Statistical mechanics of ribbons

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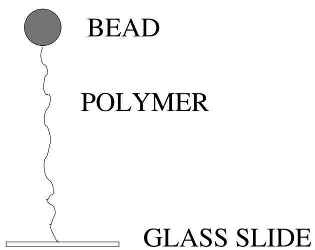
Perspective

- Recent Interest triggered by Single Molecule Experiments on Biopolymers with a view to understanding role of ELASTICITY at the cellular level (cytoskeletal network of biopolymers, packaging of DNA in a cell nucleus)
- IMAGING OF SINGLE MOLECULES (end-end distributions)
- PROBING ELASTICITY BY STRETCHING AND TWISTING (Force-Extn and Torque-Twist Curves)



- Theoretical Tools: Statistical Mechanics -(Biopolymers Subjected to Thermal Fluctuations in a cell- Competition between Energy and Entropy), Differential Geometry and Topology Of Curves.

Theoretical Analysis: WLC model

- *In the wormlike chain(WLC) model, we view the polymer as a ribbon, a framed space curve $\{\vec{x}(s), \hat{e}^i(s)\}$. $\vec{x}(s)$ describes the curve, $\hat{t}(s) = \frac{d\vec{x}}{ds}$, its tangent vector and $\hat{e}^i(s)$ the framing (the $\hat{e}^i$ s are an orthonormal frame with $\hat{e}^3 = \hat{t}$). s is the arc length parameter along the curve ranging from 0 to L, the contour length of the curve. $\vec{x}(0) = 0$ since one end is fixed at the origin. The tangent vectors at both ends $\hat{t}(0)$,$\hat{t}(L)$ are fixed to $\hat{t}_i$ and $\hat{t}_f$ respectively.*
- *We first restrict ourselves to the Pure Bend WLC model (with no twist degrees of freedom). We then probe the role of twist elasticity within the framework of the WLC model.*

The Worm Like Chain Model (Pure Bend)

- *A configuration $\mathcal{C}$ of polymer of contour length L described by a space curve $\vec{x}(s)$, with s the arc-length parameter ($0 \leq s \leq L$). The tangent vector $\hat{t} = d\vec{x}/ds$ to the curve satisfies:*

$$\hat{t}.\hat{t} = 1$$

(INEXTENSIBILITY CONSTRAINT)

- *The curvature κ is defined as follows:*

$$\kappa = |d\hat{t}/ds|$$

- *The energy $\mathcal{E}$ associated with a configuration $\mathcal{C}$ is*

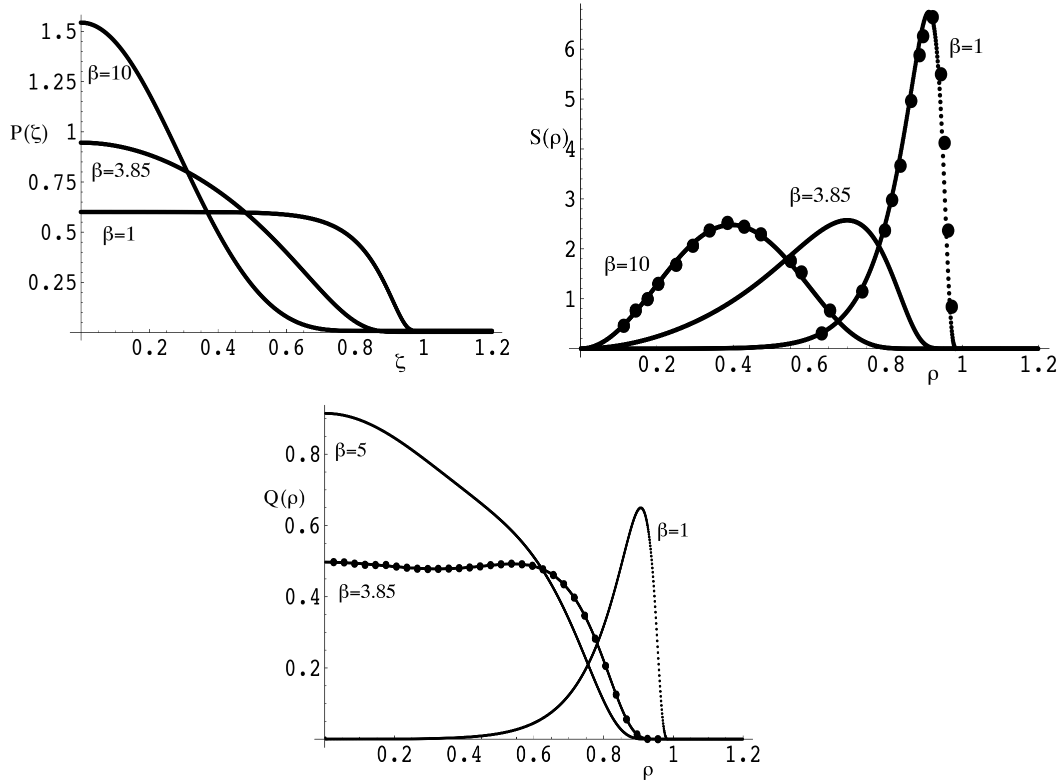
$$\mathcal{E}(\mathcal{C}) = \frac{A}{2}\int_0^L ds\kappa^2$$

where A is the bending rigidity. WLC model has shown excellent agreement (Marko-Siggia) with Force-Extn curves of DNA (a flexible biopolymer)- We extended it to ALL A.

The WLC Model (Bend):Schematic Outline

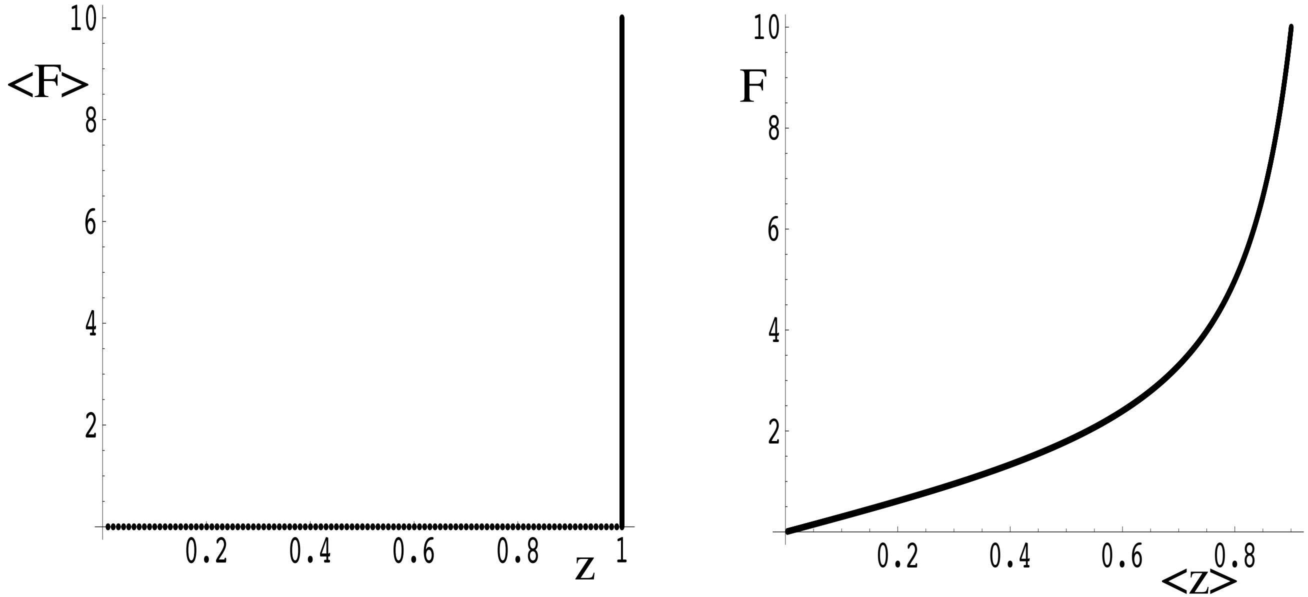
- Semiflexible polymers characterized by $\beta = L/L_P$, with $L_p = A/k_B T$, the persistence length (the length scale over which polymer is STRAIGHT)
- The central quantity of interest: $Z = \Sigma_{\mathcal{C}} \exp(-\mathcal{E}[\mathcal{C}]/k_B T)$, (The Partition Function: sum over configurations of the polymer subjected to thermal fluctuations for a given $\mathcal{E}$).
- Elastic properties contained in Z and its derivatives.
- "Exact" analysis- analytical+numerical(computable to any desired accuracy) (See Physical Review E, **66** 050801(R) (2002) - J. Samuel and S. Sinha for more detail) -pure bend+force f, $\rightarrow$ rigid rotor in a potential f.
- RESULTS: Our analytical results (end-end distance distributions and force-extension curves) have been tested against experiments on Actin Filaments (E. Frey, Loic Legoff and collaborators) and simulations(E. Frey, F. Wilhem and A. Dhar D. Chaudhury .

End-End Distribution Functions: Comparison with simulations



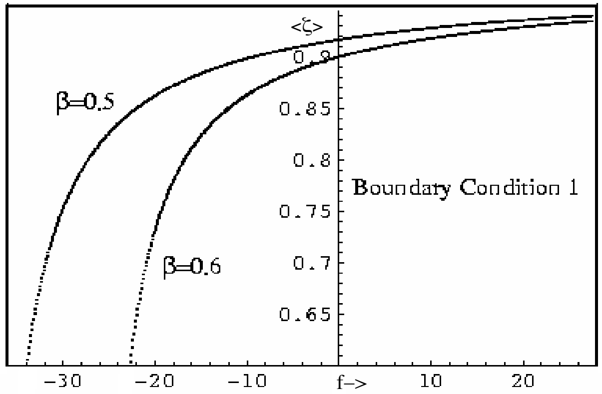
- *lines:our semi-analytical results; dots: results of simulations (Wilhelm and Frey, PRL (1996) and Dhar and Chaudhuri, PRL (2002). The three sets of graphs pertain to three distinct classes of experiments which can be also done over a range of biopolymer rigidities.*

Force-Extn Curves: Ensemble Inequivalence



- *Semiflexible polymers are of finite length (β). This leads to DISTINCT force-extension relations depending on the choice of the control parameter (force f or extension z). The figure is for $\beta = 0$. This leads to a "Free Energy of Transition (FET)" for switching between ensembles. The distinction (and also FET) disappears only in the $\beta \to \infty$ limit.* (*Physical Review E,* **71** *021104 (2005) - S. Sinha and J. Samuel*)

Stiff Polymers: Buckling



- *We have studied buckling of stiff polymers (e.g. actin filaments)(β small (finite)). In this limit we get explicit analytic results. (Physical Review E,* **76** *061801 (2007) - A. Ghosh. J. Samuel and S. Sinha)*
- *We find the following critical compressive force for buckling: $f_C = -(\pi/\beta)^2$. The compressive force needed to buckle rises sharply with stiffness $1/\beta$ (See Fig. for both ends clamped).*
- *Our results at the single molecule level has a bearing on the issue of cytoskeletal buckling under compression- of interest to biologists.*

Bend Angle Distribution

- *We analytically determine the bend angle distribution, i.e. the number of configurations with a final tangent vector* $\hat{t}_f$ *making an angle* θ *defined by* $\arccos{(\hat{t}_i.\hat{t}_f)}$ *by taking into consideration fluctuation corrections:*

(1) $$Det\mathcal{O} = L^2 \sin\theta/\theta.$$

around the classical mechanical minimum energy given by

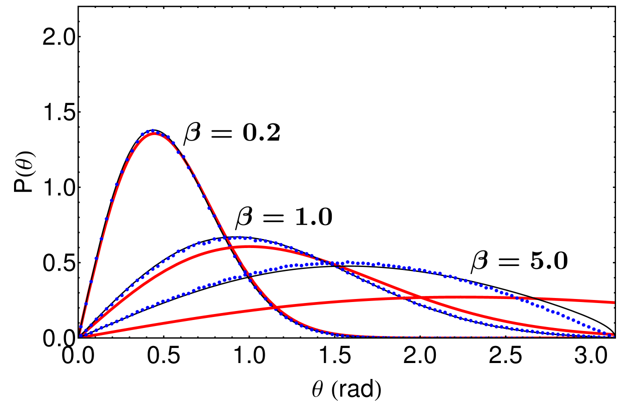
(2) $$E_{min} = A\theta^2/(2L),$$

Bend Angle Distribution (contd..):

This leads to the following approximate bend angle distribution:

(3) $$P(\theta) = \frac{\mathcal{N}}{L}\sqrt{\theta \sin\theta}\exp\left[-\frac{A\theta^2}{2LkT}\right]$$

and compare with simulation results:



- *Our predictions can be tested against AFM studies on DNA bending.*

Outline

- The WLC model (bend+twist) ignores self avoidance and views the polymer as a framed space curve $\mathcal{C} = \{\vec{x}(s), \hat{e}_i(s)\}, i = 1, 2, 3, 0 \leq s \leq L$ of contour length L, with an energy cost $\mathcal{E}(\mathcal{C})$ for bending and twisting.
- the energy $\mathcal{E}(\mathcal{C})$ of a configuration $\mathcal{C}$ is given by

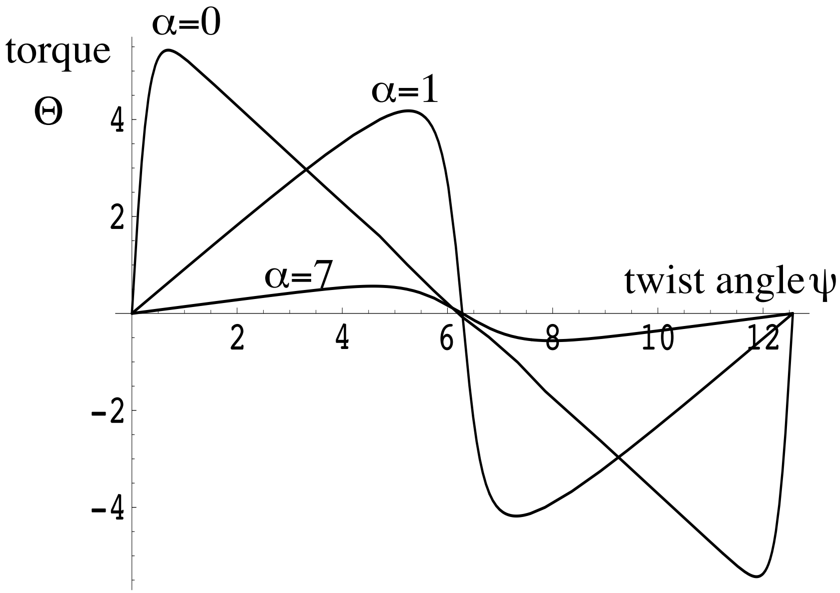
$$\mathcal{E}[\mathcal{C}] = 1/2 \int_0^L [A((\Omega_1)^2 + (\Omega_2)^2) + C(\Omega_3)^2] ds, \tag{4}$$

where A is the bending modulus and C the twist modulus.

- "Exact" analysis- analytical+numerical(computable to any desired accuracy) (See Physical Review Letters, **90** 098305 (2003) - J. Samuel and S. Sinha for more detail) -pure bend+twist $\rightarrow$ symmetric top.
- RESULTS: Torque(Θ)-Twist(ψ) relation: we compute the torque $\Theta = \partial F/\partial\psi$ needed to twist the molecule by an angle ψ. Here $F = -1/\beta Log[Z]$, with Z the pertinent partition function.

Torque-Twist relations:

- *Torque-Twist curves can be tested against experimental results and simulations.*



$\alpha = L_{BP}/L_{TP}$. L_{BP} and L_{TP} are the bend and twist persistence lengths.

- *Torque-Twist curves show periodicity- reflection of not taking into consideration self-avoidance in the model.* (can be seen in a special class of experiments in the presence of TOPOISOMERASE)

WLC with Bend and Twist:

- *The central quantity of interest:* $Z = \Sigma_{\mathcal{C}} \exp(-\mathcal{E}(\mathcal{C})/k_B T)$,

(The Partition Function: sum over configurations of the polymer subjected to thermal fluctuations for a given $\mathcal{E}$).

- *Elastic properties contained in Z and its derivatives.*
- *We first focus on the mechanics of the polymer which can be shown to be equivalent to that of a symmetric top (Kirchoff).*
- *We calculate the configurational energy as a function of the bending angle α between the initial and final tangent vectors, which is given by:*

(5)
$$\mathcal{E}_{cl}(\mu) = \frac{\tau^2 L}{2}[(\frac{1}{\mu}+1)^2 - 4]$$

where $\mu = \cos\theta$ (the cosine of an angle, appearing as a tangent vector component) and α are related via:

(6)
$$\alpha(\mu) = \arccos\left[(1-\mu^2)\cos(\frac{\tau L}{\mu}) + \mu^2\right]$$

Moment angle relns and Fluctuation corrs.

- Differentiating $\mathcal{E}_{cl}(\alpha)$ with respect to α gives us the moment-angle relation:

(7) $$M_{cl}(\alpha) = \frac{\partial \mathcal{E}_{cl}}{\partial \alpha}$$

- We compute the Van Vleck determinant to arrive at an expression for the fluctuation determinant Δ:

(8) $$\Delta^{-1} = \frac{1}{\sin\alpha} \frac{\partial}{\partial \alpha} \left[M_{cl}^2(\alpha) \right]$$

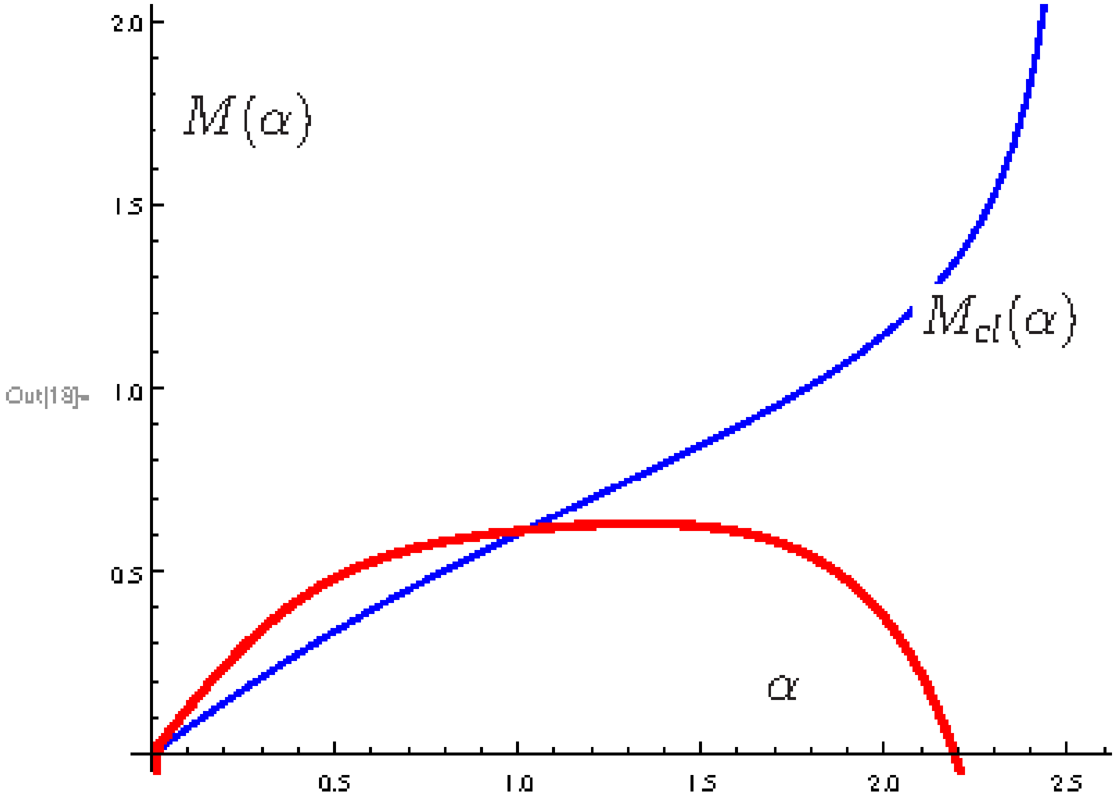
where $M_{cl}(\alpha)$ the classical Moment-angle relation.

- The thermal fluctuations are easily incorporated in using Eq. (8) in the expression for the free energy

(9) $$\mathcal{F}(\alpha(\mu)) = \mathcal{E}_{cl}(\mu) + 1/2kT \log \Delta(\mu)$$

This free energy can be differentiated to give the moment angle relations when thermal fluctuations are incorporated.

Results



- *Fig. shows Bending moment versus bending angle. blue line: mechanical elastic response and red line: includes thermal fluctuations*
- *Fig. shows initial Hookean behaviour followed by nonlinear behaviour for large bending angles. Notice softening of 'bending rigidity' due to thermal fluctuations.*

Conclusion

- *To summarize, we have studied aspects of statistical mechanics of ribbons with a view to understanding the elastic properties of DNA and other biopolymers which in turn control biological processes like packaging of DNA in a cell nucleus.*

  • *In particular, we have studied the elastic response of a semiflexible polymer with only bending degree of freedom. Then we have also looked at the role of twisting degrees of freedom.*

  • *We have studied how THERMAL FLUCTUATIONSmodify its response.*

  • *Some of these analytical results have been tested against simulations and experiments. We also have some further analytical predictions that can be tested against future experiments and simulations.*