Tumbling in an extensional flow

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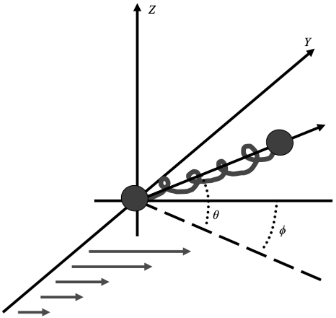
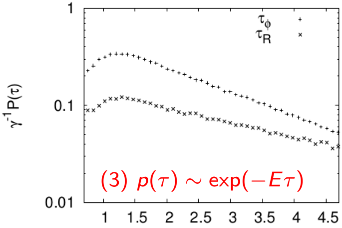
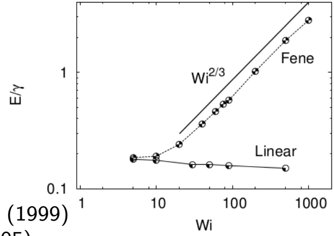
Polymer dynamics in shear flow

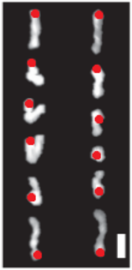


(2) shear flow: $\mathbf{u} = \gamma(0, y, 0)$



(3) $p(\tau) \sim \exp(-E\tau)$

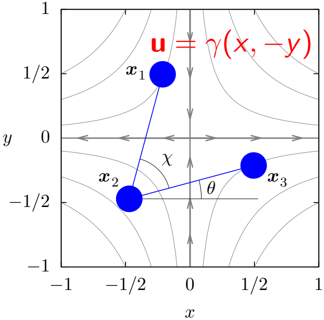




(4) DNA tumbling in shear flow $L \approx 7\mu m$

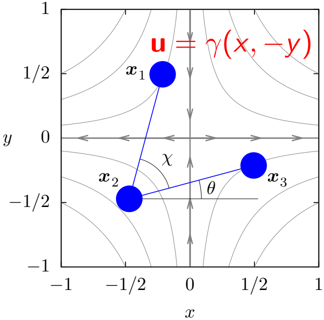
(1) Smith, Babcock and Chu. Science. (1999)
(2) Chertkov, et al. J. Fluid Mech. (2005)
(3) Celani, Puliafito and Turitsyn. Europhys. Lett. (2005)
(4) Gerashchenko and Steinberg. Phys. Rev. Lett. (2006)

The trumbbell model



1. rigid, inertialess beads and rods
2. frame of reference at $\mathbf{x}_c$: $\mathbf{r}_\nu = \mathbf{x}_c - \mathbf{x}_\nu, \nu = 1, 2, 3$
3. coordinates $\mathbf{q} = \{\theta, \chi\}$ (in 2D)
4. neglect hydrodynamical interactions
5. dilute solution

The trumbbell model



Forces at play:

- Stokes' drag with coefficient ζ
- rigidity constraint (fixed length ℓ)
- restoring potential $\phi = \mu(\chi - \pi)^2/2$
- thermal fluctuations

Langevin equations:

$$m\ddot{\mathbf{x}}_\nu = -\zeta[\dot{\mathbf{x}}_\nu - \mathbf{u}(\mathbf{x}_\nu, t)] + \mathfrak{t}_\nu + \mathbf{f}_\nu + \sqrt{D}\,\boldsymbol{\eta}_\nu(t)$$

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Diffusion Equation for p.d.f. $\psi(\theta, \chi; t)$

P.d.f. ψ satisfies (Hassager, JCP (1974)):

$$\frac{\partial \psi}{\partial t} = -\frac{\partial}{\partial \mathbf{q}^i} \left\{ G^{ij} \left[\left(\kappa^{kl}(t) \mathbf{r}^l_\nu \frac{\partial \mathbf{r}^k_\nu}{\partial \mathbf{q}^j} - \frac{1}{\zeta} \frac{\partial \phi}{\partial \mathbf{q}^j} \right) \psi - \frac{KT}{\zeta} \sqrt{h} \frac{\partial}{\partial \mathbf{q}^j} \left(\frac{\psi}{\sqrt{h}} \right) \right] \right\}$$

where

$\kappa^{ij}(t) = \partial^j u^i(\mathbf{x}_c(t), t)$, $\quad H^{ij} = \sum_{\nu,k} \frac{\partial r^k_\nu}{\partial q^i} \frac{\partial r^k_\nu}{\partial q^j}$, $\quad G = H^{-1}$, $\quad h = \det H$

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In 2D:

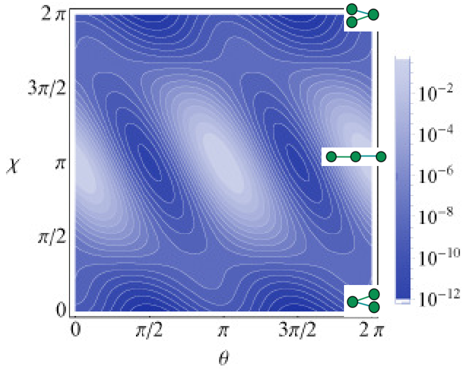
$$\begin{aligned} \dot{\theta}(t) &= V_\theta + \sqrt{D_{\theta\theta}}\, \xi_\theta(t), \\ \dot{\chi}(t) &= V_\chi + \frac{D_{\theta\chi}}{\sqrt{D_{\theta\theta}}}\, \xi_\theta(t) + \sqrt{D_{\chi\chi} - \frac{D^2_{\theta\chi}}{D_{\theta\theta}}}\, \xi_\chi(t) \end{aligned} \qquad (1)$$

where $\xi_\theta(t), \xi_\chi(t)$ are independent white noises.

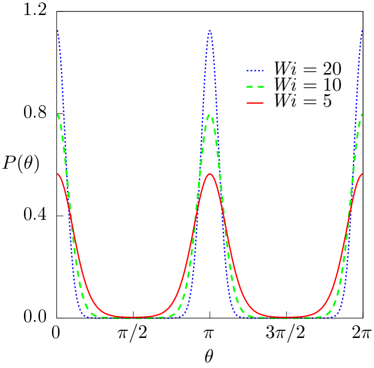
Stationary statistics with $\mathbf{u} = \gamma(x, -y)$

$$\psi_{\rm st} = N\sqrt{4-\cos^2\chi}\,\exp\left[\frac{Z\,Wi(2\cos\chi-1)\cos(2\theta+\chi)}{3} - \frac{Z(\pi-\chi)^2}{2}\right]$$

where $Wi = \gamma\zeta\ell^2/\mu, Z = \mu/KT, Pe = Z\,Wi$.

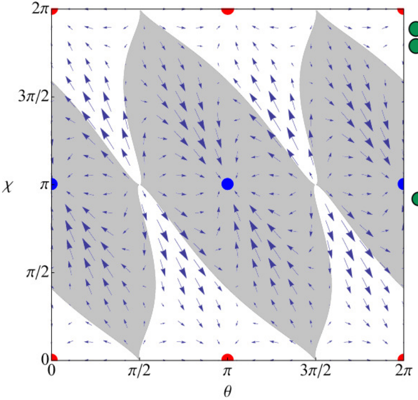


ln $\psi_{\rm st}$ for $Wi = 5, Z = 1$



marginal p.d.f. of θ

Vector plot ($Wi = Pe = \infty$)



$P_0 : (\theta = n\pi, \chi = 0, 2\pi)$

$\lambda_0^{(1)} = -2\gamma, \lambda_0^{(2)} = -4\gamma/3$

$P_\pi : (\theta = n\pi, \chi = \pi)$

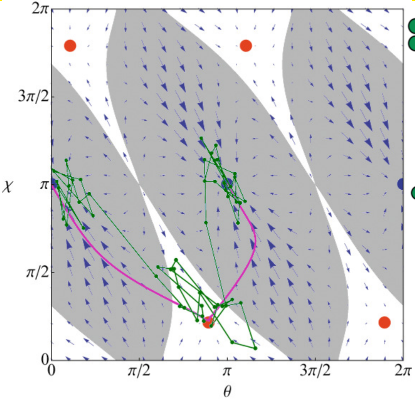
$\lambda_\pi^{(1)} = -4\gamma, \lambda_\pi^{(2)} - 2\gamma.$

$$\frac{\lambda_\pi^{(1)}}{\lambda_0^{(1)}} = 2 \text{ for all } \gamma$$

$$\dot{\theta}(t) = -\frac{\gamma}{2(4 - \cos^2\chi)} [7\sin(2\theta) + 4\cos(2\theta + \chi)\sin\chi - \sin(2(\theta + \chi))]$$

$$\dot{\chi}(t) = -\frac{4\gamma}{2 + \cos\chi} [\sin\chi \cos(2\theta + \chi)]$$

Stationary statistics ($Wi < Pe = \infty$)



$P_0 : (\theta = n\pi, \chi = 0, 2\pi)$

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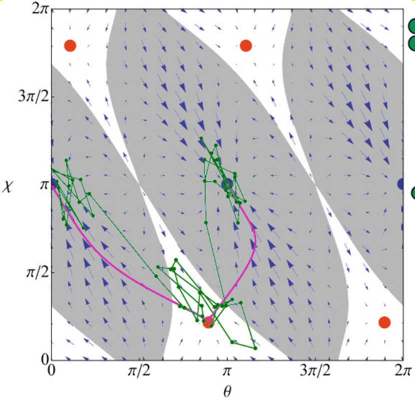
Stationary statistics ($Wi < Pe = \infty$)




$P_0 : (\theta = n\pi, \chi = 0, 2\pi)$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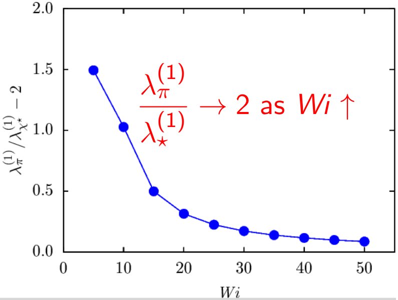
Stable points $P_\star \to P_0$ as $Wi \to \infty$

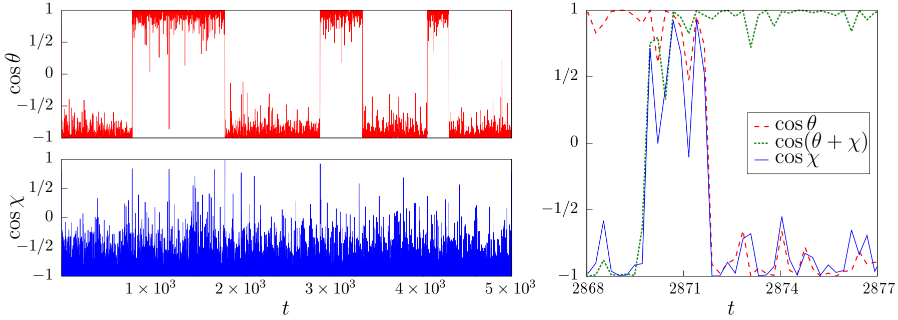


Green curve: sample trajectory

Pink curve: a minimum energy path connecting (π, π) and $(0, \pi)$

Tumbling Dynamics

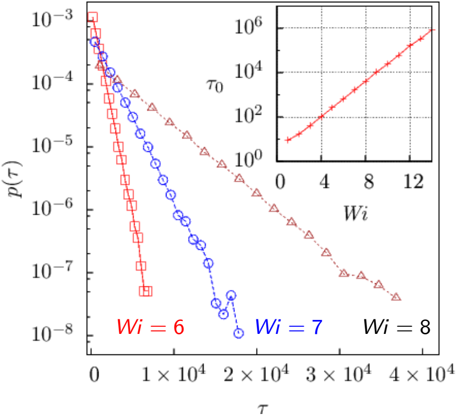
Time series of (1) for $Wi = 6, Z = 1$



Movie: 

P.d.f. of tumbling time τ

$p(\tau) \propto \exp(-\tau/\tau_0)$ for $\tau \gg \tau_0$

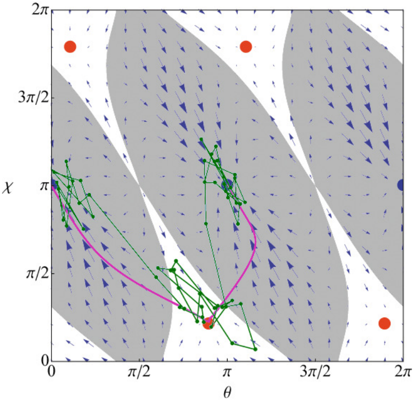


$\tau_0 \propto \exp(Wi)$

different from tumbling time in shear!

Remarks:

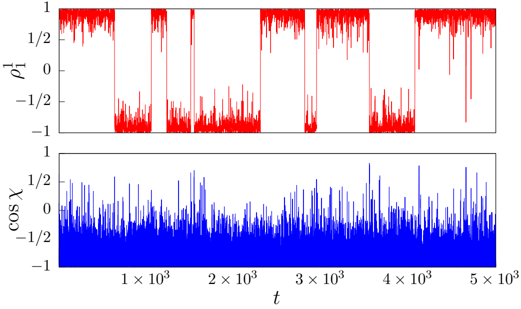
1. tumbling motion = exit from an attractive domain (large deviations theory)
2. p(exit)=exponential with ↑ mean as noise ↓
3. Minimum energy paths (most probable transition path) show tumbling-through-folding motion
4. reminiscent of buckling instabilities, but the dynamics are different[1]

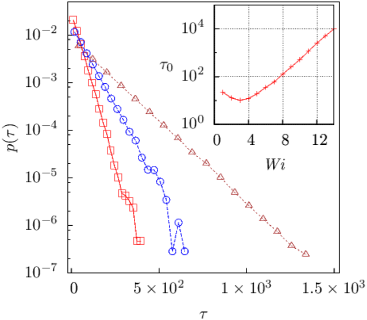


[1] Lindner and Shelley. In Fluid-Structure Interactions in Low Reynolds-Number Flows. (2014)

Trumbbell model in 3D

Flow: $\mathbf{u} = \gamma(x, -y, 0)$





Coordinates: $\mathbf{q}$ = three Euler angles and $\chi \to$ singularity in equations

Equivalent formulation: $\dot{\boldsymbol{\rho}}_1 = \dot{\mathbf{x}}_1 - \dot{\mathbf{x}}_2$ and $\dot{\boldsymbol{\rho}}_3 = \dot{\mathbf{x}}_3 - \dot{\mathbf{x}}_2$

$\to$ system of Stratonovich SDEs

Conclusions

1. Semi-flexible polymers perform tumbling-through-folding motion in an extensional flow
2. Two dimensional analysis $\leftrightarrow$ planar 3D flow.
3. Tumbling time $p(\tau) \propto exp(-\tau/\tau_0)$ with $\uparrow \tau_0$ as $\uparrow Wi$
4. Use of large deviations theory

Questions: Increase degrees of freedom? Effect of dynamics on flow? Hydrodynamic interactions?

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Thank you for your attention!

References

1. A. Celani, A. Pulifiato and K. Turitsyn. *Polymers in linear shear flows: A numerical study*. Europhys. Lett., **70**(4), 464-470 (2005).
2. M. Chertkov, I. Kolokolov, V. Lebedev and K. Turitsyn. *Polymer statistics in a random flow with mean shear*. J. Fluid Mech. **531**. (2005)
3. S. Gerashchenko and V. Steinberg. *Statistics of Tumbling of a Single Polymer in Shear Flow*. Phys. Rev. Lett. **96**, 038304 (2006).
4. O. Hassager. *Kinetic theory and rheology of bead-rod models for macromolecular solutions*. J. Chem. Phys. **60**, 5 (1974).
5. D. Smith, H. Babcock and S. Chu. *Single polymer dynamics in steady shear flow*. Science. **283** (1999)

Appendix

Drift coefficients of the Fokker–Planck equation in 2D:

$$\begin{aligned} V_\theta &= -\frac{6KT\sin\chi}{\zeta\ell^2(2-\cos\chi)(2+\cos\chi)^2} - \frac{3\mu(\pi-\chi)}{\zeta\ell^2(2+\cos\chi)} - \\ &\frac{1}{4-\cos^2\chi}\{[2\sin\chi\cos^2(\theta+\chi)+\cos\theta(4\sin\theta-\cos\chi\sin(\theta+\chi))]\kappa^{11}(t) + \\ &[2\cos\chi\sin^2(\theta+\chi)-\sin\theta(2+\cos\chi)\sin(\theta+\chi)+4\sin^2\theta]\kappa^{12}(t) + \\ &[-2\cos\chi\cos^2(\theta+\chi)+\cos\theta(2+\cos\chi)\cos(\theta+\chi)-4\cos^2\theta]\kappa^{21}(t) + \\ &[2\cos\theta(\sin(\theta+\chi)-2\sin\theta)+\cos\chi(\sin\theta\cos(\theta+\chi)-\sin(2(\theta+\chi)))]\kappa^{22}(t)\} \end{aligned}$$

$$\begin{aligned} V_\chi &= \frac{12KT\sin\chi}{\zeta\ell^2(2-\cos\chi)(2+\cos\chi)^2} + \frac{6\mu(\pi-\chi)}{\zeta\ell^2(2+\cos\chi)} + \frac{\sin\chi}{2+\cos\chi}\{[1-2\cos(2\theta+\chi)]\kappa^{11}(t) \\ &-2\sin(2\theta+\chi)[\kappa^{12}(t)+\kappa^{21}(t)]+[1+2\cos(2\theta+\chi)]\kappa^{22}(t)\} \end{aligned}$$

Noise coefficients:

$$D_{\theta\theta} = \frac{12KT}{\zeta\ell^2(4-\cos^2\chi)}, \qquad D_{\theta\chi} = -\frac{6KT}{\zeta\ell^2(2+\cos\chi)}, \qquad D_{\chi\chi} = \frac{12KT}{\zeta\ell^2(2+\cos\chi)}$$