Euler's elastica and their application to DNA, nucleosomes and chromatin fibers

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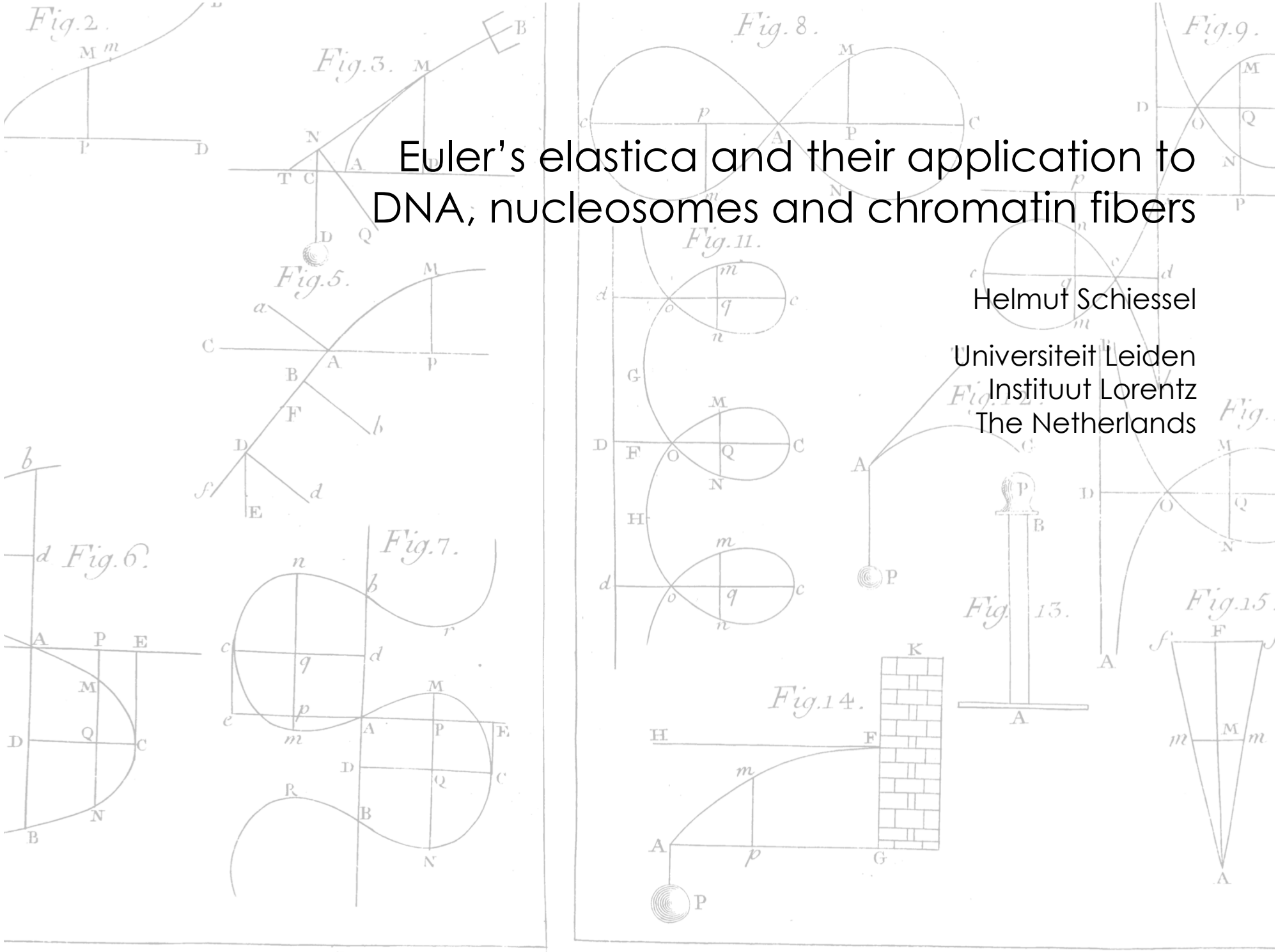
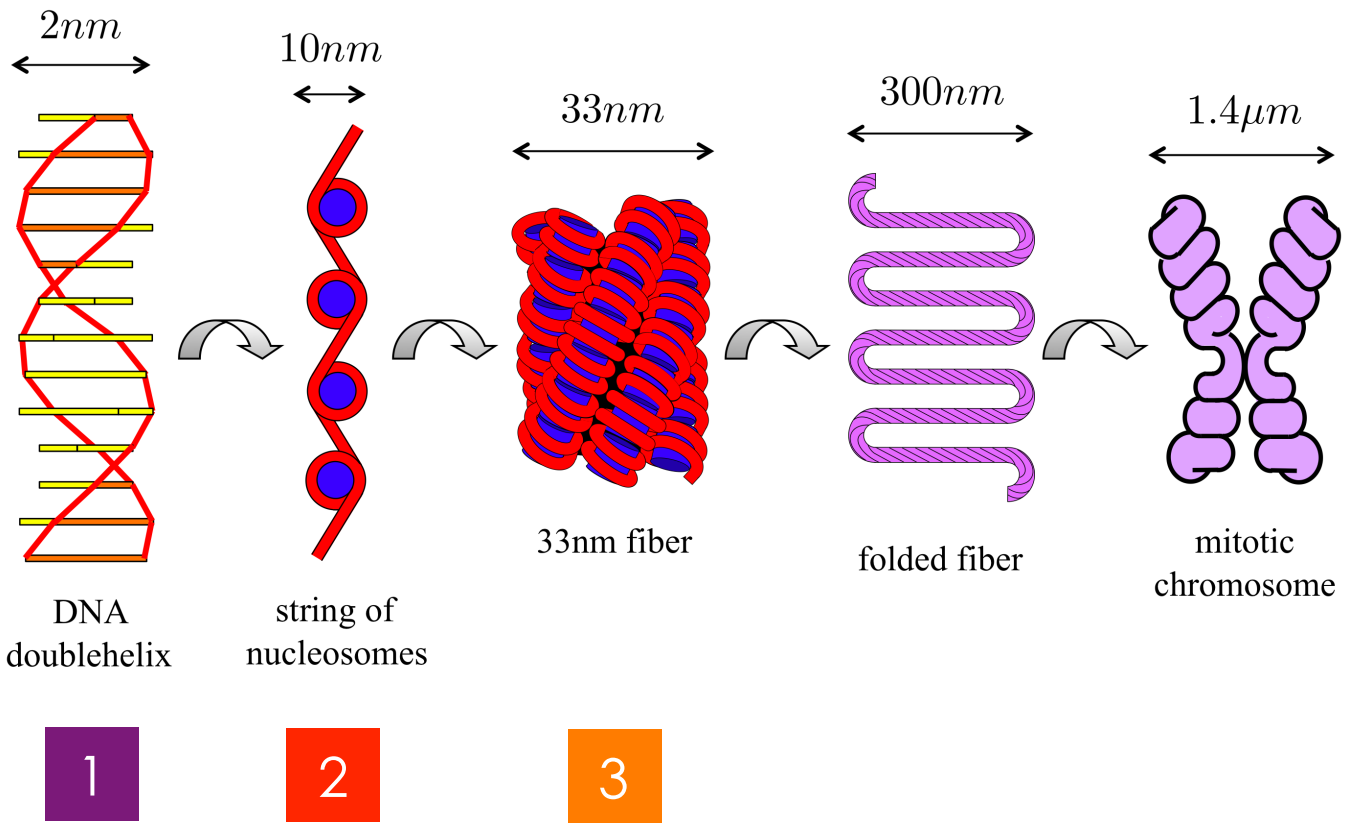


Overview


2nm
10nm
33nm
300nm
1.4μm
DNA doublehelix
string of nucleosomes
33nm fiber
folded fiber
mitotic chromosome
1
2
3

Galileo Galilei

1564-1642

Discorsi, 1638:

DISCORSI
E
DIMOSTRAZIONI
MATEMATICHE,
intorno à due nuoue scienze
Attenenti alla
MECANICA & I MOVIMENTI LOCALI,
del Signor
GALILEO GALILEI LINCEO,
Filosofo e Matematico primario del Sereniſſimo
Grand Duca di Toſcana.
Con vna Appendice del centro di gravità d'alcuni Solidi.

IN LEIDA,
Appreſſo gli Elſevirii. M. D. C. XXXVIII.

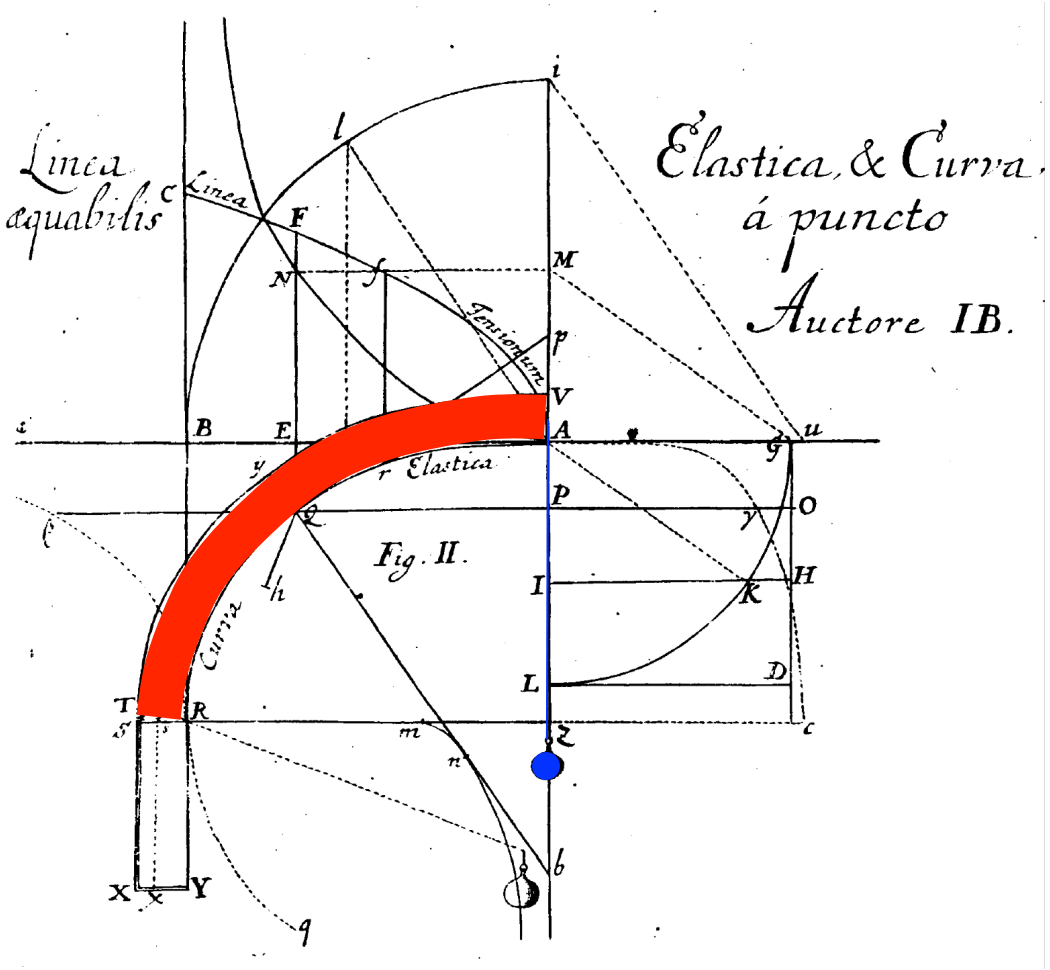
114 DIALOGO SECONDO

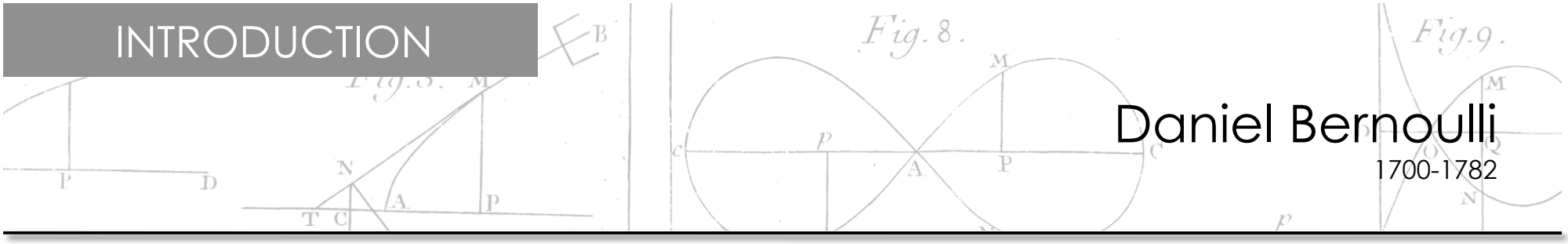
ſin quì dichiarate, non ſarà difficile l'intender la ragione, onde auuenga, che vn Priſma, ò Cilindro ſolido di vetro, acciaio, legno, ò altra materia frangibile, che ſoſpeſo per lungo ſolterrà graviſſimo peſo, che gli ſia attaccato, mà in trauerſo (come poco fà dicemmo) da minor peſo aſſai potrà tal volta eſſere ſpezzato, ſecondo che la ſua lunghezza eccederà la ſua groſſezza. Imperò che figuriamoci il Priſma ſolido A B, C D *fitto in vn muro dalla parte* A B, *e nell' altra eſtremità s'intenda la forza del Peſo* E, *(intendendo ſempre il muro eſſer eretto all' Orizonte, & il Priſma, ò Cilindro fitto nel muro ad angoli retti) è manifeſto che douendoſi ſpezzare ſi romperà nel luogo* B, *done il taglio del muro ſerue per ſoſtegno, e la* B C *per la parte della Leua, doue ſi pone la forza, e la groſſezza del ſolido* B A *è l'altra parte della Leua, nella quale è poſta la reſiſtenza, che conſiſte nello ſtaccamento, che s' hà da fare della parte del ſolido* B D, *che è fuor del muro, da quella che è dentro, e per le coſe dichiarate il momento della forza poſta in* C *al momento della reſiſtenza che ſtà nella*

Jacob Bernoulli

1654-1705

Curvatura Laminae Elasticae, 1694:





Daniel Bernoulli

1700-1782

Letter to Euler, October 1742:

I'd like to know whether you might not solve the curvature of the elastic lamina under this condition, that on the length of the lamina on two points the position is fixed, and that the tangents at these points are given.

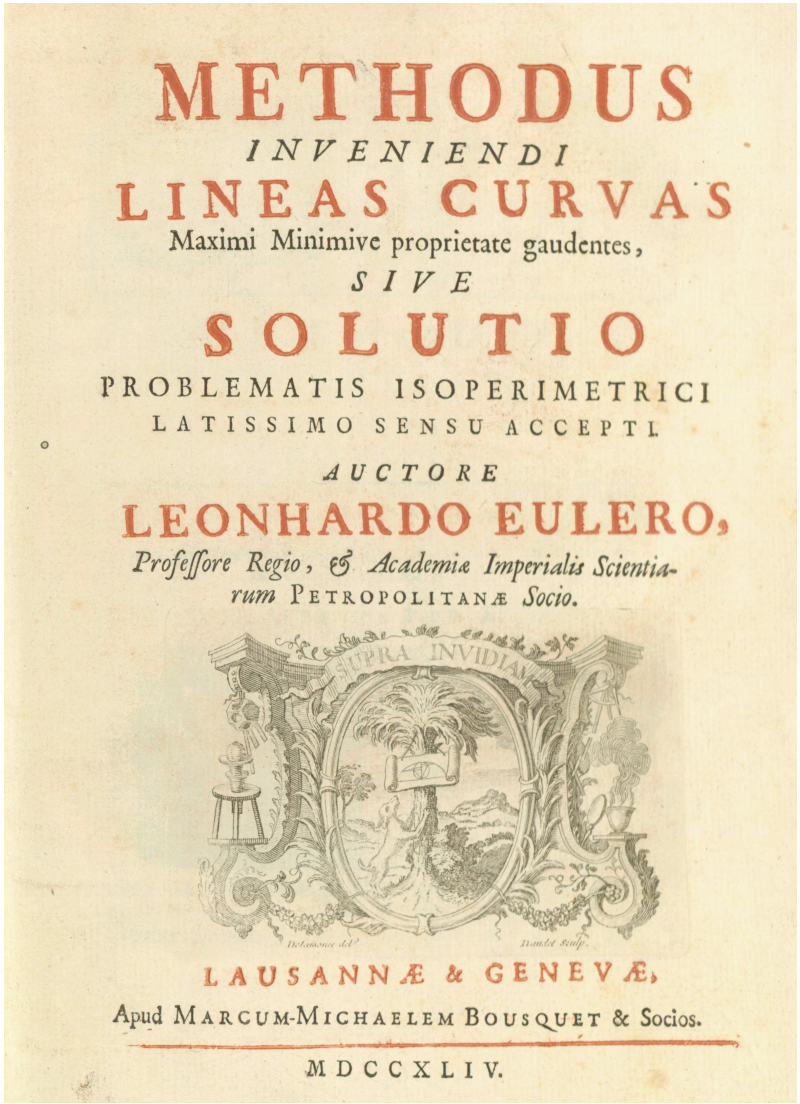
[…]

I'd express the potential energy of a curved elastic lamina (which is straight when in its natural position) through $\int \frac{ds}{RR}$, assuming the element ds is constant and indicating the radius of curvature by *R*. There is nobody as perfect as you for easily solving the problem....

Leonard Euler

1707-1793

Euler, 1744:



METHODUS
INVENIENDI
LINEAS CURVAS
Maximi Minimive proprietate gaudentes,
SIVE
SOLUTIO
PROBLEMATIS ISOPERIMETRICI
LATISSIMO SENSU ACCEPTI
AUCTORE
LEONHARDO EULERO,
Professore Regio, & Academiæ Imperialis Scientiarum PETROPOLITANÆ Socio.

SUPRA INVIDIAM

LAUSANNÆ & GENEVÆ,
Apud MARCUM-MICHAELEM BOUSQUET & Socios.
MDCCXLIV.

Tabula III.

Additamentum.

Fig. 1.

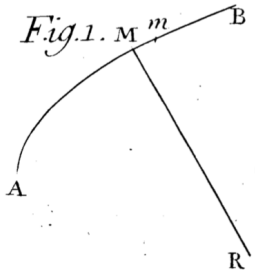


Fig. 2.

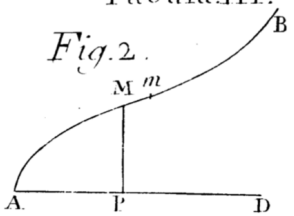


Fig. 3.

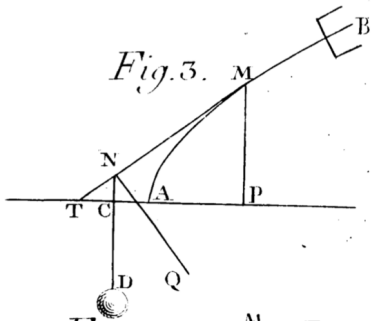


Fig. 4.

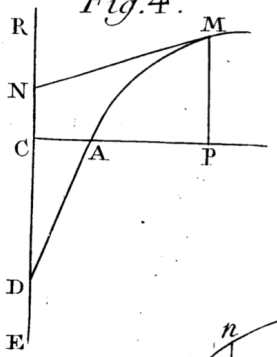


Fig. 5.

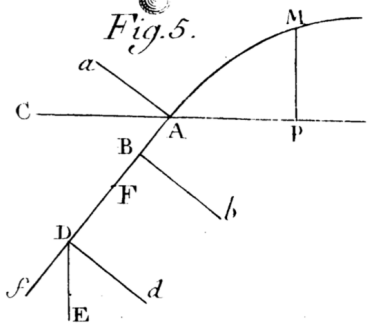


Fig. 6.

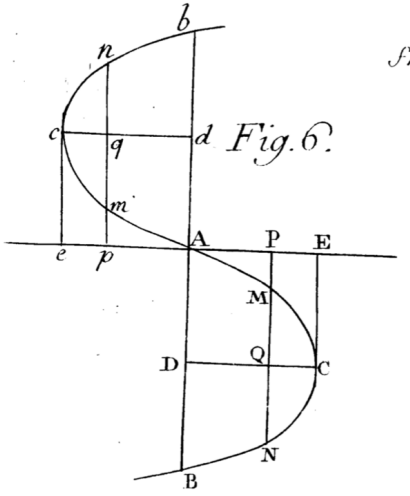
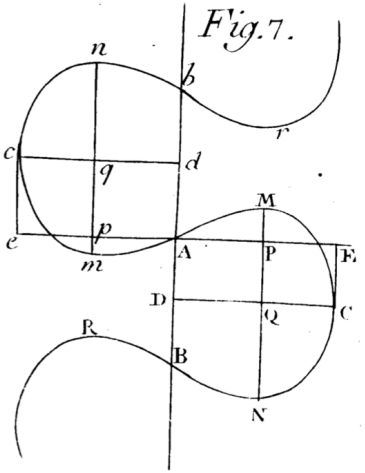


Fig. 7.



Tabula IV.

Additamentum.

Fig. 8.

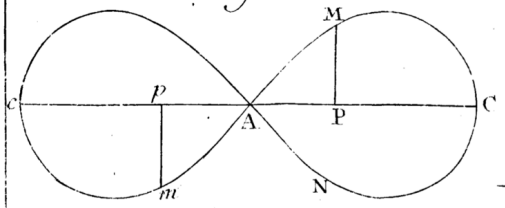


Fig. 9.

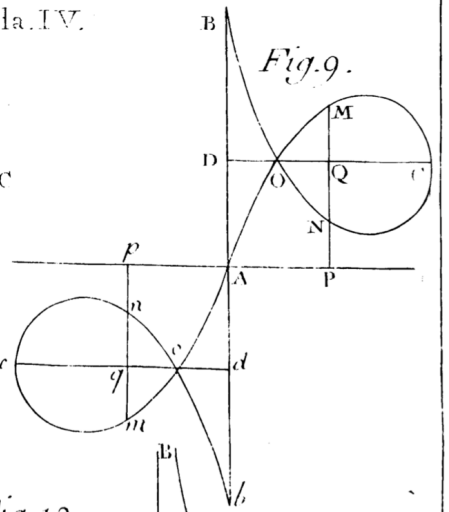


Fig. 11.

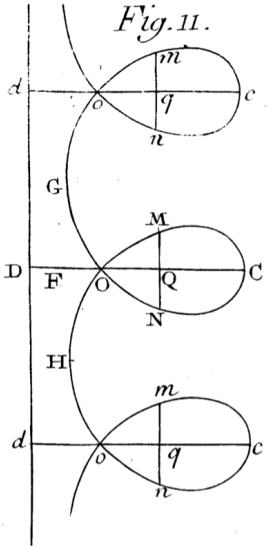


Fig. 12.

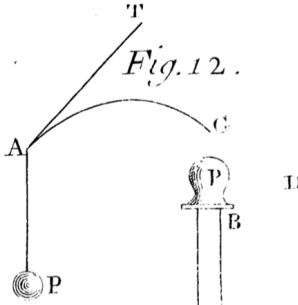


Fig. 13.

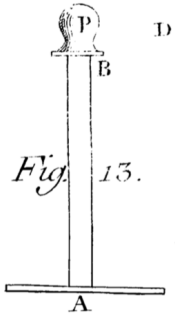


Fig. 10.

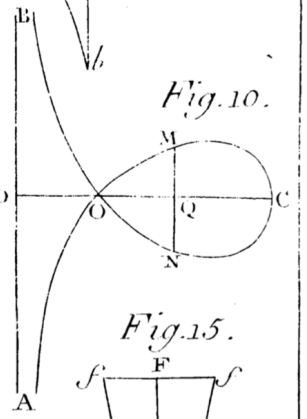


Fig. 14.

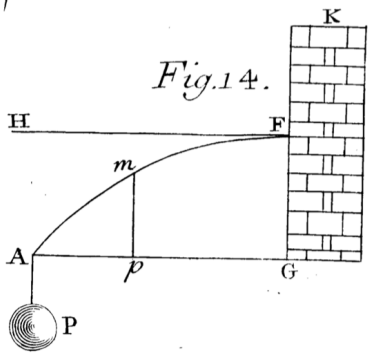
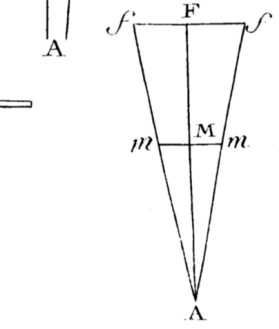
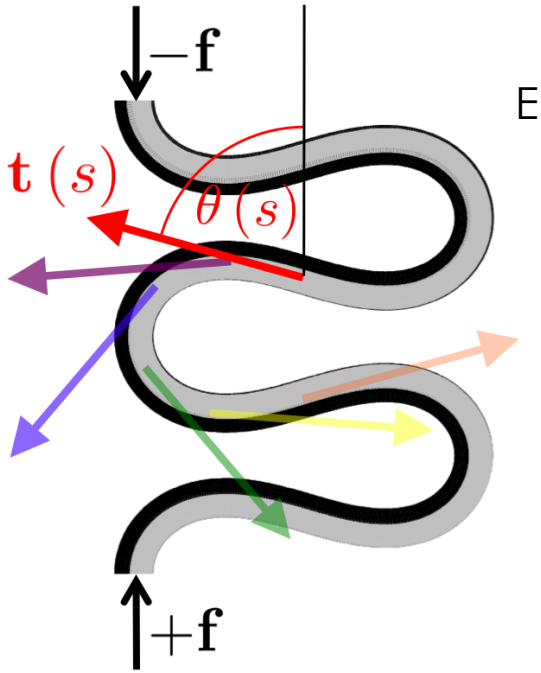


Fig. 15.



Gustav Kirchhoff
1824-1887

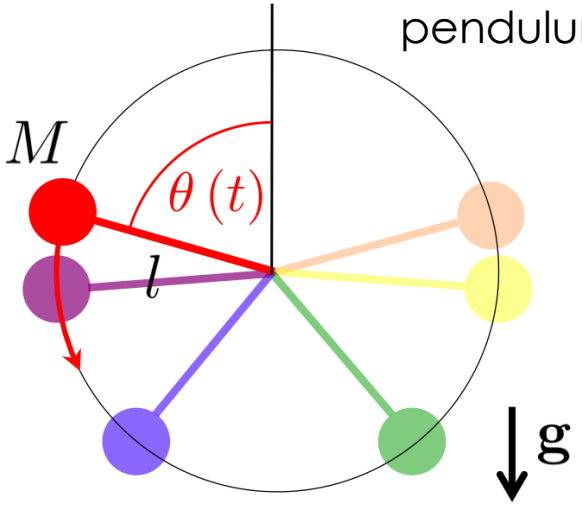
Kirchhoff kinetic analogy (1859):



Euler elastica

1 : 1

pendulum



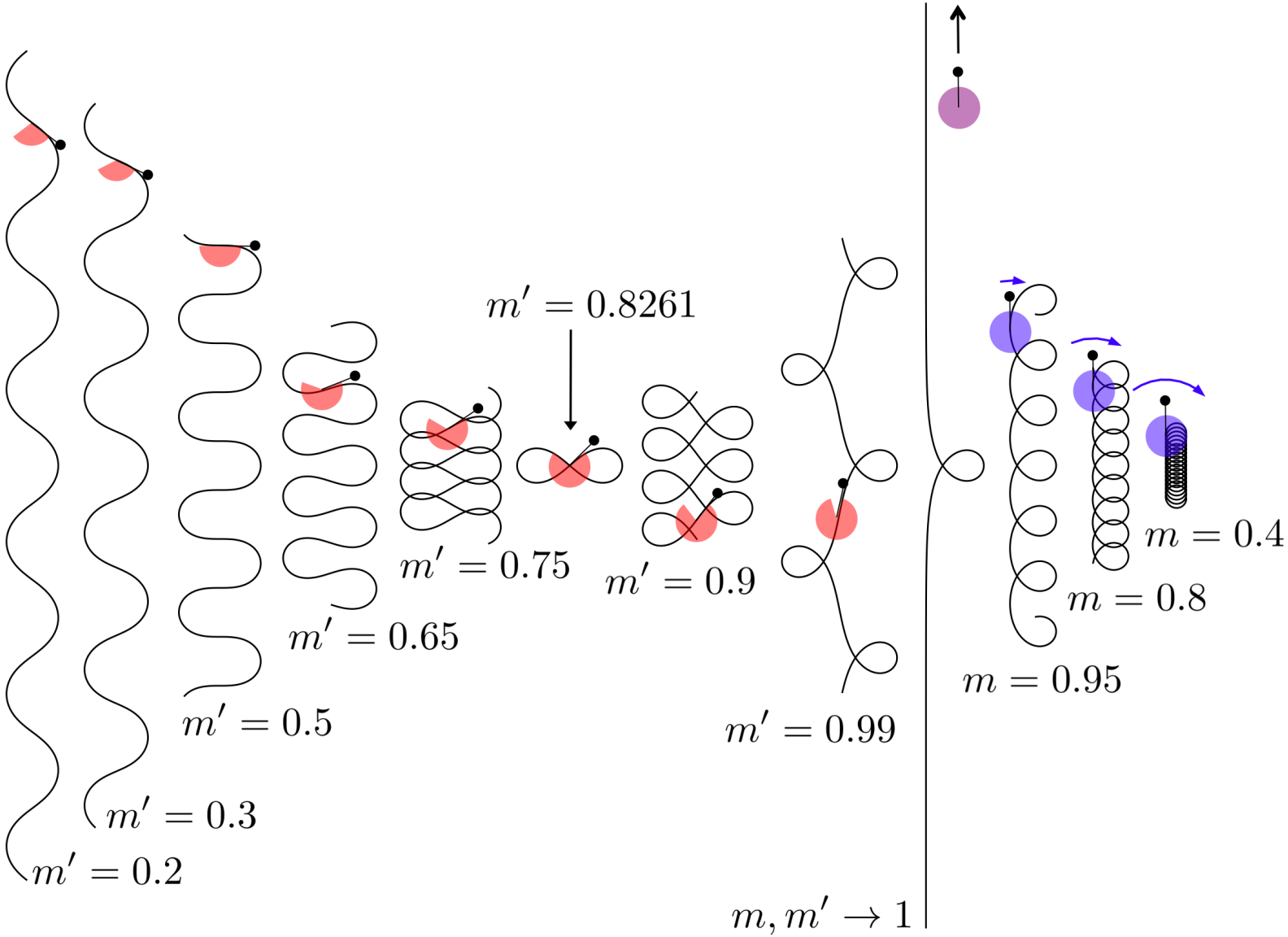
Hamiltonian (wormlike chain model):

$$H = \int_0^L ds \left[\frac{A}{2} \dot{\theta}^2 - f \cos\theta \right]$$

Lagrangian action:

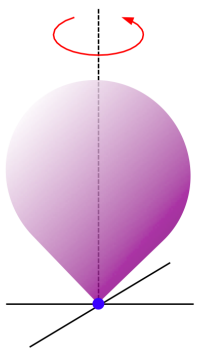
$$S = \int_0^T d\tau \left[\frac{Ml^2}{2} \dot{\theta}^2 - Mgl \cos\theta \right]$$

Examples

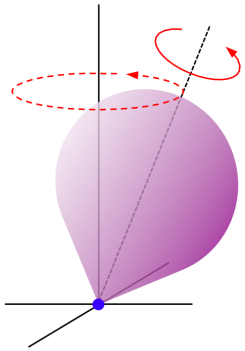


Full kinetic analogy

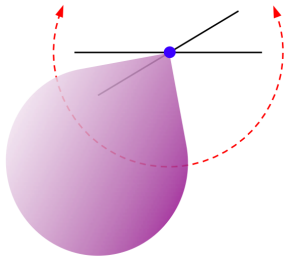
Kirchhoff, J. Reine Angew. Math **56** (1859) 285-313



sleeping top



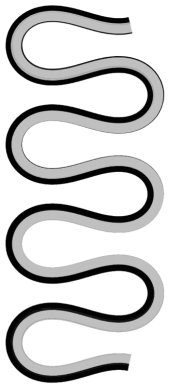
regular precession



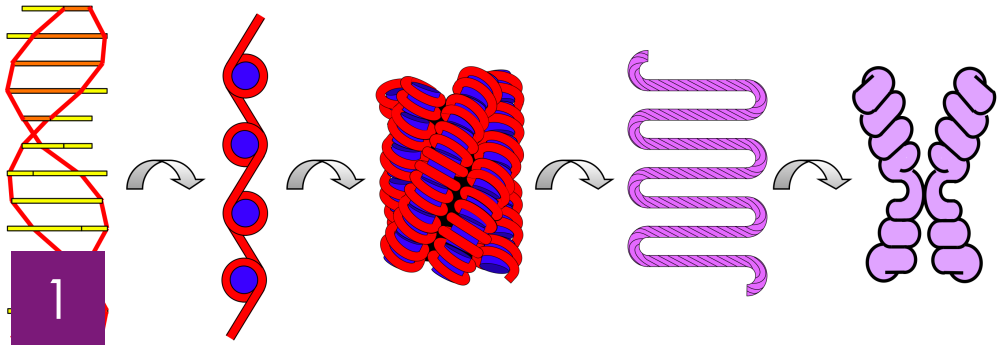
pendulum

twisted rod

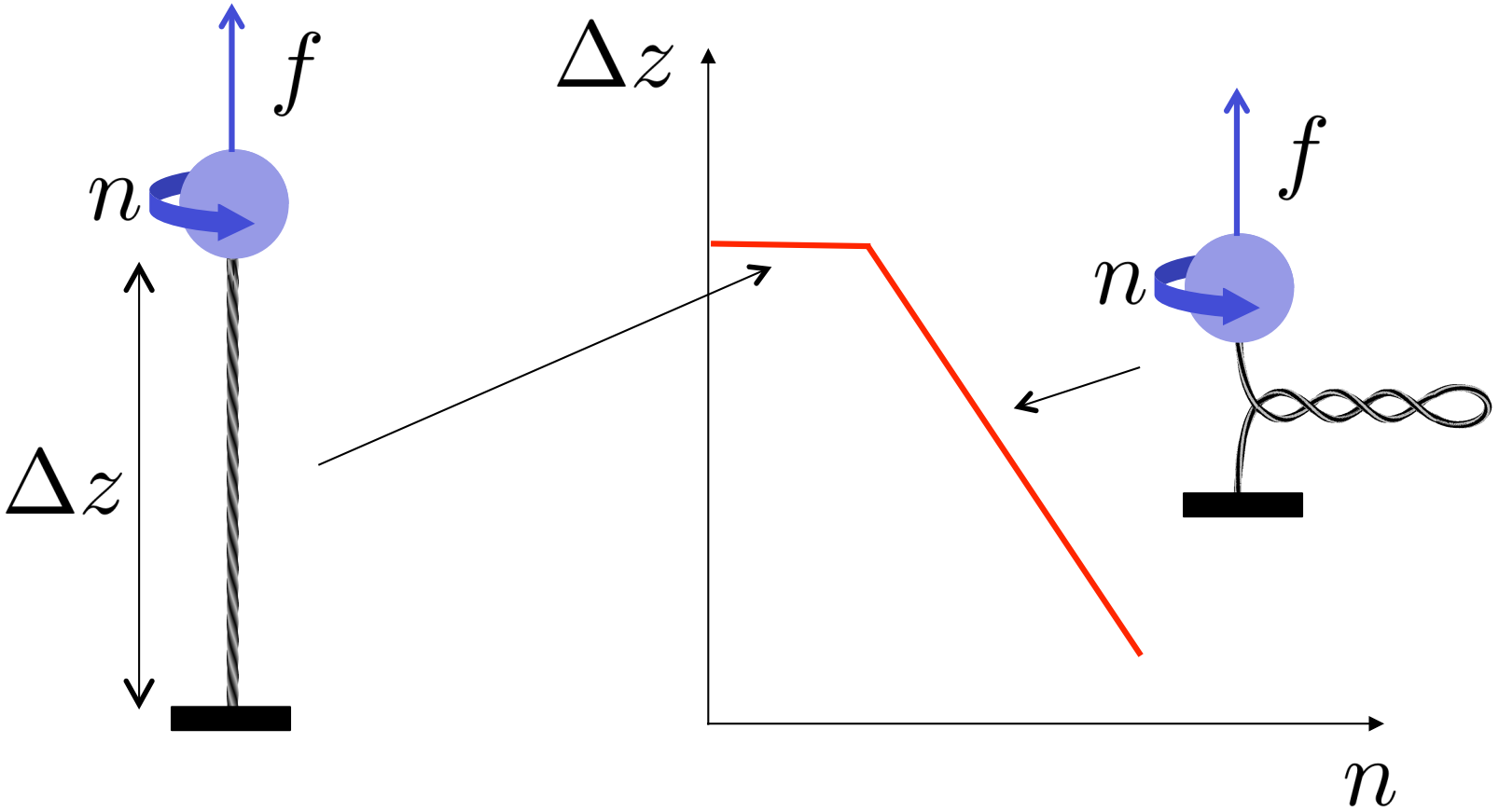
helix



planar filament



Twisting DNA under tension

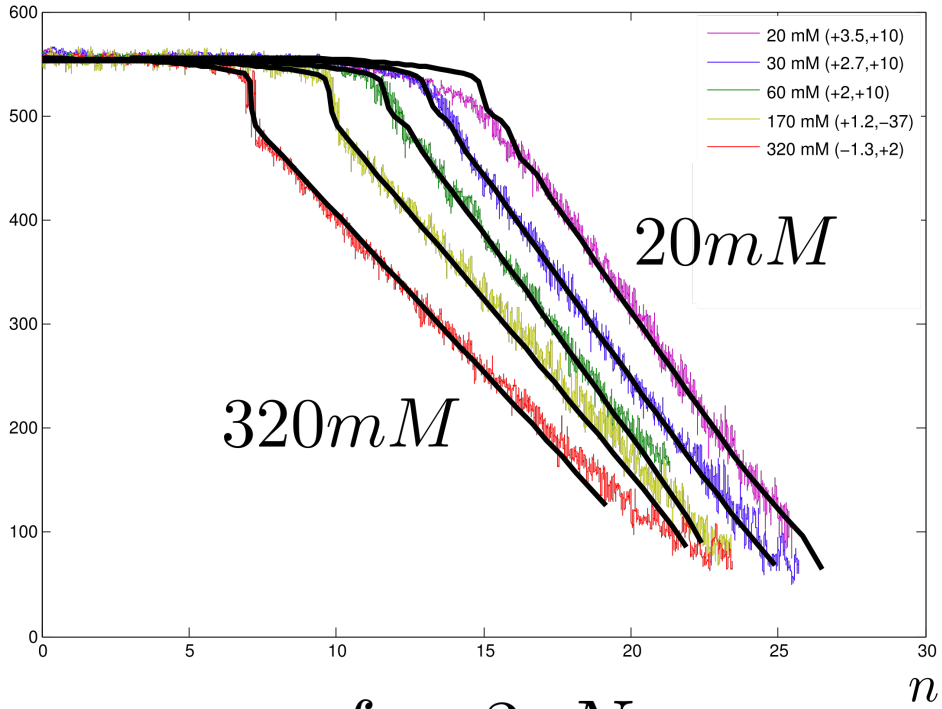


Theories: Marko, Phys. Rev. E **76** (2007) 021926
Clauvelin, Audoly & Neukirch, Biophys. J. **96** (2009) 3716
Maffeo, Schopflin, Brutzer, Stehr, Aksimentiev, Wedemann & Seidel, PRL 105, 158101

Comparison experiment/theory

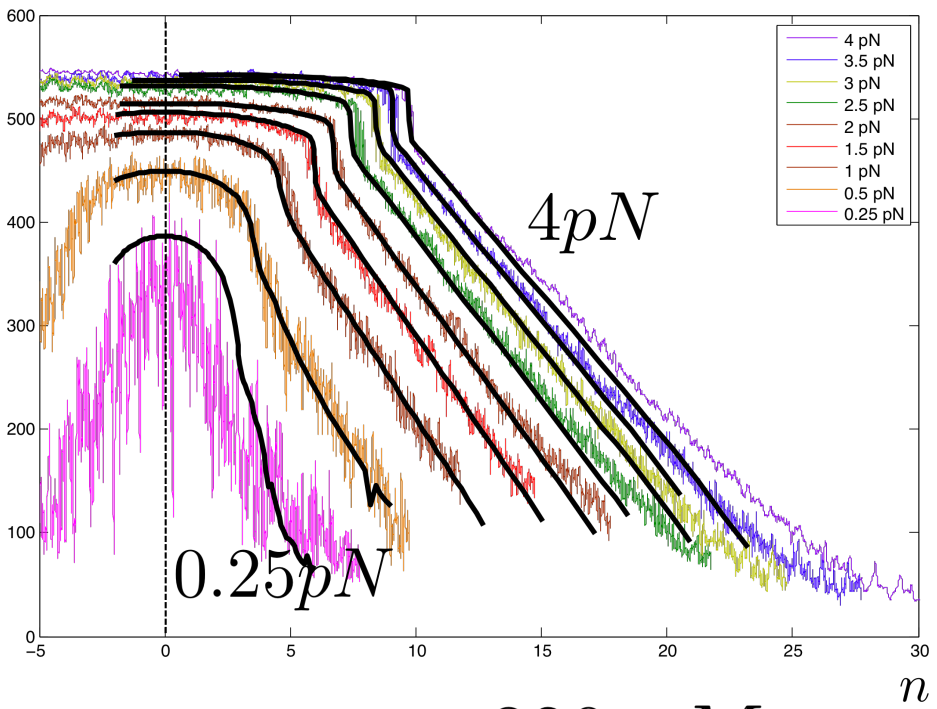
Ralf Seidel lab, Dresden

$\Delta z\,[nm]$



$f = 3pN$

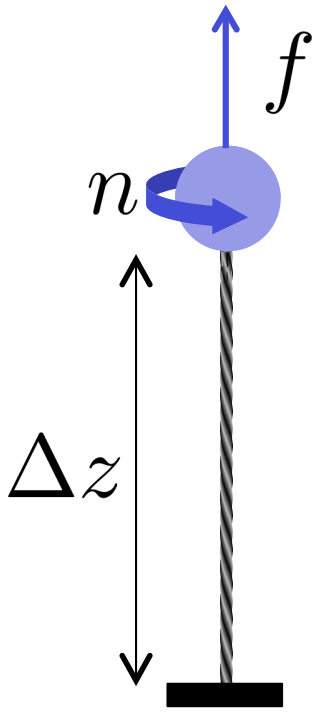
$\Delta z\,[nm]$

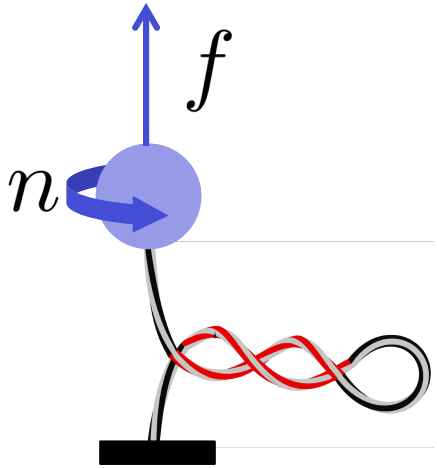


$c_s = 320mM$

$L = 600nm$

Twisting DNA under tension

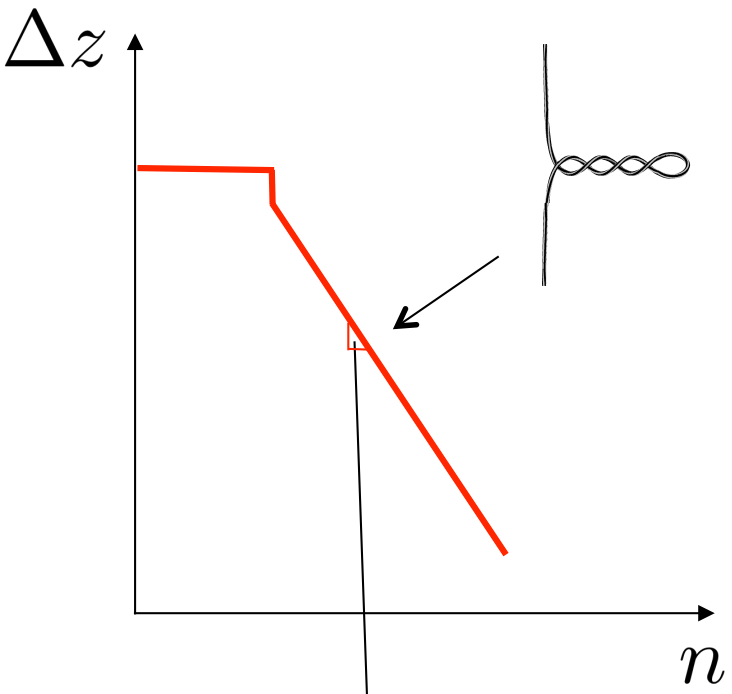




total energy:

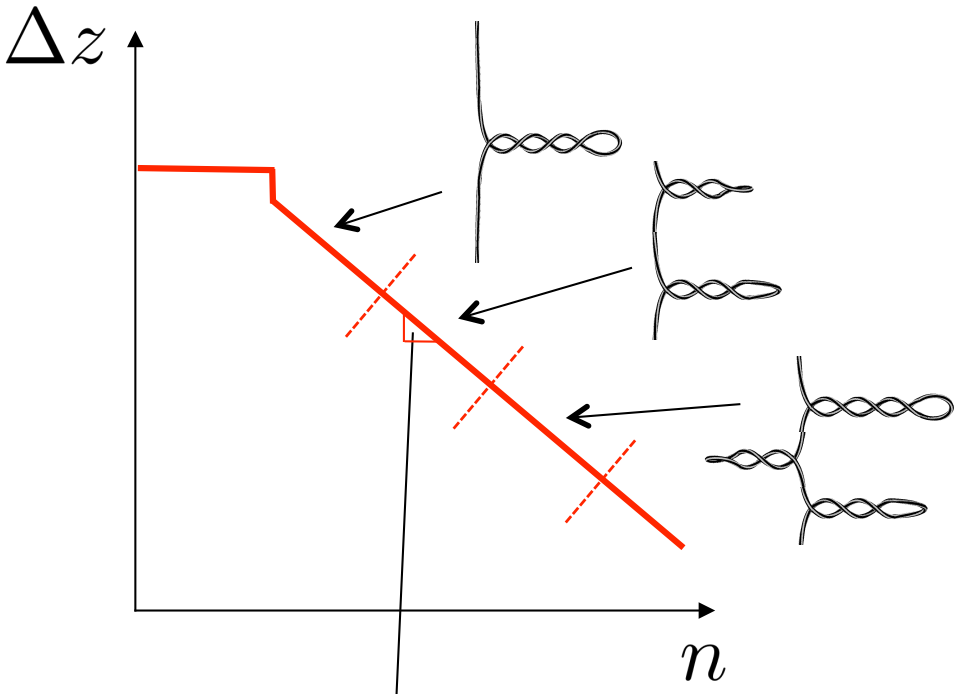
$$E_{\mathrm{tot}} = \underbrace{\frac{A}{2}\int_0^L \frac{ds}{R^2(s)}}_{\text{DNA bending}} + \underbrace{\frac{C}{2}\int_0^L \Delta\psi^2(s)\,ds}_{\text{DNA twisting}} \underbrace{- f\Delta z}_{\text{external force}} \underbrace{- 2\pi n\left([\mathbf{t}, \Delta\psi]\right)\tau_f}_{\text{external twist}} + \underbrace{U_{\mathrm{el}}\left([\mathbf{t}]\right)}_{\text{electrostatic contribution}}$$

Multiplectoneme formation



slope:

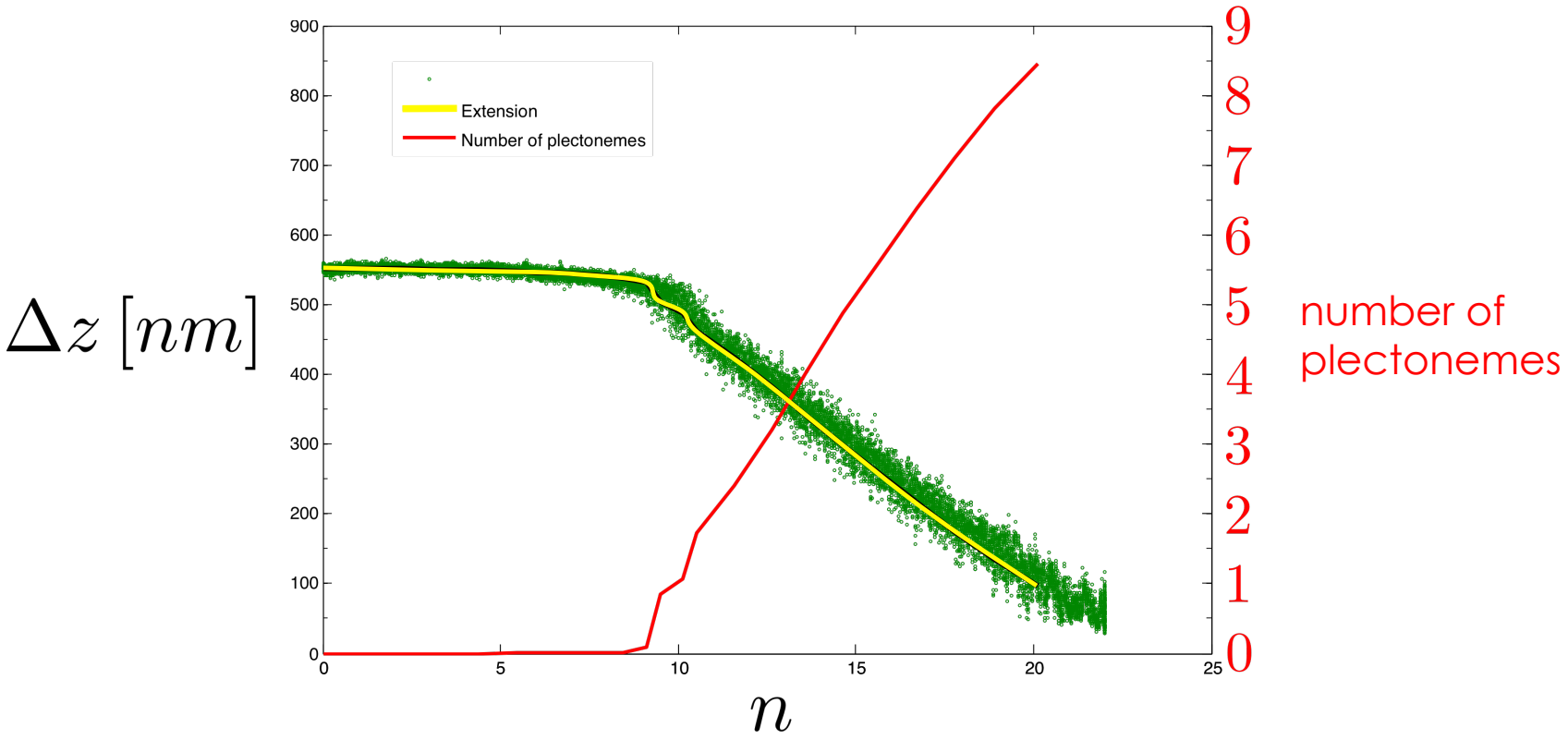
$$\frac{\partial \Delta z}{\partial n} = -\frac{\rho}{\rho_{pl}\mathrm{wr}}$$

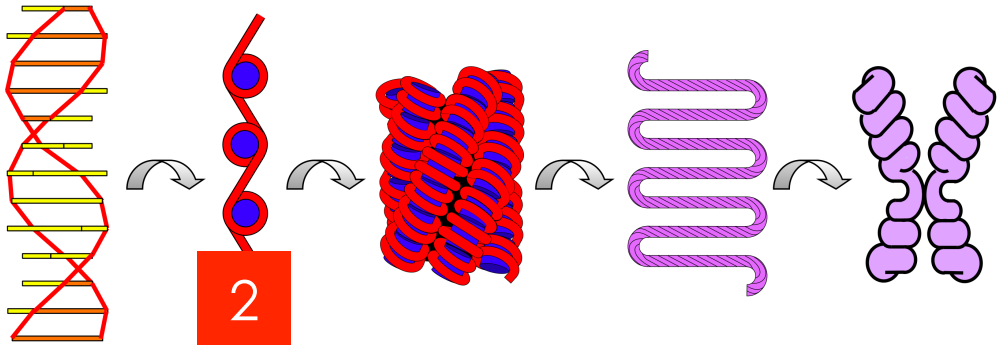


$$\frac{\partial \Delta z}{\partial n} = -\frac{\rho}{\rho_{pl}\mathrm{wr}} + \frac{\partial m}{\partial n}\left(\frac{\rho}{\rho_{pl}\mathrm{wr}} - l_{\mathrm{loop}}\right)$$

Example

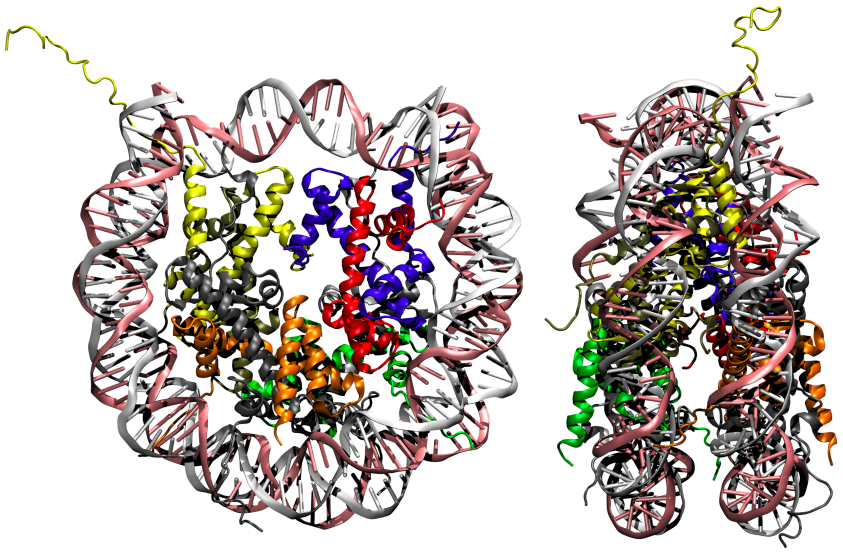
$$L = 600nm \quad f = 3pN \quad c_s = 30mM$$





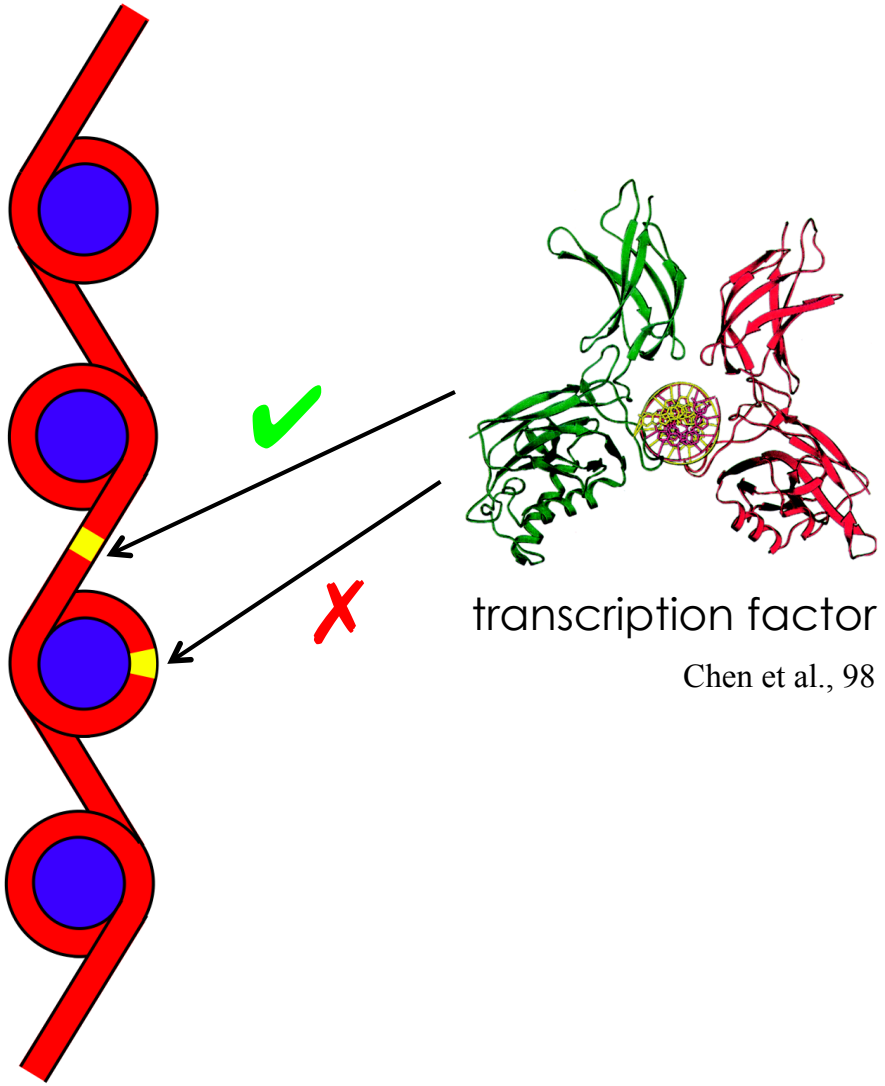
Nucleosomes under tension

nucleosome core particle:



Luger et al., 97

- 1 ¾ turns
- 147 bp, 50nm
- 14 binding sites

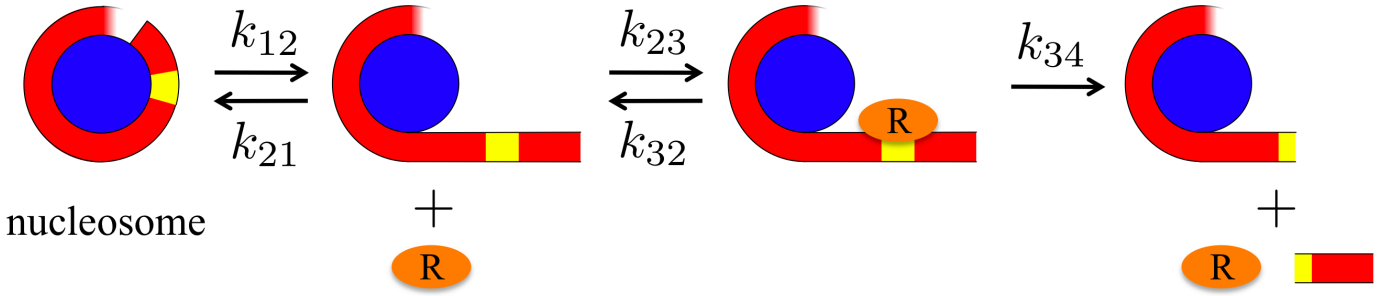


transcription factor

Chen et al., 98

Nucleosome breathing

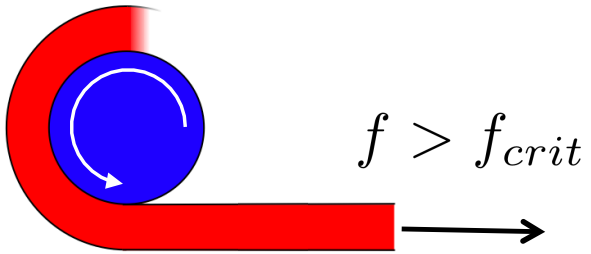
Polach & Widom, J. Mol. Biol. **254** (1995) 130



adsorption energy per length:

Prinsen & HS, Biochimie **92** (2010) 1722

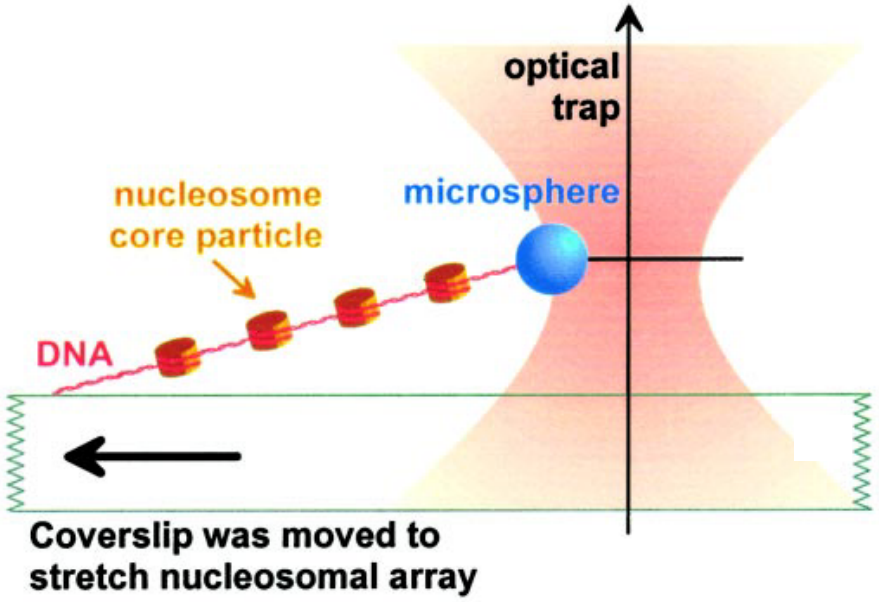
$$f_{\text{crit}} \approx \frac{15 k_B T}{50 nm} = 1.2 pN$$

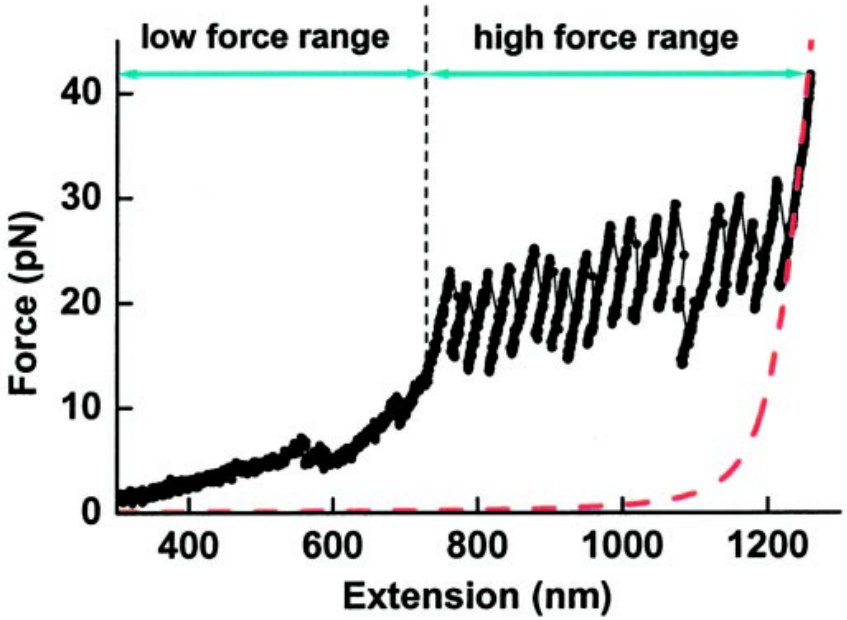


Force-induced unwrapping

Brower-Toland et al., PNAS **99** (2002) 1960

17 nucleosomes under tension:

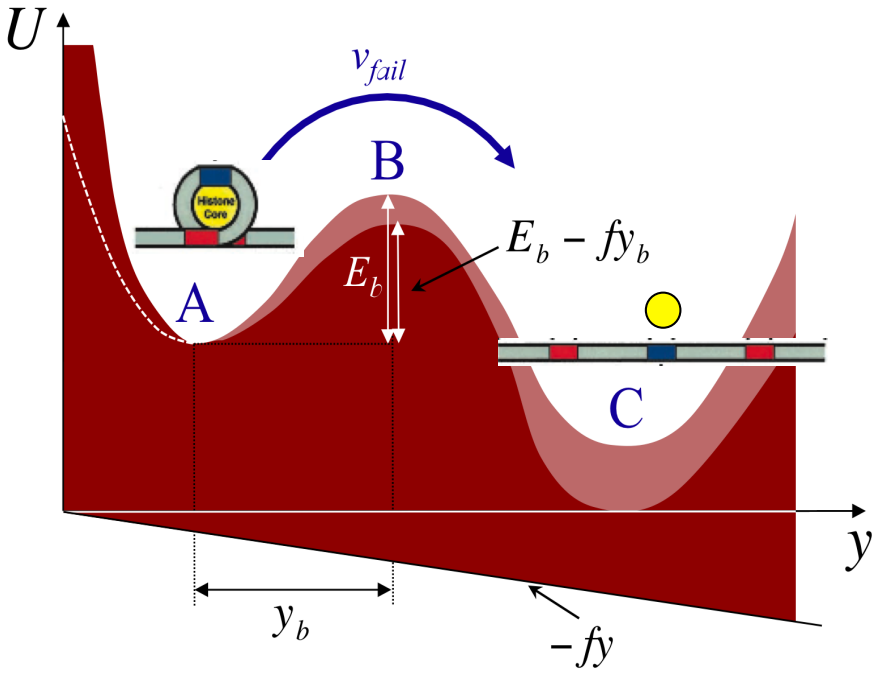


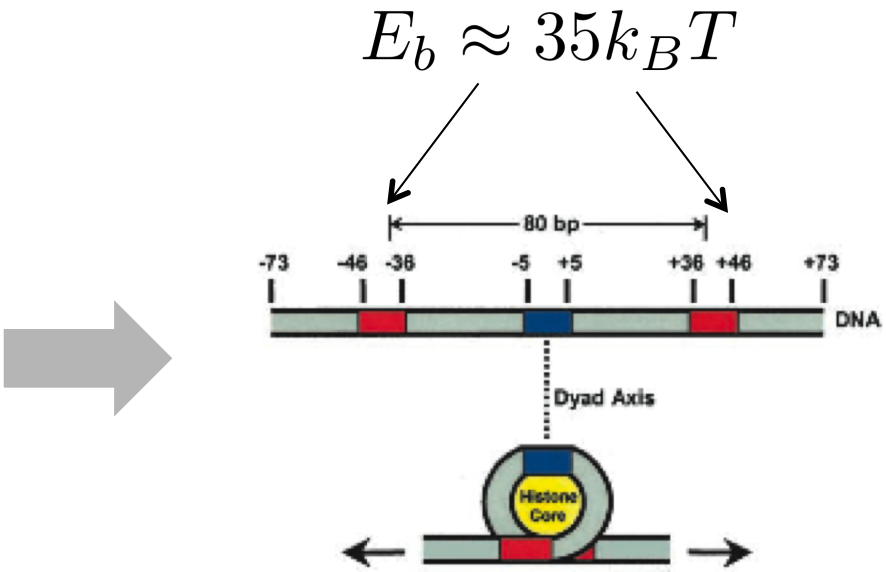


But: $f_{\text{crit}} \approx \frac{15 k_B T}{50nm} = 1.2pN$

Super binding sites

Brower-Toland et al., PNAS **99** (2002) 1960

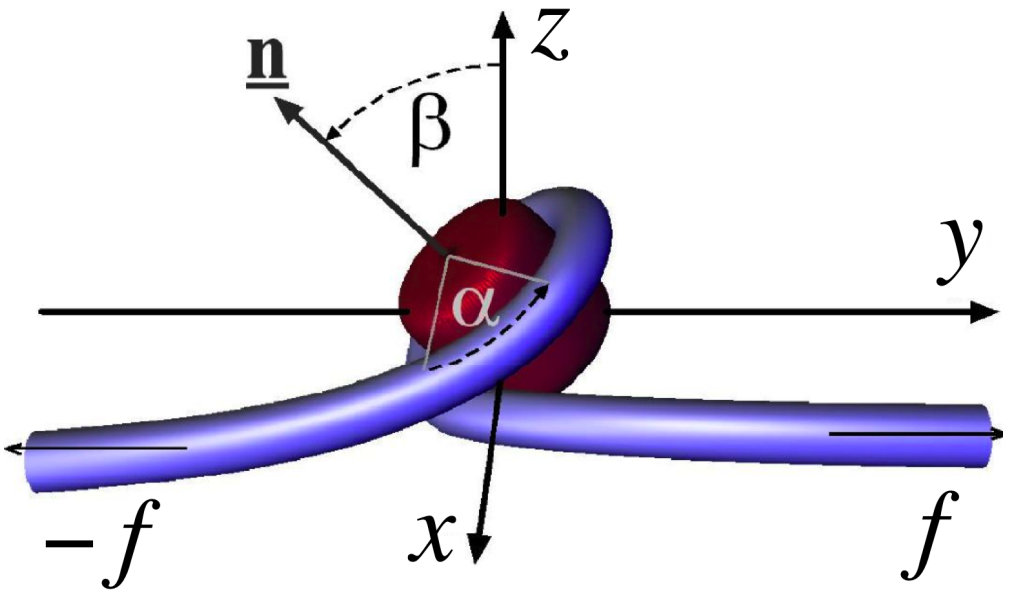




But: $E_{complex} \approx 15k_BT$

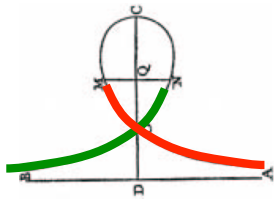
Model

Kulic & HS, Phys. Rev. Lett. **92** (2004) 228101



α : unwrapping angle

β : tilting angle

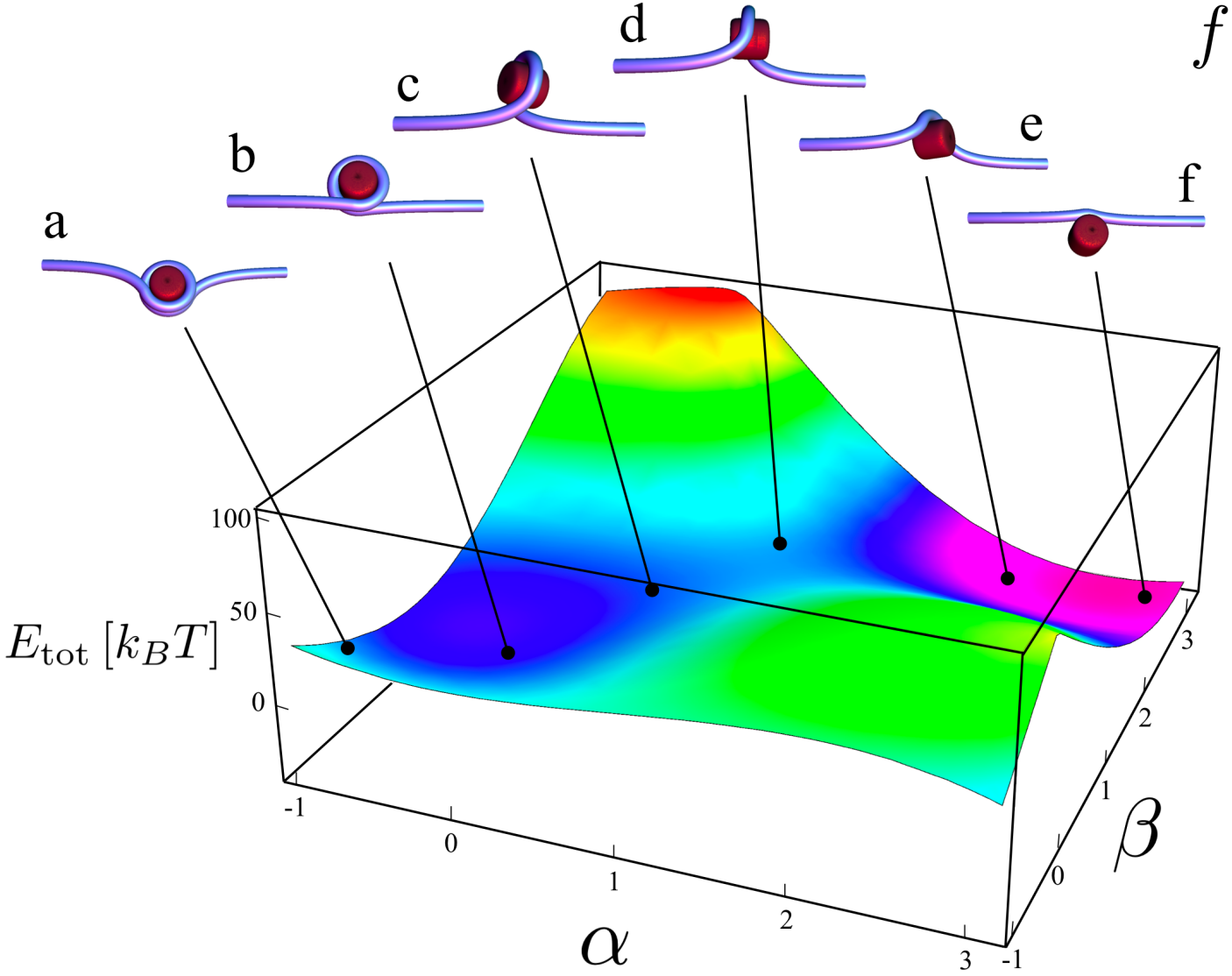


total energy:

$$E_{\mathrm{tot}} = \underbrace{\frac{A}{2}\int_0^L ds \left(\frac{1}{R(s)}\right)^2}_{\text{DNA bending}} \underbrace{- f L_{EE}}_{\text{external force}} \underbrace{+ 2R_0 f_{\mathrm{crit}} \alpha}_{\text{DNA adsorption}}$$

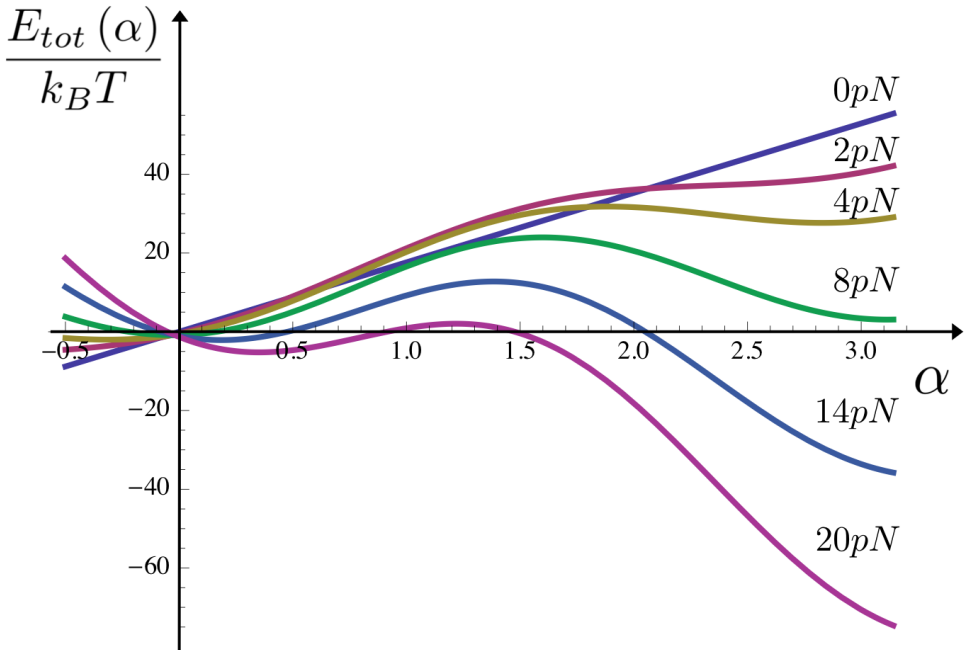
Energy landscape

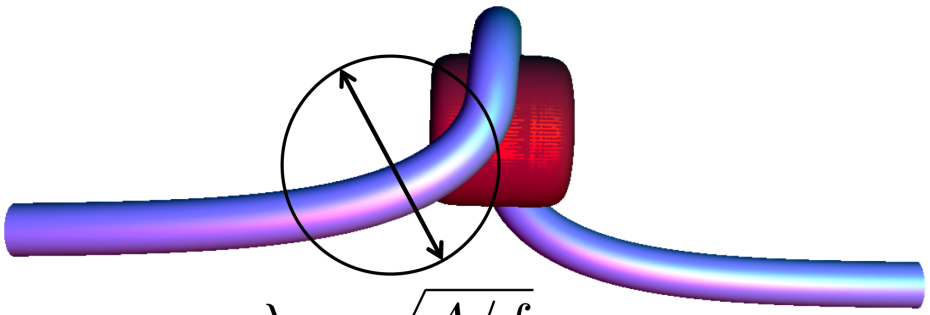
$f = 14pN$



The origin of the barrier

$$E_{\mathrm{tot}}(\alpha) \approx \underbrace{2R_0\left(f_{\mathrm{crit}} - f\right)\alpha}_{\text{tilting term}} \underbrace{- \frac{2}{\sqrt{3}}\sqrt{Af}\cos 2\alpha}_{\text{barrier term}}$$

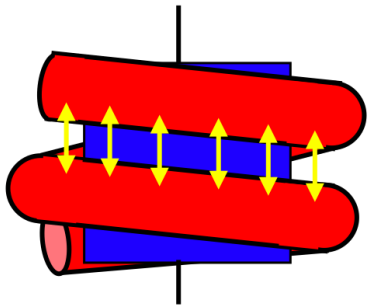


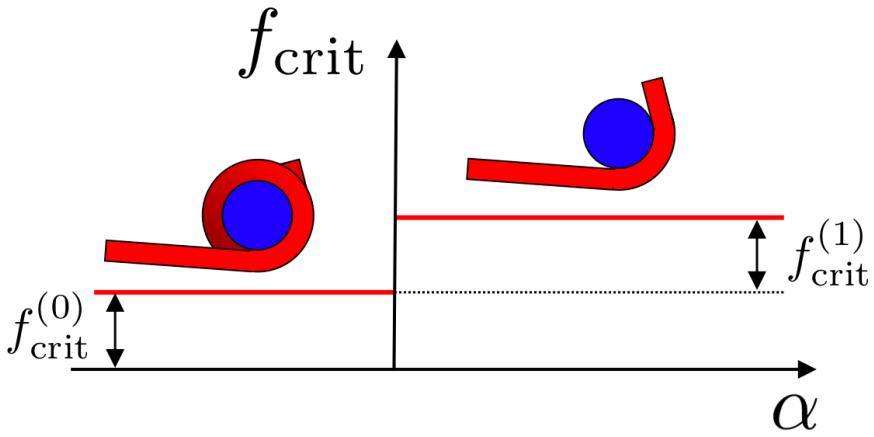


$$\lambda = \sqrt{A/f}$$

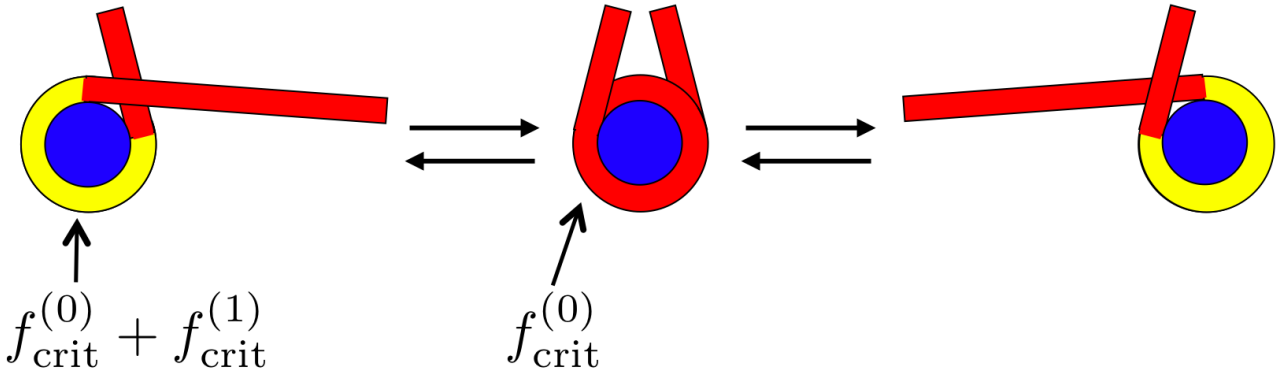
$$E_b \approx \frac{A\lambda}{\lambda^2} = \sqrt{Af}$$

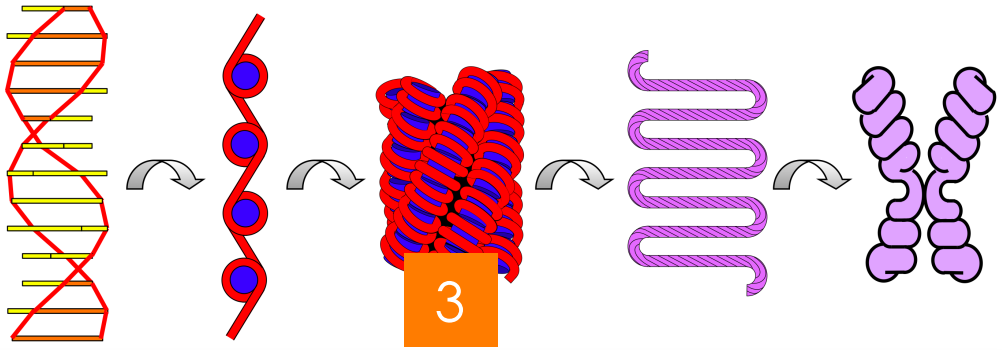
The first-second round difference



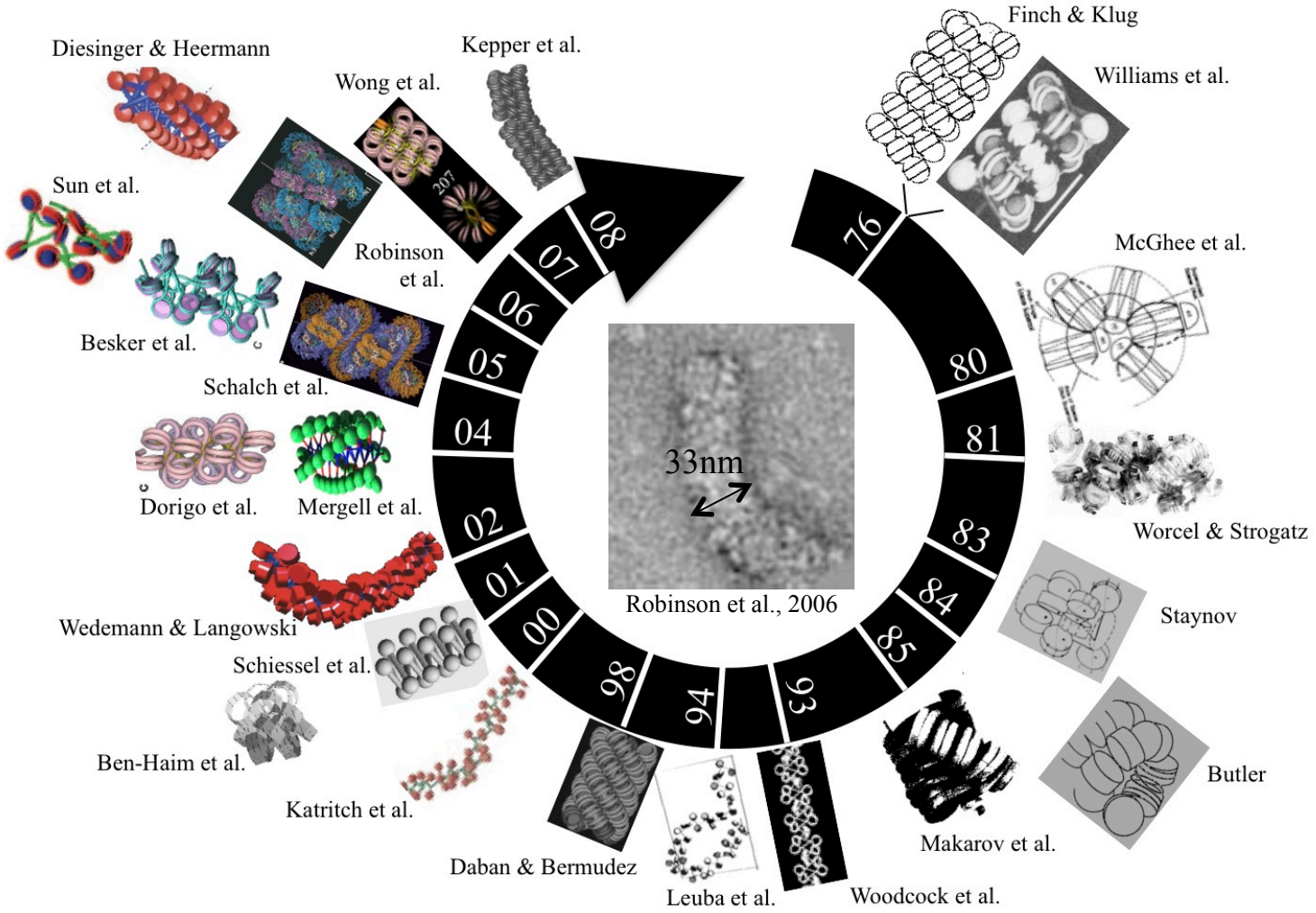


Two turn design combines accessibility and stability:





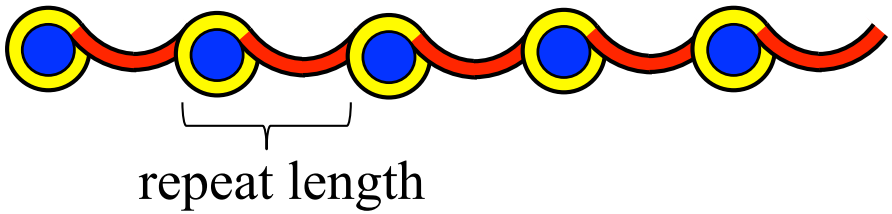
Chromatin fiber timeline

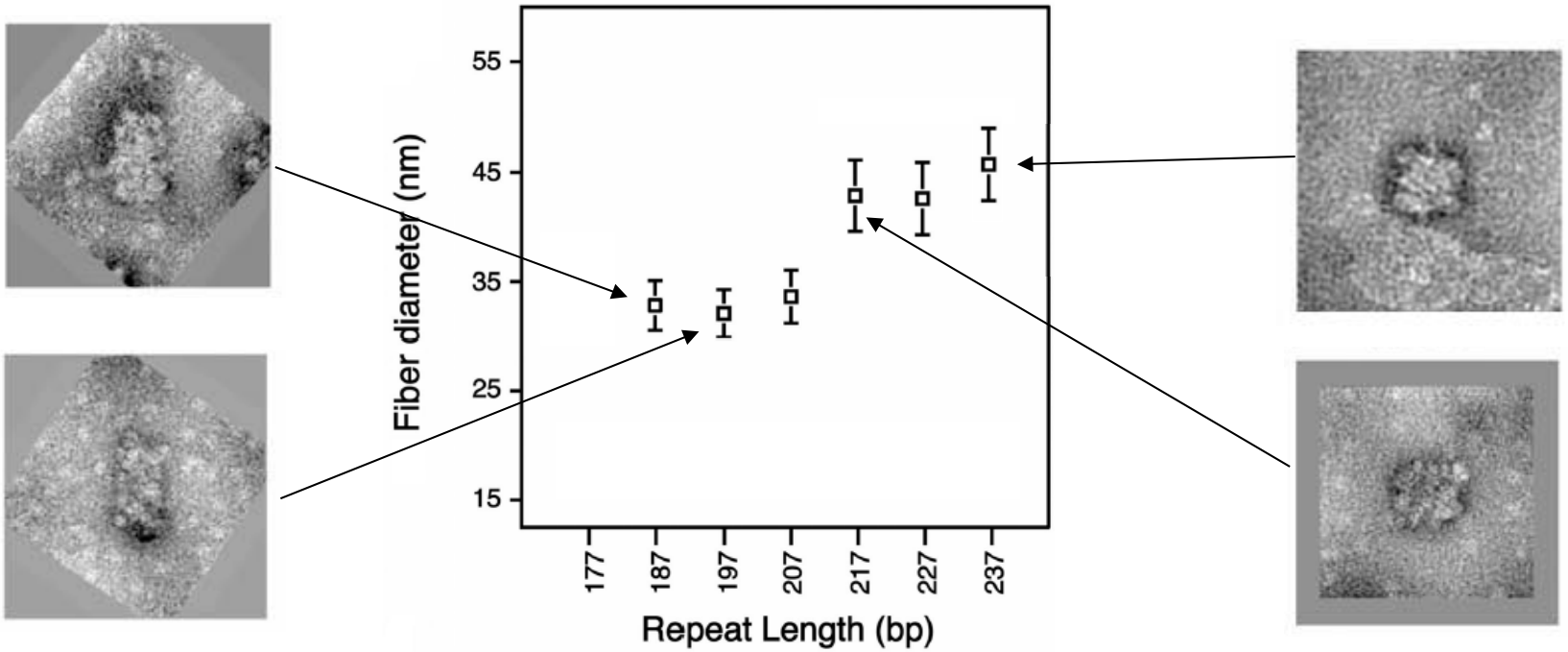


Ideal fibers

Robinson *et al.*, PNAS **17** (2006) 6506

long arrays of 50 to 70 nucleosomes:

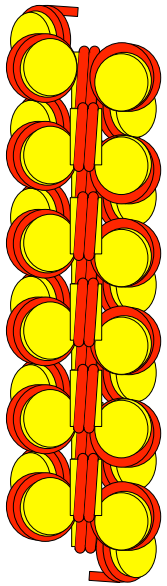




Bent vs. straight linkers

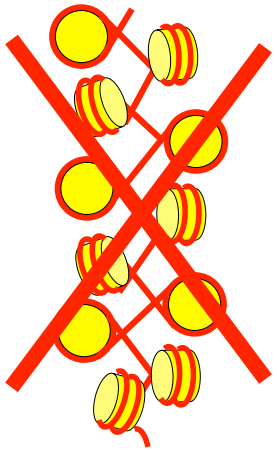
Alberts et al. "Molecular Biology of the Cell":

1994



solenoid model

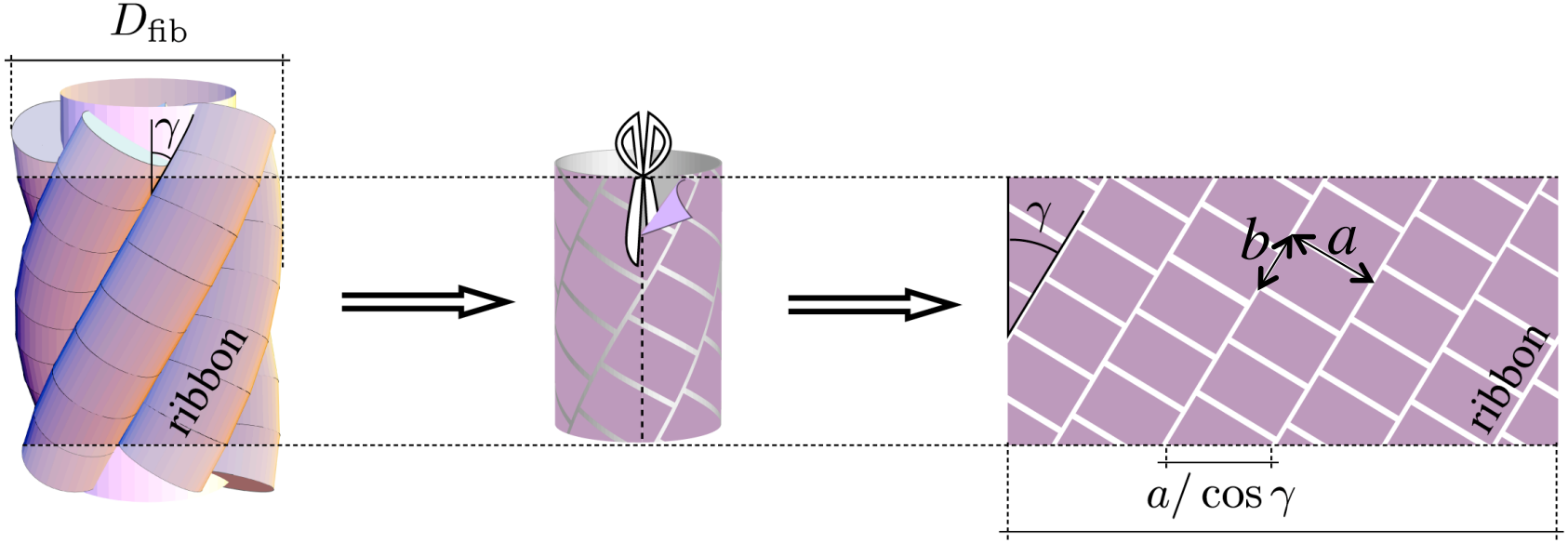
2002

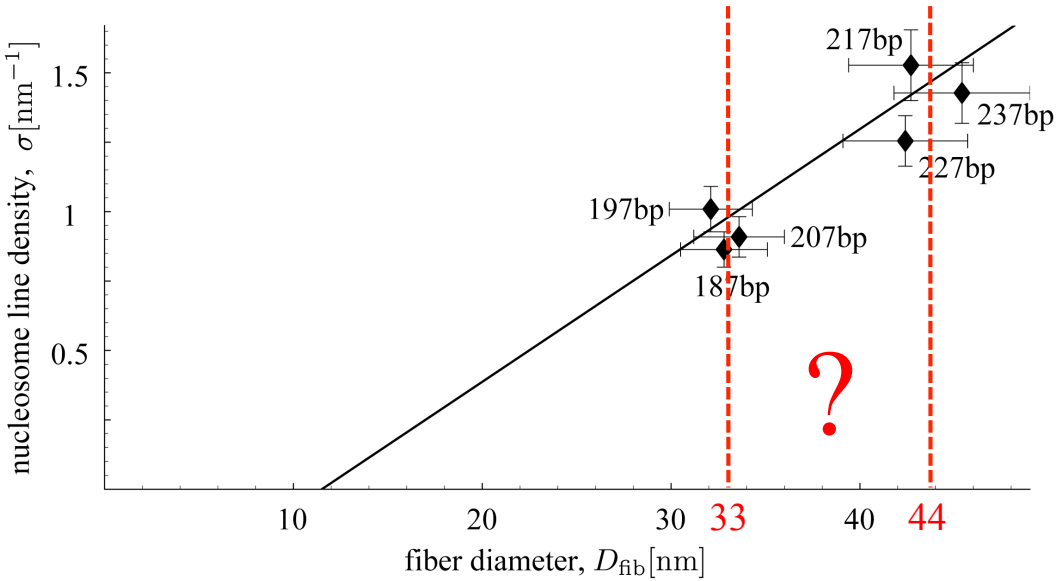


crossed-linker model

Dense packing of nucleosomes

M. Depken & HS, Biophys. J. **96** (2009) 777





dense packing:

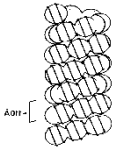
$$\sigma = \frac{\pi\,(D_{\mathrm{fib}} - a)}{ab}$$

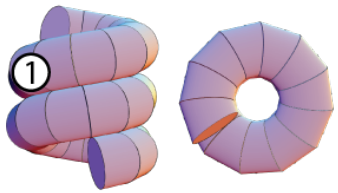
nucleosome line density

Splay angle

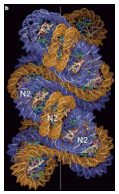
M. Depken & HS, Biophys. J. **96** (2009) 777

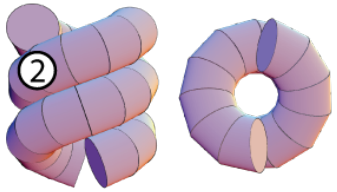
1976



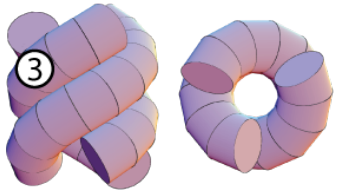


2005

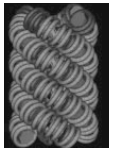


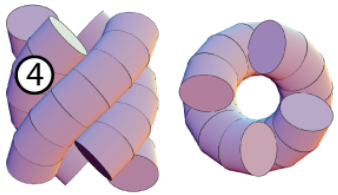


1985

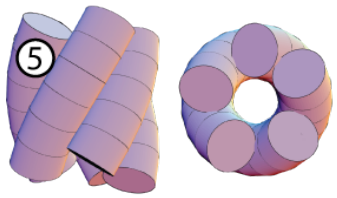


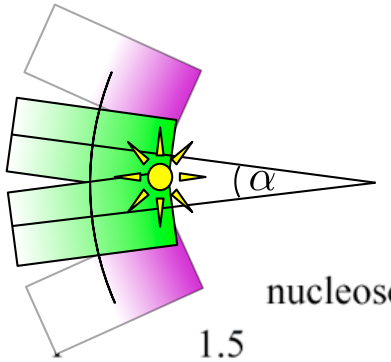
1998



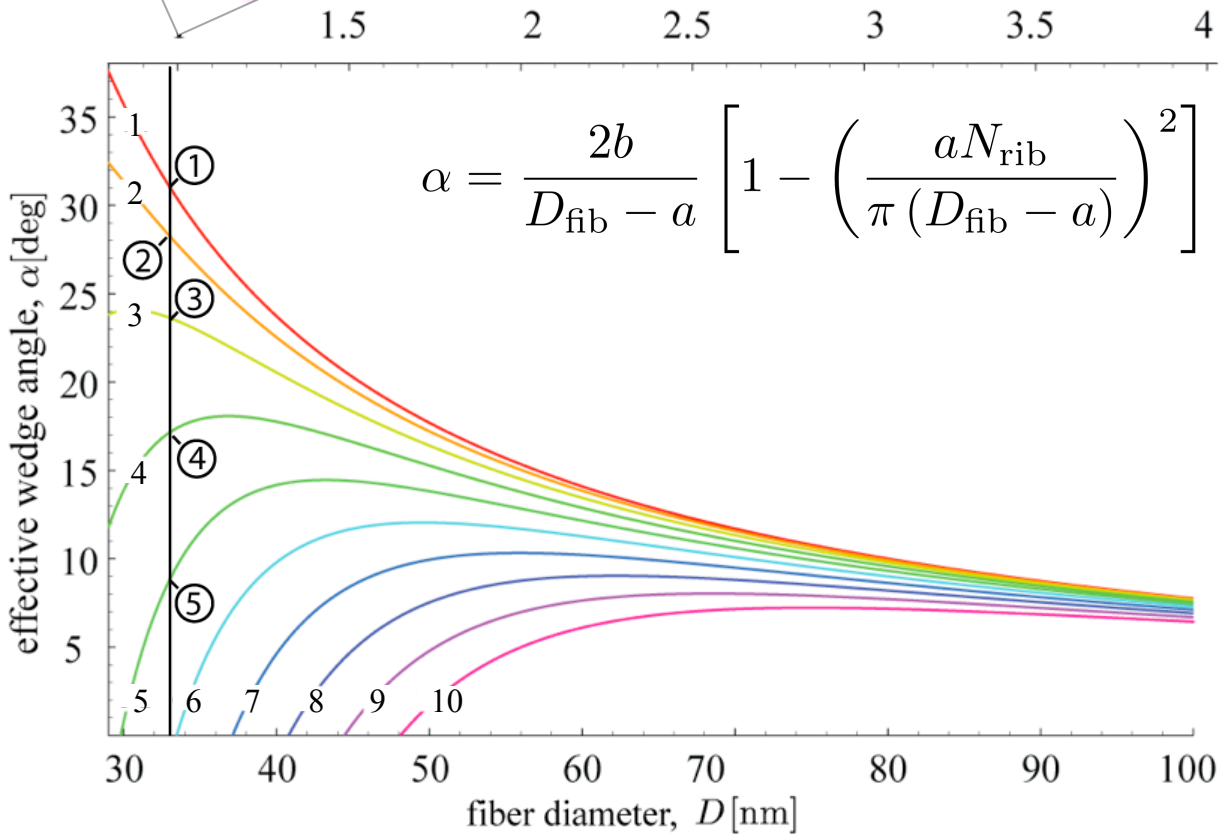


2007





$$\alpha = \frac{2b}{D_{\mathrm{fib}} - a}\left[1 - \left(\frac{aN_{\mathrm{rib}}}{\pi\,(D_{\mathrm{fib}} - a)}\right)^2\right]$$

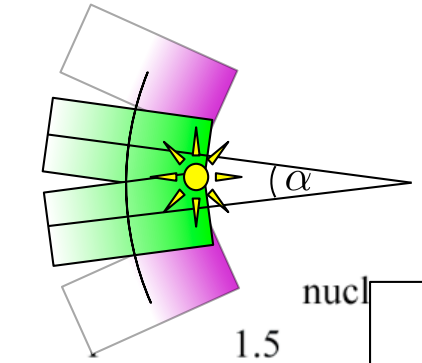


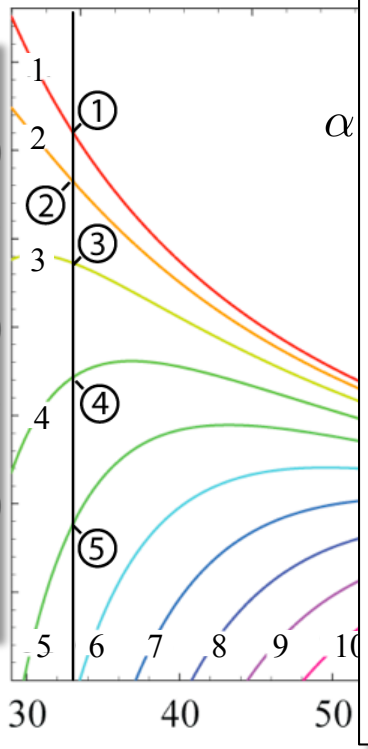
Splay angle

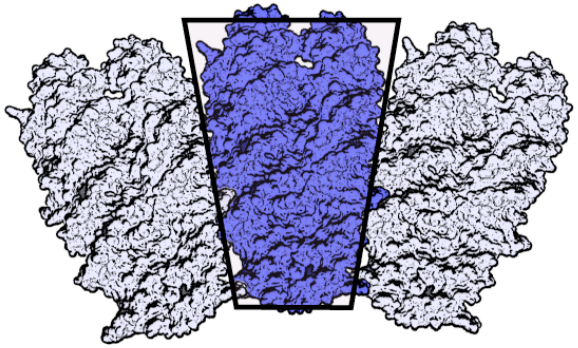
M. Depken & HS, Biophys. J. **96** (2009) 777

1976

2005

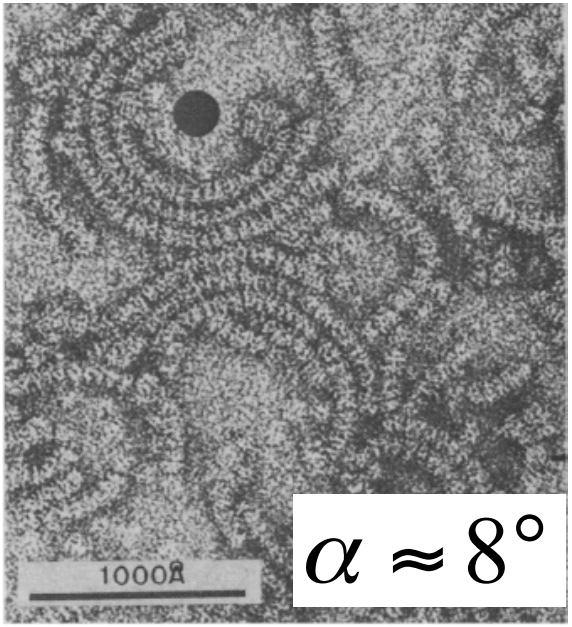






crystal structure

Luger et al., Nature (1997)

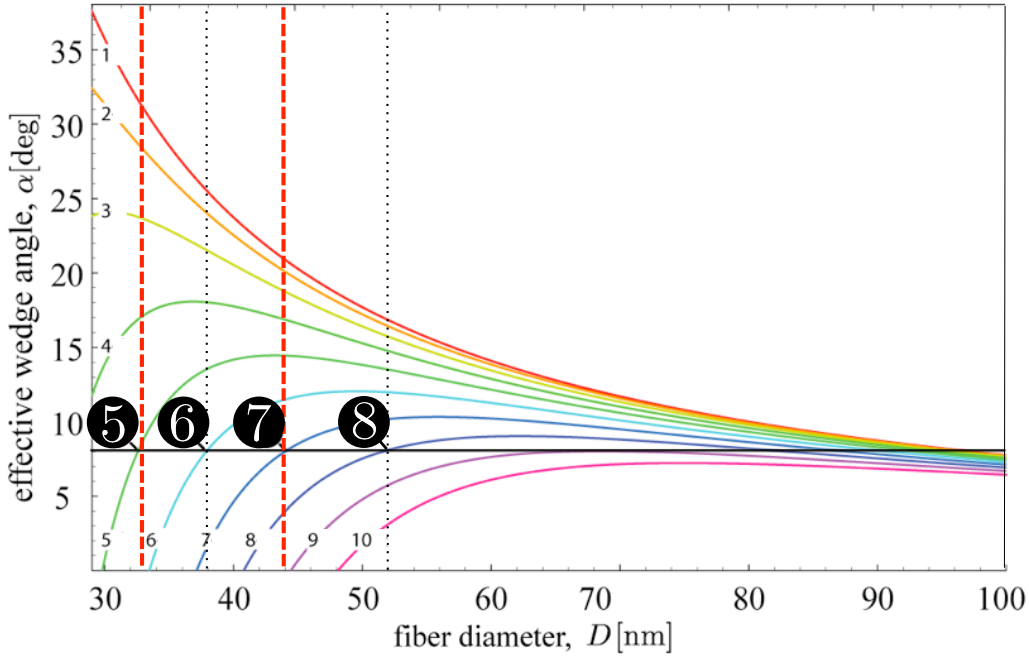


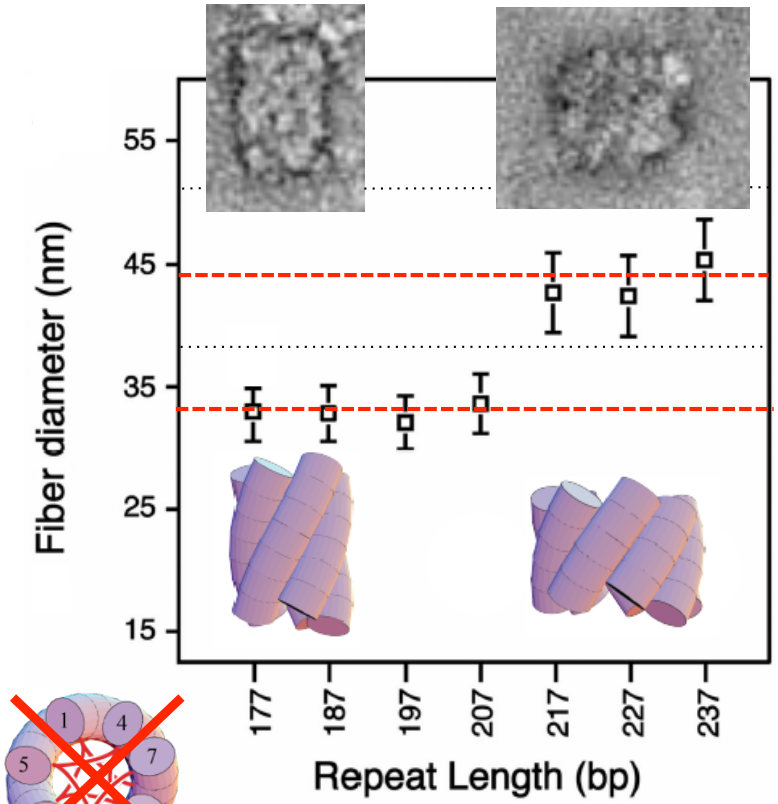
nucleosome arcs

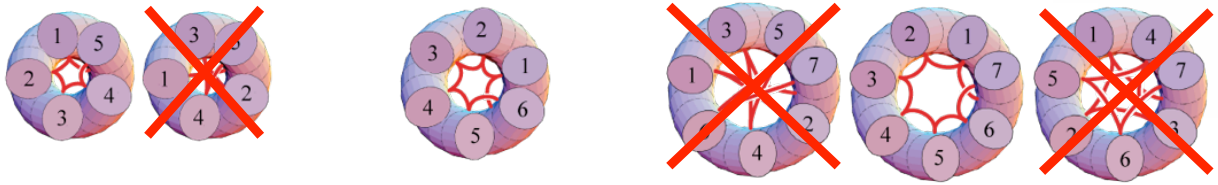
Dubochet & Noll, Science (1978)

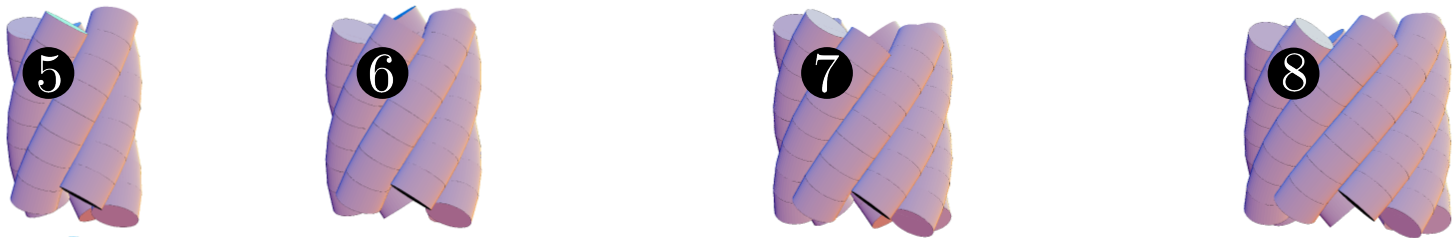
Magical nucleosome shells

M. Depken & HS, Biophys. J. **96** (2009) 777



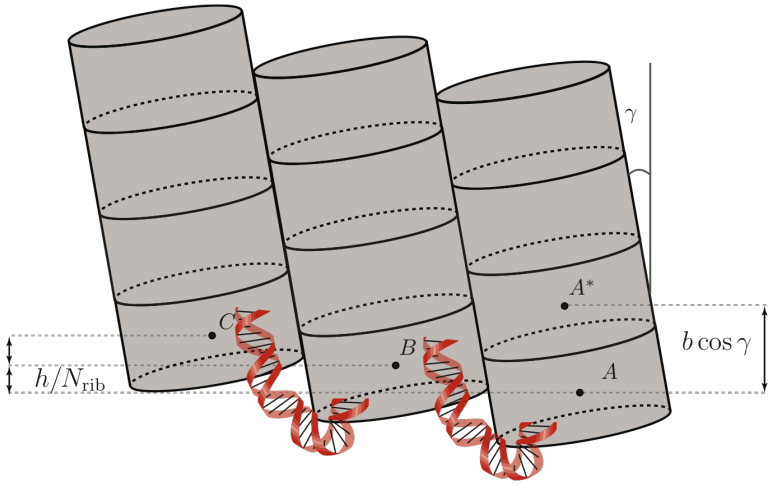


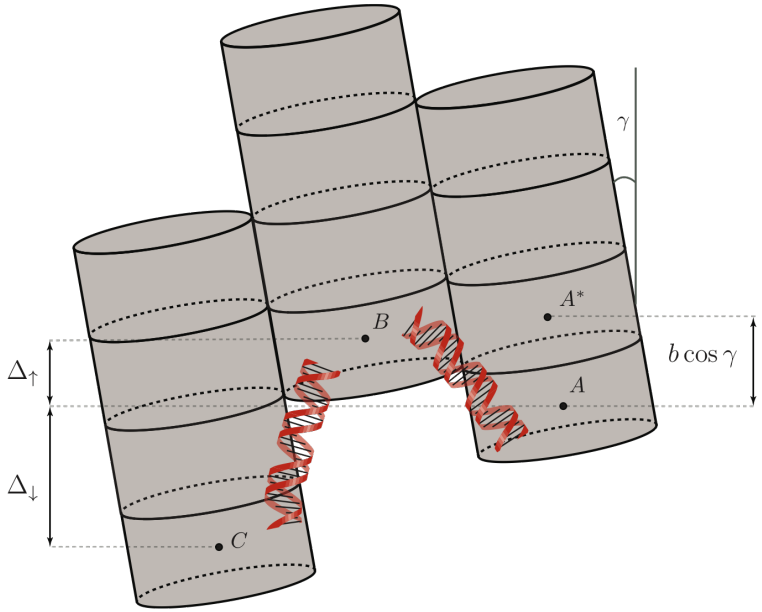




Sliding ribbons out-of-register

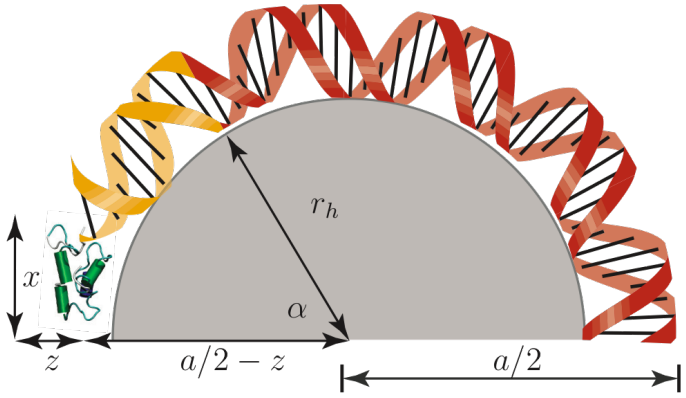
G. Lanzani & HS, submitted



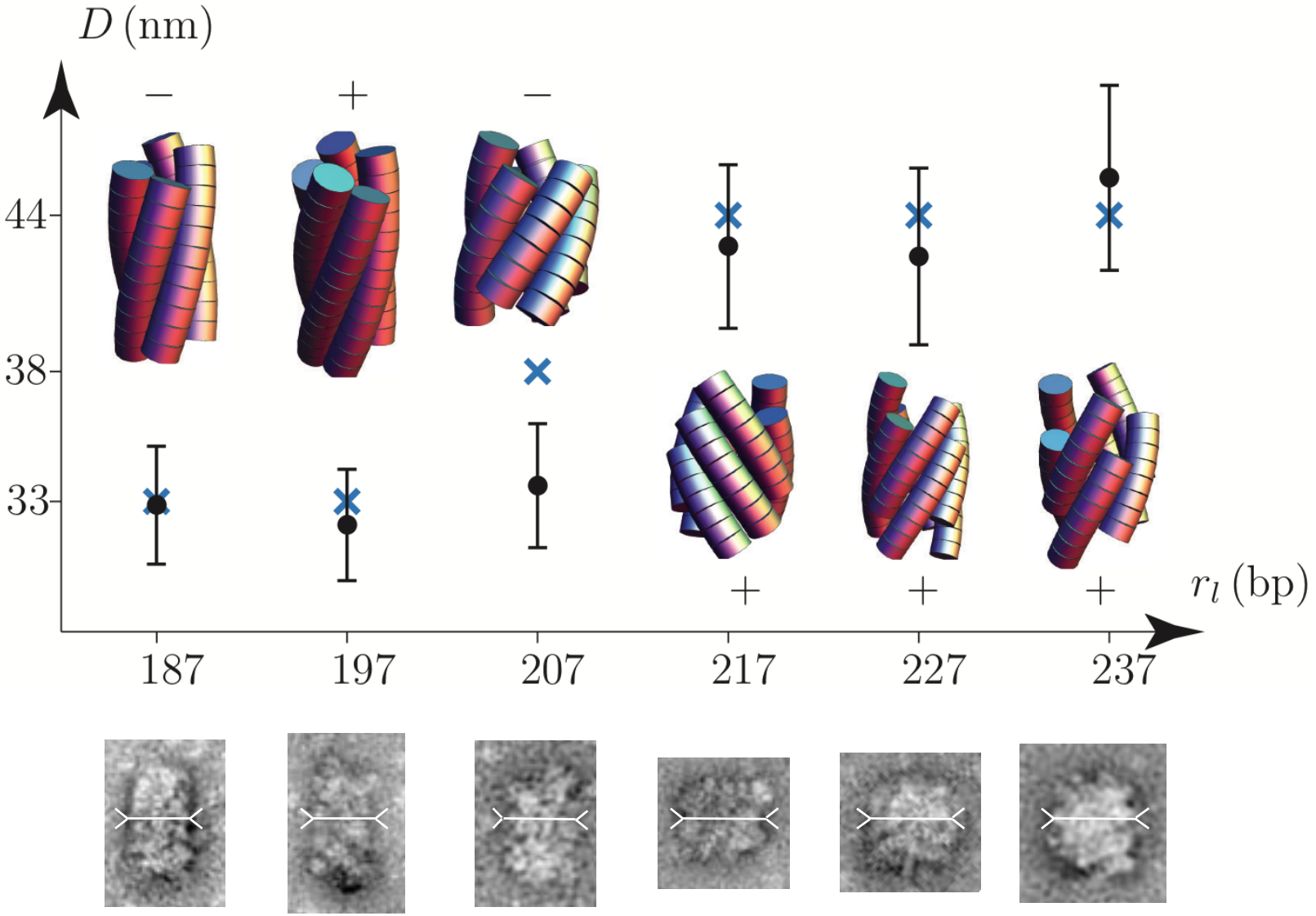


$$\approx 40 k_B T$$

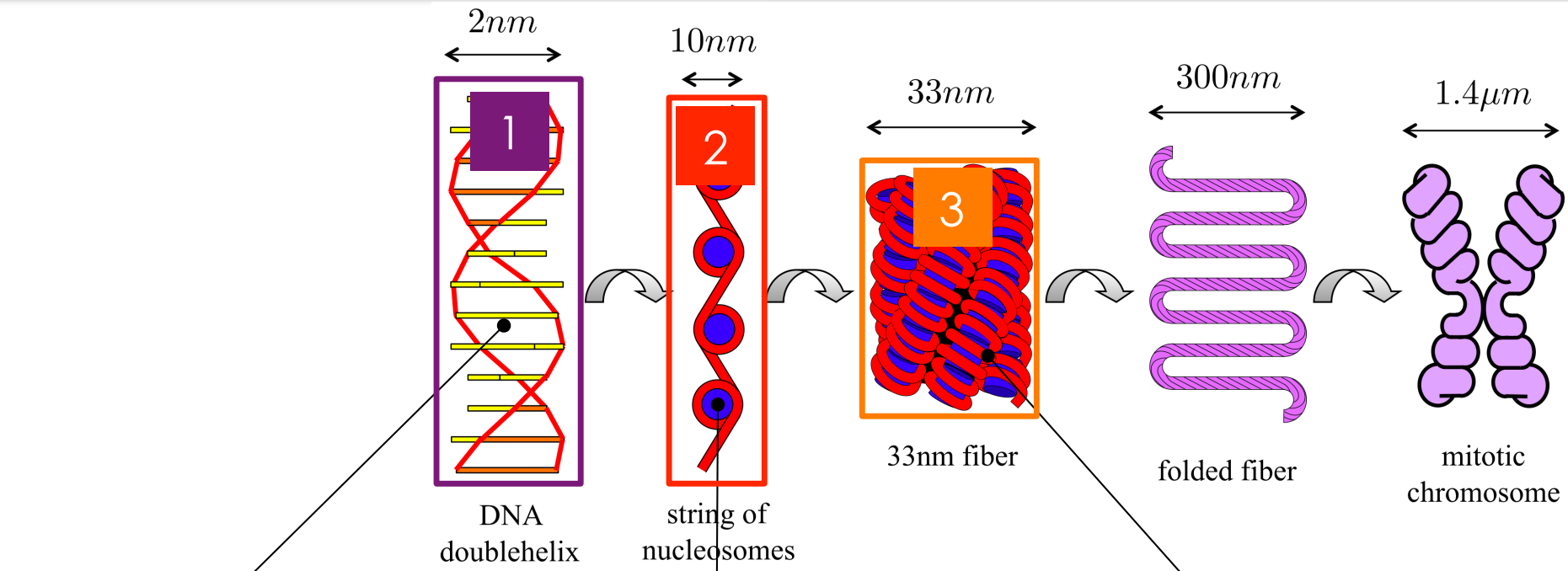
$$\approx 1 k_B T$$



Optimal fibers



Acknowledgements

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