

# Semiflexible Polymer Dynamics: elasticity, geometry, constraint

QuickTime™ and a  
decompressor  
are needed to see this picture.

Image:  
Neil  
Melndelson,  
U Arizona

Chris Wiggins  
Applied Math, Columbia U  
NYC  
Feb 13 2002

elasticity

## Bending

- Review: energy

$$\mathcal{E}_{\text{bending}} = \frac{1}{2} A \int ds (\mathbf{r}'')^2$$

# elasticity

## Boundary Conditions

- From the Energy
- Forcelessness
- Torquelessness

$$\mathcal{E}_{\text{bending}} = \frac{1}{2} A \int ds (\mathbf{r}'')^2$$

$$\delta \mathcal{E} = A \left\{ \mathbf{r}'' \delta \mathbf{r}' | - \mathbf{r}''' \delta \mathbf{r} | + \int \mathbf{r}'''' \delta \mathbf{r} \right\}$$

# elasticity

## Diffusion?

- Analogy with random walks

$$\begin{aligned} \rho &\propto e^{-\frac{1}{2} A \int d\hat{\mathbf{t}}' r'^2} \delta(\hat{\mathbf{t}}^2 - 1) \\ &\sim e^{-\frac{1}{2} \frac{1}{D} \int \dot{x}^2 dt} \end{aligned}$$

- Schroedinger eqn. gives  $t(s)t(0)$  correlation

## geometry

---

Geometry

---

- Another perspective.....

$$\begin{aligned}\hat{\mathbf{t}}' &= \kappa \hat{\mathbf{n}} \\ \hat{\mathbf{n}}' &= -\kappa \hat{\mathbf{t}}\end{aligned}$$

- or

$$\begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{n}} \end{pmatrix}' = \begin{pmatrix} 0 & \kappa \\ -\kappa & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{n}} \end{pmatrix}$$

## geometry

---

Geometric Frames

---

- What about 3D?

$$\begin{aligned}\hat{\mathbf{n}}' &= -\kappa \hat{\mathbf{t}} + \tau \hat{\mathbf{b}} \\ \hat{\mathbf{b}}' &= \quad \quad \quad - \tau \hat{\mathbf{n}}\end{aligned}$$

- Extension (Frenet):

$$\begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{n}} \\ \hat{\mathbf{b}} \end{pmatrix}' = \begin{pmatrix} 0 & \kappa & 0 \\ -\kappa & 0 & \tau \\ 0 & -\tau & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{n}} \\ \hat{\mathbf{b}} \end{pmatrix}$$

## geometry

---

Material Frames

---

- In general...

$$\begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_2 \end{pmatrix}' = \begin{pmatrix} 0 & \Omega_2 & \Omega_1 \\ -\Omega_2 & 0 & \Omega_3 \\ -\Omega_1 & -\Omega_3 & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_2 \end{pmatrix}$$

- New term in the energy: twist!

$$E_{\text{twist}} = \frac{1}{2} C \int ds \Omega_3^2$$

## geometry

---

Natural Frames

---

- Frame equations

$$\begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_2 \end{pmatrix}' = \begin{pmatrix} 0 & a & b \\ -a & 0 & 0 \\ -b & 0 & 0 \end{pmatrix} \begin{pmatrix} \hat{\mathbf{t}} \\ \hat{\mathbf{e}}_1 \\ \hat{\mathbf{e}}_2 \end{pmatrix}$$

cf. R.L. Bishop, Amer. Math. Monthly 1975.

## geOmetry

## Natural Frames

- Construction

$$\begin{aligned}\hat{\mathbf{e}}_{\perp} &= \hat{\mathbf{e}}_1^{(n)} + i\hat{\mathbf{e}}_2^{(n)} \\ &= (\hat{\mathbf{n}} + i\hat{\mathbf{b}}) e^{i \int^s ds \tau} \\ &= (\hat{\mathbf{e}}_1^{(m)} + i\hat{\mathbf{e}}_2^{(m)}) e^{i \int^s ds \Omega_3}\end{aligned}$$

## geOmetry

## Natural Frames

- Construction

$$\begin{aligned}\psi &= a + ib \\ &= \kappa e^{i \int^s ds \tau} \\ &= (\Omega_1 + i\Omega_2) e^{i \int^s ds \Omega_3}\end{aligned}$$

cf. Hasimoto 1972

geometry

## Natural Frames

- Elastic Force

$$\mathcal{F}_\perp = -A(\psi'' + \frac{1}{2}|\psi|\psi) + iC(\Omega\psi)' - \Lambda\psi$$

- Meaning of terms is qualitatively clear

cf. Shi & Hearst 1994, Goldstein et al. 1998

geometry

$$\dot{\mathcal{L}}k = \dot{\mathcal{T}}w + \dot{\mathcal{W}}r$$

spinning vs twisting

$\omega'$  vs  $\dot{\Omega}$

$\partial_s(\hat{\mathbf{e}}_2 \cdot \partial_t \hat{\mathbf{e}}_1)$  vs  $\partial_t(\hat{\mathbf{e}}_2 \cdot \partial_s \hat{\mathbf{e}}_1)$

$(\hat{\mathbf{e}}_2 \dot{\hat{\mathbf{e}}}_1)'$  vs  $\dot{\hat{\mathbf{e}}}_2 \hat{\mathbf{e}}_1'$

$\hat{\mathbf{e}}_2' \dot{\hat{\mathbf{e}}}_1 + \hat{\mathbf{e}}_2 \dot{\hat{\mathbf{e}}}_1'$  vs  $\dot{\hat{\mathbf{e}}}_2 \hat{\mathbf{e}}_1' + \hat{\mathbf{e}}_2 \dot{\hat{\mathbf{e}}}_1'$

# geometry

$$\dot{\mathcal{L}}k = \dot{\mathcal{T}}w + \dot{\mathcal{W}}r$$

- Spinning vs twisting

$$\omega' = \dot{\Omega} + \dot{\hat{\mathbf{e}}}_2 \hat{\mathbf{e}}'_1 - \hat{\mathbf{e}}'_2 \dot{\hat{\mathbf{e}}}_1$$

$$\omega' = \dot{\Omega} + (\dot{\hat{\mathbf{e}}}_3 \hat{\mathbf{e}}_2)(\hat{\mathbf{e}}_1 \hat{\mathbf{e}}'_3) - (\hat{\mathbf{e}}'_3 \hat{\mathbf{e}}_2)(\hat{\mathbf{e}}_1 \dot{\hat{\mathbf{e}}}_3)$$

$$\omega' = \dot{\Omega} + \hat{\mathbf{t}} \cdot (\hat{\mathbf{t}}' \times \dot{\hat{\mathbf{t}}})$$

- Local lk=tw+wr

cf. Kamien 1998

# geometry

## Dynamics

- Physics says:  $\zeta_{\text{trans}} \dot{\mathbf{r}} = -\frac{\delta \mathcal{E}}{\delta \mathbf{r}}$   
 $\zeta_{\text{rot}} \dot{\chi} = -\frac{\delta \mathcal{E}}{\delta \chi},$

- ergo e.o.m:

$$\zeta_{\text{trans}} \psi_t = -A \psi''' + iC\Omega \psi''' + \Lambda \psi'' + h.o.t$$

$$\Omega_t = \frac{C}{\zeta_{\text{rot}}} \Omega'' - \frac{1}{\zeta_{\text{trans}}} \Im \mathcal{F}_\perp \psi^*$$

geometry

## Geometric Untwisting

QuickTime™ and a  
decompressor  
are needed to see this picture.

cf. Goldstein 1998

geometry

## Geometric Untwisting

QuickTime™ and a  
decompressor  
are needed to see this picture.

Image: Neil Mendelson, U. Arizona

## constraint

---

Constraints

---

- Energy:

$$E_{\text{stretch}} = \frac{1}{2} \int ds \Lambda \mathbf{r}'^2$$

- BC's

## constraint

---

Toy Problem: Chain

---

$$\begin{aligned}\mathbf{f} &= m\mathbf{a} \\ \rho_1 \ddot{\mathbf{r}} &= \partial_s(\Lambda \hat{\mathbf{t}}) \\ \rho_1 \ddot{\hat{\mathbf{t}}} &= \partial_s^2 \Lambda \hat{\mathbf{t}} \\ \rho_1 \partial_t^2 e^{i\theta} &= \partial_s^2 \Lambda e^{i\theta} \\ \ddot{\theta} &= \Lambda \theta'' + 2\theta' \Lambda \\ (\partial_s^2 - \theta'^2) \Lambda &= -(\dot{\theta})^2\end{aligned}$$

cf. Belmonte et. al. 2001

constraint

## Toy Problem: Chain

QuickTime™ and a  
decompressor  
are needed to see this picture.

Image: A. Belmonte, Penn State

constraint

## Toy Problem: Chain

QuickTime™ and a  
decompressor  
are needed to see this picture.

Image: A. Belmonte, Penn State

# constraint

## Toy Problem: Chain

QuickTime™ and a decompressor are needed to see this picture.

# constraint

## Experimental Constraints

- tethering
- driving

# numerics

## Spectral Numerics?

- Eigenfunctions

$$\Lambda = \Omega = \psi = \psi' = 0$$

- Stiffness

$$\dot{\theta} = D\theta'' + f$$

$$\dot{\theta}_q = -Dq^2\theta$$

$$\theta^{n+1} = (1 - Dq^2\Delta t)\theta^n$$

$$\theta^{n+1} = e^{-Dq^2\Delta t}(\theta^n + \int_{t_n}^{t_{n+1}} dt' e^{Dq^2 t'} f(t'))$$

# stochastics

kT

QuickTime™ and a  
Video decompressor  
are needed to see this picture.

Image courtesy J. Howard, Max Planck Institute of Molecular Cell Biology and Genetics, Dresden

# stochastics

$kT$

- Constraints
- Metric Forces
- Time Scales