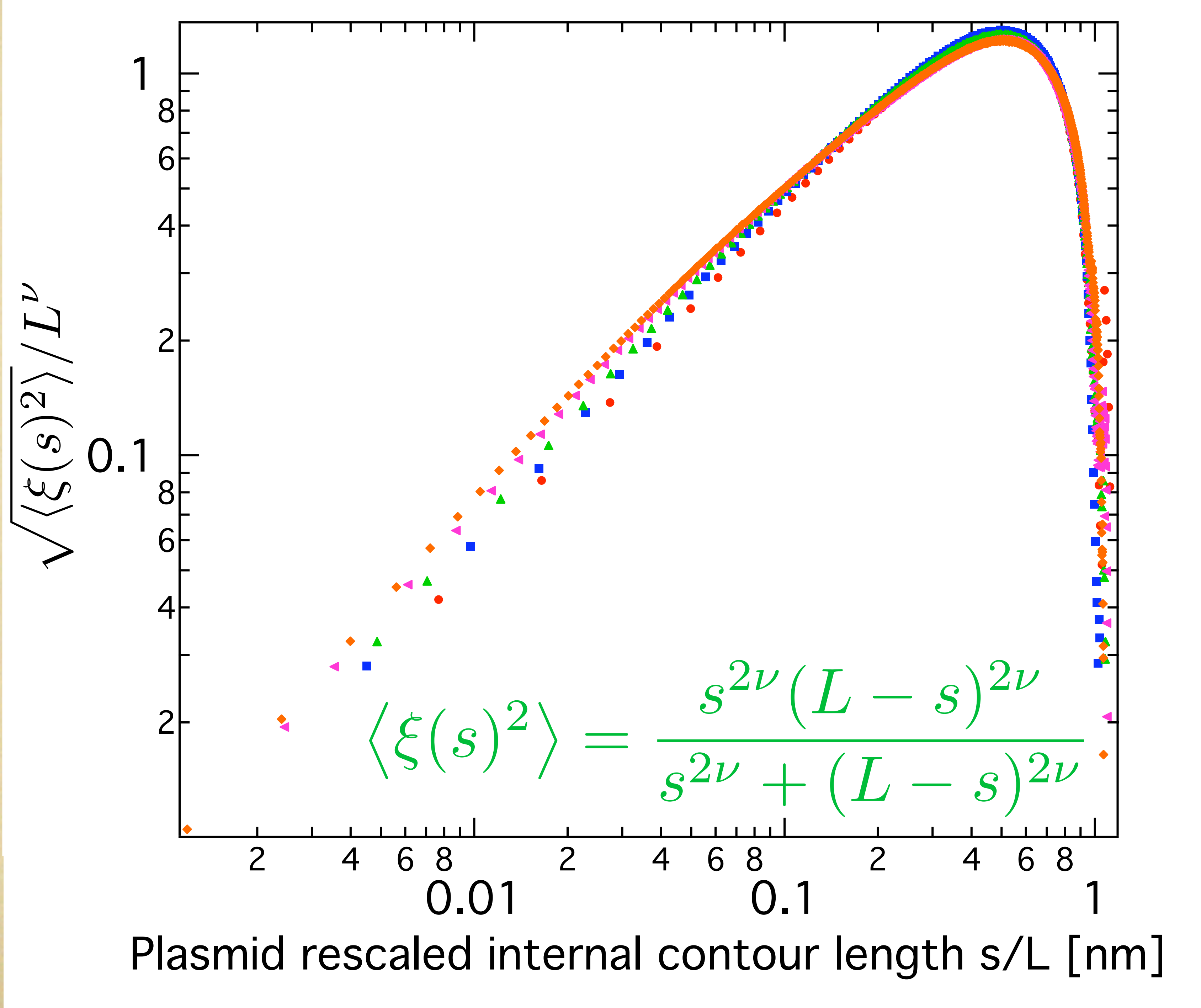
Internal End-to-End Distance for Circular DNA

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



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

Rescaled Data



Statistical properties of DNA

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Scaling of the internal End-to-end distance

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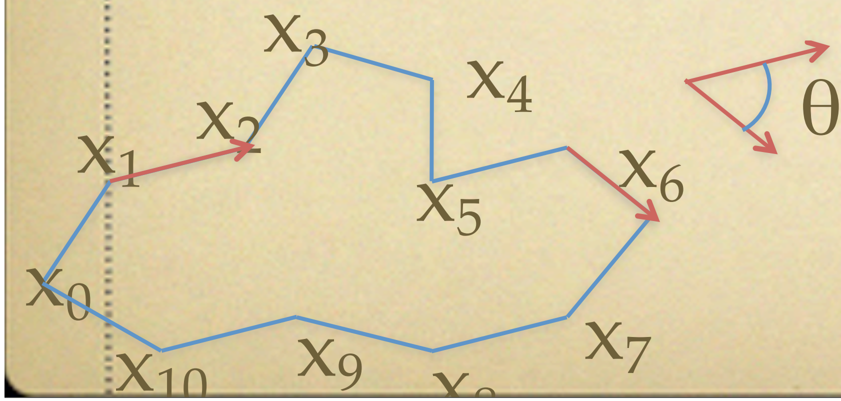
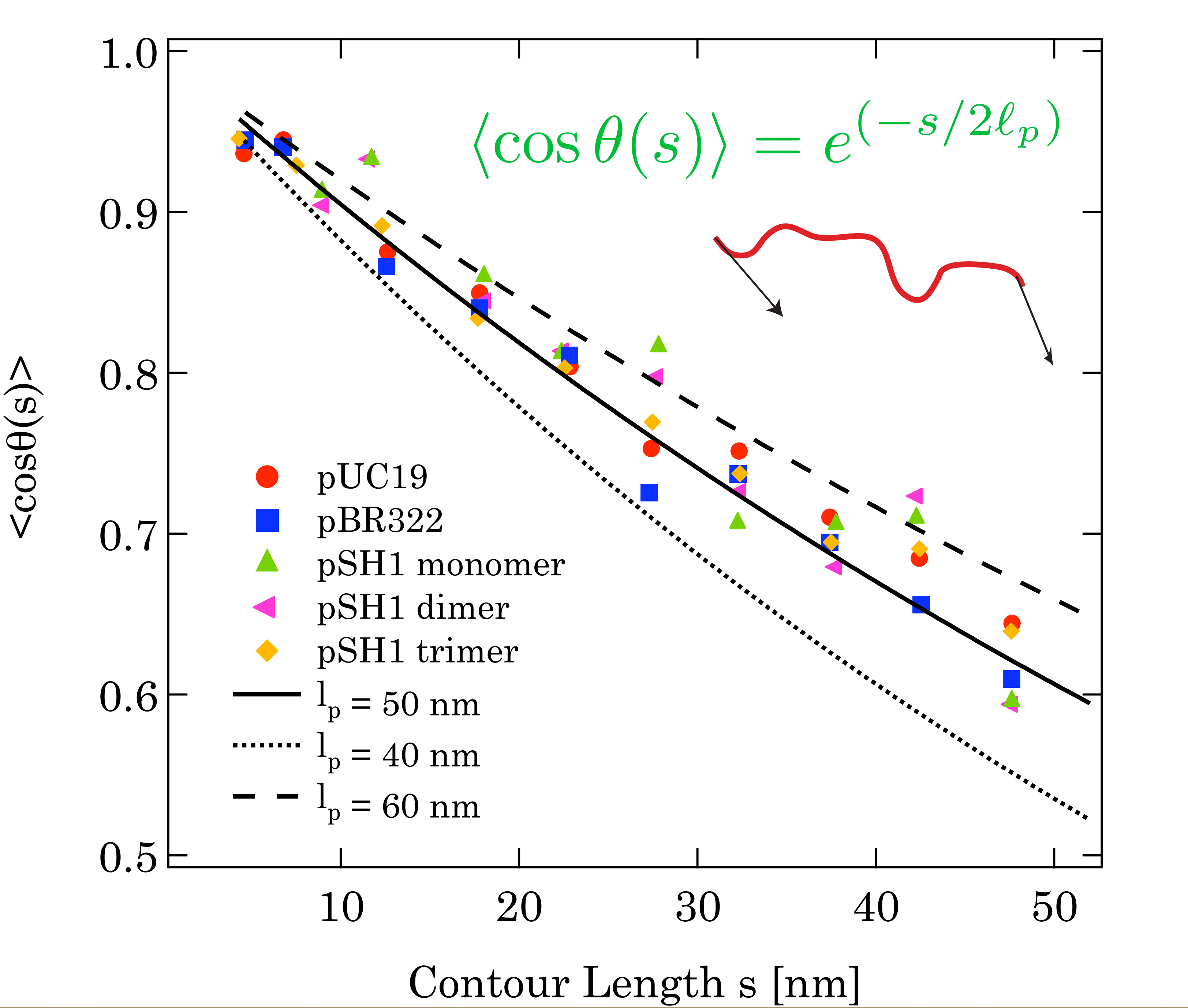


Shape properties: asphericity

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

Bond Correlation Function



Statistical properties of DNA

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

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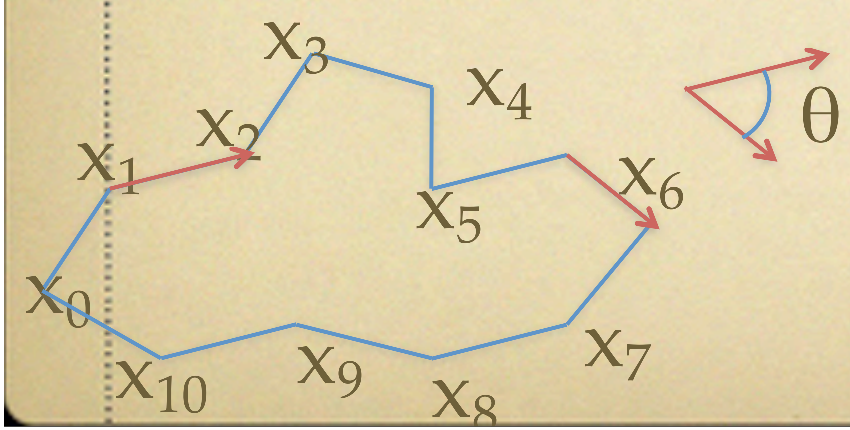
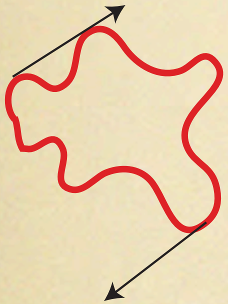


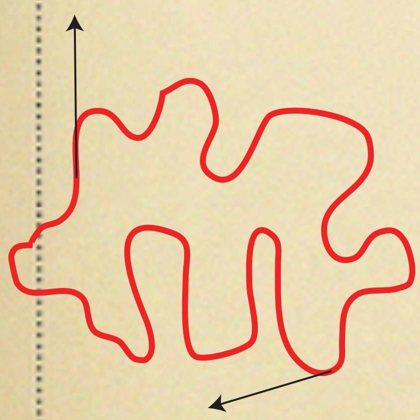
Shape properties: asphericity

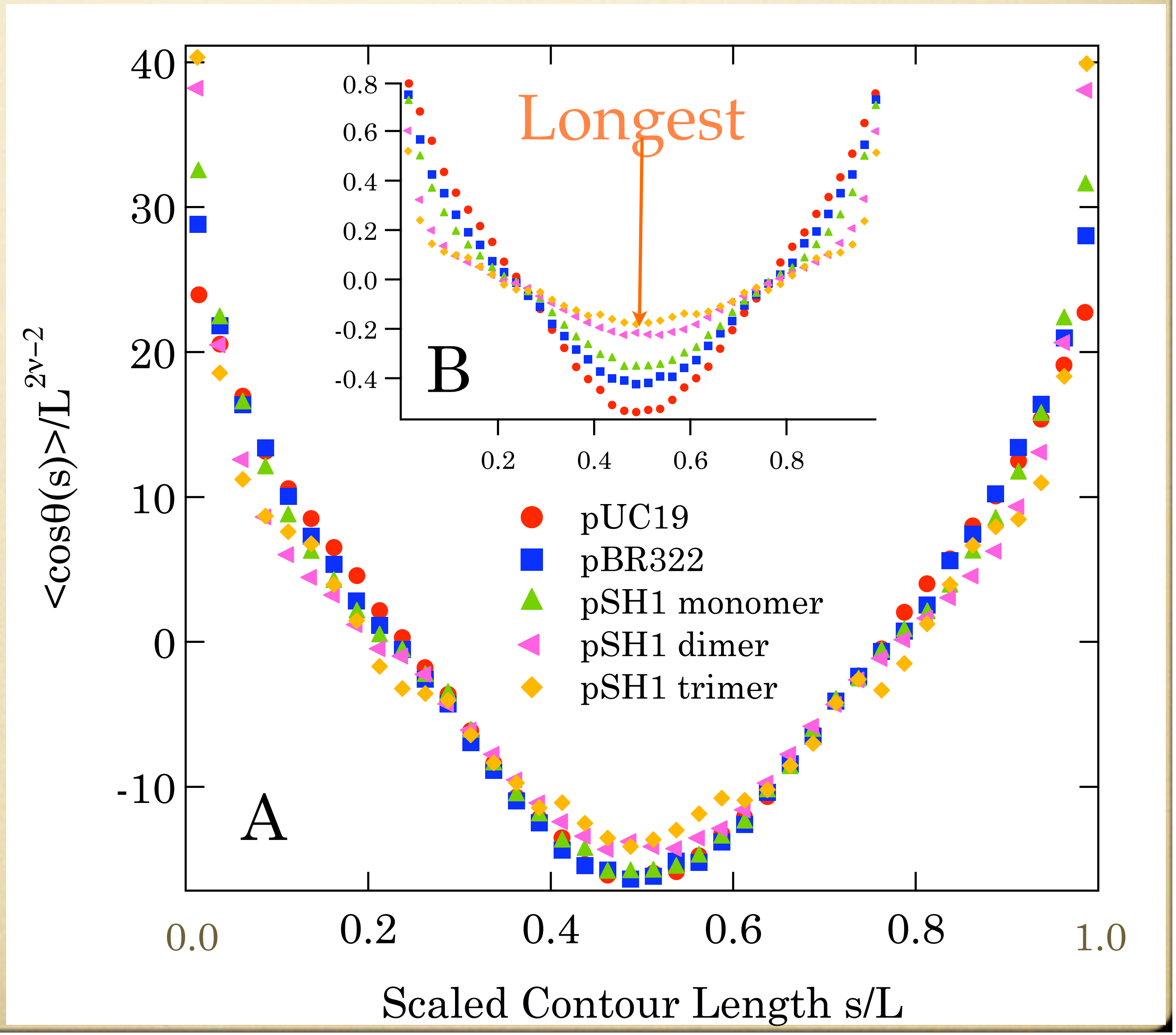
$$A = \left\langle \left(\frac{\lambda_1 - \lambda_2}{\lambda_1 + \lambda_2} \right)^2 \right\rangle$$

Bond Correlation Function of DNA

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



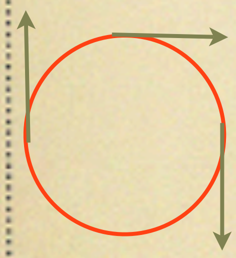


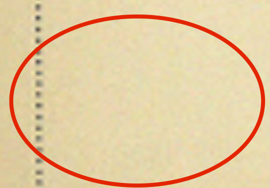


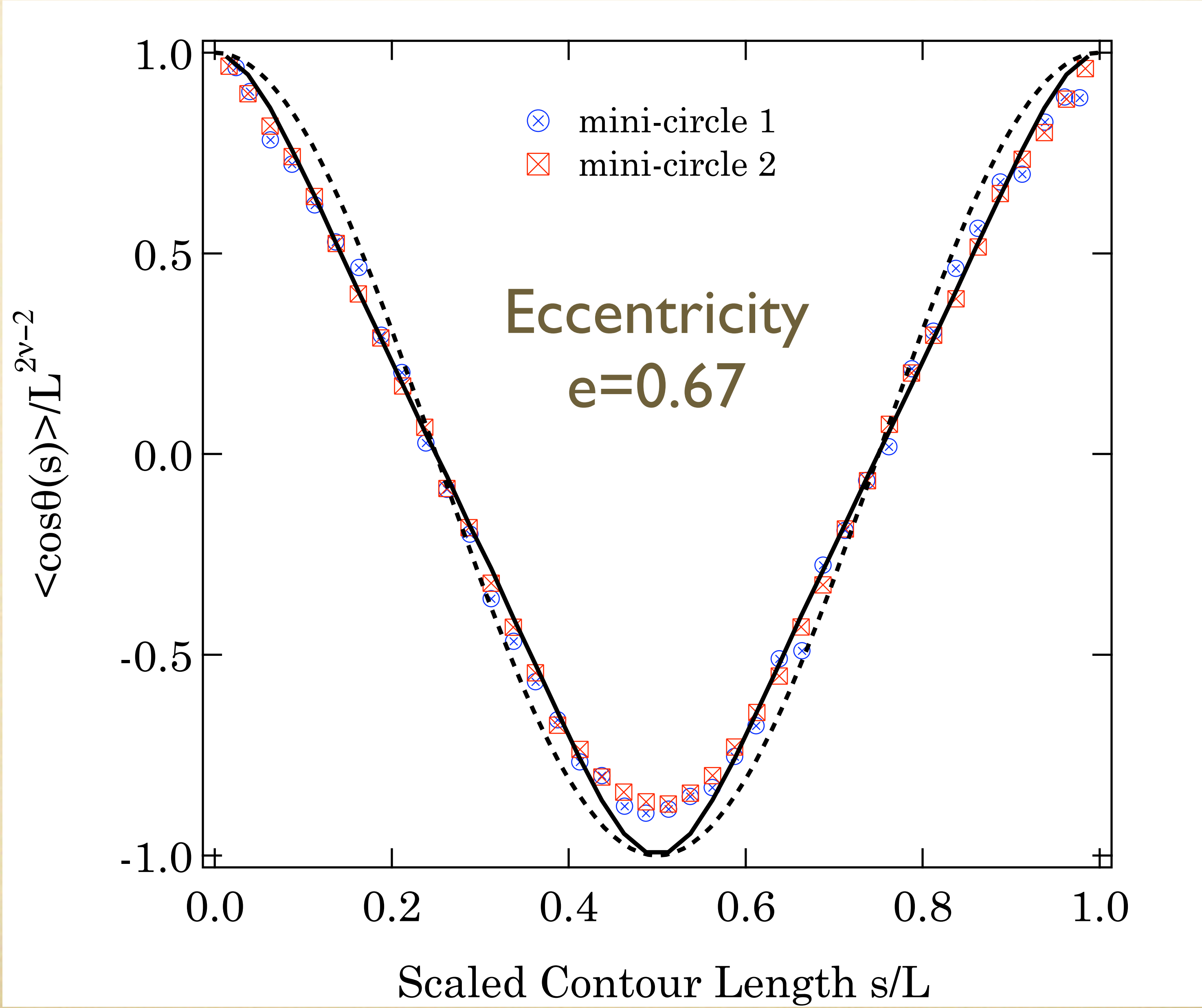
A. Baumgärtner,
J. Chem. Phys., **76**,
4275 (1982).

Bond Correlation Function of DNA mini-circles

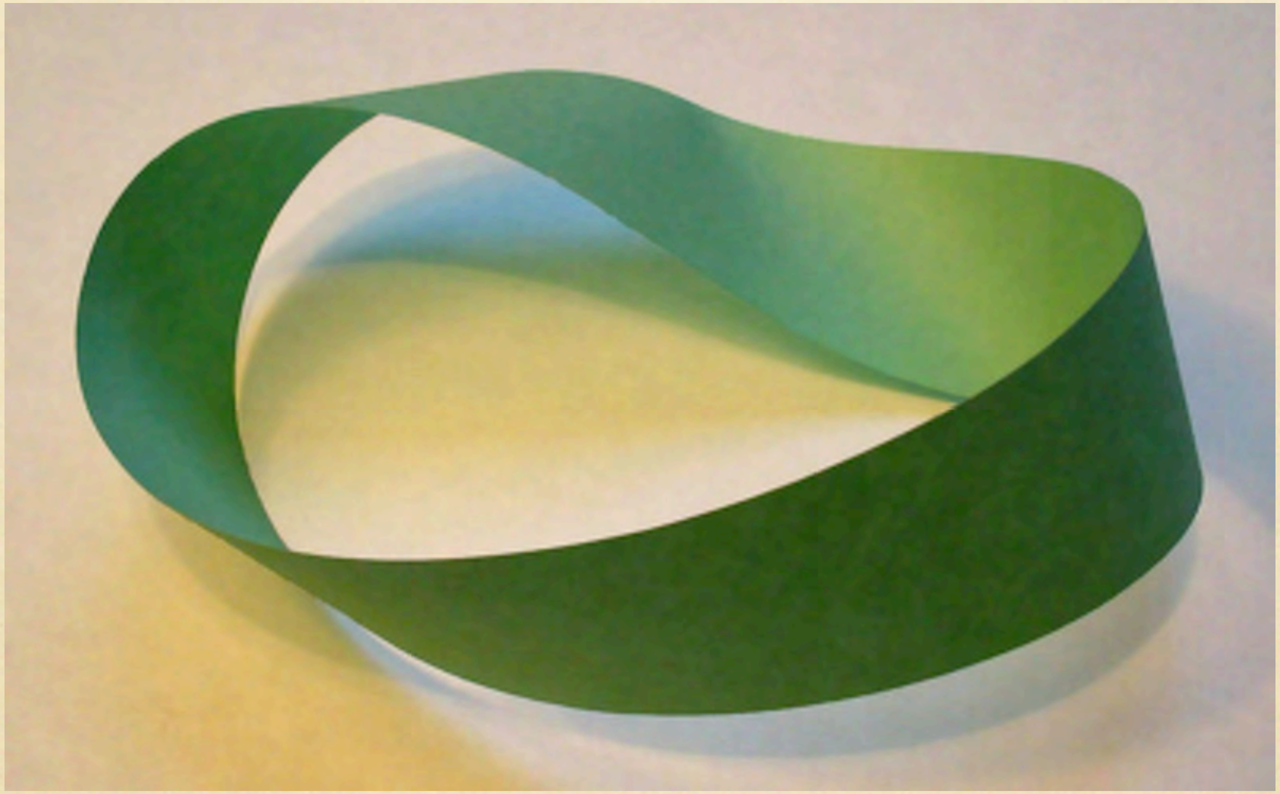
241 bp
676 bp







The double Helix Determines the Shape of Small DNA Circles



Asphericity

Gyration Tensor

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

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

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

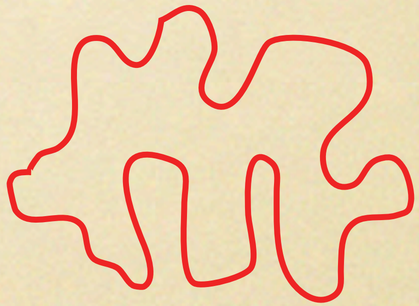
$$A_2 = \frac{(\lambda_2 - \lambda_1)^2}{(\lambda_1 + \lambda_2)^2} \qquad A_2 = \left\langle \frac{(\lambda_2 - \lambda_1)^2}{(\lambda_1 + \lambda_2)^2} \right\rangle$$

Results for Circular DNA

Theoretical Values	Ring SAW 0.206	Ring RW 0.279	Bishop 1988

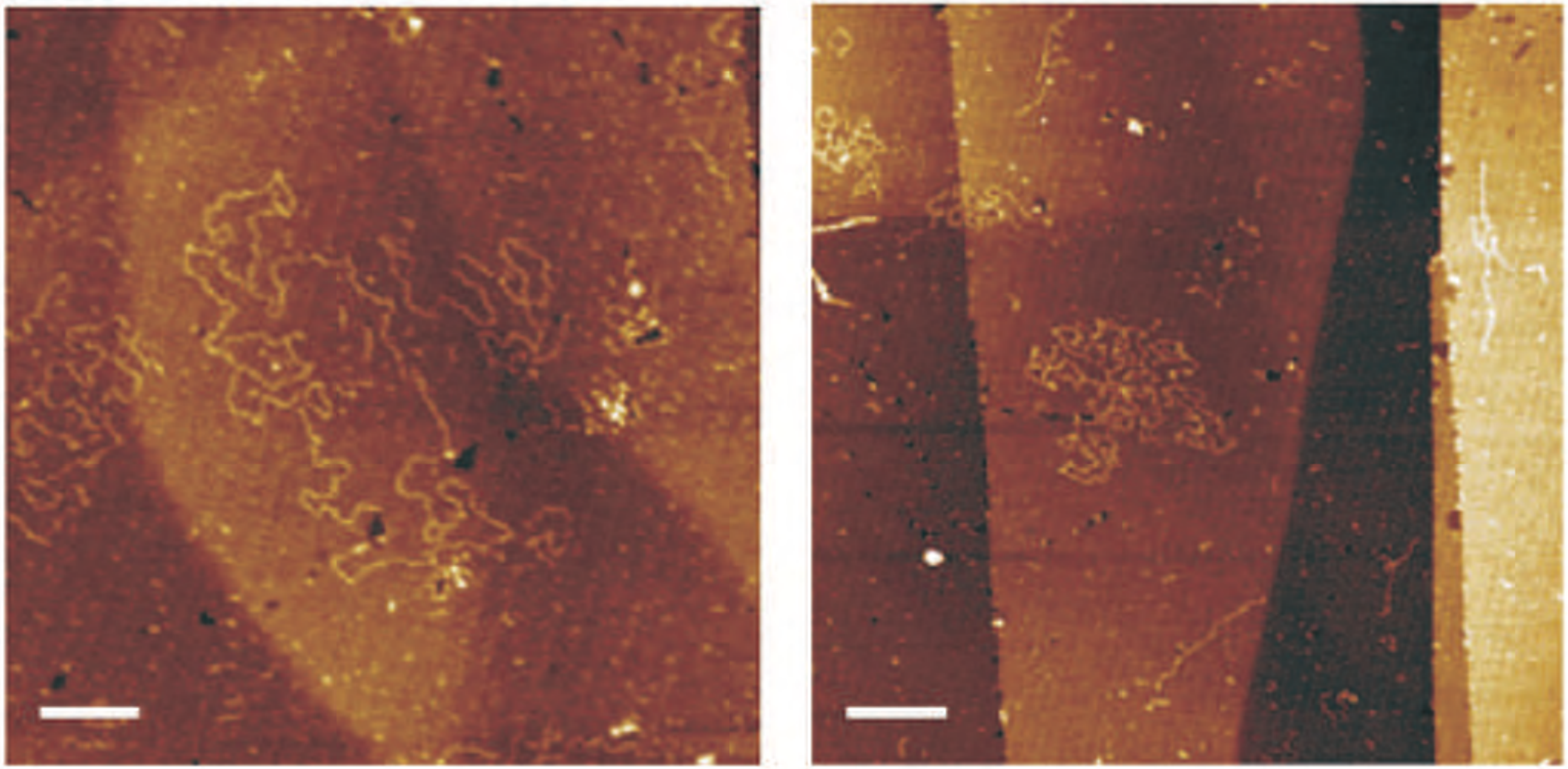
Experimental Values

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



2 D Properties of circular ssDNA : one length (sorry !)

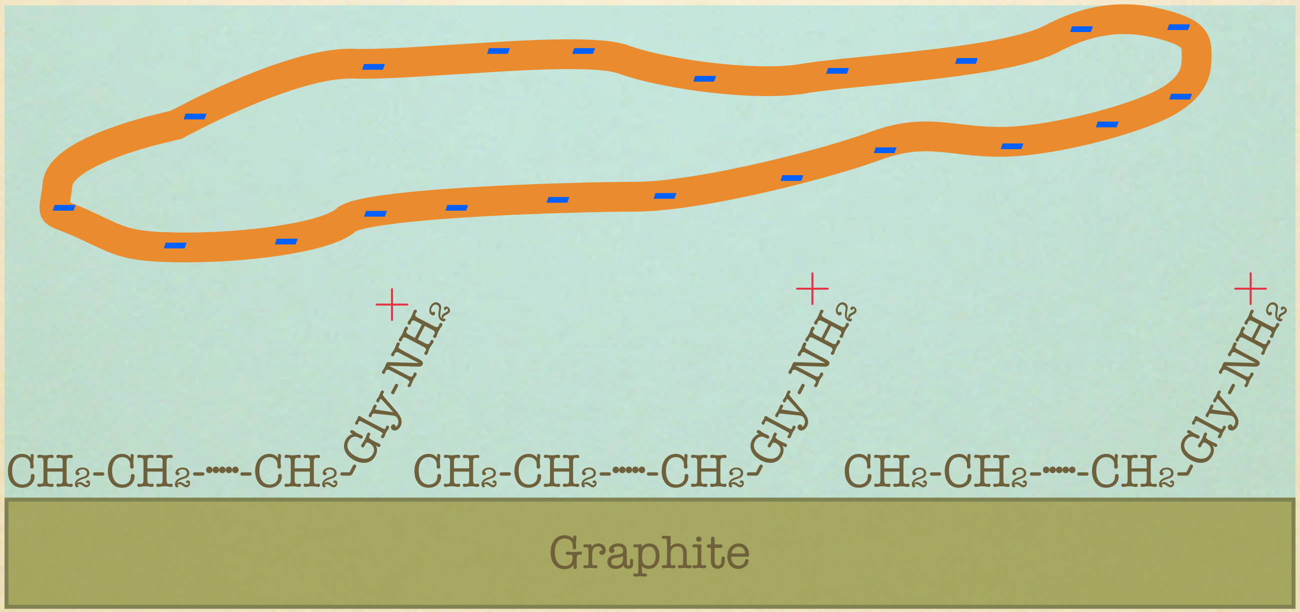
AFM Images of ssDNA



100 nm 0 mM NaCl 100 nm 10 mM NaCl

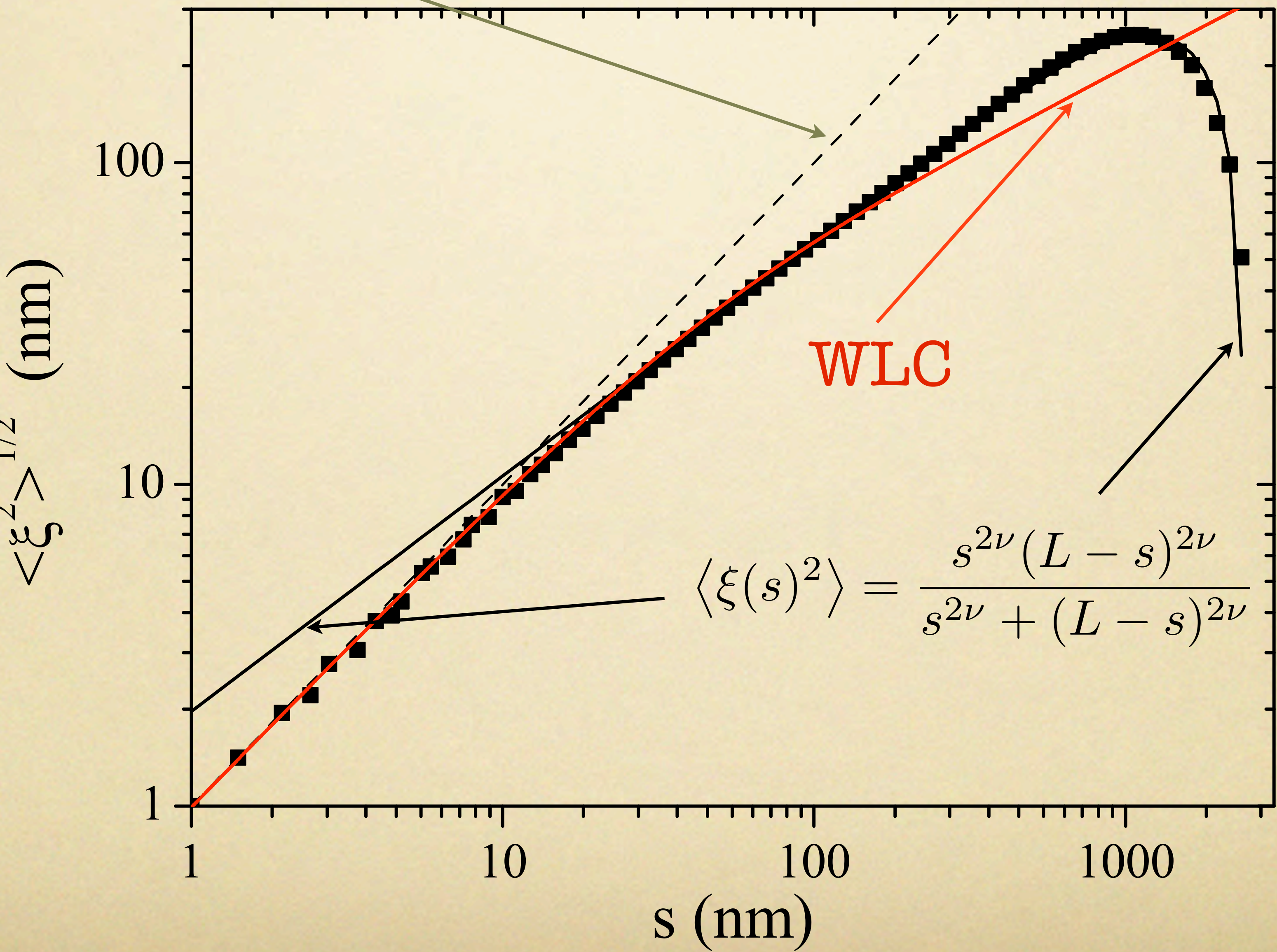
Virion ϕ x174 : 5386 bp 10 mM Tris-HCl buffer, pH 7.8

2 D deposition of ssDNA



Internal End-to-End Distance

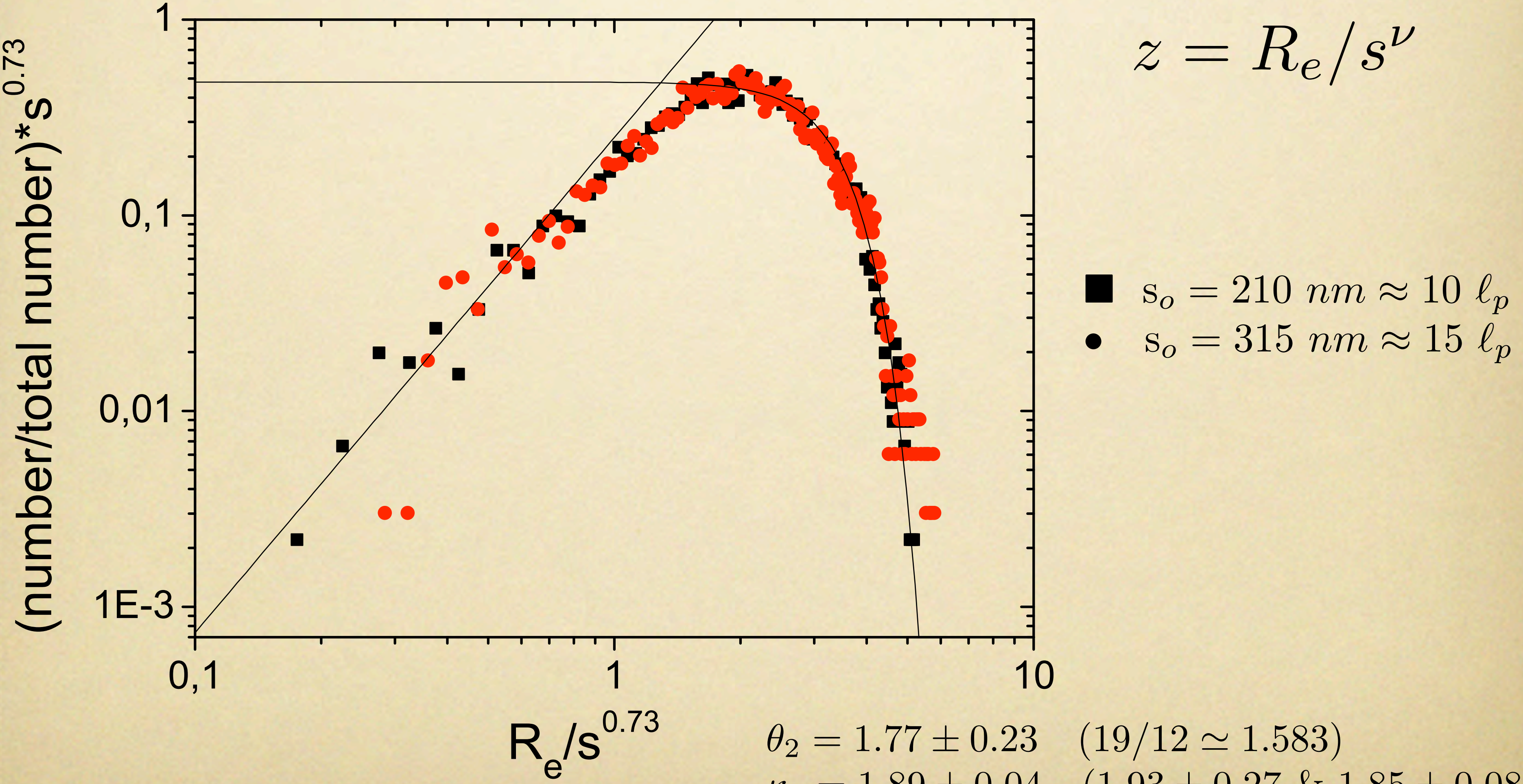
Rigid Rod Regime (RRR)



Distribution of the Internal End-to-End Distance for s large >> lp

$$f_s(z) = \begin{cases} a z^{d-1+\kappa} \exp(-b z^{\delta}) & \text{if } z \gg 1, \\ c z^{d-1+\theta_2} & \text{if } z \ll 1 \end{cases}$$

$$z = R_e / s^{\nu}$$

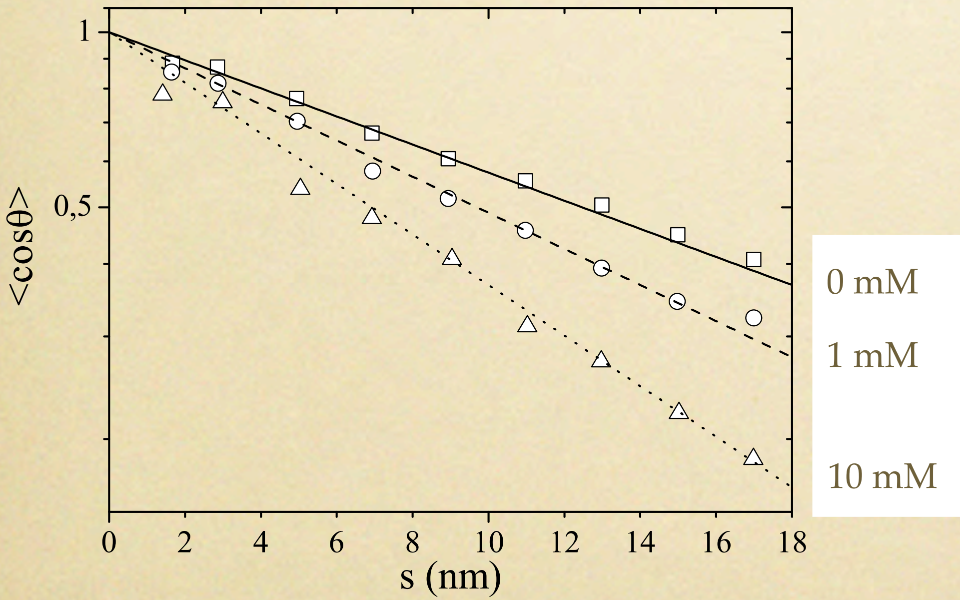


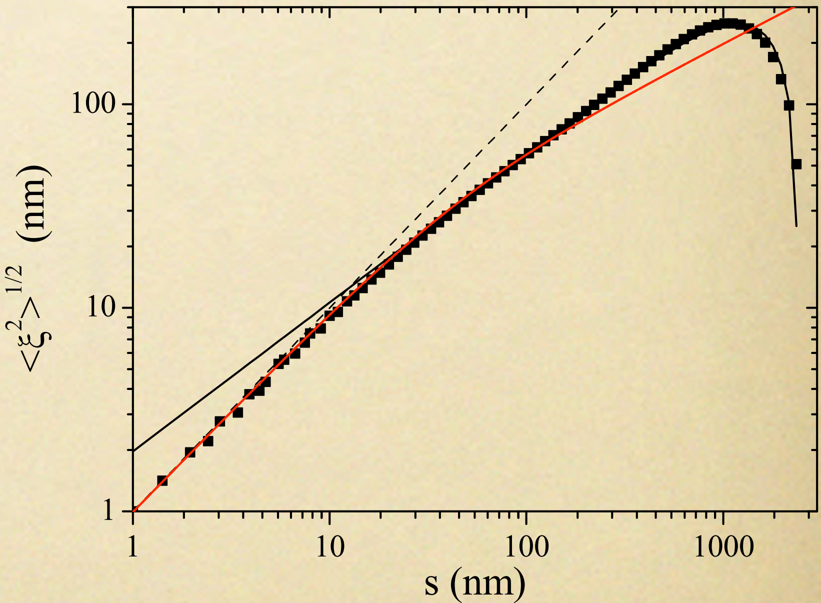
$\theta_2 = 1.77 \pm 0.23 \quad (19/12 \simeq 1.583)$

$\kappa_2 = 1.89 \pm 0.04 \quad (1.93 \pm 0.27 \ \& \ 1.85 \pm 0.08)$

Persistence Length from small s (approx lp)

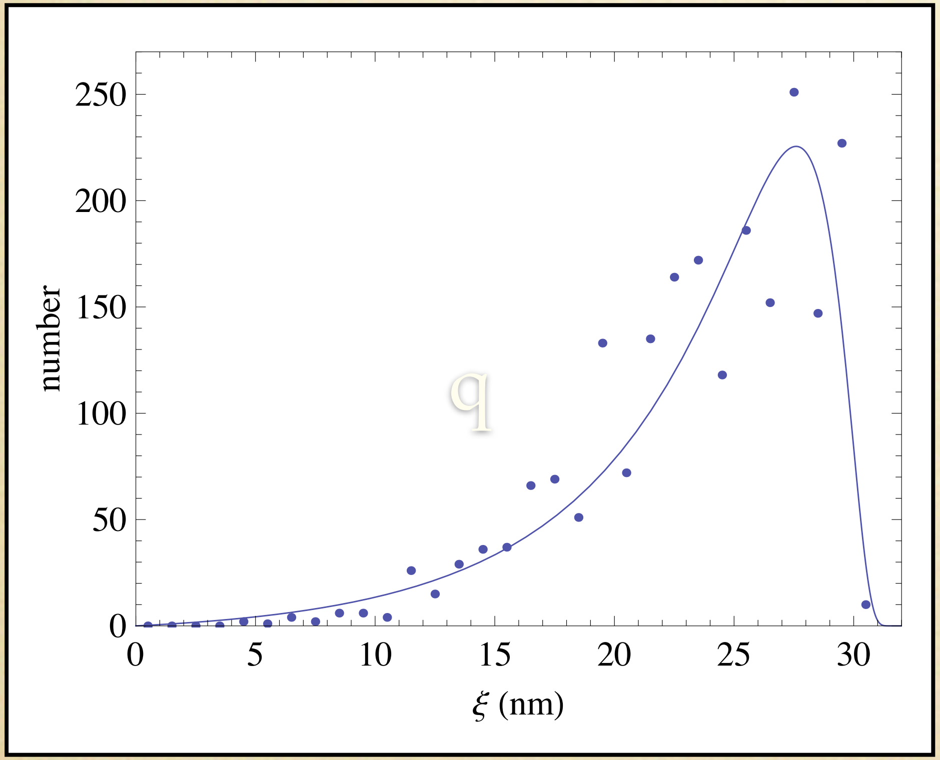
- Correlation Function
- End-to-End Distance
- Ent-to-End Distance Distribution





Persistence Length

- Correlation Function
- End-to-End Distance
- End-to-End Distance Distribution



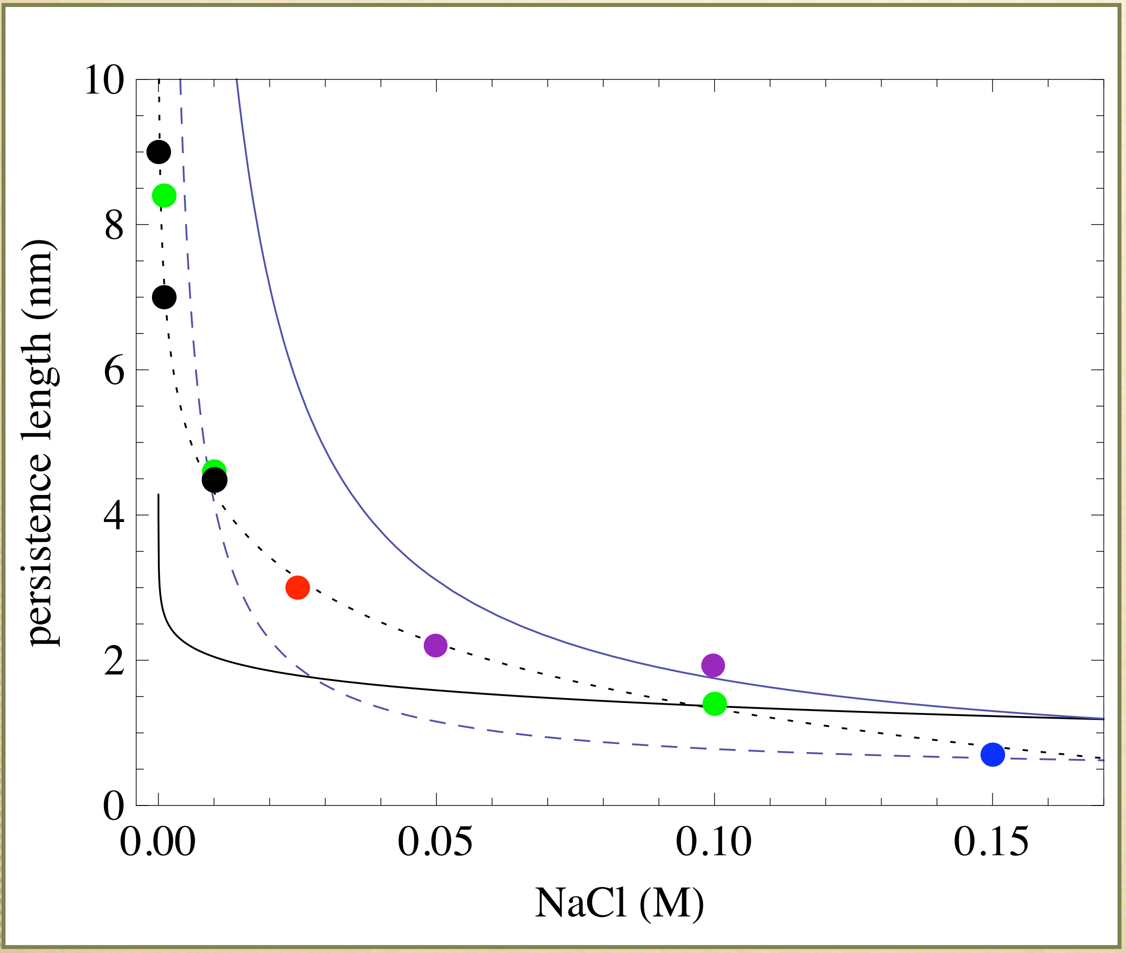
s = 32 nm ~ 5 lp

$$G(r) = \frac{1}{2\pi\mathcal{N}}\frac{2\kappa}{\sqrt{\pi}}\sum_{\ell=0}^{\infty}\frac{(2\ell-1)!!}{2^{\ell}\ell!}\frac{1}{[2\kappa(1-r)]^{5/4}} \times exp\left[-\frac{(\ell+1/4)^2}{2\kappa(1-r)}\right] D_{3/2}\left[2\frac{\ell+1/4}{\sqrt{2\kappa(1-r)}}\right]$$

$$\ell_p = \frac{2\kappa}{k_B T}$$

Wilhem & Frey, PRL, **77**, 2581 (1996)

Persistence Length vs. salt concentration



Experiments

- Present Work
- Tinland, Pluen, Sturm, Weill
- Murphy, Rasnik, Cheng, Lohman, Ha
- Smith, Cui, Bustamante

Theory

- Manning, 1996
- Odijk, 1977
- Toan & Micheletti, 2006

Collaborators

- Francesco Valle, ISMN CNR, Bologna
- Mélanie Favre, EPFL
- Jozef Adamcik, EPFL
- Erika Ercolini, EPFL
- Guillaume Witz, EPFL
- Kristian Rechendorff, EPFL
- Paolo De Los Rios, EPFL
- Ralf Metzler, TU Munich
- Joaquim Roca, Barcelona
- Andrzej Stasiak, Uni Lausanne
- Erwin Frey, LMU, Munich
- Bertrand Duplantier, Ecole Polytechnique, Paris
- Hirofumi Wada, Kyoto University,

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