An Overview of the Oseen-Frank Elastic Model

~~plus Some Symmetry Aspects of the Straley~~

~~Mean-Field Model for Biaxial Nematic Liquid Crystals~~

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Background

- macroscopic continuum model, equilibrium states, orientational properties
- variational, phenomenological
- nematic LC mesophase: orientational order, no positional order
- flavors of the model: uniaxial nematic ("nematic"), chiral nematic ("cholesteric")
- assumes uniform degree of order, constant temperature, constant mass density
- *director*: $\boldsymbol{n} = \boldsymbol{n}(x), \ |\boldsymbol{n}(x)| = 1, \ \forall x \in \Omega$
  - average orientation of distinguished molecular axis
  - distinguished eigenvector of uniaxial $\mathbf{Q}$

Free Energy Functional:

$$\min_{\boldsymbol{n}\in\mathcal{N}} \mathcal{F}[\boldsymbol{n}], \quad \mathcal{N} = \text{admissible (regularity, BCs, } |\boldsymbol{n}| = 1)$$

$$\mathcal{F}[\boldsymbol{n}] = \int_\Omega W_{\mathrm{e}}(\boldsymbol{n}, \nabla\boldsymbol{n})\, dV, \quad W_{\mathrm{e}} = \text{distortional elastic energy density}$$

W_{e} penalizes distortions from “ground state” (e.g., parallel $\leftrightarrow$ steric, Van der Waals)

additional terms:

magnetic and/or electric fields

surface anchoring potential

flexoelectric polarization

Modeling Assumptions

- continuum: $|\nabla\boldsymbol{n}| \ll \dfrac{1}{\text{molecular length scale}}$
- frame indifference: $W_{\mathrm{e}}(\mathbf{Q}\boldsymbol{n}, \mathbf{Q}\nabla\boldsymbol{n}\mathbf{Q}^T) = W_{\mathrm{e}}(\boldsymbol{n}, \nabla\boldsymbol{n}), \quad \forall\mathbf{Q} \in SO(3)$
- material symmetry (nematic only): ” , $\forall\mathbf{Q} \in O(3)$
- evenness: $-\boldsymbol{n} \leftrightarrow \boldsymbol{n} \;\Rightarrow\; W_{\mathrm{e}}(-\boldsymbol{n}, -\nabla\boldsymbol{n}) = W_{\mathrm{e}}(\boldsymbol{n}, \nabla\boldsymbol{n})$
- quadratic in $\nabla\boldsymbol{n}$
- non-negative: $W_{\mathrm{e}}(\boldsymbol{n}, \nabla\boldsymbol{n}) \geq 0$ ($W_{\mathrm{e}} = 0$ on “ground state” . . . usually)

Nematic Model

$$2W_{\text{nem}} = K_1(\operatorname{div}\boldsymbol{n})^2 + K_2(\boldsymbol{n}\cdot\operatorname{curl}\boldsymbol{n})^2 + K_3|\boldsymbol{n}\times\operatorname{curl}\boldsymbol{n}|^2 + (K_2+K_4)\big[\operatorname{tr}\big((\nabla\boldsymbol{n})^2\big) - (\operatorname{div}\boldsymbol{n})^2\big]$$

$$K_i = K_i(T), \quad 0 \le K_1, K_2, K_3, \quad 0 \le K_2 + K_4 \le 2K_1$$

Ground State: uniform field

$$\boldsymbol{n} = \text{const} \quad \Rightarrow \quad \operatorname{div}\boldsymbol{n} = 0, \ \operatorname{curl}\boldsymbol{n} = \boldsymbol{0} \quad \Rightarrow \quad W_{\text{nem}} = 0$$

Surface Term / Null Lagrangian:

$$\operatorname{tr}\big((\nabla\boldsymbol{n})^2\big) - (\operatorname{div}\boldsymbol{n})^2 = \operatorname{div}\big[\operatorname{curl}\boldsymbol{n}\times\boldsymbol{n} - (\operatorname{div}\boldsymbol{n})\boldsymbol{n}\big]$$

often zero or an additive constant . . .

Equal Elastic Constants: $K_1 = K_2 = K_3 = K, \quad K_4 = 0$

$$W_{\text{nem}} = \frac{K}{2}|\nabla\boldsymbol{n}|^2 = \frac{K}{2}\sum_{i,j=1}^{3}\Big(\frac{\partial n_i}{\partial x_j}\Big)^2$$

Cholesteric Model

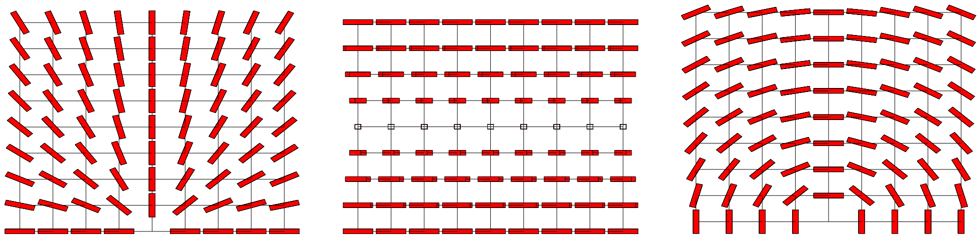
$$2W_{\text{chol}} = K_1(\operatorname{div}\boldsymbol{n})^2 + K_2(\boldsymbol{n}\cdot\operatorname{curl}\boldsymbol{n} + q_0)^2 + K_3|\boldsymbol{n}\times\operatorname{curl}\boldsymbol{n}|^2$$

$$0 \le K_1, K_2, K_3, \qquad \pm q_0, \qquad \frac{2\pi}{|q_0|} = \text{cholesteric pitch}$$

ground state: Beltrami field

$$\boldsymbol{n} = \cos q_0 z\, \boldsymbol{e}_x + \sin q_0 z\, \boldsymbol{e}_y \ \Rightarrow \ \operatorname{div}\boldsymbol{n} = 0, \ \operatorname{curl}\boldsymbol{n} = -q_0\boldsymbol{n} \ \Rightarrow \ W_{\text{chol}} = 0$$

Interpretation



Splay (K_1) Twist (K_2) Bend (K_3)

$\boldsymbol{n} = \boldsymbol{e}_r$ $\boldsymbol{n} = \cos qz\, \boldsymbol{e}_x + \sin qz\, \boldsymbol{e}_y$ $\boldsymbol{n} = \boldsymbol{e}_\theta$

K_{24} . . . “Saddle Splay” . . . ?

Dimensions and Scales

Dimensions:

$$[\mathcal{F}] = \text{energy}, \quad [W_\text{e}] = \frac{\text{energy}}{\text{volume}}, \quad [K_i] = \frac{\text{energy}}{\text{length}} = \text{force}, \quad [q_0] = \frac{1}{\text{length}}$$

Typical Values: 5CB ($26°$C)

$$K_1 = 6.2 \times 10^{-12}\,\text{J/m}, \quad K_2 = 3.9 \times 10^{-12}\,\text{J/m}, \quad K_3 = 8.2 \times 10^{-12}\,\text{J/m}$$

$$K_i \approx 10\,\text{pN}, \qquad K_1 \approx K_3, \qquad K_2 \approx \frac{1}{2} K_{1,3}$$

Intrinsic Length Scales:

cholesteric pitch

boundary extrapolation length

magnetic/electric coherence lengths

generally not of molecular order (vs Landau-de Gennes, “mesoscopic”) . . .

Electric Field

Typical Situation: capacitor, constant voltage

$$\boldsymbol{E} = -\nabla U, \quad U = \text{electrostatic potential}$$
$$\boldsymbol{D} = \varepsilon_0 \boldsymbol{E} + \boldsymbol{P} = \text{electric displacement / flux}$$
$$\boldsymbol{P} = \varepsilon_0 \boldsymbol{\chi}(\boldsymbol{n}) \boldsymbol{E} = \text{induced polarization}$$
$$\Rightarrow \quad \boldsymbol{D} = \boldsymbol{\varepsilon}(\boldsymbol{n}) \boldsymbol{E}, \quad \boldsymbol{\varepsilon}(\boldsymbol{n}) = \varepsilon_0 \big(\mathbf{I} + \boldsymbol{\chi}(\boldsymbol{n})\big) = \text{dielectric tensor}$$

$$[\boldsymbol{\varepsilon}] = \varepsilon_0 \begin{bmatrix} \varepsilon_\perp & & \\ & \varepsilon_\perp & \\ & & \varepsilon_\parallel \end{bmatrix}_{\boldsymbol{l},\boldsymbol{m},\boldsymbol{n}} \quad \leftrightarrow \quad \boldsymbol{\varepsilon} = \varepsilon_0 \big[\varepsilon_\perp \mathbf{I} + \varepsilon_{\mathsf{a}} \boldsymbol{n} \otimes \boldsymbol{n}\big], \quad \varepsilon_{\mathsf{a}} := \varepsilon_\parallel - \varepsilon_\perp$$

Electrostatics: Gauss's Law

$$\operatorname{div} \boldsymbol{D} = 0 \;\Rightarrow\; \operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n}) \nabla U\big) = 0 \;\leftrightarrow\; \sum_{i,j=1}^{3} \frac{\partial}{\partial x_i} \left(\varepsilon_{ij} \frac{\partial U}{\partial x_j} \right) = 0$$

Perturbative Effect:

$$\operatorname{div} \boldsymbol{D} = 0 \;\Rightarrow\; \Delta U + \frac{\varepsilon_{\mathsf{a}}}{\varepsilon_\perp} \operatorname{div}\big((\nabla U \cdot \boldsymbol{n}) \boldsymbol{n}\big) = 0, \quad \frac{\varepsilon_{\mathsf{a}}}{\varepsilon_\perp} = \frac{\varepsilon_\parallel - \varepsilon_\perp}{\varepsilon_\perp} = O(1).$$

Free Energy:

$$\mathcal{F}[\boldsymbol{n}, U] = \int_\Omega \big[W_{\mathsf{e}}(\boldsymbol{n}, \nabla \boldsymbol{n}) - W_{\mathsf{elec}}(\boldsymbol{n}, \nabla U)\big]$$
$$W_{\mathsf{elec}} = \frac{1}{2} \boldsymbol{D} \cdot \boldsymbol{E} = \frac{1}{2} \boldsymbol{\varepsilon}(\boldsymbol{n}) \nabla U \cdot \nabla U = \frac{1}{2} \varepsilon_0 \big[\varepsilon_\perp |\nabla U|^2 + \varepsilon_{\mathsf{a}} (\nabla U \cdot \boldsymbol{n})^2\big]$$
$$\delta_U \mathcal{F} = 0 \;\Rightarrow\; \operatorname{div} \boldsymbol{D} = \operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n}) \nabla U\big) = 0$$

Equilibrium:

$$\min_{\boldsymbol{n}} \max_{U} \mathcal{F}[\boldsymbol{n}, U] \;\leftrightarrow\; \min_{\boldsymbol{n}} \mathcal{F}[\boldsymbol{n}, U(\boldsymbol{n})], \;\text{ subject to } \operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n}) \nabla U\big) = 0$$

Influence:

$$\varepsilon_{\mathsf{a}} > 0 \;\Rightarrow\; \boldsymbol{n} \parallel \boldsymbol{E} \quad \text{vs} \quad \varepsilon_{\mathsf{a}} < 0 \;\Rightarrow\; \boldsymbol{n} \perp \boldsymbol{E}$$

Magnetic Field

similar, but . . .

Free Energy:

$$\mathcal{F}[\boldsymbol{n}] = \int_\Omega \left[W_{\mathrm{e}}(\boldsymbol{n}, \nabla\boldsymbol{n}) - W_{\mathrm{mag}}(\boldsymbol{n})\right], \quad W_{\mathrm{mag}} = \frac{1}{2}\boldsymbol{B}\cdot\boldsymbol{H}$$

$$\boldsymbol{B} = \mu_0(\boldsymbol{M} + \boldsymbol{H}), \quad \boldsymbol{M} = \boldsymbol{\chi}(\boldsymbol{n})\boldsymbol{H}$$

$$\Rightarrow \quad \boldsymbol{B}\cdot\boldsymbol{H} = \mu_0(1+\chi_\perp)H^2 + \mu_0\chi_{\mathrm{a}}(\boldsymbol{H}\cdot\boldsymbol{n})^2, \quad \chi_{\mathrm{a}} := \chi_\parallel - \chi_\perp$$

$$\frac{\chi_{\mathrm{a}}}{1+\chi_\perp} = \frac{\chi_\parallel - \chi_\perp}{1+\chi_\perp} = O(10^{-6}) \quad \Rightarrow \quad \boldsymbol{H} \approx \text{const}$$

Typical Form Taken:

$$\mathcal{F}[\boldsymbol{n}] = \int_\Omega \left[W_{\mathrm{e}}(\boldsymbol{n}, \nabla\boldsymbol{n}) - \frac{1}{2}\mu_0\chi_{\mathrm{a}}(\boldsymbol{H}\cdot\boldsymbol{n})^2\right]$$

Equilibrium:

$$\min_{\boldsymbol{n}} \mathcal{F}[\boldsymbol{n}], \qquad \boldsymbol{H} = \text{uniform field}$$

intrinsic length scale:

$$\frac{1}{H}\sqrt{\frac{K}{\mu_0\chi_{\mathrm{a}}}} = \text{magnetic coherence length}$$

Flexoelectricity

distortion-induced polarization . . . Meyer (1969)

$$\mathbf{P}_{\mathsf{f}}(\boldsymbol{n}) = e_1(\operatorname{div}\boldsymbol{n})\boldsymbol{n} + e_3\boldsymbol{n}\times\operatorname{curl}\boldsymbol{n}$$

$e_1, e_3 =$ flexoelectric coefficients (Lagerwall sign convention)

free-energy density: $W_{\text{total}} = \cdots - \mathbf{P}_{\mathsf{f}}\cdot\boldsymbol{E}$

electrostatics: $\boldsymbol{D} = \boldsymbol{\varepsilon}(\boldsymbol{n})\boldsymbol{E} + \mathbf{P}_{\mathsf{f}} \;\Rightarrow\; \operatorname{div}\big(\boldsymbol{\varepsilon}(\boldsymbol{n})\nabla U\big) = \operatorname{div}\mathbf{P}_{\mathsf{f}}(\boldsymbol{n})$

Surface Anchoring Potential

"weak anchoring" vs "strong anchoring" . . .

$$\mathcal{F} = \int_\Omega W_{\text{vol}} + \int_{\partial\Omega} W_{\text{surf}}, \quad W_{\text{surf}} = W_{\text{surf}}(\boldsymbol{n}, \boldsymbol{\nu}, \ldots)$$

various forms . . . e.g., Rapini-Papoular (1969)

$$W_{\text{surf}} = \pm\frac{1}{2}W_0(\boldsymbol{n}\cdot\boldsymbol{\nu})^2$$

enters natural BCs . . .

dimensions: $[W_{\text{surf}}] = \dfrac{\text{energy}}{\text{area}}$

typical values: $W_0 = 10^{-6}$ to 10^{-4} J/m^2

intrinsic length scale:

$$\frac{K}{W_0} = \text{surface extrapolation length}$$

Equilibrium Equations

various forms . . .

Ex: director components, no E-field

$$\mathcal{F}[\boldsymbol{n}] = \int_\Omega W_{\text{vol}}(\boldsymbol{n}, \nabla\boldsymbol{n})\, dV + \int_{\Gamma_1} W_{\text{surf}}(\boldsymbol{n})\, dS, \quad \partial\Omega = \Gamma_0 \cup \Gamma_1, \quad \Gamma_0 \text{“strong”}$$

$$\delta\mathcal{F}[\boldsymbol{n}_0](\boldsymbol{u}) = \int_\Omega \Big[\frac{\partial W_{\text{vol}}}{\partial \boldsymbol{n}} \cdot \boldsymbol{u} + \frac{\partial W_{\text{vol}}}{\partial \nabla\boldsymbol{n}} \cdot \nabla\boldsymbol{u} \Big] + \int_{\Gamma_1} \frac{\partial W_{\text{surf}}}{\partial \boldsymbol{n}} \cdot \boldsymbol{u}$$

weak form #1:

$$\delta\mathcal{F}[\boldsymbol{n}_0](\boldsymbol{u}) = 0, \quad \forall \boldsymbol{u} \in \{\boldsymbol{n}_0 \cdot \boldsymbol{u} = 0 \text{ in } \Omega, \boldsymbol{u} = \boldsymbol{0} \text{ on } \Gamma_0\} =: T_{\boldsymbol{n}_0}$$

weak form #2:

$$\delta\mathcal{F}[\boldsymbol{n}_0](\boldsymbol{v}) = \int_\Omega \lambda_0 \boldsymbol{n}_0 \cdot \boldsymbol{v} + \int_{\Gamma_1} \mu_0 \boldsymbol{n}_0 \cdot \boldsymbol{v}, \quad \forall \boldsymbol{v} \in \{\boldsymbol{v} = \boldsymbol{0} \text{ on } \Gamma_0\}$$

strong form:

$$-\operatorname{div}\Big(\frac{\partial W_{\text{vol}}}{\partial \nabla\boldsymbol{n}}\Big) + \frac{\partial W_{\text{vol}}}{\partial \boldsymbol{n}} = \lambda_0 \boldsymbol{n}_0, \quad \text{in } \Omega$$

$$\Big(\frac{\partial W_{\text{vol}}}{\partial \nabla\boldsymbol{n}}\Big)\boldsymbol{\nu} + \frac{\partial W_{\text{surf}}}{\partial \boldsymbol{n}} = \mu_0 \boldsymbol{n}_0, \quad \text{on } \Gamma_1$$

Stability:

$$\delta^2\mathcal{F}[\boldsymbol{n}_0](\boldsymbol{u}) - \int_\Omega \lambda_0 |\boldsymbol{u}|^2 - \int_{\Gamma_1} \mu_0 |\boldsymbol{u}|^2 \geq 0, \quad \forall \boldsymbol{u} \in T_{\boldsymbol{n}_0}$$

more complicated with coupled E-field . . .

Orientation Angles

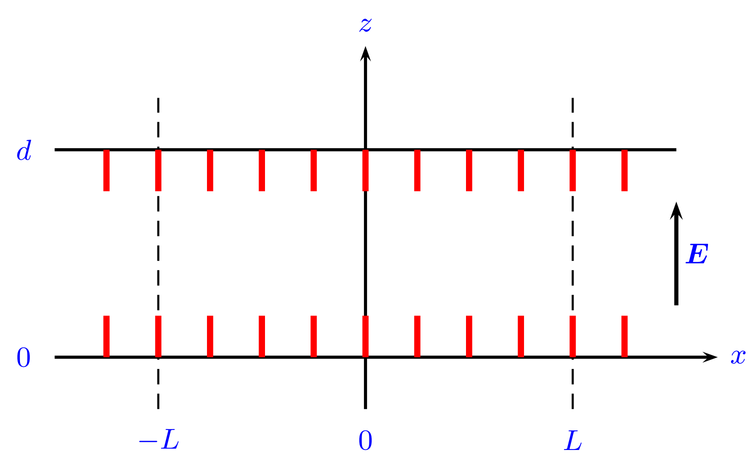
deal with $|\boldsymbol{n}| = 1$ pointwise constraint . . . e.g.,

$$\boldsymbol{n} = \sin\theta\cos\phi\,\boldsymbol{e}_1 + \sin\theta\sin\phi\,\boldsymbol{e}_2 + \cos\theta\,\boldsymbol{e}_3$$
$$\theta = \theta(x), \quad \phi = \phi(x), \quad \forall x \in \Omega$$
$$\mathcal{F}[\boldsymbol{n}] = \mathcal{F}[\theta,\phi] = \int_\Omega W(\theta, \nabla\theta, \phi, \nabla\phi) \;\; \ldots$$

1-D Example

System:

- chiral nematic film
- electric field + negative dielectric anisotropy
- strong homeotropic anchoring



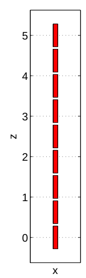
Influences:

BCs $\Rightarrow$ $\boldsymbol{n} = \boldsymbol{e}_z$

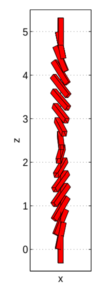
q_0 $\Rightarrow$ $\boldsymbol{n}$ = helical twist $(P = 2\pi/q_0 =$ "pitch"$)$

$\varepsilon_{\mathrm{a}} < 0$ $\Rightarrow$ $\boldsymbol{n} \perp \boldsymbol{E}$

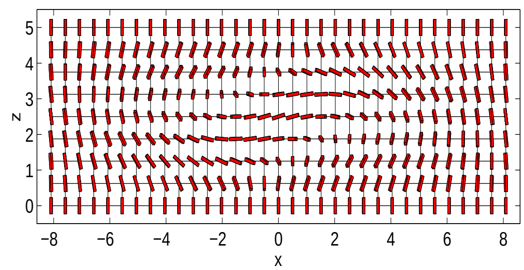
Phases:



Homeotropic



Translation Independent Cholesteric (TIC)



Cholesteric Finger Type 1 (CF1)

1-D Analysis

Assumption: $\boldsymbol{n} = \boldsymbol{n}(z)$, $U = U(z)$ (includes Homeotropic and TIC, *not* CF1)

Free Energy Density: $\angle$ representation, $\theta = \theta(z)$, $\phi = \phi(z)$

$$2W = \left(K_1 \sin^2\theta + K_3 \cos^2\theta\right) \theta_z^2 + \left(K_2 \sin^2\theta + K_3 \cos^2\theta\right) \sin^2\theta \, \phi_z^2 \\ - 2K_2 q_0 \sin^2\theta \, \phi_z + K_2 q_0^2 - \varepsilon_0 \left(\varepsilon_\perp \sin^2\theta + \varepsilon_\parallel \cos^2\theta\right) U_z^2$$

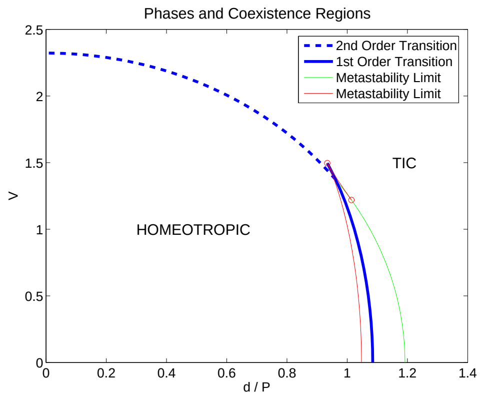
Equilibrium Equations: $\theta(z) = 0,\ U(z) = V z/d$ $\leftrightarrow$ Homeotropic

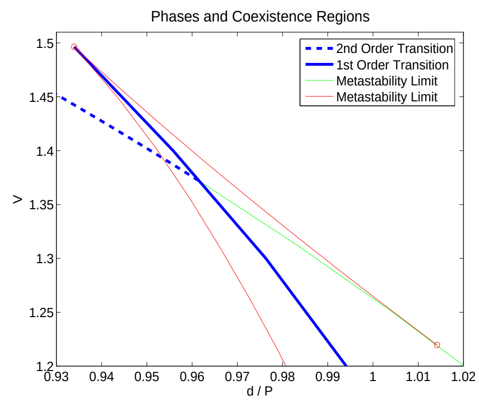
$$\frac{d}{dz}\left[\left(K_1 \sin^2\theta + K_3 \cos^2\theta\right) \theta_z\right] = \sin\theta\cos\theta \Big\{ (K_1 - K_3)\theta_z^2 \\ + \left[(2K_2 - K_3)\sin^2\theta + K_3 \cos^2\theta\right] \phi_z^2 - 2K_2 q_0 \phi_z + \varepsilon_0 \varepsilon_{\mathrm{a}} U_z^2 \Big\}$$

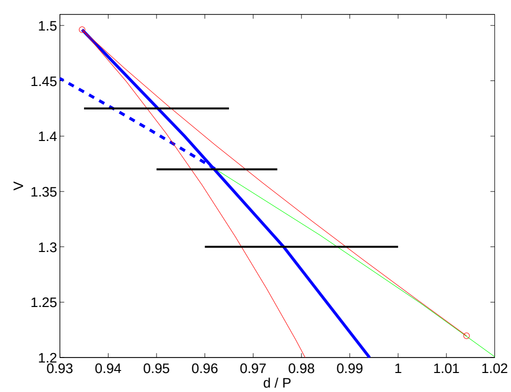
$$\frac{d}{dz}\Big\{ \sin^2\theta \left[\left(K_2 \sin^2\theta + K_3 \cos^2\theta\right) \phi_z - K_2 q_0\right] \Big\} = 0$$

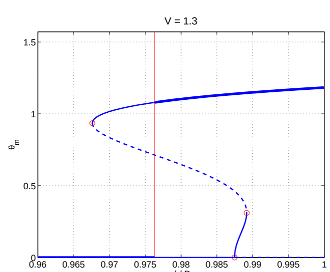
$$\frac{d}{dz}\left[\left(\varepsilon_\perp \sin^2\theta + \varepsilon_\parallel \cos^2\theta\right) U_z\right] = 0$$

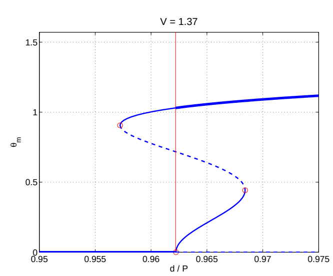
Phase Diagram

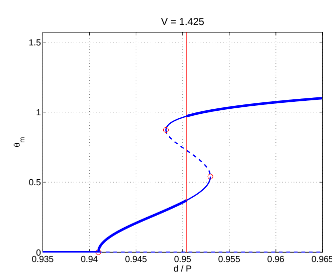






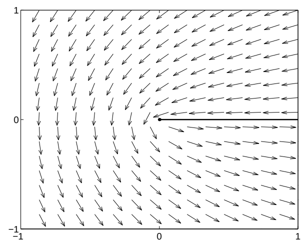






Notes and Issues

- Effective for modeling many problems at device or experiment scale
- Consistent with Ericksen-Leslie hydrostatics, provided . . .
- Admits point defects ($\boldsymbol{n} = \boldsymbol{e}_r$ spherical $\Rightarrow$ $\mathcal{F} < \infty$) . . .
  but does *not* admit line defects ($\boldsymbol{n} = \boldsymbol{e}_r$ cylindrical $\Rightarrow$ $\mathcal{F} = \infty$)
- Parity issues:
  - "globally" OK:
    $\mathcal{F}[-\boldsymbol{n}] = \mathcal{F}[\boldsymbol{n}]$
  - "locally"? . . .
    workarounds ($\boldsymbol{n} \mapsto \boldsymbol{n} \otimes \boldsymbol{n}$)

  Ball and Zarnescu (2011)
- $|n(x)| = 1$ pointwise constraint a *nuisance*.
- Math analysis: Hardt-Kinderlehrer-Lin (1986)
- References (books): Virga (1994), Stewart (2004)