Mechanical actions on nanocylinders in nematic liquid crystals

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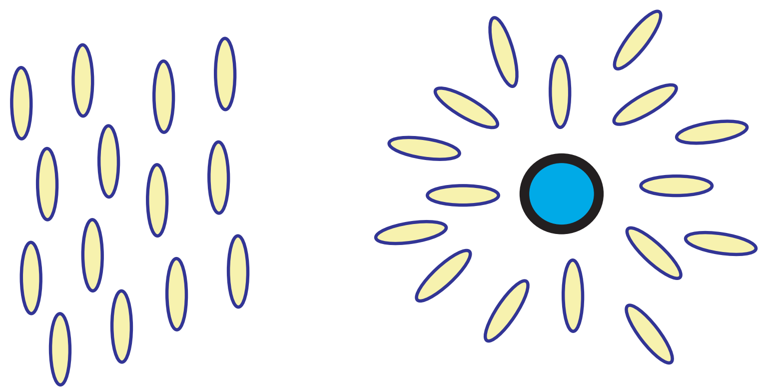
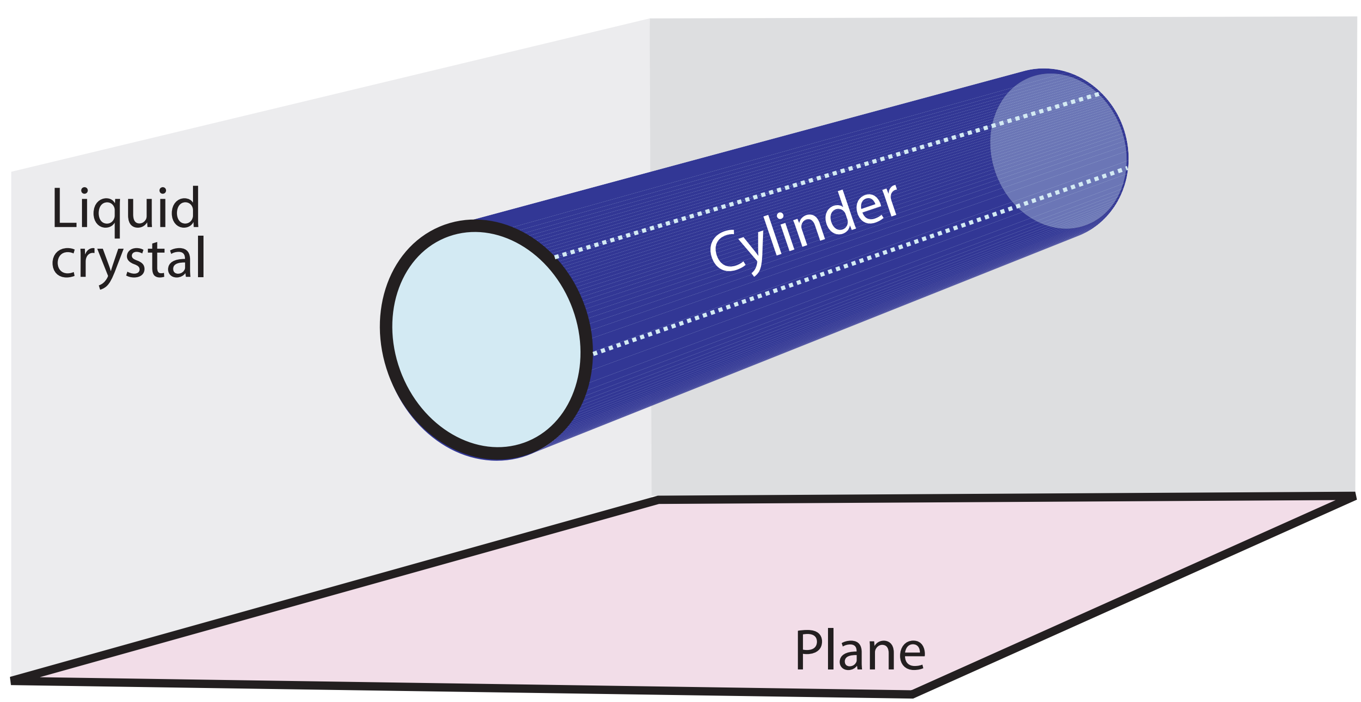
Introduction

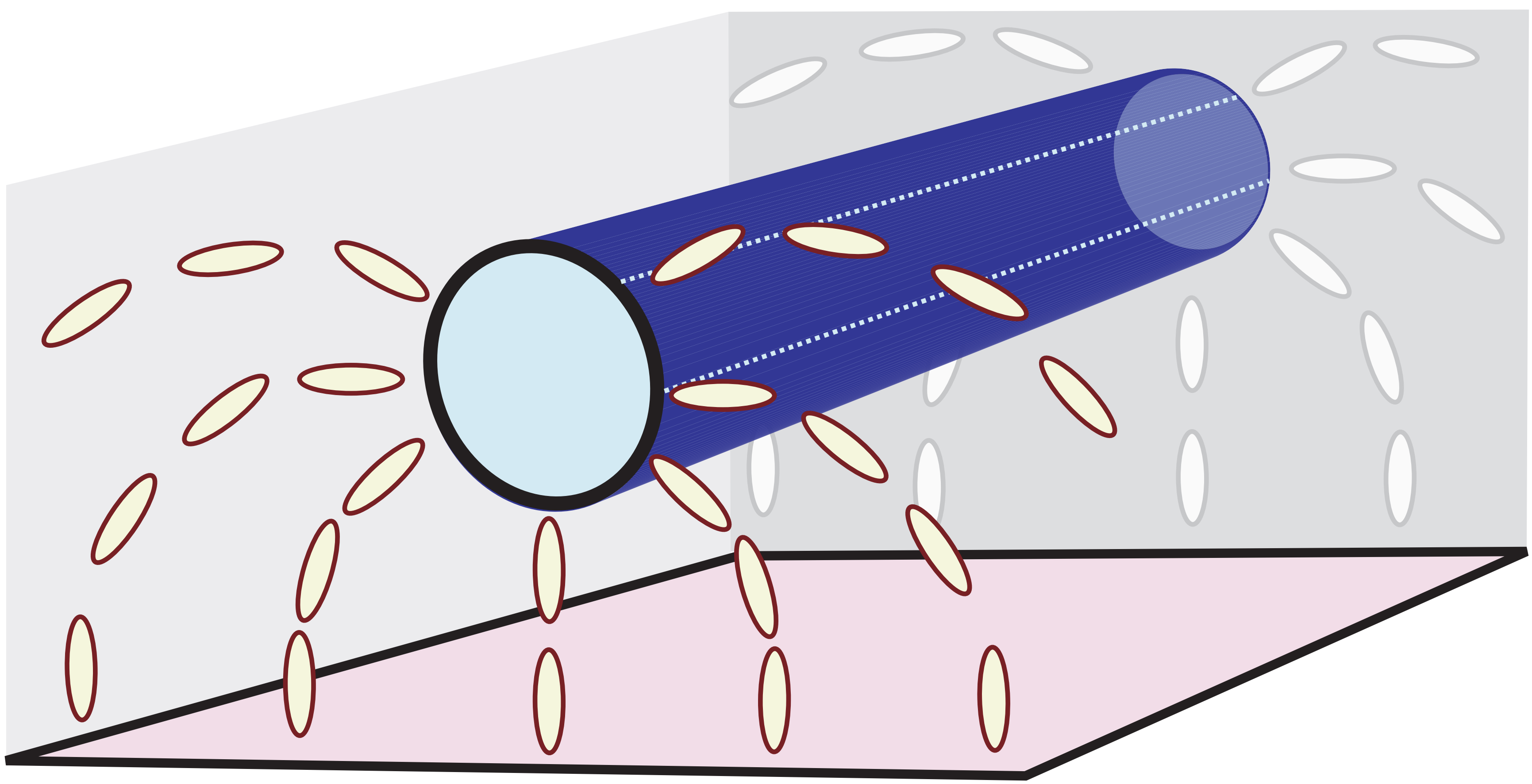


The molecular ordering of liquid crystals can be affected by the boundaries of submerged particles.

The particles can experience ***forces and torques*** due to the change in ordering.



- The cylinder and the wall both prescribe homeotropic alignment on the liquid crystal molecules.



Energy

- To describe alignment of molecules on the mesoscopic scale we employ Landau - de Gennes theory employing a full second-rank tensor $\underset{\sim}{Q}$.

- $\underset{\sim}{Q}$ is traceless, rank 2, with eigenvalues in range $\left[-\frac{1}{3}, \frac{2}{3}\right]$.

- When two eigenvalues are equal, $\underset{\sim}{Q} = s\left(\underset{\sim}{n} \otimes \underset{\sim}{n} - \frac{1}{3}I\right).$

  $s \in \left[-\frac{1}{2}, 1\right]$ is the scalar order parameter.

- Three distinct eigenvalues:

$$\underset{\sim}{Q} = s_1 \underset{\sim}{e}_1 \otimes \underset{\sim}{e}_1 + s_2 \underset{\sim}{e}_2 \otimes \underset{\sim}{e}_2 - (s_1 + s_2) \underset{\sim}{e}_3 \otimes \underset{\sim}{e}_3.$$

An invariant measure of biaxiality is given by

$$\beta^2 = 1 - 6\frac{\left(\operatorname{tr} \underset{\sim}{Q}^3\right)^2}{\left(\operatorname{tr} \underset{\sim}{Q}^2\right)^3}.$$

This parameter ranges in $[0, 1]$ and ***vanishes precisely*** for all uniaxial states of $\underset{\sim}{Q}$.

- For temperature $T < T_{NI}$, the state naturally preferred by a nematic comprising cylindrical molecules would be uniaxial.

- We adopt the bulk potential

$$f_b(\underset{\sim}{Q}) = \frac{A}{2}\operatorname{tr}\underset{\sim}{Q}^2 - \frac{B}{3}\operatorname{tr}\underset{\sim}{Q}^3 + \frac{C}{4}(\operatorname{tr}\underset{\sim}{Q}^2)^2.$$

$A = a(T - T^*)$ where a is a positive constant,

$T^* < T_{NI}$ is the ***supercooling*** temperature,

B and C are positive scalars.

- Both relative and absolute minimizers of f_b satisfy $\beta^2 = 0$.

- When the tensor field $\underset{\sim}{\boldsymbol{Q}}$ is not uniform in space, the free energy $\boldsymbol{W}$ per unit volume is

$$\boldsymbol{W} \;=\; \frac{\boldsymbol{L}}{\boldsymbol{2}}|\boldsymbol{\nabla}\underset{\sim}{\boldsymbol{Q}}|^{\boldsymbol{2}} + \boldsymbol{f_b}(\underset{\sim}{\boldsymbol{Q}}),$$

  where elastic constant $\boldsymbol{L}(>\mathbf{0})$ is independent of temperature.

- The total free energy stored in $\boldsymbol{\mathcal{B}}$,

$$\mathbb{F}(\boldsymbol{\mathcal{B}}) \;=\; \int_{\boldsymbol{\mathcal{B}}} \boldsymbol{W}\,\mathbf{d}\boldsymbol{V}.$$

- In the absence of body torques exerted by external causes, an equilibrium configuration for $\mathbb{F}(\mathcal{B})$ satisfies

$$\mathbf{div}\, \mathbf{T}^{(E)} = \underset{\sim}{\mathbf{0}},$$

where

$$\mathbf{T}^{(E)} \;=\; W\boldsymbol{I} - \nabla \underset{\sim}{\boldsymbol{Q}} \odot \frac{\partial W}{\partial \nabla \underset{\sim}{\boldsymbol{Q}}}$$

$$\left(\nabla \underset{\sim}{\boldsymbol{Q}} \odot \frac{\partial W}{\partial \nabla \underset{\sim}{\boldsymbol{Q}}}\right)_{ij} \;=\; Q_{hk,i} \frac{\partial W}{\partial Q_{hk,j}}.$$

- $\mathbf{T}^{(E)}$ is the form of Ericksen's stress tensor. It represents the distribution of contact forces in $\mathcal{B}$.

- For a body $\mathcal{P}$ submerged in $\mathcal{B}$, the total force $F(\mathcal{P})$ transmitted by the liquid crystal through the boundary $\partial\mathcal{P}$ is

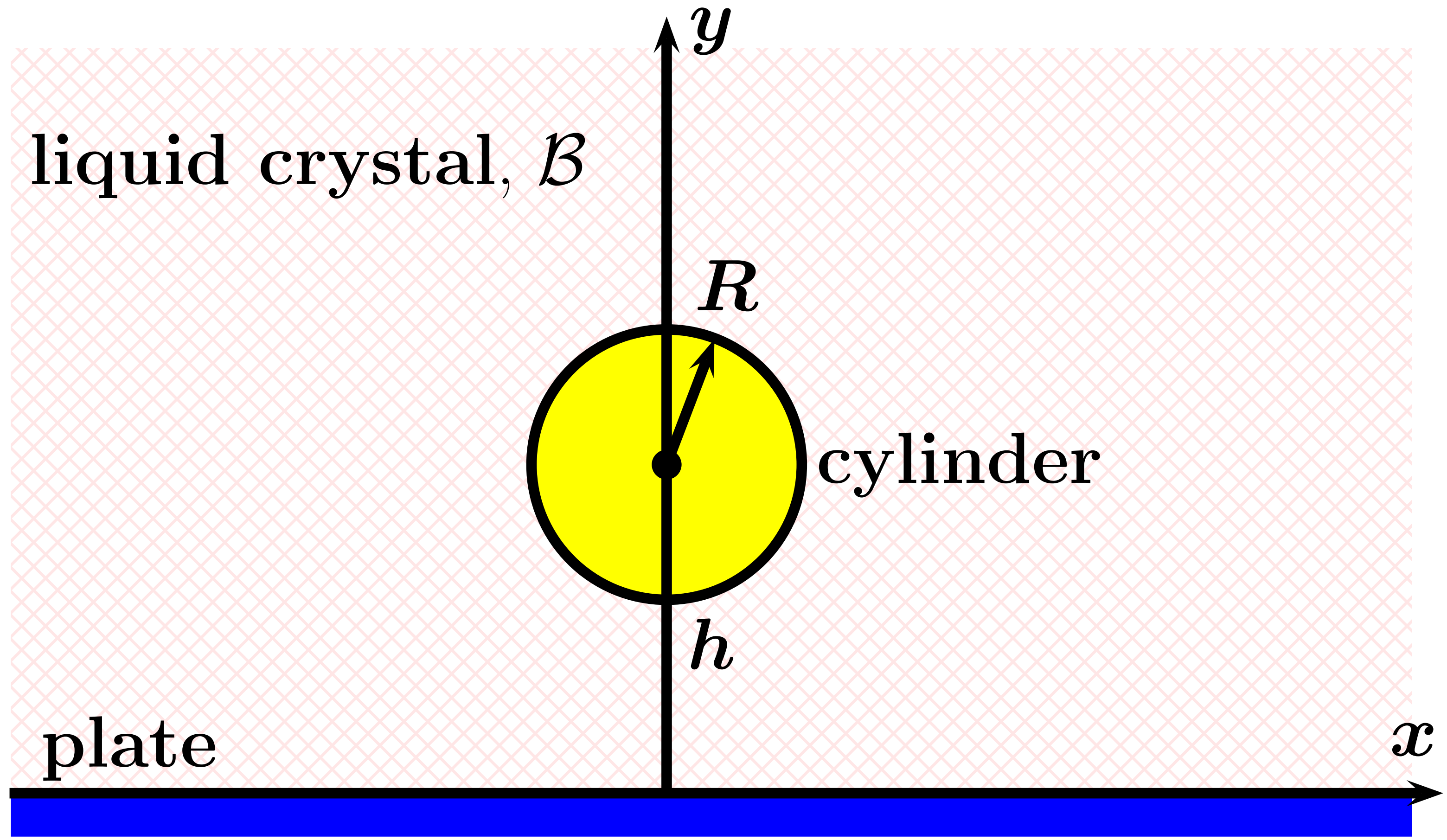
$$\boldsymbol{F}(\mathcal{P}) = \int_{\partial\mathcal{P}} \mathbf{T}^{(E)} \underset{\sim}{\boldsymbol{\nu}} \, \mathrm{d}S.$$

- Distribution of contact torques is described by the couple stress tensor

$$L_{ij} = 2\varepsilon_{ikl} Q_{km} \frac{\partial W}{\partial Q_{ml,j}}.$$

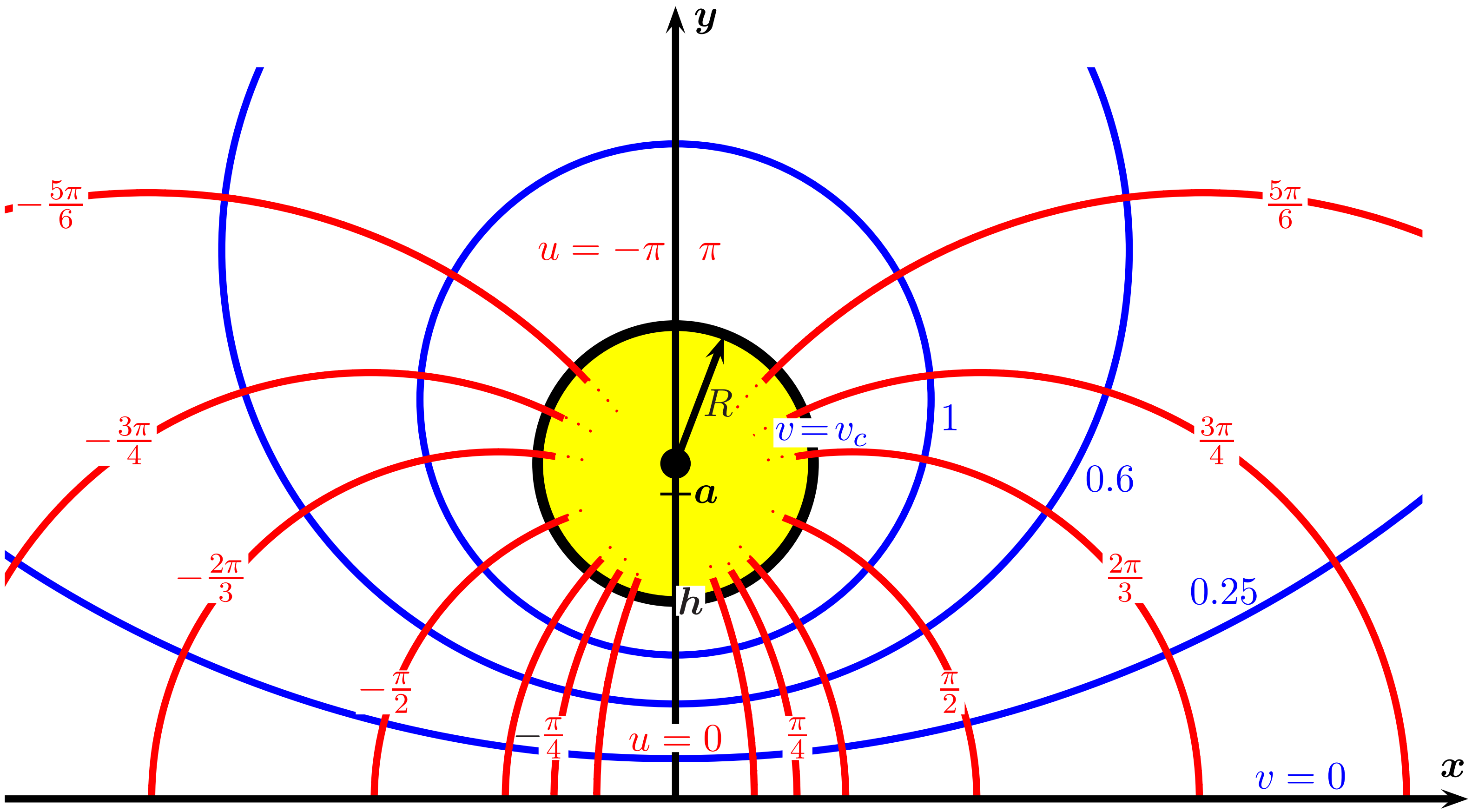
- The total torque transmitted on a submerged body $\mathcal{P}$ by the surrounding liquid crystal is

$$\boldsymbol{M}(\mathcal{P}) = \int_{\partial\mathcal{P}} \mathbf{L} \underset{\sim}{\boldsymbol{\nu}} \, \mathrm{d}S.$$



Cross-section of cylinder, radius R.

Separation between cylinder and plate is h.



$$\frac{\boldsymbol{a}}{\boldsymbol{R}} := \sqrt{\left(\frac{\boldsymbol{h}}{\boldsymbol{R}}\right)^{2} + 2\frac{\boldsymbol{h}}{\boldsymbol{R}}}.$$

- We introduce *bipolar* coordinates (u, v) via

$$x = a\frac{\sin u}{\cos u + \cosh v}, \qquad y = a\frac{\sinh v}{\cos u + \cosh v},$$

- Cylinder boundary corresponds to $v_c = \sinh^{-1}\frac{a}{R}$.

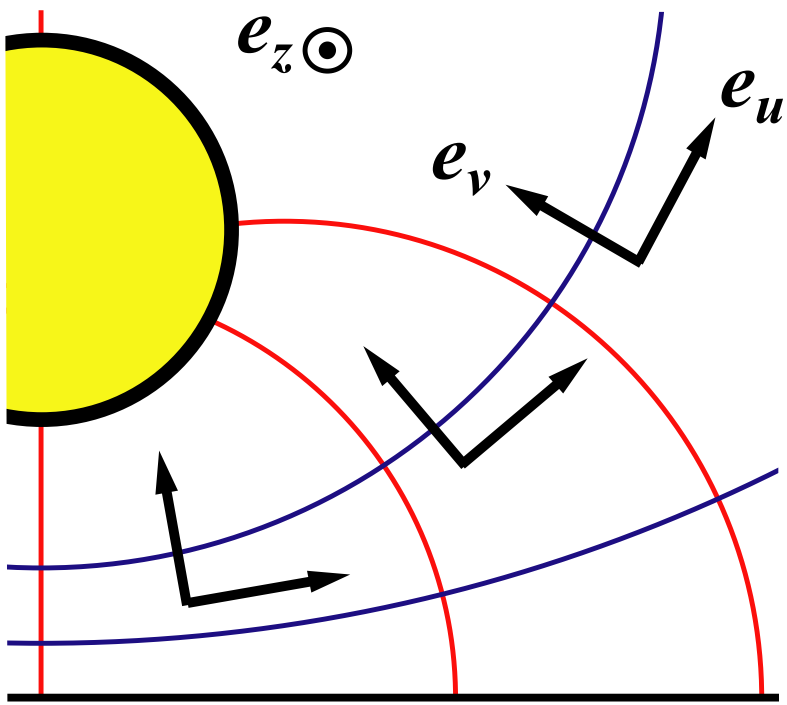
- Coordinates lines in the (u, v) plane are families of orthogonal (Apollonian) circles in the (x, y) plane.

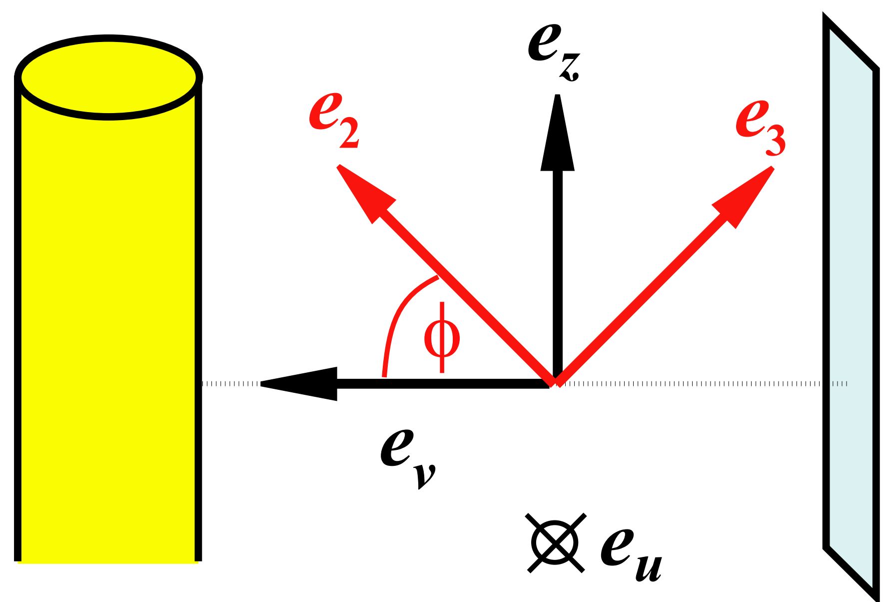
Mechanical Actions

$$\underset{\sim}{Q} = s_1 \underset{\sim}{e}_u \otimes \underset{\sim}{e}_u + s_2 \underset{\sim}{e}_2 \otimes \underset{\sim}{e}_2 - (s_1 + s_2) \underset{\sim}{e}_3 \otimes \underset{\sim}{e}_3,$$

$$\underset{\sim}{e}_2 = \cos\phi\, \underset{\sim}{e}_v + \sin\phi\, \underset{\sim}{e}_z, \qquad \underset{\sim}{e}_3 = -\sin\phi\, \underset{\sim}{e}_v + \cos\phi\, \underset{\sim}{e}_z,$$

s_1, s_2, and ϕ are all ***functions of*** v ***alone***.





Biaxial coherence length

$$\xi_b = \sqrt{\frac{4CL}{B^2(1+\sqrt{1-\theta})}},$$

where $\theta = \dfrac{24AC}{B^2}$ is temperature dependent.

- Rescaling: $\eta = \dfrac{v}{v_c}, \qquad 0 \le \eta \le 1.$

- Homeotropic nematic uniaxial ordering on both the plane and the boundary of cylinder, $s_b = 1 + \sqrt{1-\theta}$,

$$s_1\Big|_{\partial\mathcal{B}} = -\frac{1}{3}s_b, \qquad s_2\Big|_{\partial\mathcal{B}} = \frac{2}{3}s_b, \qquad \phi\Big|_{\partial\mathcal{B}} = 0.$$

Aim

- Our aim is to compute both the force and the torque exerted by the plane at $z = 0$ on the cylinder through the intervening liquid crystal.

- We will examine the role played in this interaction by the biaxial states that are likely to arise in response to the geometric frustration, especially in the vicinity of the cylinder's surface.

- Due to symmetry of the boundary conditions, the same force and torque would be exchanged between ***two parallel cylinders*** of equal radius R at the distance $2h$ (applicable to surface force apparatus).

Equilibrium textures

- Our BVP has been studied numerically for

$$1 < R/\xi_b < 10^3,$$

  i.e. cylinders in the nano-to-microscale range.

- Smaller values of R/ξ_b would be unphysical since ξ_b is the smallest length scale in the problem.

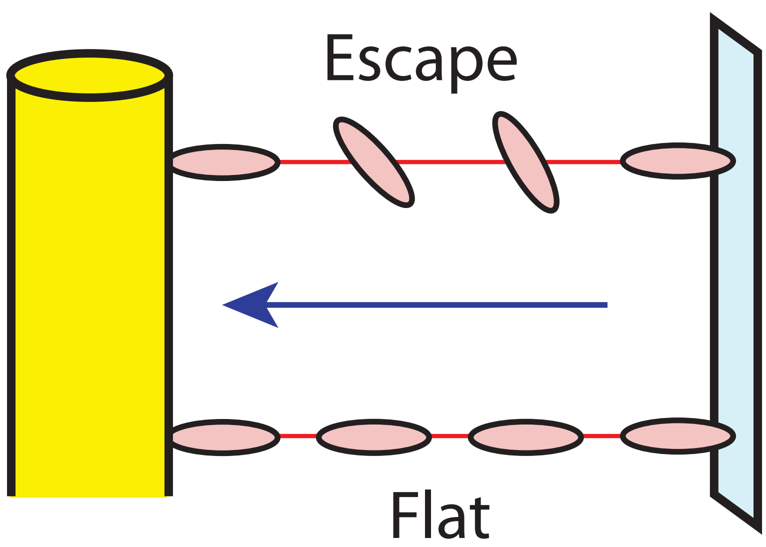
- Larger values of R/ξ_b were more problematic for our numerical methods.

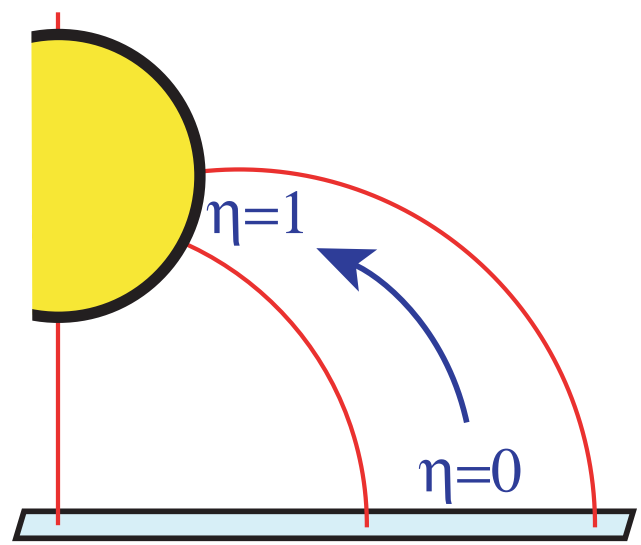
Two types of solution

- For all values of ξ_b, there exists a solution such that $\phi(\eta) = \mathbf{0}$ for all $\eta \in [\mathbf{0},\ \mathbf{1}]$ (the ***flat*** solution).

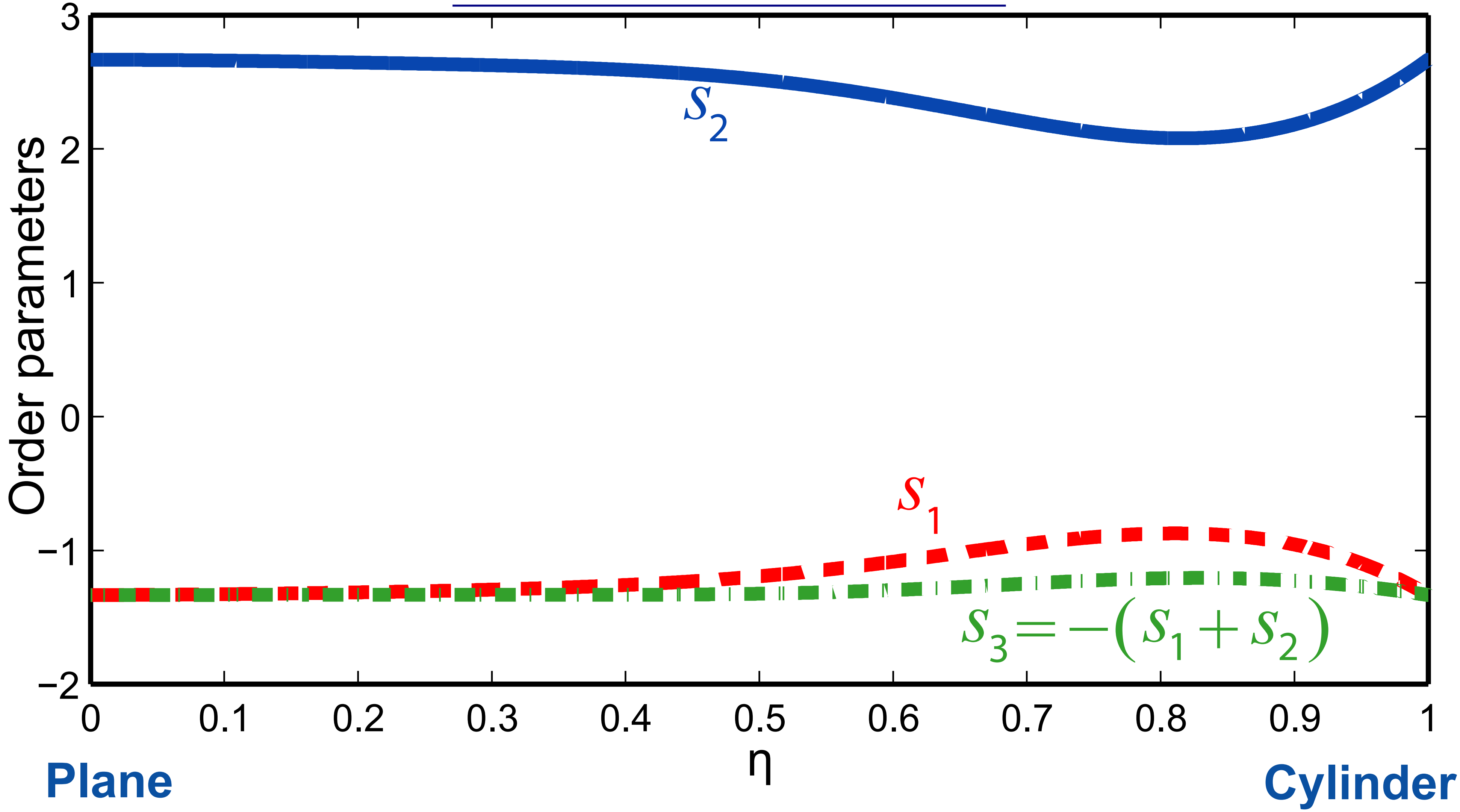
- However, for separation lengths h above some critical value, h_c, there exists a second type of solution with ϕ ***not identically zero***.

- Uniaxial ordering on the cylinder and plate, with an ***escape*** into the z-direction in the bulk.



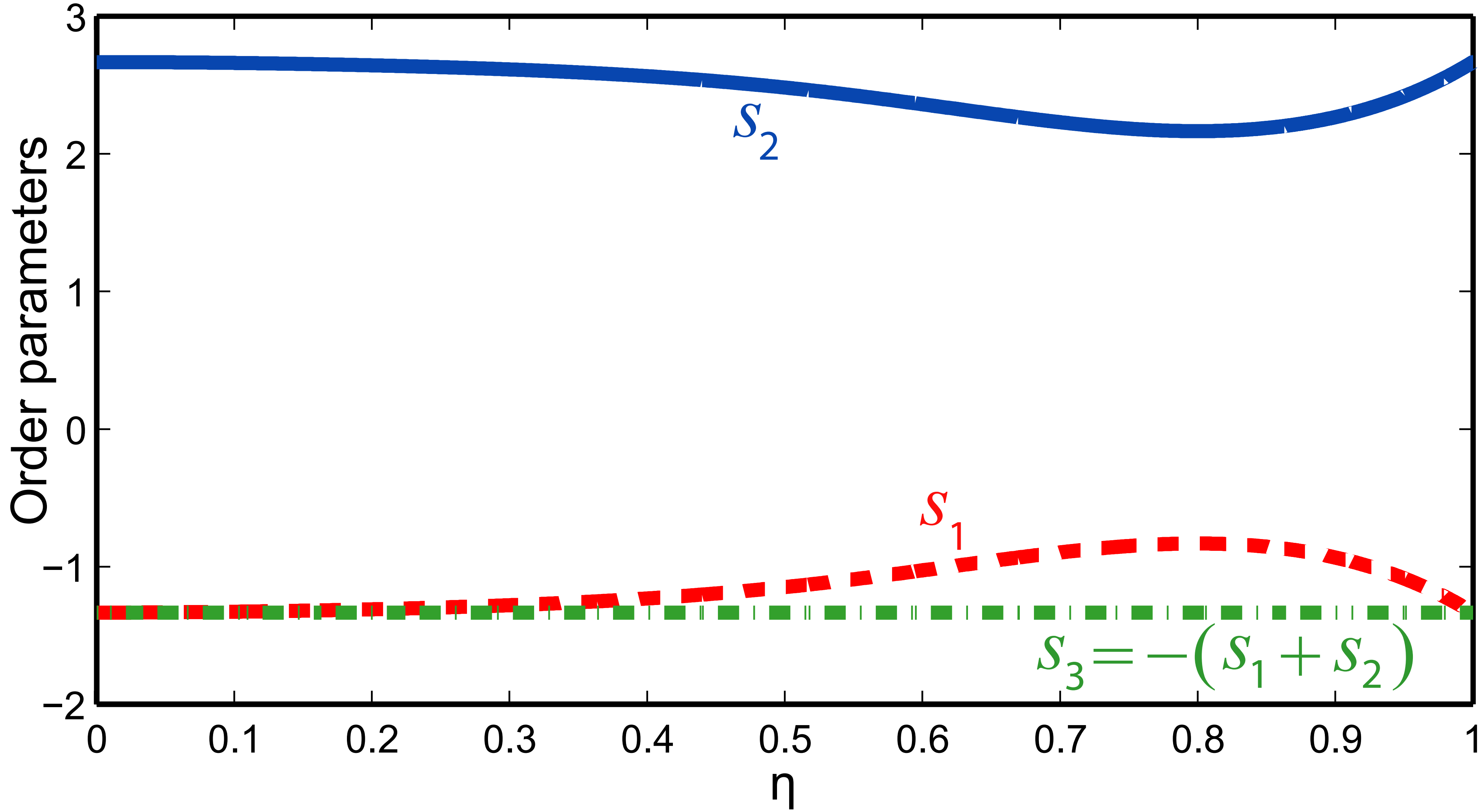


The escape solution

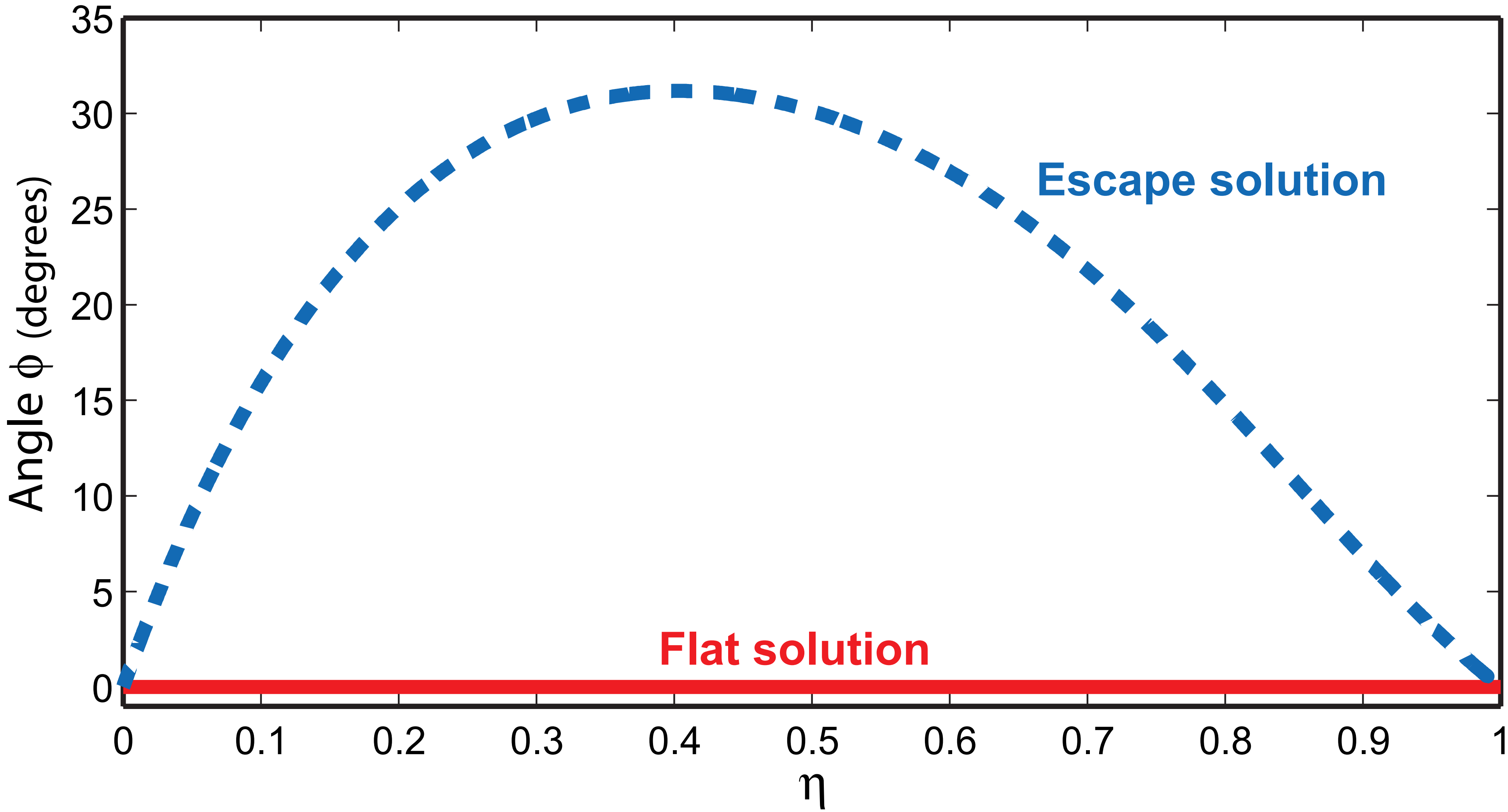


$$h = 5R, \quad R = 2\xi_b, \quad \theta = -8.$$

Flat solution

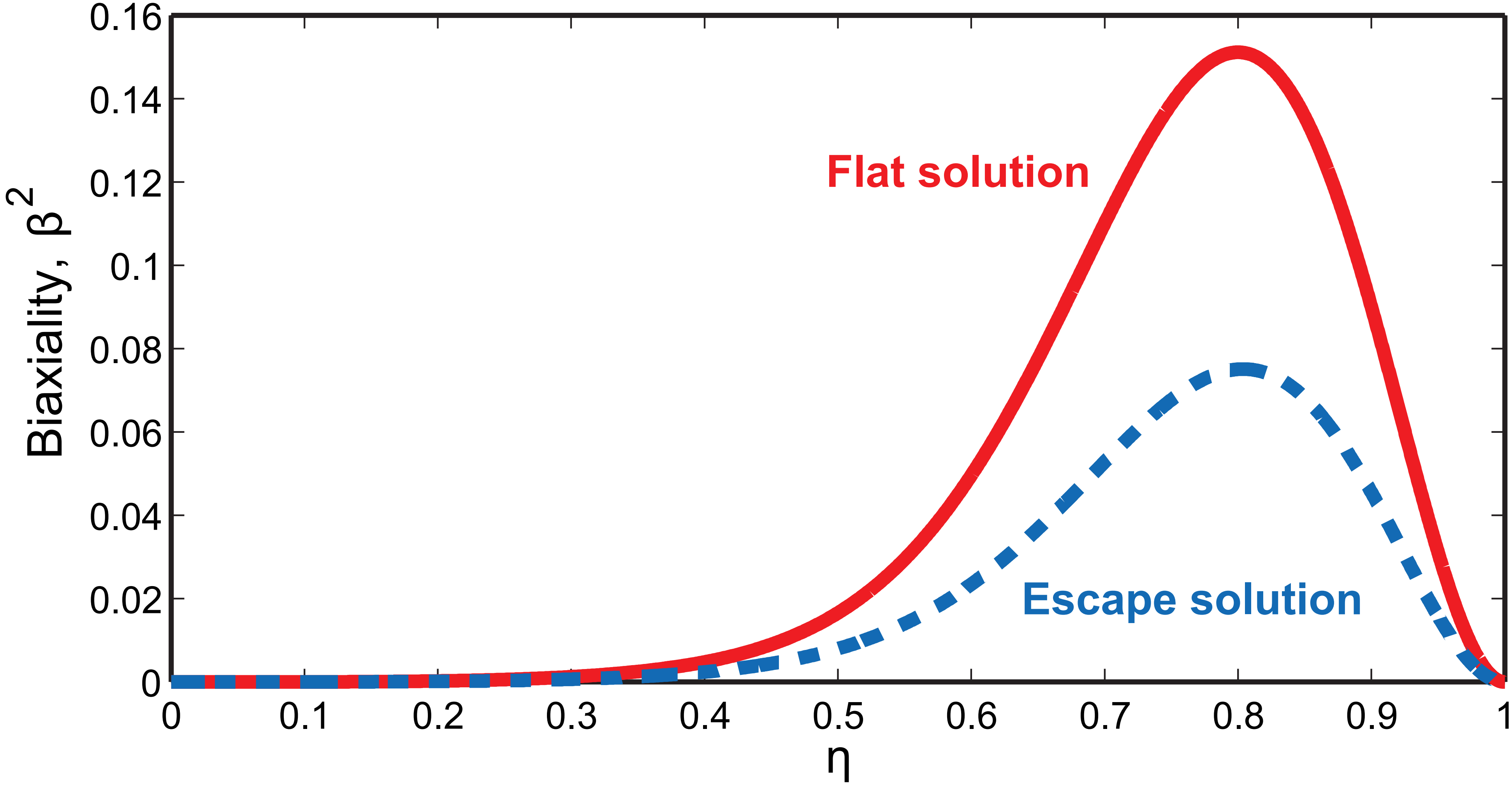


Angle ϕ



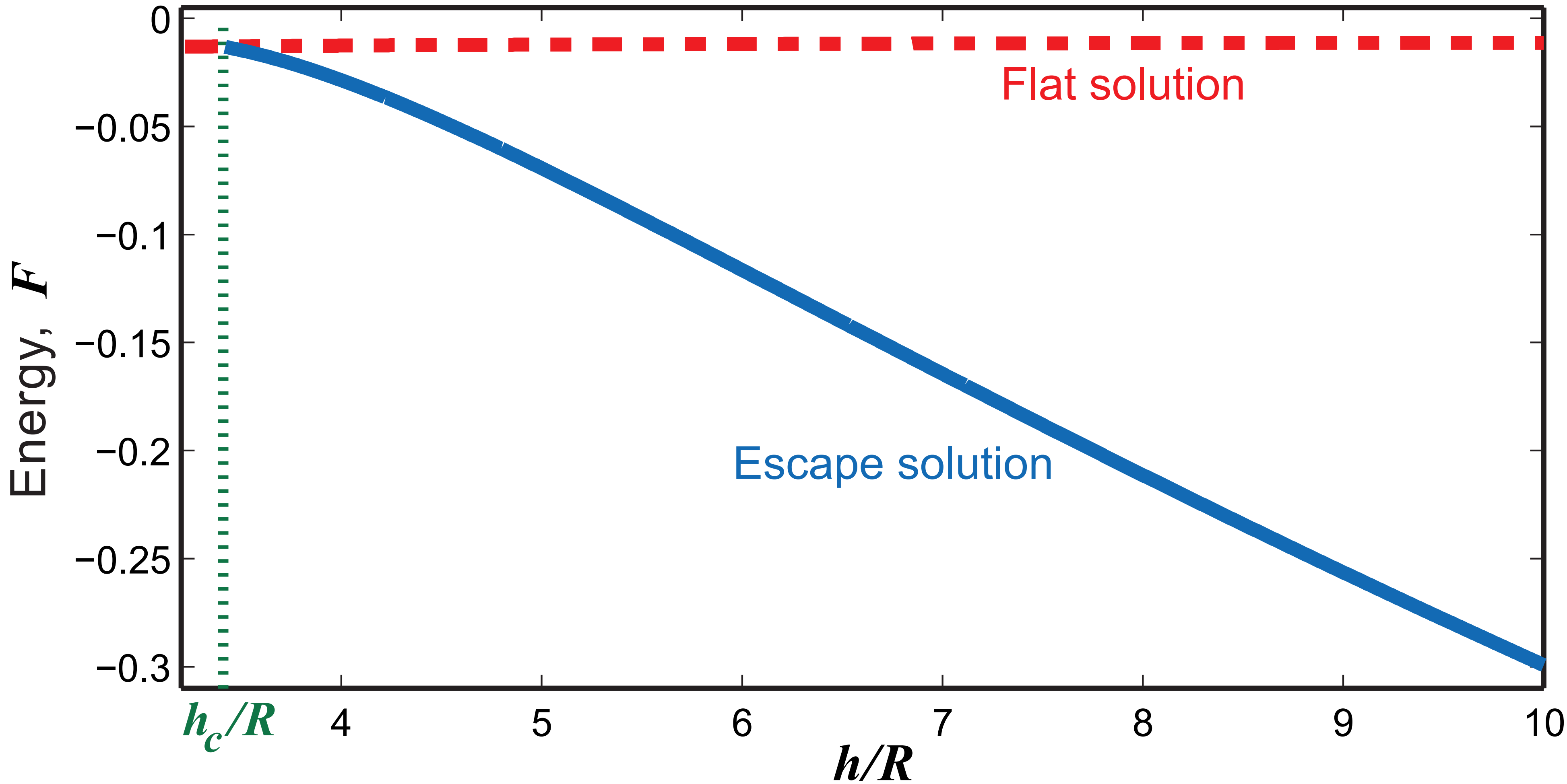
Escape solution
Flat solution
Angle ϕ (degrees)
η
35
30
25
20
15
10
5
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

Biaxiality

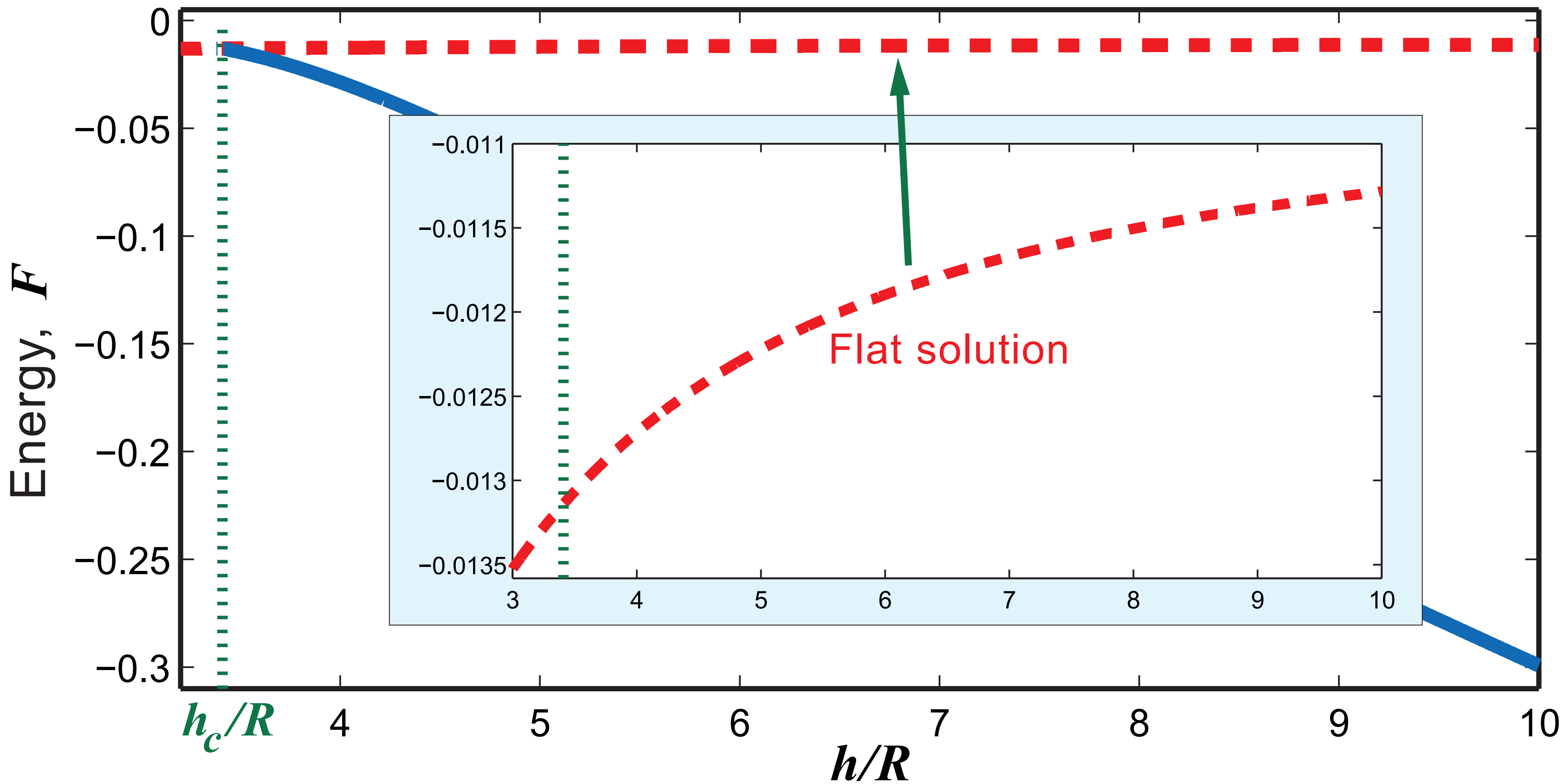


If separation is large enough the director can escape into the third dimension in an attempt to retain its uniaxiality throughout the sample.

Energy

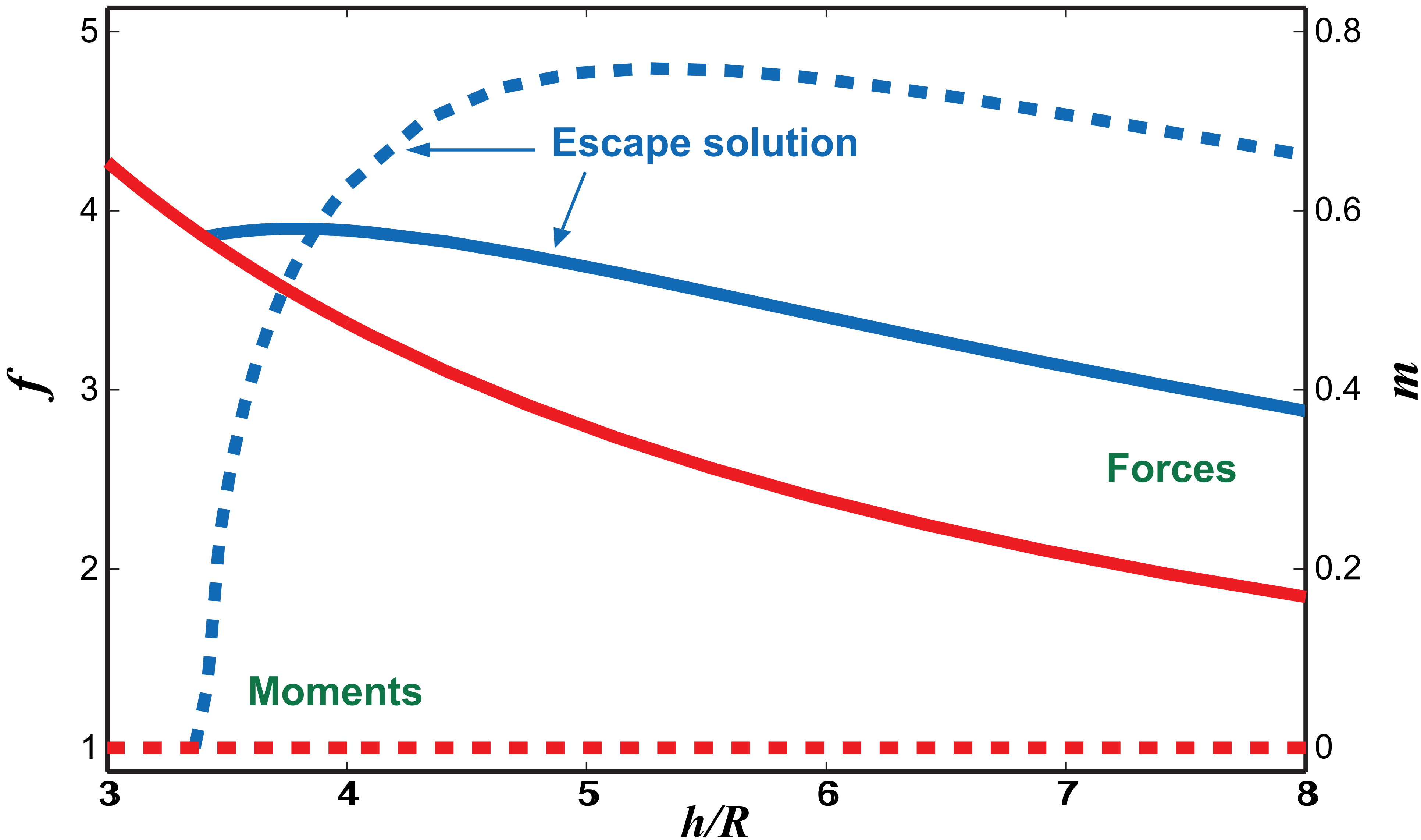


For $h \geq h_c$, the escape texture is energetically favourable.

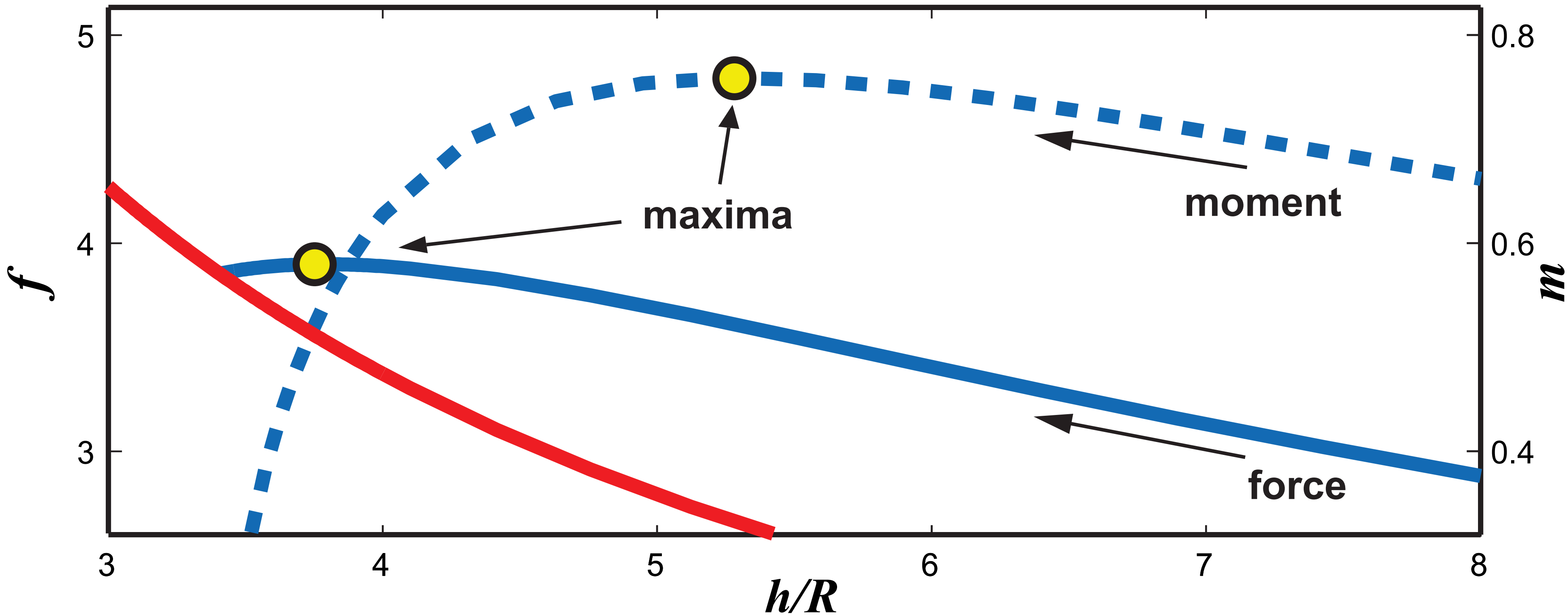


The energy for the flat solution is a slowly increasing function of h/R.

Force and Torque per unit height



Snapping instabilities



- Lack of monotonicity would impact upon experimental apparatus.
- The predicted instability would be more easily detected by a *torque* machine.
- A tiny hysteresis loop is associated with the force snapping instability.

Behaviour of the force

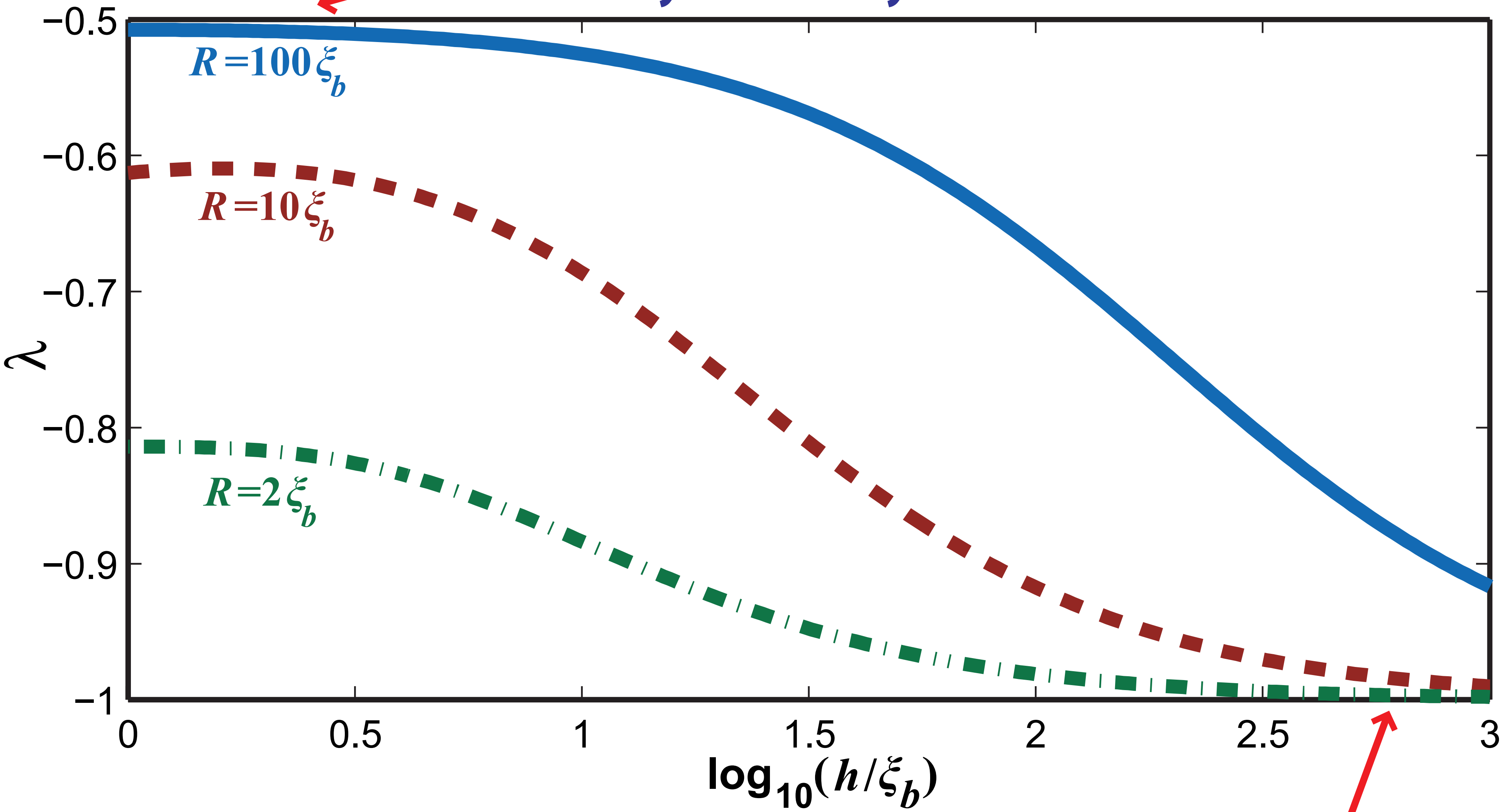
- The flat solution at small separations resembles an in-plane solution obtained via a ***director theory***.

- Sonnet & Gruhn showed that the elastic force on a cylinder per unit length due to a uniaxial nematic liquid behaves like $1/\sqrt{h}$ for h small.

- We assume that the force and the separation are related via $f \propto h^{\lambda}$.

Exponent of force for flat solution

Influence of curvature on concentration of biaxiality around cylinder is weaker



Consistent with force experienced by +1 disclination far from a plate

Conclusions

- We predict a snapping instability with an associated hysteresis loop in the force diagram, which should occur upon steadily reducing h.
- The bifurcation and the snapping instability are ***driven by the cylinder's curvature.***
- A similar instability was predicted in a twist cell at a critical thickness - ***order reconstruction***.

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