DNA INSPIRED PHYSICS

Sanjay Kumar
Department of Physics
Banaras Hindu University
Varanasi - 221005

Collaborators:

Garima Mishra
Rakesh Kumar Mishra
Ravinder Kumar
Sadhana Singh
Anurag Mishra
W. Janke
D. Giri
SM Bhattacharjee

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Simons Foundation, ICTP, Italy

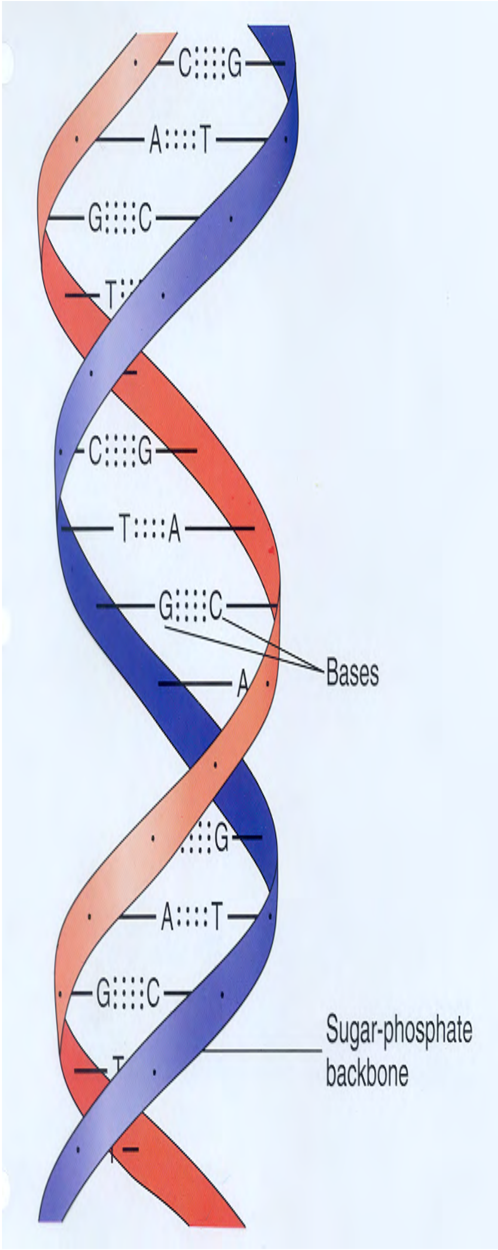
Thanks: Y. Singh, D. Dhar

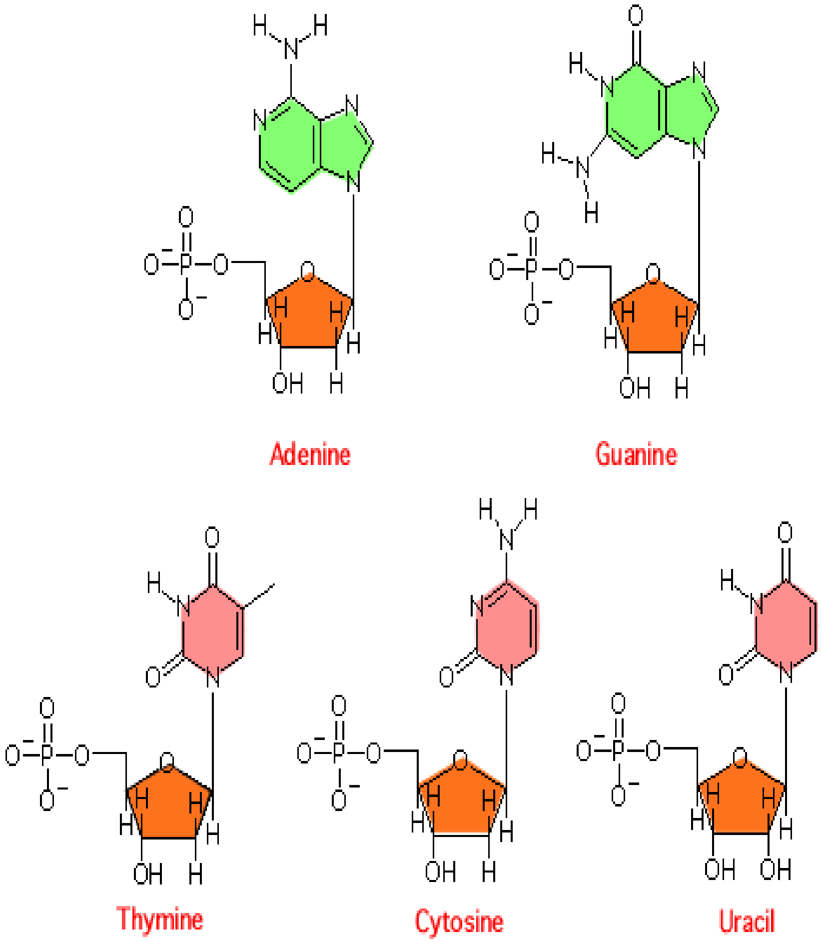
DNA

Fundamental building blocks

DNA

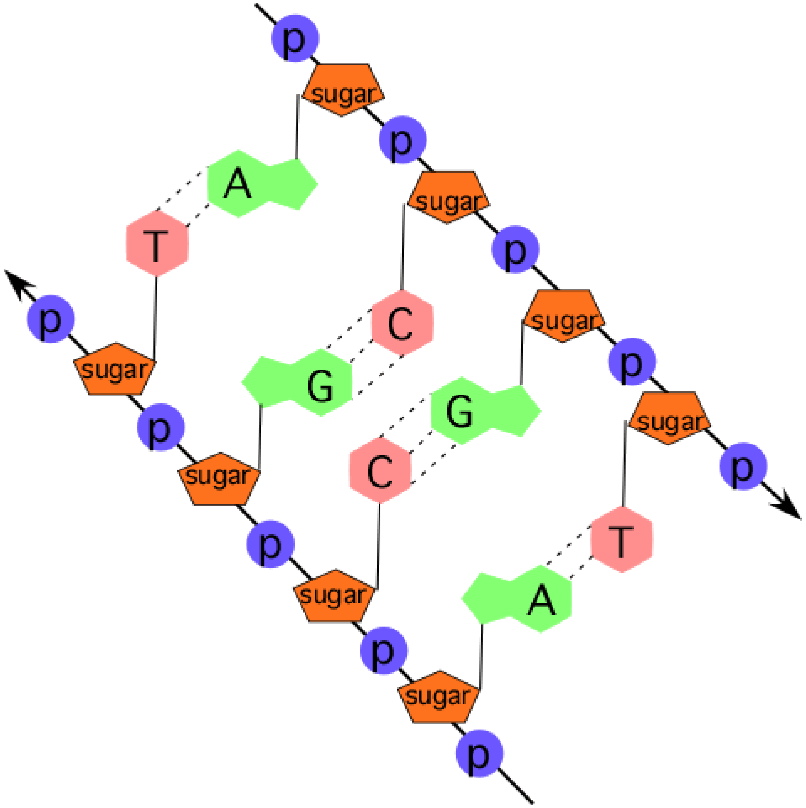
Combination of chemical species





DNA

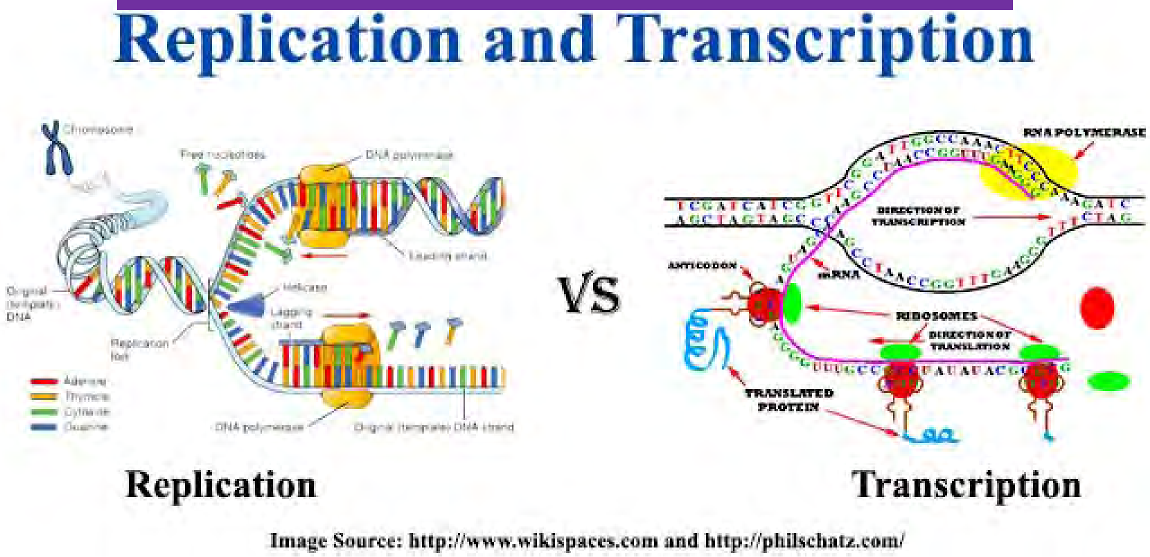
A tool by which theoretical models can be tested and that gives you the predicting power

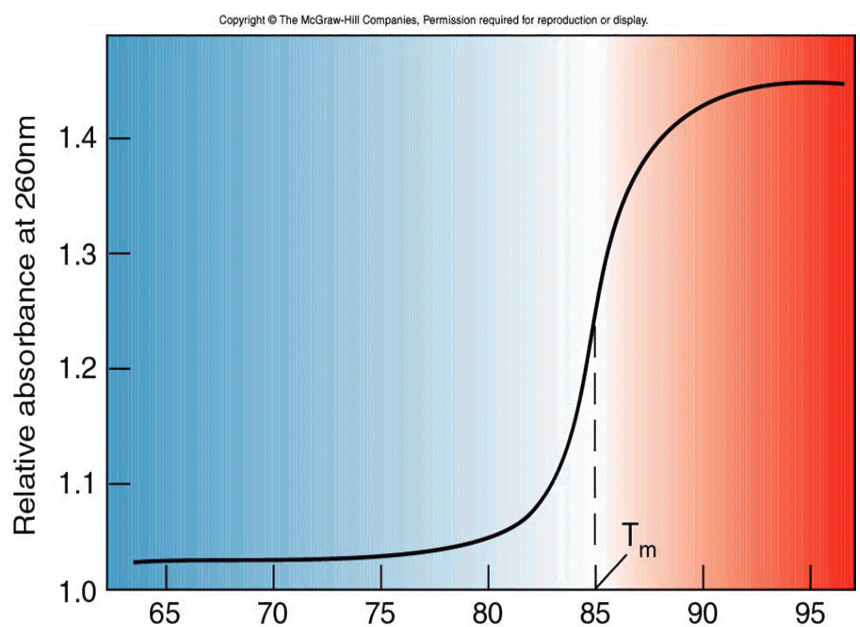


Outline

- Introduction
- Motivation
- Models
- Methods
- Brief Review of work@BHU

Two important biological processes



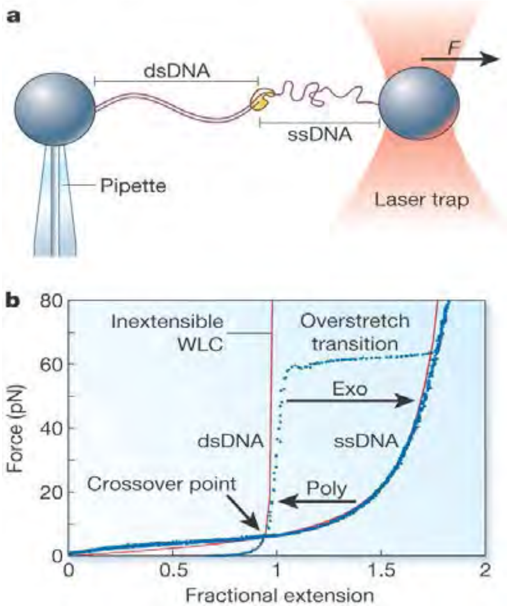



Nucleus
www.FreeScienceLectures.com

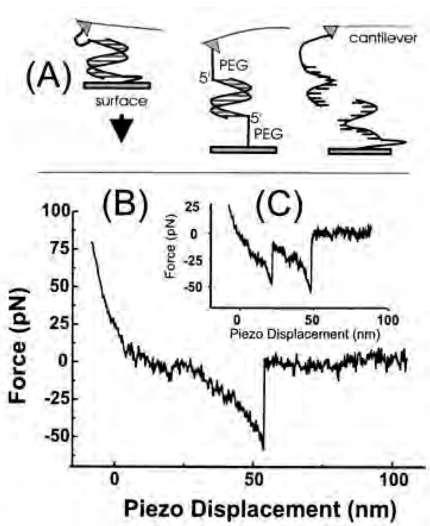
Single molecule force spectroscopy

Arthur Ashkin’s optical tweezers: the Nobel Prize-winning technology that changed biology.

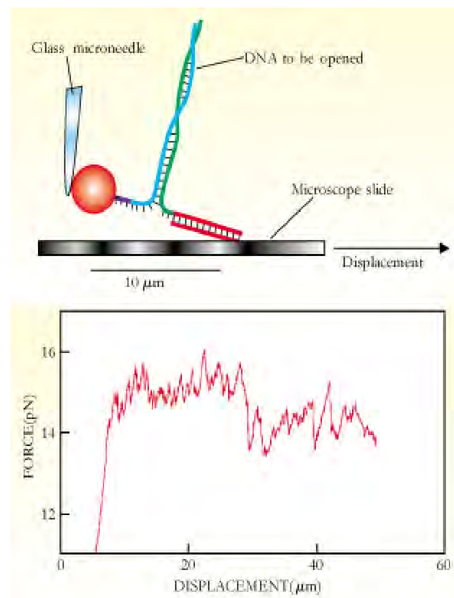
Force has been used as a thermodynamic parameter



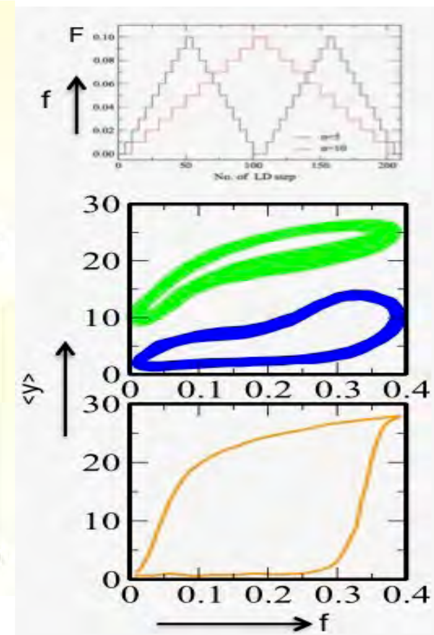
Rief et al. Science, **276**, 1112, (1997)
Bustamante et al. Nature, **421**, 423, (2003)



Lee et al. Science, **266**, 771 (1994)
Strunz et al PNAS, **96**, 11277, (1999)

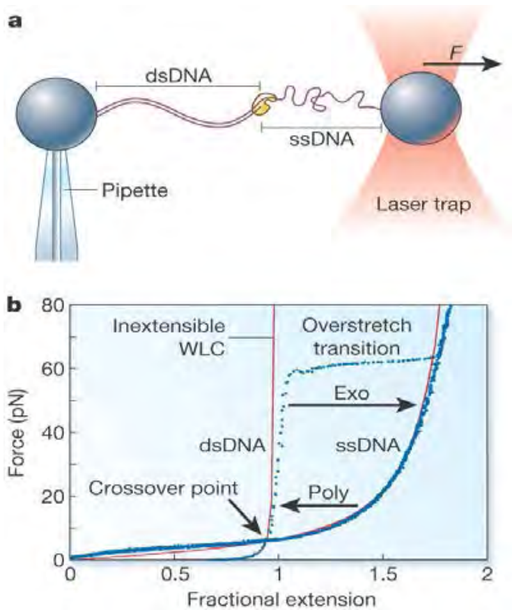


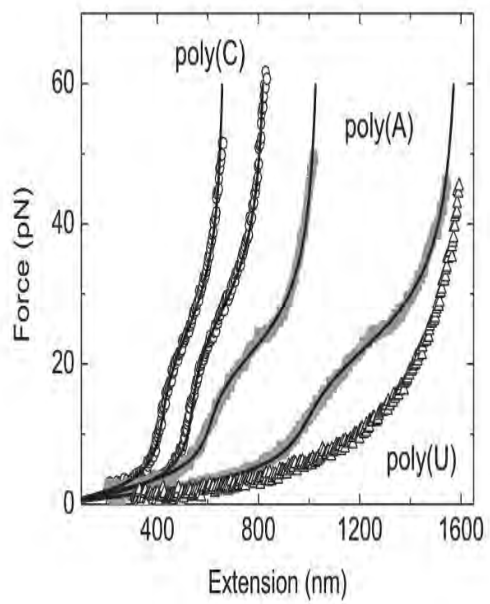
Bockelmann et al. Phys. Rev. Lett. **79**, 4489 (1997)

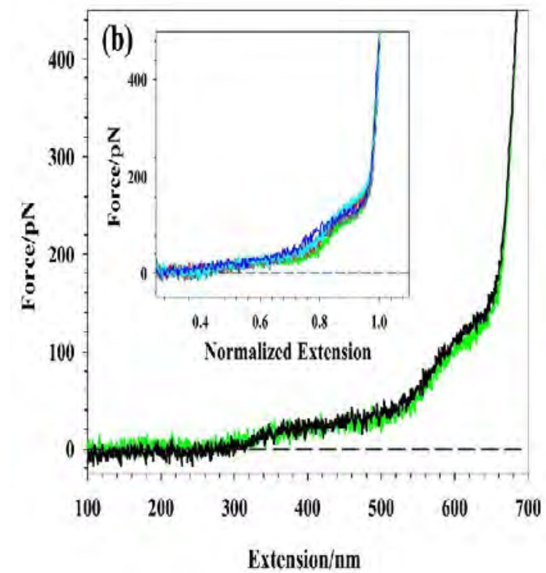


Kumar & Mishra Phys. Rev. Lett. **100,** 258102 (2013)

DNA Stretching: ssDNA





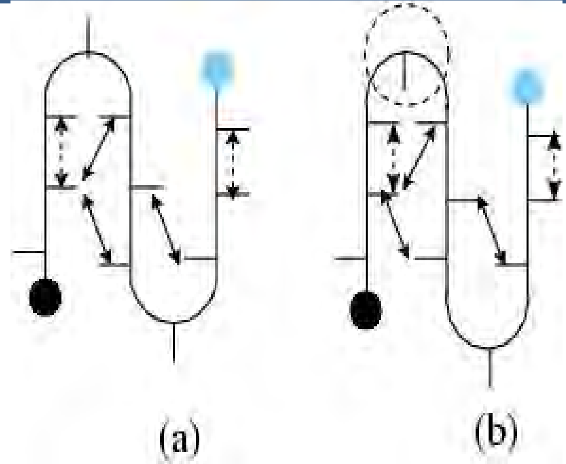


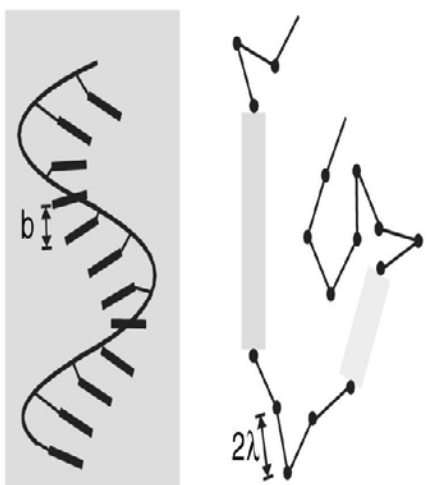
Rief et al. Science, **276**, 1112 (1997)
Bustamante et al. Nature, **421**, 423 (2003)

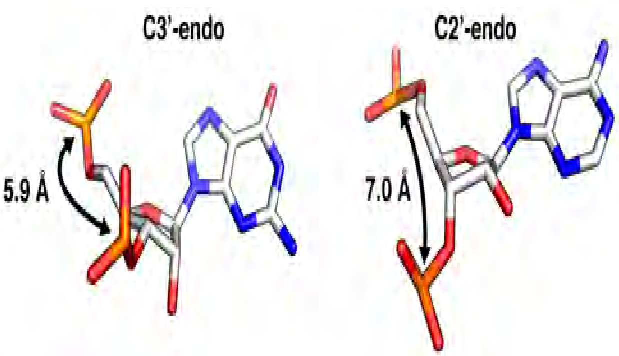
Seol et al. Phys. Rev. Lett. **98**, 158103 (2007)

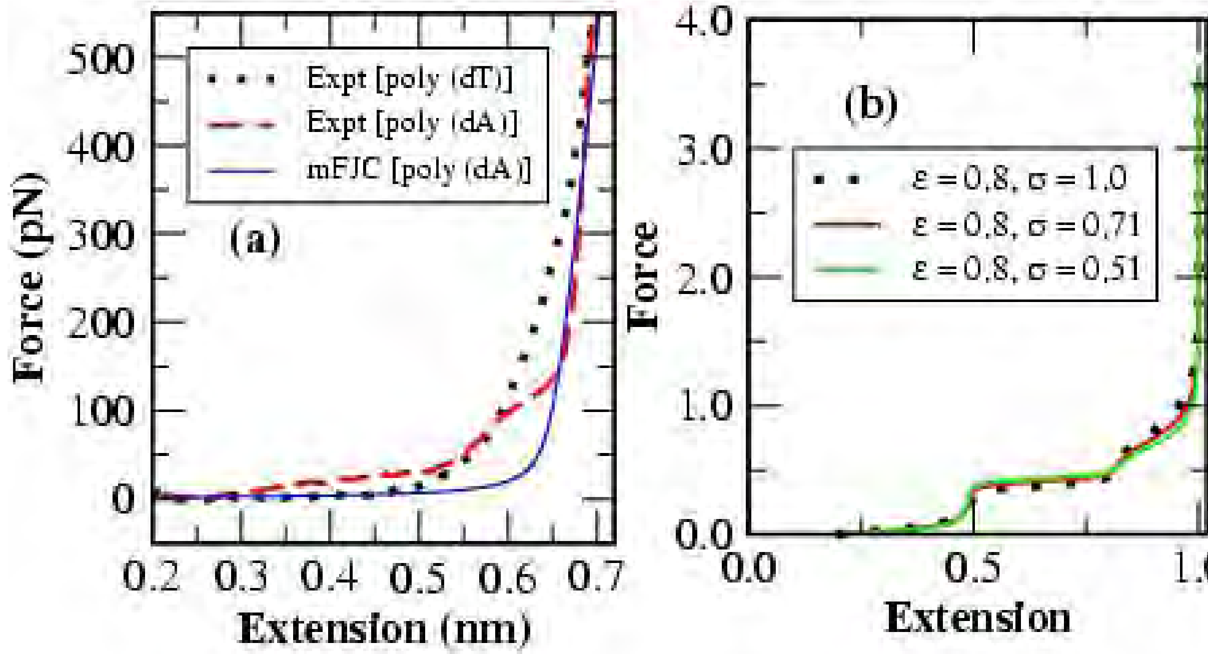
Ke et al. Phys. Rev. Lett, **99**, 018302, (2007)

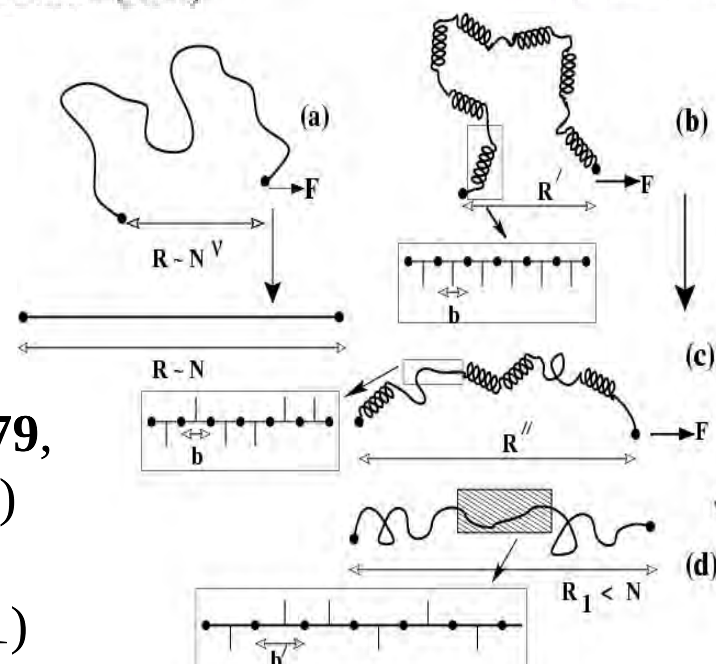
DNA Stretching: Evidence of Structural Transition





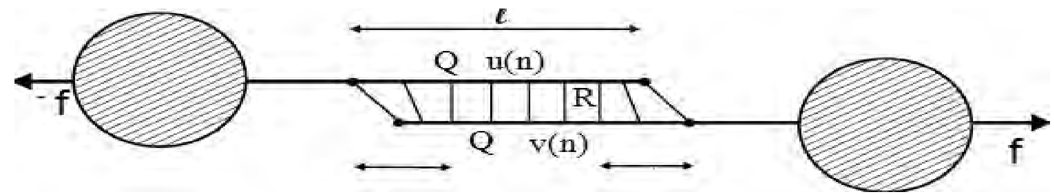






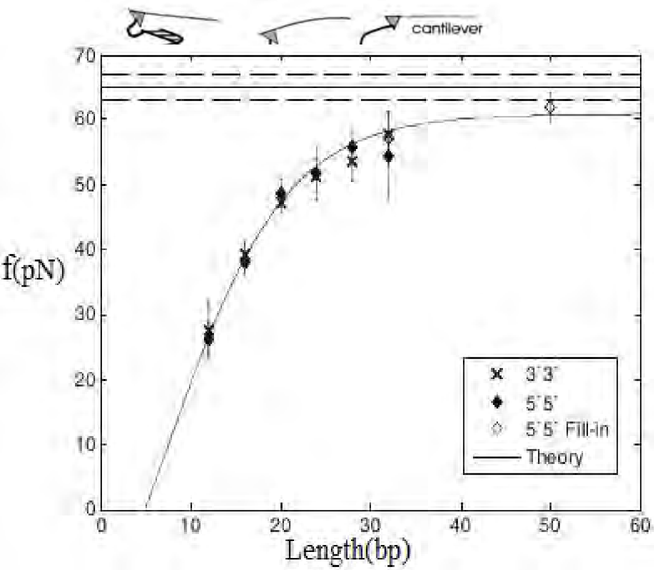
Phys. Rev. E **79**, 031930 (2009)
Soft Matter **7**, 4595 (2011)

Stretching of dsDNA Rupture: Rupture



Q= Elastic constant for the backbone

R= Elastic constant for base pairs



$$H = \sum_{-l/2}^{\infty} \tfrac{1}{2} Q(u_{n+1} - u_n)^2 + \sum_{-\infty}^{l/2} \tfrac{1}{2} Q(v_{n+1} - v_n)^2$$

$$+ \sum_{-l/2}^{l/2} \tfrac{1}{2} R(u_n - v_n)^2$$

Lee et.al. Science, **266**, 771 (1994)

Strunz et al PNAS, **96**, 11277, (1999)

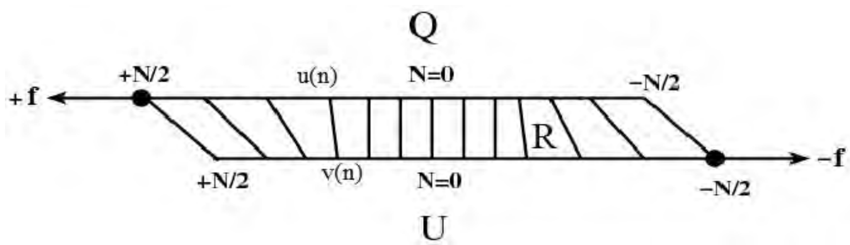
Hatch *et al.* Phys. Rev. E **78**, 011920(2008)

$$f_c = 2 f_1 (\chi^{-1} \tanh(\chi \frac{l}{2}))$$

$$\chi^{-1} = \sqrt{Q/2R}$$

de Gennes, C. R. Acad. Sci. Paris, **1505** (2001)

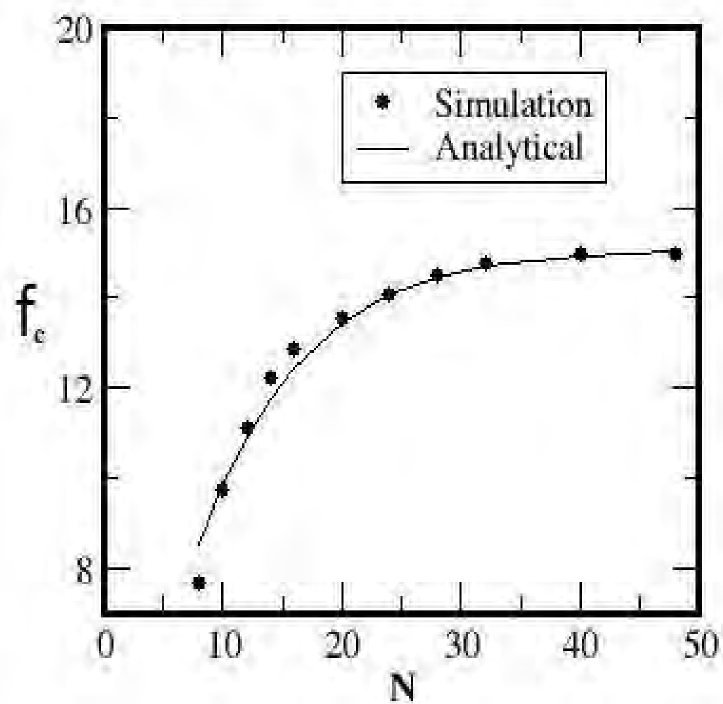
Stretching of dsDNA Rupture: Rupture



$$H = \sum_{n=-N/2}^{\infty} \tfrac{1}{2} Q(u_n - u_{n+1})^2 + \sum_{-\infty}^{N/2} \tfrac{1}{2} U(v_n - v_{n+1})^2 + \sum_{n=-N/2}^{N/2} \tfrac{1}{2} R(v_n - u_n)^2$$

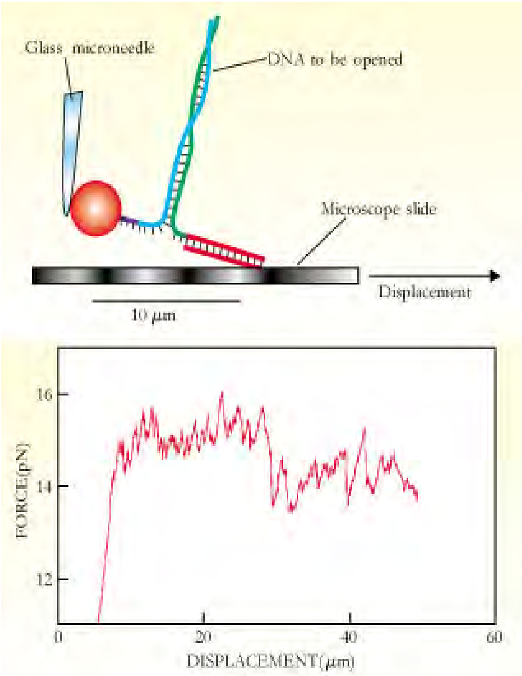
$$\frac{f_C}{f1} = \frac{2\tanh\left(\frac{\chi N}{2}\right)}{\chi\left(1 + \frac{(Q-U)}{(Q+U)}\left[\frac{\chi + \tanh\left(\frac{\chi N}{2}\right)}{1 + \chi \tanh\left(\frac{\chi N}{2}\right)}\right]\tanh\left(\frac{\chi N}{2}\right)\right)}$$

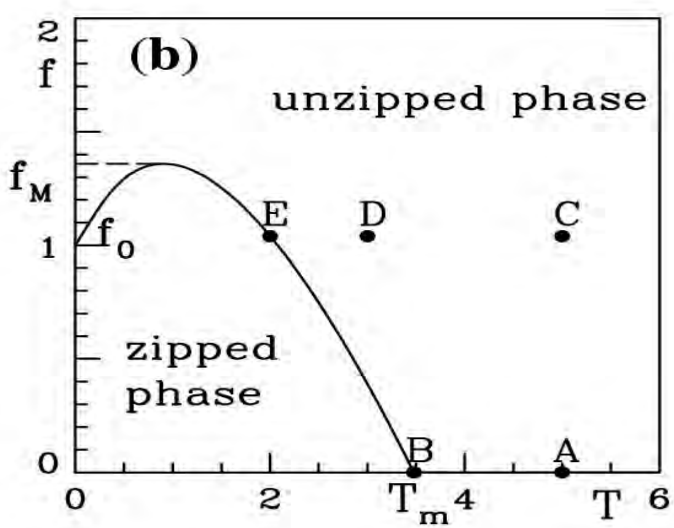
$$\chi^{-1} = \sqrt{\frac{QU}{R(Q+U)}}$$

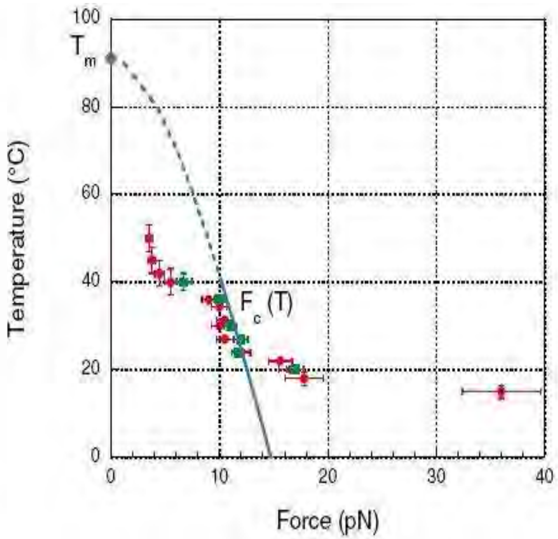


J. Chem. Phys, ,**139**, 165101 (2013)

DNA unzipping: puzzle, solution and more







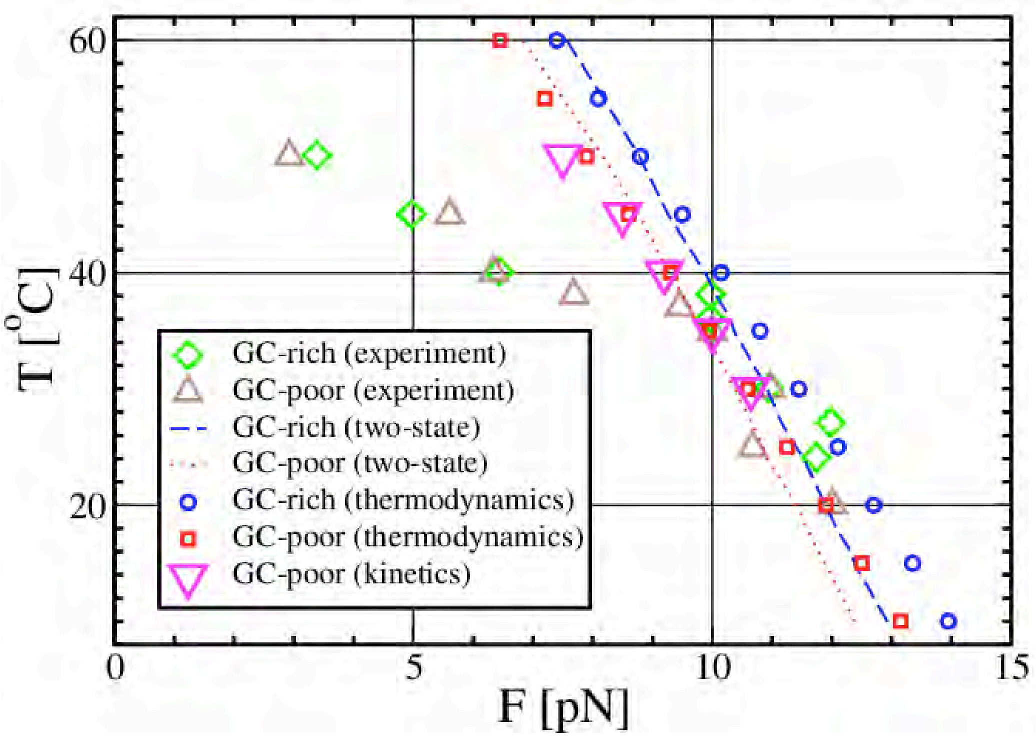
Bockelmann et al. Phys. Rev. Lett. **79**, 4489, 1997

Marenduzzo et al, Phys. Rev. Lett. **88** 28102 (2002)

C. Danilowicz *et al*, Phys. Rev. Lett. **93**, 078101, 2004

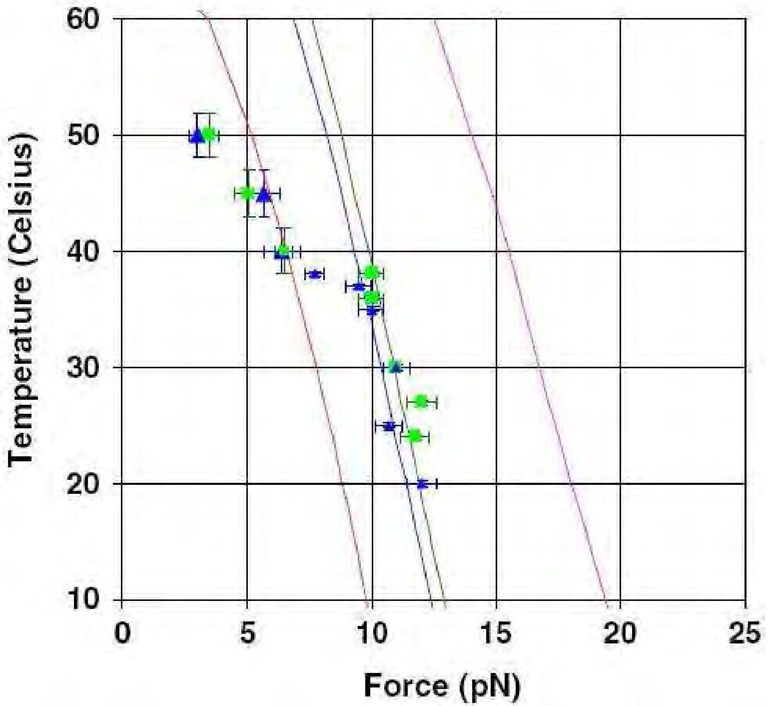
Theoretical efforts

Equilibrium effect



Bundschuh and Gerland
EPJE **19**, 347, 2006

Sequence effect



C. H. Lee *et al,*
EPJE **19**, 339, 2006

Comment

A puzzle in DNA biophysics

R. Bundschuh[1,a] and U. Gerland[2]

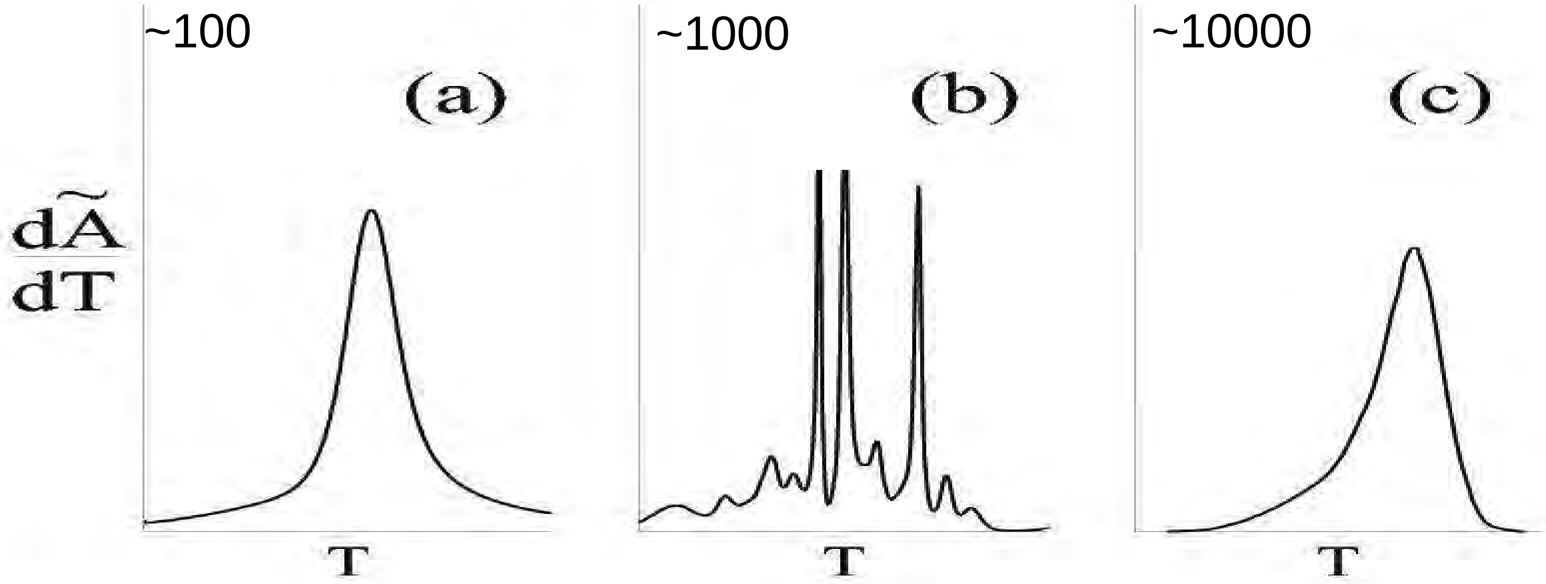
[1] Department of Physics, The Ohio State University, 191 W. Woodruff Avenue, Columbus, OH 43210-1117, USA
[2] Arnold-Sommerfeld Center for Theoretical Physics and Center for Nanoscience (CeNS), LMU München, Theresienstrasse 37, 80333 München, Germany

Received 20 December 2005 /
Published online: 13 February 2006 –

Abstract. In this issue, Lee *et al.* report the experimental temperature-dependence of the unzipping force for two natural DNA sequences. For both sequences, the curves show an anomaly at temperatures around 40 °C. In this brief contribution, we stress that the anomaly is not easily explained within the established theoretical models for the biophysics of DNA. As this puzzle questions our basic understanding of DNA, it must be resolved, most likely by a combination of additional experiments and new theoretical work.

PACS. 87.14.Gg DNA, RNA

Role of loop entropy



Blossey and Carlon
Phys. Rev. E **68**, 061911(2003)

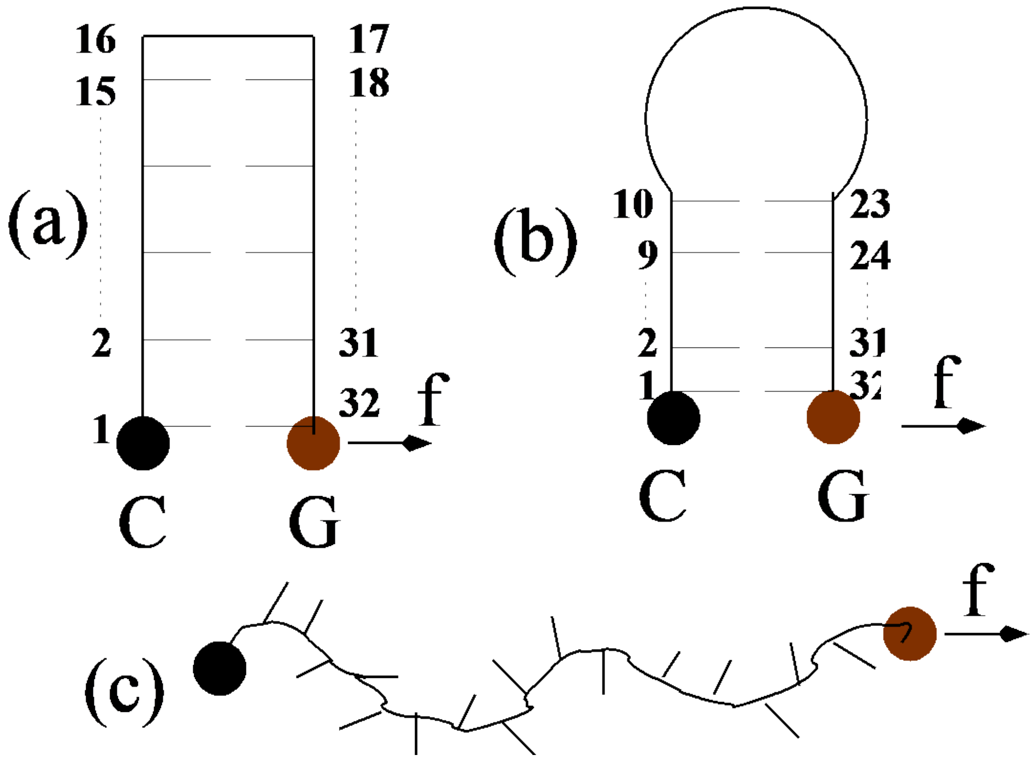
- Loop entropy play an important role.
- Stretched state must be taken in account and the bond length should not be fixed.

dsDNA *vs* DNA hairpin

- **One can study a long chain with implicit bubbles**

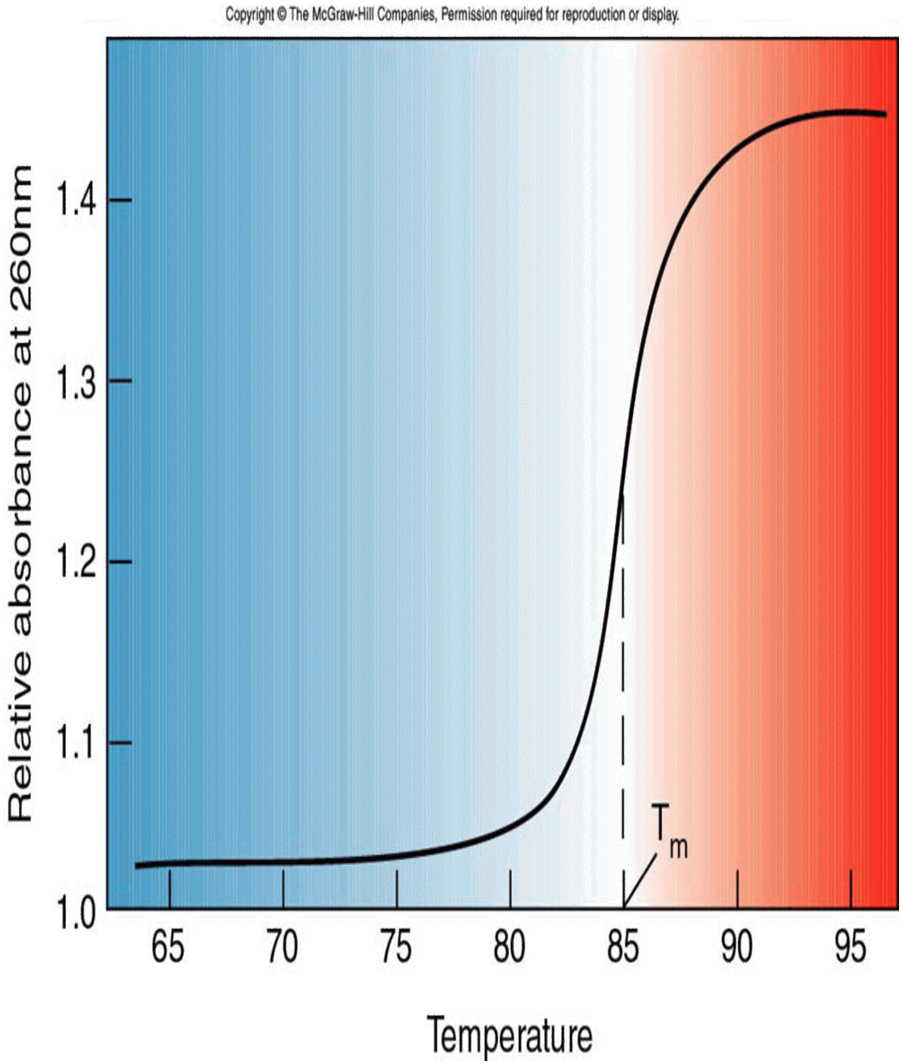
or

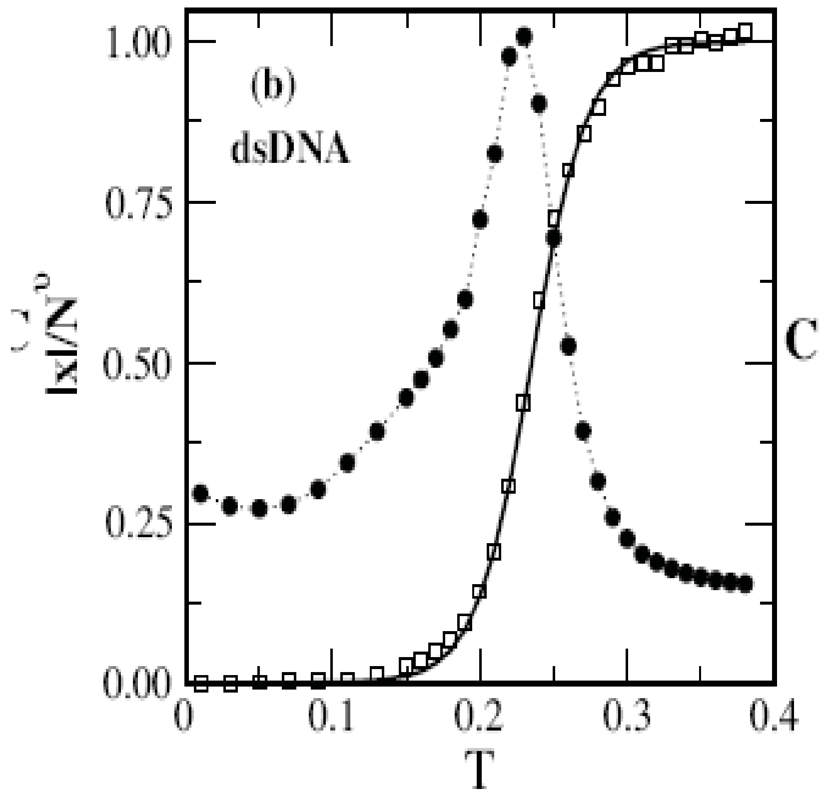
- **A premade bubble in the form of DNA hairpin in short chain.**



$$E = \sum_{i=1}^{N-1} k(d_{i,i+1} - d_0)^2 + \sum_{i=1}^{N-2} \sum_{j>i+1}^{N} 4\left(\frac{C}{d_{i,j}^{12}} - \frac{A_{ij}}{d_{i,j}^{6}}\right)$$

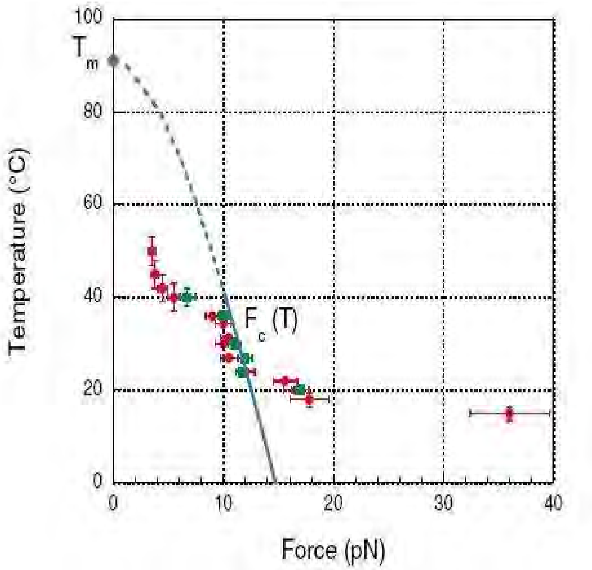
Melting Profile

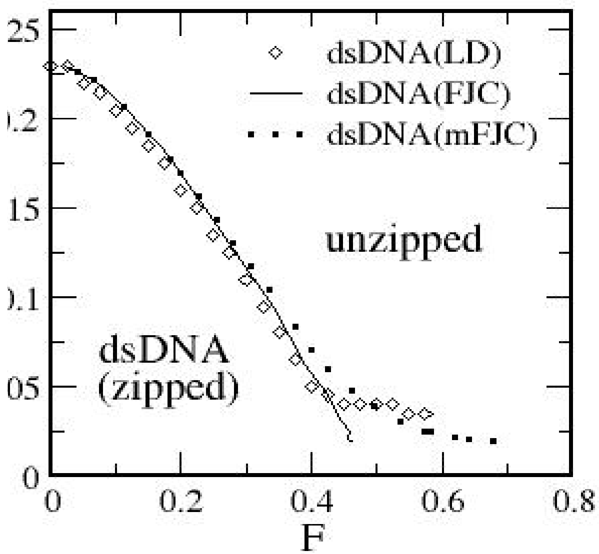


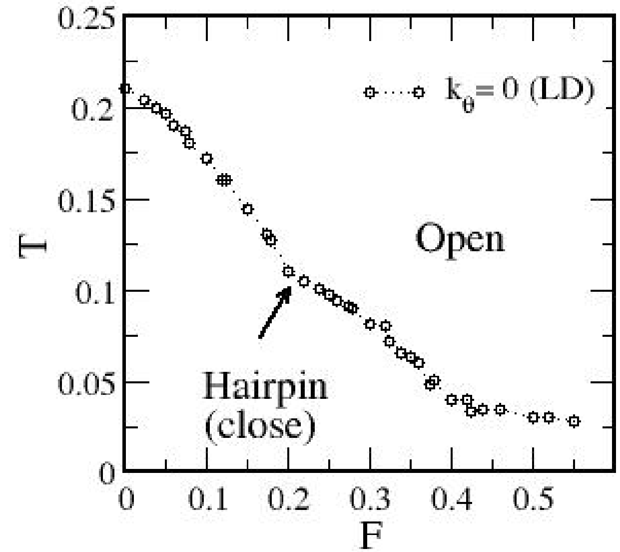


J. Chem. Phys. Vol. 135 035102 (2011)

Force-Temperature diagram for hairpin





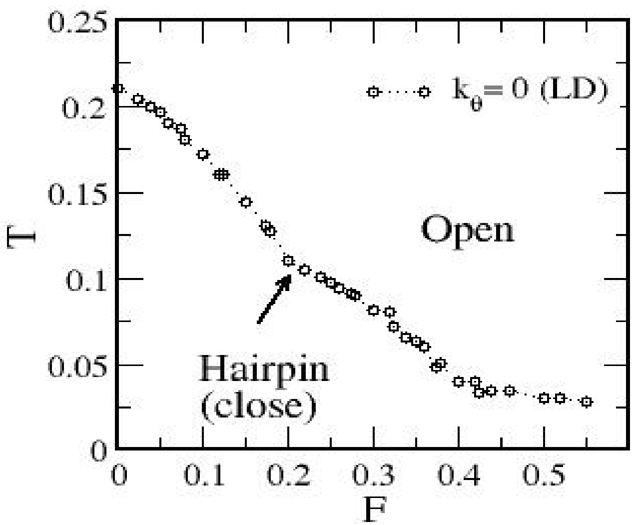


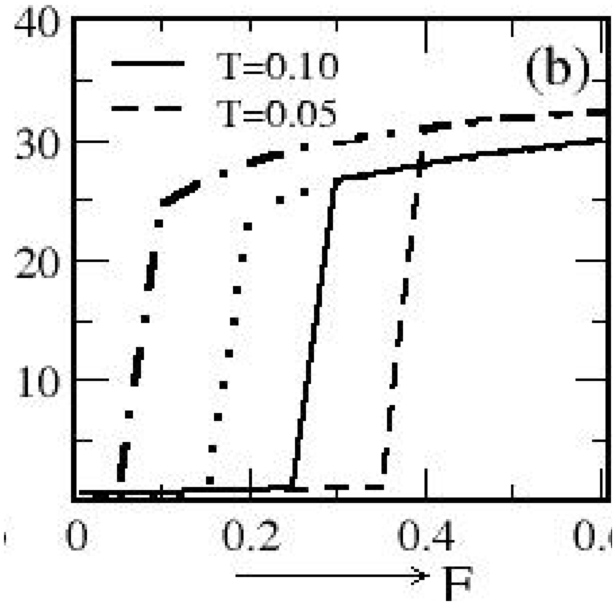
C. Danilowicz *et al*, Phys. Rev. Lett. **93**, 078101, 2004

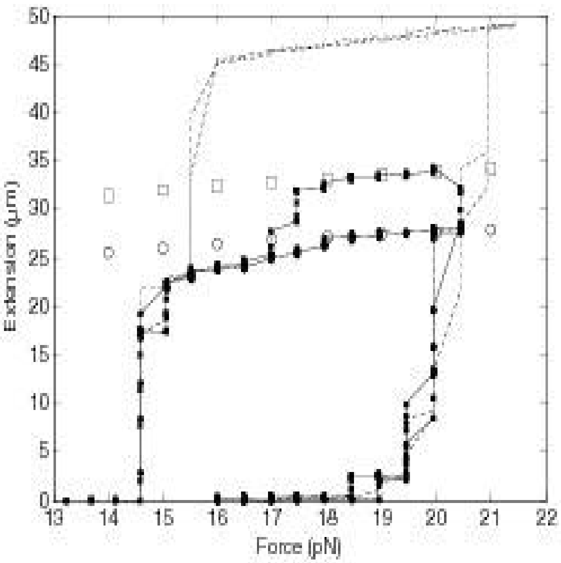
J. Chem. Phys **135,** 035102, 2011

A step forward

- Living systems are open systems and hence never at equilibrium.
- Biological processes such as transcription and replication *in vivo* occur at non-equilibrium condition.
- Part of the force temperature diagram exhibits hysteresis and thus further investigation in this reason may provide a better understanding of these processes.







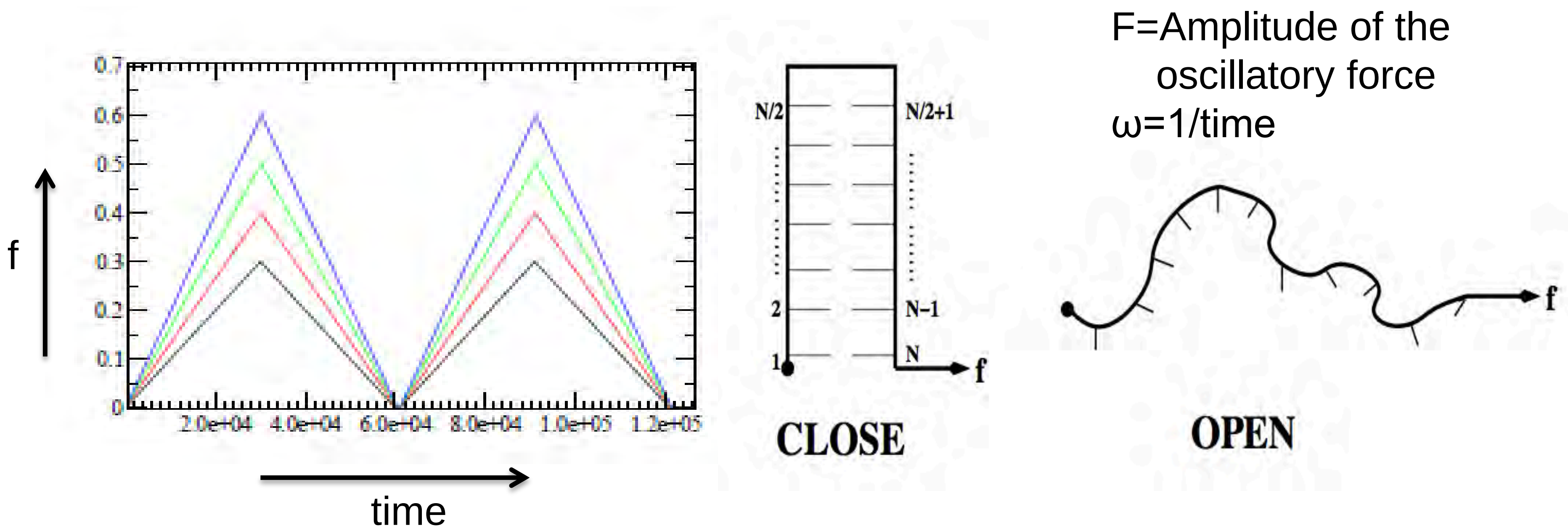
J. Chem. Phys
135, 035102, 2011

Hatch et al.
Phys. Rev. E
75, 051908, 2007

DNA under oscillatory force

In vivo, DNA is opened by helicases which are motors that move along the DNA. Both, the motion and the opening processes, require constant supply of energy. The periodic ATP consumption suggests that a helicase type molecular machine goes through cycles of action and rest, thereby creating an oscillatory, not steady, force on the DNA. In view of this, we focus our study on the effect of oscillatory force applied at one end of DNA.

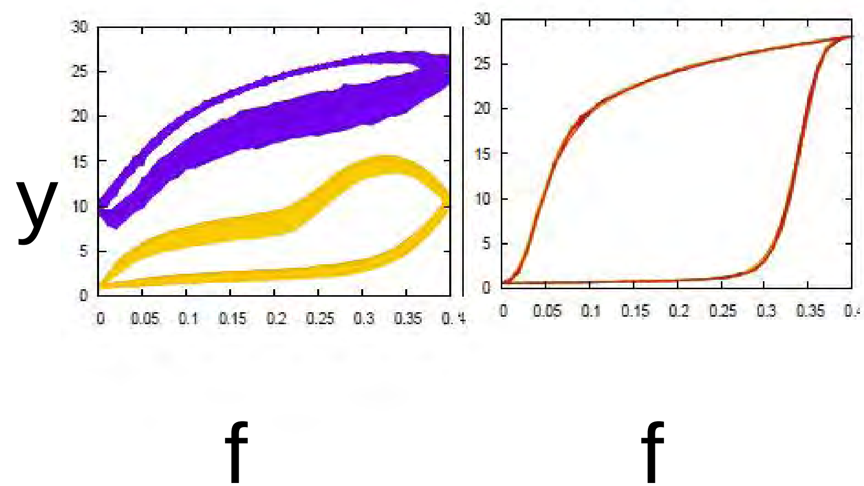
F=Amplitude of the oscillatory force
ω=1/time



Dynamical Order Parameter

The observable in presence of the applied force f(t) is the extension y(t). We define the dynamical order parameter as

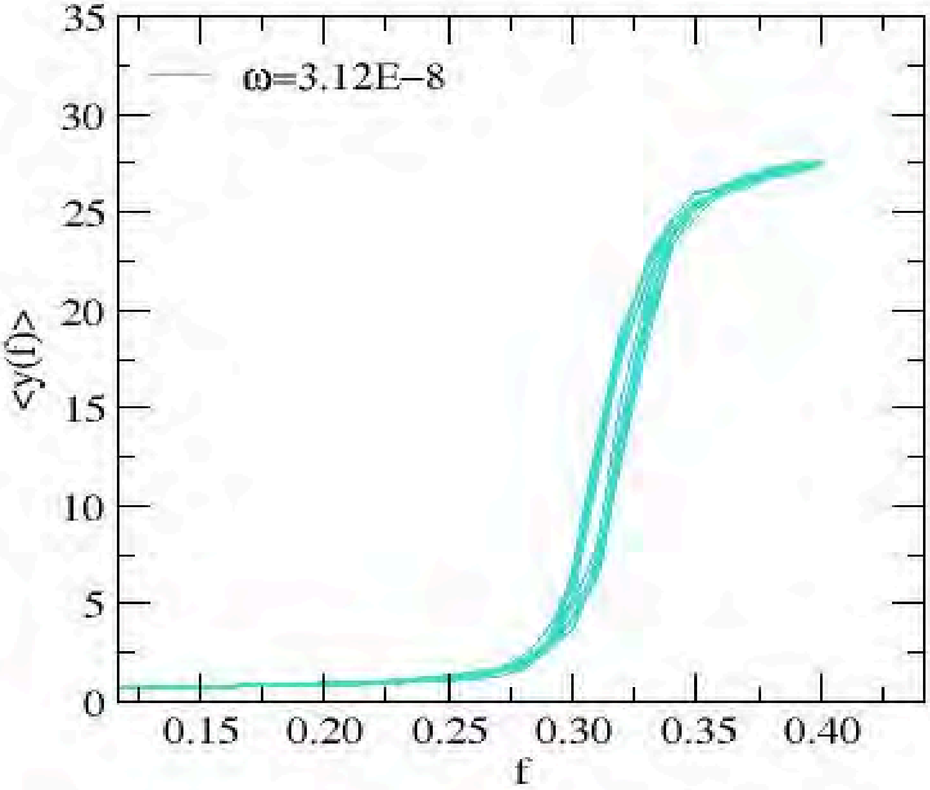
$$A = \oint y\, df$$

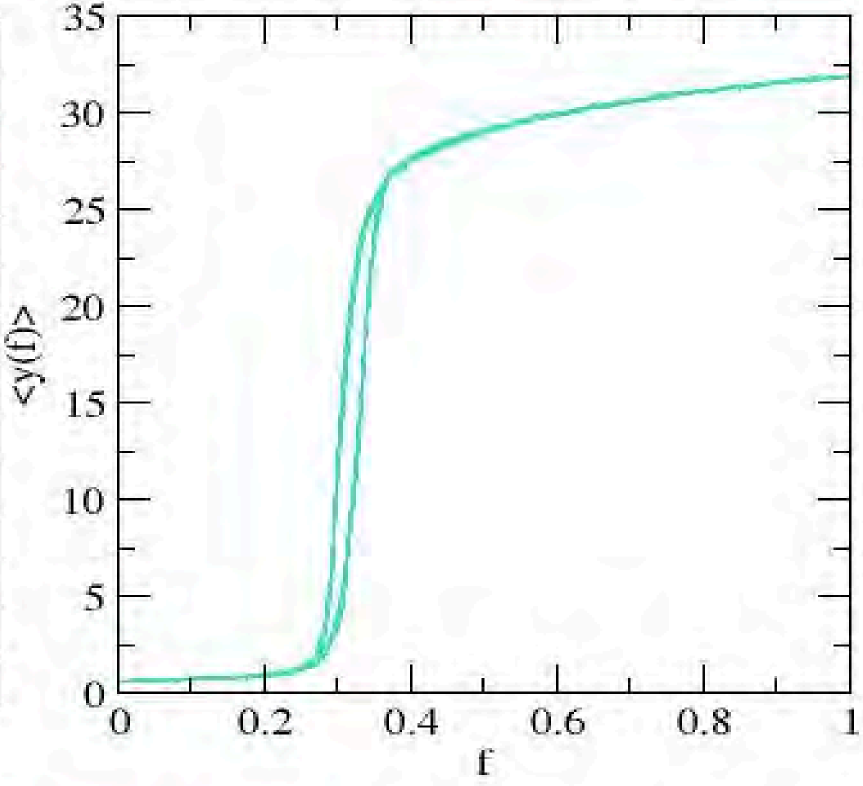


This is similar to the one defined in case magnetization under oscillatory field. Here f(t) and y(t) correspond to h(t) and m(t), respectively.

B. K.Chakrabarty,
Rev. Mod. Phys.
71, 847, (1999)

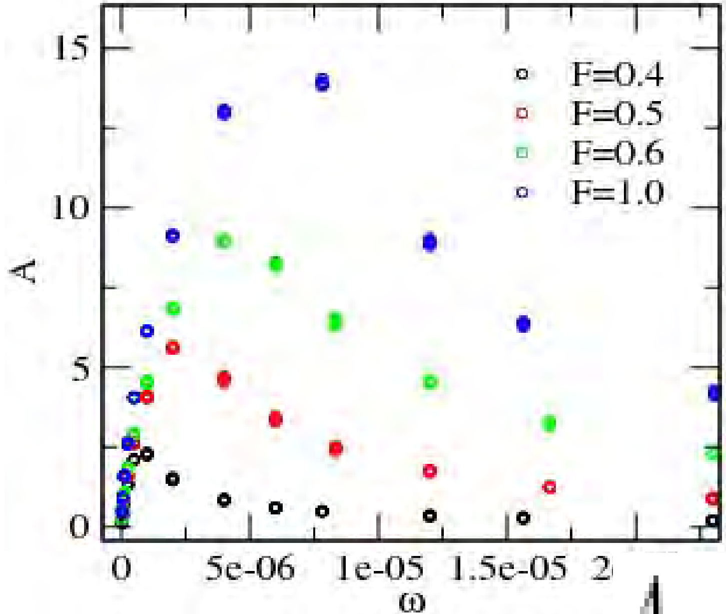
Response of oscillatory force

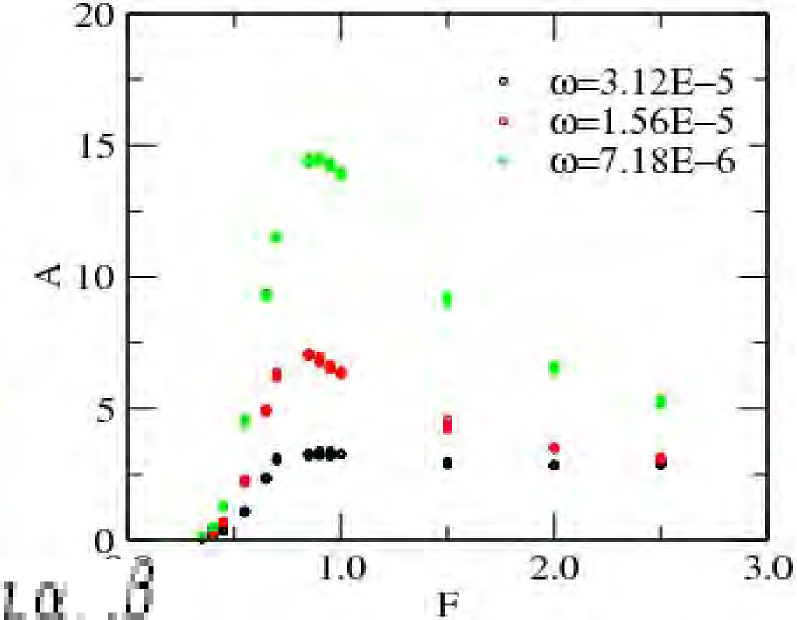




Phys. Rev. Lett. Vol 110 258102 (2013)

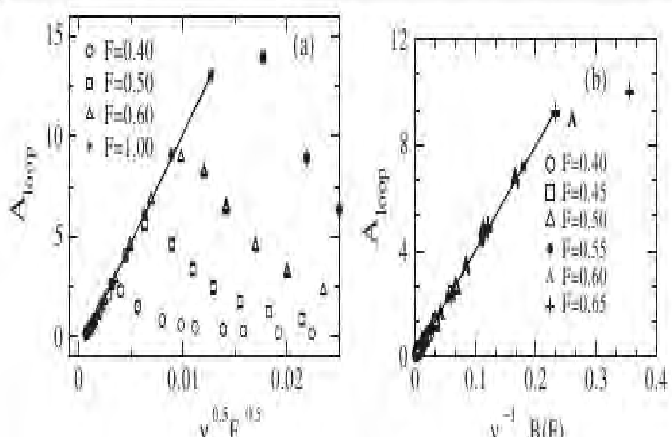
How area of the loop grows?

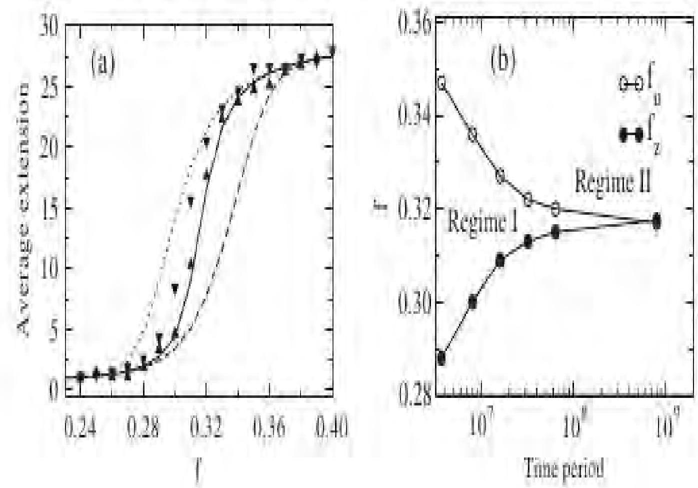




$$A \sim h^{\alpha}\omega^{\beta}$$

PRL **110,** 258102 (2013) PHYSICAL REVIEW LETTERS week ending 21 JUNE 2013





Conclusions:

•We briefly discussed SMFS experiments and showed that the simple model of polymer can capture essential physics behind them.

•We have shown the existence of Dynamical transition, where without changing the physiological conditions, DNA may be brought from the zipped or open state to a new dynamic state.


Thank you