Distortion-induced effects in nematic liquid crystals

Ferroelectric phenomena in liquid crystals
Kent State University

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Outline

- Introduction to nematic liquid crystals

- Effective weak anchoring
  - Statement of the problem
  - Surface melting
  - Effective surface tilt angle
  - Effective weak anchoring

- Induced biaxiality
  - Statement of the problem
  - Elastic energy
  - Examples

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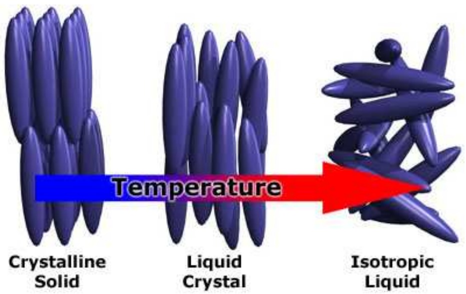
Nematic liquid crystals



- Orientational probability distribution $f_p : \mathbb{S}^2 \to \mathbb{R}_+$
- Tensor order parameter:
  $\mathbf{Q} = \langle \mathbf{m} \otimes \mathbf{m} - \frac{1}{3}\mathbf{I} \rangle =$
  $s\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{I}\right) + \beta\left(\mathbf{e}_+ \otimes \mathbf{e}_+ - \mathbf{e}_- \otimes \mathbf{e}_-\right)$
- $s \in [-\frac{1}{2}, 1]$ is the degree of orientation, $\mathbf{n}$ is the director (local preferred orientation if $s > 0$), β measures the degree of biaxiality
- The phase can be isotropic ($s = \beta = 0$), uniaxial ($s \neq 0$, $\beta = 0$) or biaxial ($s \neq 0$, $\beta \neq 0$)

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Free energy functional

- Free energy density: $\Psi = \frac{K}{2}|\nabla \mathbf{Q}|^2 + A\,\mathrm{tr}\mathbf{Q}^2 - B\,\mathrm{tr}\mathbf{Q}^3 + C\,\mathrm{tr}\mathbf{Q}^4$
- Ψ is the sum of the elastic term and the Landau-de Gennes potential
- Elastic term penalizes distortions, Landau-de Gennes potential is minimized when $\mathbf{Q}$ is uniaxial with fixed degree of orientation
- In the uniaxial case ($\beta = 0$)

$$|\nabla \mathbf{Q}|^2 = \frac{2}{3}|\nabla s|^2 + 2s^2|\nabla \mathbf{n}|^2$$

$$\Psi_{LdG}(s) = \frac{2}{9}Cs^4 - \frac{2}{9}Bs^3 + \frac{2}{3}As^2$$

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- Anchoring = boundary conditions
  - Strong, free anchoring $\leftrightarrow$ Dirichlet, Neumann b.c.
  - Weak anchoring $\leftrightarrow$ surface potential favouring a direction

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Effective weak anchoring

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Statement of the problem

- Anchoring potential can be viewed as the result of molecular interactions
- Anchoring is commonly imposed by rubbing $\Rightarrow$ the geometry of the problem affects the anchoring potential!
- Another effect: decrease of s close to a rough-surface
- This decrease affects the director distribution (coupling given by $s^2|\nabla \mathbf{n}|^2$)
- Our aim is to investigate the roughness influence on anchoring potential. A singular perturbation approach, new to the problem, is used

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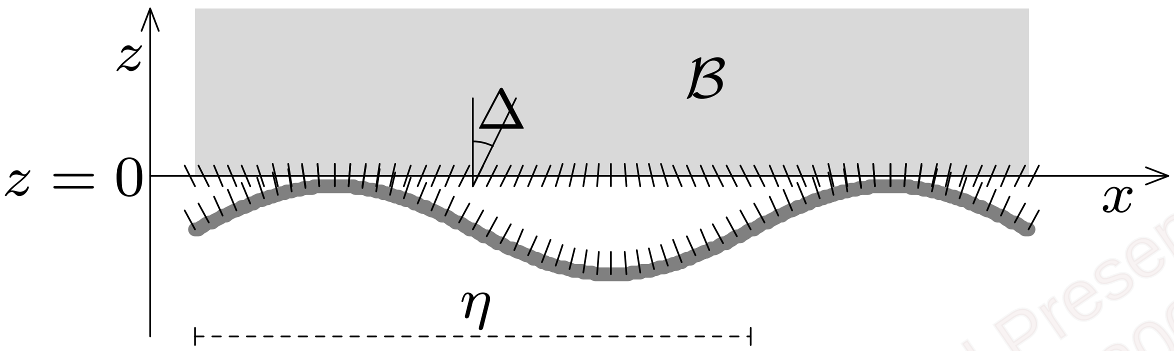
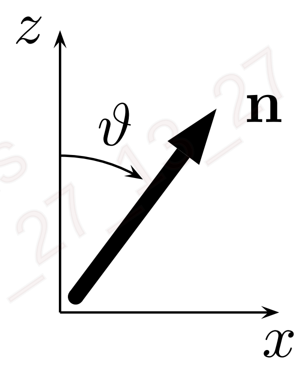
Modeling a rough boundary





We assume first a single wavelength.

We expand in the roughness amplitude Δ.

At first order we obtain a sinusoidal modulation of ϑ along the x axis.

This modulation has wavelength η and amplitude linearly dependent on Δ.

The amplitude Δ and the wavelength η characterizing the grooves will be crucial parameters in our results.

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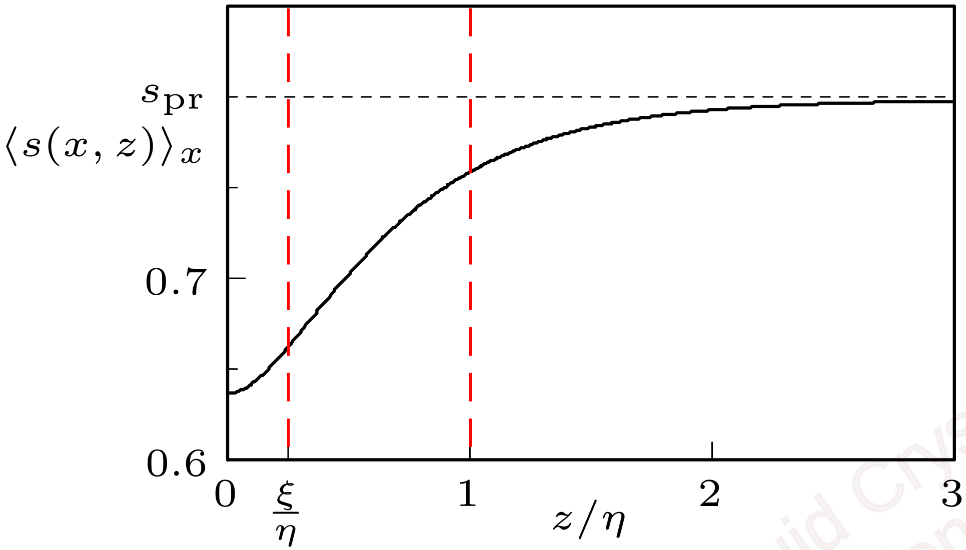
Surface melting (Neumann)



Rough surface

$$\langle s(x,0)\rangle_x \approx s_{\rm pr}\left(1 - \frac{{\rm m}^2\xi^2}{\omega^2} - \frac{\Delta^2\xi^2}{\omega^2\eta^2}\right)$$

m is the slope of the *outer* solution at the boundary

$\xi = \sqrt{9K/C}$ is the nematic coherence length

ω^2 measures the potential depth of $f_{\rm LdG}(s_{\rm pr})$: $f''_{\rm LdG}(s_{\rm pr}) = K\omega^2/\xi^2$.

- Two scale analysis: *two* boundary layers, of thickness ξ, η. Physical situation: $\xi \ll \eta$
- Outer solution: uniform decrease of s triggered by m

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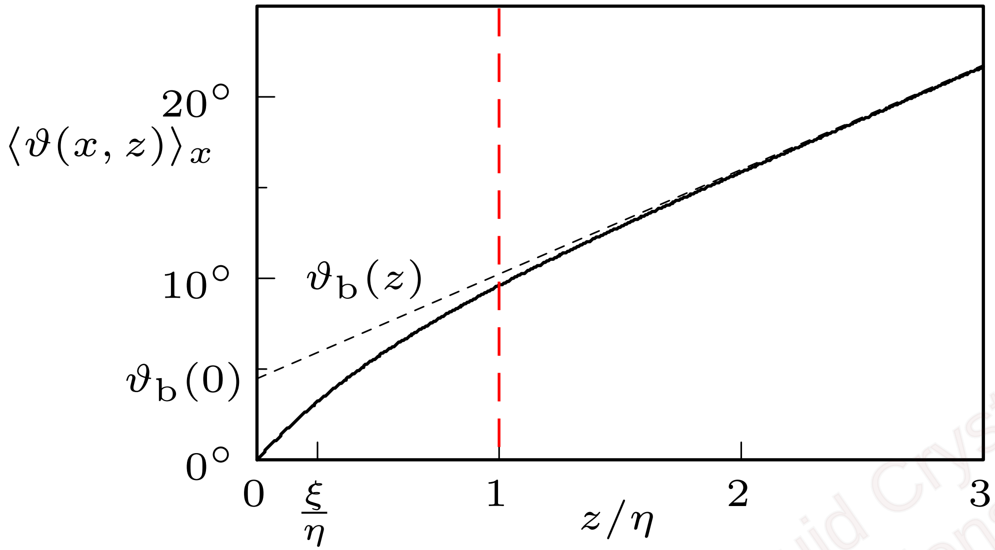
Effective surface angle (Neumann)



Rough surface

$$\vartheta_{\mathrm{b}}(0) \approx \frac{2\,\mathrm{m}\,\xi^2\,\Delta^2}{\eta\,\omega^2}$$

m is the slope of the *outer* solution at the boundary

$\xi = \sqrt{9K/C}$ is the nematic coherence length

ω^2 measures the potential depth of $f_{\mathrm{LdG}}(s_{\mathrm{pr}})$: $f''_{\mathrm{LdG}}(s_{\mathrm{pr}}) = K\omega^2/\xi^2$.

A coarse observation of the nematic configuration measures a surface tilt angle slightly different from the homeotropic prescription $\vartheta_{\mathrm{surf}} = 0$.

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Effective weak anchoring

We want to compare our results with a classical weak-anchoring model

- A tilt angle $\vartheta_{\rm b}(0) \neq 0$ may also be modeled through a weak anchoring potential $W f_{\rm w}$, where W is the anchoring strength
- Define the surface extrapolation length $\zeta = \dfrac{K}{W f''_{\rm w}(0)}$
- Comparison with our result relates ζ to the microscopic roughness parameters
- s free at the surface $\Rightarrow$ $\dfrac{\zeta}{\xi} = \dfrac{2\Delta^2}{\omega^2}\dfrac{\xi}{\eta} + \mathcal{O}\left(\dfrac{\xi^2}{\eta^2}\right)$

  Anchoring strength increases when either the roughness amplitude Δ decreases or the roughness wavelength η increases

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Conclusions - Part I

- The roughness induces a partial melting (decrease of s) close to the surface in a layer of thickness η
- This decrease favours a steep shape of ϑ
- Comparison with effective weak anchoring allows to relate the anchoring potential with surface parameters

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Induced biaxiality

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Predicting Biaxiality (I)

- Within de Gennes' theory, nematics have three different phases: isotropic, uniaxial and biaxial
- The free energy favors a uniaxial ground state, but biaxial domains have been predicted and observed
- It is well known that defects are often a source of biaxiality!
- Early theory, employing only the director **n** as order parameter, cannot take biaxiality into account
- When this is a good approximation?

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- When this is a good approximation?

Can we predict where the biaxiality is most likely to arise (if any), once we know the director distribution?

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Elastic free energy

$$\frac{K}{2}|\nabla \mathbf{Q}|^2 = K\Big[\tfrac{1}{3}|\nabla s|^2 + |\nabla\beta|^2 + s^2|\nabla \mathbf{n}|^2 + \beta^2\Big(|\nabla\mathbf{n}|^2 + 4|(\nabla\mathbf{e}_+)^T\mathbf{e}_-|^2\Big)$$
$$- 2s\beta\Big(\mathbf{e}_+\cdot\mathbf{S}\mathbf{e}_+ - \mathbf{e}_-\cdot\mathbf{S}\mathbf{e}_-\Big)\Big], \text{ where } \quad \boxed{\mathbf{S} = (\nabla\mathbf{n})(\nabla\mathbf{n})^T}$$

- $\mathbf{S}$ is symmetric and $\mathbf{n}$ is an eigenvector (with null eigenvalue)

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Elastic free energy

$$\frac{K}{2}|\nabla \mathbf{Q}|^2 = K\Big[\boxed{\tfrac{1}{3}|\nabla s|^2 + |\nabla \beta|^2} + s^2|\nabla \mathbf{n}|^2 + \beta^2\Big(|\nabla \mathbf{n}|^2 + 4|(\nabla \mathbf{e}_+)^T \mathbf{e}_-|^2\Big) - 2s\beta\Big(\mathbf{e}_+ \cdot \mathbf{S}\mathbf{e}_+ - \mathbf{e}_- \cdot \mathbf{S}\mathbf{e}_-\Big)\Big], \text{ where } \quad \mathbf{S} = (\nabla \mathbf{n})(\nabla \mathbf{n})^T$$

- $\mathbf{S}$ is symmetric and $\mathbf{n}$ is an eigenvector (with null eigenvalue)
- First two terms penalize spatial variations

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Elastic free energy

$$\frac{K}{2}|\nabla\mathbf{Q}|^2 = K\Big[\tfrac{1}{3}|\nabla s|^2 + |\nabla\beta|^2 + \boxed{s^2|\nabla\mathbf{n}|^2} + \beta^2\Big(|\nabla\mathbf{n}|^2 + 4|(\nabla\mathbf{e}_+)^T\mathbf{e}_-|^2\Big) - 2s\beta\Big(\mathbf{e}_+\cdot\mathbf{S}\mathbf{e}_+ - \mathbf{e}_-\cdot\mathbf{S}\mathbf{e}_-\Big)\Big], \quad \text{where} \quad \mathbf{S} = (\nabla\mathbf{n})(\nabla\mathbf{n})^T$$

- $\mathbf{S}$ is symmetric and $\mathbf{n}$ is an eigenvector (with null eigenvalue)
- First two terms penalize spatial variations
- Third term decreases s whenever $|\nabla\mathbf{n}| \neq 0$, studied before!

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Elastic free energy

$$\frac{K}{2}|\nabla\mathbf{Q}|^2 = K\Big[\tfrac{1}{3}|\nabla s|^2 + |\nabla\beta|^2 + s^2|\nabla\mathbf{n}|^2 + \boxed{\beta^2\Big(|\nabla\mathbf{n}|^2 + 4|(\nabla\mathbf{e}_+)^T\mathbf{e}_-|^2\Big)}$$

$$- 2s\beta\Big(\mathbf{e}_+\cdot\mathbf{S}\mathbf{e}_+ - \mathbf{e}_-\cdot\mathbf{S}\mathbf{e}_-\Big)\Big], \quad \text{where} \quad \mathbf{S} = (\nabla\mathbf{n})(\nabla\mathbf{n})^T$$

- $\mathbf{S}$ is symmetric and $\mathbf{n}$ is an eigenvector (with null eigenvalue)
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- Fourth term is positive definite $\Rightarrow$ pushes the solution toward $\beta = 0$

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Elastic free energy

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- Third term decreases s whenever $|\nabla\mathbf{n}| \neq 0$, studied before!
- Fourth term is positive definite $\Rightarrow$ pushes the solution toward $\beta = 0$
- Last term is what shifts biaxiality away from $\beta = 0$

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Elastic free energy

$$\frac{K}{2}|\nabla \mathbf{Q}|^2 = K\Big[\tfrac{1}{3}|\nabla s|^2 + |\nabla \beta|^2 + s^2|\nabla \mathbf{n}|^2 + \beta^2\Big(|\nabla \mathbf{n}|^2 + 4|(\nabla \mathbf{e}_+)^T \mathbf{e}_-|^2\Big)$$

$$\boxed{-2s\beta\Big(\mathbf{e}_+ \cdot \mathbf{S}\mathbf{e}_+ - \mathbf{e}_- \cdot \mathbf{S}\mathbf{e}_-\Big)}\Big], \quad \text{where} \quad \mathbf{S} = (\nabla \mathbf{n})(\nabla \mathbf{n})^T$$

- $\mathbf{S}$ is symmetric and $\mathbf{n}$ is an eigenvector (with null eigenvalue)
- First two terms penalize spatial variations
- Third term decreases s whenever $|\nabla \mathbf{n}| \neq 0$, studied before!
- Fourth term is positive definite $\Rightarrow$ pushes the solution toward $\beta = 0$
- Last term is what shifts biaxiality away from $\beta = 0$
- It is minimum when $\{\mathbf{e}_+, \mathbf{e}_-\}$ coincide with the two eigenvectors of $\mathbf{S}$ that are orthogonal to $\mathbf{n}$

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Predicting biaxiality (II)

Consider the symmetric tensor $\mathbf{S} = (\nabla \mathbf{n})(\nabla \mathbf{n})^T$. It always possesses a null eigenvalue (with eigenvector $\mathbf{n}$). Whenever its other two eigenvalues do not coincide, biaxiality is naturally induced in the system, and the optimal eigendirections of $\mathbf{Q}$ coincide with those of $\mathbf{S}$.

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Planar fields

- Planar fields $\Rightarrow$ $$\begin{aligned} \mathbf{n} &= \cos\theta\,\mathbf{e}_x + \sin\theta\,\mathbf{e}_y \\ \mathbf{n}_\perp &= -\sin\theta\,\mathbf{e}_x + \cos\theta\,\mathbf{e}_y \end{aligned}$$
- $\nabla\mathbf{n} = \mathbf{n}_\perp \otimes \nabla\theta \Rightarrow \mathbf{S} = |\nabla\theta|^2\,\mathbf{n}_\perp \otimes \mathbf{n}_\perp$
- There is spontaneous biaxiality whenever the tilt angle is not uniform

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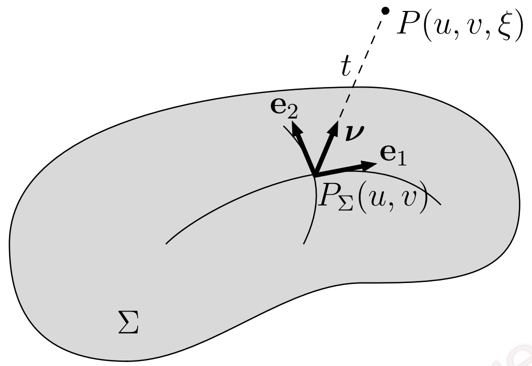
Surface biaxiality



Suppose that a liquid crystal is limited by a surface and homeotropic boundary conditions $\mathbf{n} \equiv \boldsymbol{\nu}$ are assumed.

$$\mathbf{S} = \frac{\kappa_1^2}{(1-\kappa_1 t)^2}\,\mathbf{e}_1 \otimes \mathbf{e}_1 + \frac{\kappa_2^2}{(1-\kappa_2 t)^2}\,\mathbf{e}_2 \otimes \mathbf{e}_2$$

$\kappa_1,\ \kappa_2$ are the principal curvatures
$\mathbf{e}_1,\ \mathbf{e}_2$ are the principal axis

- Biaxiality arises along the principal axis
- The effect is triggered by the difference between the principal curvatures
- The preferred direction is the one with higher positive curvature

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Escape in the third dimension

- Cylinder of radius R with homeotropic boundary conditions (Cladis and Kléman [a])
- $\mathbf{n} = \cos\phi(r)\,\mathbf{e}_r + \sin\phi(r)\,\mathbf{e}_z$
  $\mathbf{n}_\perp = -\sin\phi(r)\,\mathbf{e}_r + \cos\phi(r)\,\mathbf{e}_z$
- $\mathbf{S} = \dfrac{\cos^2\phi}{r^2}\,\mathbf{e}_\theta \otimes \mathbf{e}_\theta + \phi'^2\,\mathbf{n}_\perp \otimes \mathbf{n}_\perp$
- Cladis and Kléman solution is $\phi(r) = \dfrac{\pi}{2} - 2\arctan\dfrac{r}{R} \Rightarrow$
  $\phi'^2 = \cos^2\phi / r^2$
- The escape in the third dimension is one example of spatially varying fields which do not induce any biaxiality

[a] P. Cladis and M. Kléman, J. Physique **33**, 591 (1972).

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Conclusions - Part II

- We have given an easy way to determine the "natural" directions of biaxiality
- Those are given by the eigenvectors of $\mathbf{S} = (\nabla \mathbf{n})(\nabla \mathbf{n})^T$
- Examples show for instance that surface biaxiality in the homeotropic case is ruled by the difference between the principal curvatures of the surface

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[2] P. Biscari, G. Napoli, S. Turzi *Bulk and surface biaxiality in nematic liquid crystals*, Phys. Rev E **74** (2006), 031708

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