

Liquid Crystal Director Models with Coupled Electric Fields

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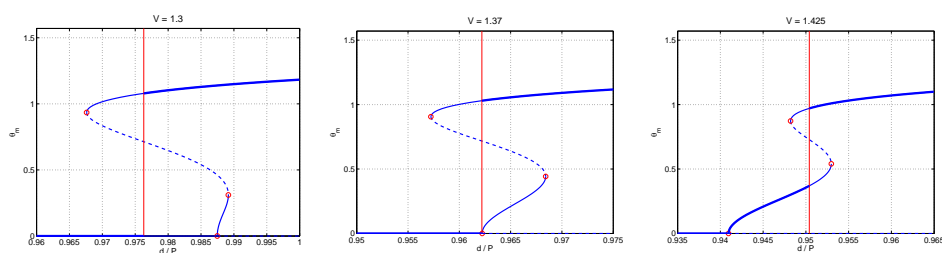
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Motivation

- Numerical modeling of devices and experiments: equilibrium orientational properties, coupled electric fields, Oseen-Frank.
- Numerical bifurcation and phase analysis:
 - discretized free energy (finite differences or finite elements or ...):
 $f = f(\mathbf{n}, \varphi)$, $\mathbf{n} = \{\mathbf{n}_i\} = \text{directors}$, $\varphi = \{\varphi_i\} = \text{electric potential}$
 - Lagrangian: $L(\mathbf{n}, \varphi, \lambda) = f(\mathbf{n}, \varphi) + \sum \lambda_i (|\mathbf{n}_i|^2 - 1)$
 - paths of equilibria ($\nabla L = \mathbf{0}$) via parameter continuation
 - bifurcation and branch switching
 - local stability assessment



Questions and Issues

- Characterization of local stability.
- Extension from discrete setting to continuum setting.
- Effect of $\mathbf{n} - \mathbf{E}$ coupling on electric-field-induced instabilities, e.g., Fréedericksz-transition thresholds.
- Anomalous behavior of the electric-field bend-Fréedericksz transition.

Free Energy

Typical Situation: capacitor, constant voltage, $\mathbf{E} = -\nabla\varphi = \text{local electric field}$

$$\mathcal{F}[\mathbf{n}, \varphi] = \int_{\Omega} W(\mathbf{n}, \nabla\mathbf{n}, \nabla\varphi) dV + \int_{\Gamma_1} W_b(\mathbf{n}) dS$$

$$W(\mathbf{n}, \nabla\mathbf{n}, \nabla\varphi) = W_e(\mathbf{n}, \nabla\mathbf{n}) - W_E(\mathbf{n}, \nabla\varphi)$$

Distortional Elasticity: e.g., $W_e = \frac{1}{2}K|\nabla\mathbf{n}|^2$, $\mathbf{n} = \text{“director field”}$, $|\mathbf{n}| = 1$

Electrostatic Energy: $W_E = \frac{1}{2}\mathbf{D} \cdot \mathbf{E} = \frac{1}{2}\varepsilon(\mathbf{n})\nabla\varphi \cdot \nabla\varphi$

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

Surface Anchoring Potential: e.g., $W_b = -\frac{1}{2}W_0(\mathbf{n} \cdot \boldsymbol{\nu})^2$, $\boldsymbol{\nu} = \text{unit normal}$

$$\partial\Omega = \Gamma_0 \cup \Gamma_1, \quad \Gamma_0 \text{ “strong anchoring” } (\mathbf{n} = \mathbf{n}_b), \quad \Gamma_1 \text{ “weak anchoring” } (W_b)$$

General Form:

$$\mathcal{F}[\mathbf{n}, \varphi] = \int_{\Omega} \left[W_e(\mathbf{n}, \nabla \mathbf{n}) - \frac{1}{2} \varepsilon(\mathbf{n}) \nabla \varphi \cdot \nabla \varphi \right] + \int_{\Gamma_1} W_b(\mathbf{n})$$

Prototype:

$$\begin{aligned} \mathcal{F}[\mathbf{n}, \varphi] &= \frac{1}{2} \int_{\Omega} [K |\nabla \mathbf{n}|^2 - \varepsilon(\mathbf{n}) \nabla \varphi \cdot \nabla \varphi] \\ &= \frac{1}{2} \int_{\Omega} \left\{ K |\nabla \mathbf{n}|^2 - \varepsilon_0 [\varepsilon_{\perp} |\nabla \varphi|^2 + \varepsilon_a (\nabla \varphi \cdot \mathbf{n})^2] \right\} \end{aligned}$$

Influence:

$$\varepsilon_a > 0 \Rightarrow \mathbf{n} \parallel \mathbf{E} \quad \text{vs} \quad \varepsilon_a < 0 \Rightarrow \mathbf{n} \perp \mathbf{E}$$

Boundary Conditions: various possibilities ... for simplicity

$$\mathbf{n} = \mathbf{n}_b \text{ on } \Gamma_0, \quad \varphi = \varphi_b \text{ on } \partial\Omega$$

Equilibria

Globally Stable Phase: $\mathbf{n}_0 \in \mathcal{N}_b$, $\varphi_0 \in \Phi_b$ (admissible fields) such that

$$\mathcal{F}[\mathbf{n}_0, \varphi_0] = \min_{\mathbf{n} \in \mathcal{N}_b} \max_{\varphi \in \Phi_b} \mathcal{F}[\mathbf{n}, \varphi]$$

equivalently

$$\min_{\mathbf{n} \in \mathcal{N}_b} \mathcal{F}[\mathbf{n}, \varphi], \quad \text{subject to } \operatorname{div}(\varepsilon(\mathbf{n}) \nabla \varphi) = \sum_{i,j=1}^3 \frac{\partial}{\partial x_i} \left(\varepsilon_{ij} \frac{\partial \varphi}{\partial x_j} \right) = 0$$

where

$$\begin{aligned} \mathcal{N}_b &= \{ \mathbf{n} \mid |\mathbf{n}| = 1 \text{ in } \Omega, \mathbf{n} = \mathbf{n}_b \text{ on } \Gamma_0 \} \\ \Phi_b &= \{ \varphi \mid \varphi = \varphi_b \text{ on } \partial\Omega \} \end{aligned}$$

Point: intrinsic *minimax* nature \leftrightarrow PDE-constrained minimization

1st-Order Conditions: $(\mathbf{n}_0, \varphi_0) \in \mathcal{N}_b \times \Phi_b$ equilibrium pair \Rightarrow

weak form #1: $\mathcal{U}_0 := \{\mathbf{u} \mid \mathbf{n}_0 \cdot \mathbf{u} = 0, \mathbf{u} = \mathbf{0} \text{ on } \Gamma_0\}$, $\Phi_0 := \{\psi \mid \psi = 0 \text{ on } \partial\Omega\}$

$$\delta_{\mathbf{n}} \mathcal{F}[\mathbf{n}_0, \varphi_0](\mathbf{u}) = 0, \quad \forall \mathbf{u} \in \mathcal{U}_0$$

$$\delta_{\varphi} \mathcal{F}[\mathbf{n}_0, \varphi_0](\psi) = 0, \quad \forall \psi \in \Phi_0$$

weak form #2: λ_0, μ_0 Lagrange multiplier fields, $\mathcal{V}_0 := \{\mathbf{v} \mid \mathbf{v} = \mathbf{0} \text{ on } \Gamma_0\}$

$$\delta_{\mathbf{n}} \mathcal{F}[\mathbf{n}_0, \varphi_0](\mathbf{v}) = \int_{\Omega} \lambda_0 \mathbf{n}_0 \cdot \mathbf{v} + \int_{\Gamma_1} \mu_0 \mathbf{n}_0 \cdot \mathbf{v}, \quad \forall \mathbf{v} \in \mathcal{V}_0$$

$$\int_{\Omega} \varepsilon(\mathbf{n}_0) \nabla \varphi_0 \cdot \nabla \psi = 0, \quad \forall \psi \in \Phi_0$$

strong form:

$$-\operatorname{div} \left(\frac{\partial W_e}{\partial \nabla \mathbf{n}} \right) + \frac{\partial W_e}{\partial \mathbf{n}} = \lambda_0 \mathbf{n}_0 + \varepsilon_0 \varepsilon_a (\nabla \varphi_0 \cdot \mathbf{n}_0) \nabla \varphi_0 \text{ in } \Omega$$

$$\mathbf{n}_0 = \mathbf{n}_b \text{ on } \Gamma_0, \quad \left(\frac{\partial W_e}{\partial \nabla \mathbf{n}} \right) \boldsymbol{\nu} + \frac{\partial W_b}{\partial \mathbf{n}} = \mu_0 \mathbf{n}_0 \text{ on } \Gamma_1$$

$$\operatorname{div}(\varepsilon(\mathbf{n}_0) \nabla \varphi_0) = 0 \text{ in } \Omega, \quad \varphi_0 = \varphi_b \text{ on } \partial\Omega$$

Question: 2nd-order conditions? local stability?

Deflated Free Energy

$$\tilde{\mathcal{F}}[\mathbf{n}] := \max_{\varphi \in \Phi_b} \mathcal{F}[\mathbf{n}, \varphi] = \mathcal{F}[\mathbf{n}, T(\mathbf{n})], \quad \text{where } \varphi = T(\mathbf{n}) = \text{solution to}$$

$$\delta_{\varphi} \mathcal{F}[\mathbf{n}, \varphi] = 0 \Leftrightarrow \int_{\Omega} \varepsilon(\mathbf{n}) \nabla \varphi \cdot \nabla \psi = 0, \quad \varphi \in \Phi_b, \quad \forall \psi \in \Phi_0$$

H^1 -ellipticity:

$$\varepsilon_0 \min\{\varepsilon_{\perp}, \varepsilon_{\parallel}\} \int_{\Omega} |\nabla \varphi|^2 \leq \int_{\Omega} \varepsilon(\mathbf{n}) \nabla \varphi \cdot \nabla \varphi \leq \varepsilon_0 \max\{\varepsilon_{\perp}, \varepsilon_{\parallel}\} \int_{\Omega} |\nabla \varphi|^2$$

Derivative: $\psi = DT(\mathbf{n}_0)\mathbf{v}$ = solution to: $\psi \in \Phi_0$,

$$\int_{\Omega} \varepsilon(\mathbf{n}_0) \nabla \psi \cdot \nabla \chi = \int_{\Omega} \mathbf{d}_0 \cdot \nabla \chi, \quad \forall \chi \in \Phi_0 \Leftrightarrow \operatorname{div}(\varepsilon(\mathbf{n}_0) \nabla \psi) = \operatorname{div} \mathbf{d}_0$$

$$\mathbf{d}_0 := \varepsilon_0 \varepsilon_a (\mathbf{n}_0 \otimes \mathbf{v} + \mathbf{v} \otimes \mathbf{n}_0) \mathbf{E}_0, \quad \mathbf{E}_0 = -\nabla \varphi_0, \quad \varphi_0 = T(\mathbf{n}_0)$$

Interpretation:

$$\mathbf{d}_0 = \text{1st-order change in } \mathbf{D}_0 = \varepsilon(\mathbf{n}_0) \mathbf{E}_0 \text{ associated with } \mathbf{n}_0 \mapsto \mathbf{n}_0 + \mathbf{v}$$

Alternately: $\operatorname{div}(\boldsymbol{\varepsilon}(\mathbf{n}_0)\nabla\varphi_0) = 0$, $\boldsymbol{\varepsilon}(\mathbf{n}) = \varepsilon_0[\varepsilon_\perp\mathbf{I} + \varepsilon_a(\mathbf{n} \otimes \mathbf{n})]$

$$\operatorname{div}(\boldsymbol{\varepsilon}(\mathbf{n}_0 + \mathbf{v})\nabla(\varphi_0 + \psi)) = 0 + \operatorname{div}(\boldsymbol{\varepsilon}(\mathbf{n}_0)\nabla\psi) - \operatorname{div}\mathbf{d}_0 + \dots$$

Alternately: $\delta^2\mathcal{F} = \delta_{\mathbf{nn}}^2\mathcal{F} + 2\delta_{\mathbf{n}\varphi}^2\mathcal{F} + \delta_{\varphi\varphi}^2\mathcal{F}$

$$\delta^2\mathcal{F}[\mathbf{n}_0, \varphi_0]((\mathbf{v}, \psi), (\mathbf{v}, \psi)) =$$

$$\delta_{\mathbf{nn}}^2\mathcal{F}[\mathbf{n}_0, \varphi_0](\mathbf{v}, \mathbf{v}) + 2 \int_{\Omega} \mathbf{d}_0 \cdot \nabla\psi - \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{n}_0)\nabla\psi \cdot \nabla\psi$$

Globally Stable Phase: $\tilde{\mathcal{F}}$ is coercive! ... $\mathbf{n}_0 \in \mathcal{N}_b$ such that

$$\tilde{\mathcal{F}}[\mathbf{n}_0] = \min_{\mathbf{n} \in \mathcal{N}_b} \tilde{\mathcal{F}}[\mathbf{n}] \leftrightarrow \text{equilibrium pair } (\mathbf{n}_0, \varphi_0) \text{ of "Least Free Energy"}$$

1st-Order and 2nd-Order Conditions (in terms of $\tilde{\mathcal{F}}$):

$$\delta\tilde{\mathcal{F}}[\mathbf{n}_0](\mathbf{v}) = \int_{\Omega} \lambda_0 \mathbf{n}_0 \cdot \mathbf{v} + \int_{\Gamma_1} \mu_0 \mathbf{n}_0 \cdot \mathbf{v}, \quad \forall \mathbf{v} \in \mathcal{V}_0$$

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

Calculus: relate $\delta\tilde{\mathcal{F}}, \delta^2\tilde{\mathcal{F}}$ to $\delta\mathcal{F}, \delta^2\mathcal{F}$...

$$\begin{aligned} \delta\tilde{\mathcal{F}}[\mathbf{n}_0](\mathbf{v}) &= \delta_{\mathbf{n}}\mathcal{F}[\mathbf{n}_0, T(\mathbf{n}_0)](\mathbf{v}) + \delta_{\varphi}\mathcal{F}[\mathbf{n}_0, T(\mathbf{n}_0)](DT(\mathbf{n}_0)\mathbf{v}) \\ &= \delta_{\mathbf{n}}\mathcal{F}[\mathbf{n}_0, T(\mathbf{n}_0)](\mathbf{v}), \quad \text{using } \delta_{\varphi}\mathcal{F}[\mathbf{n}_0, T(\mathbf{n}_0)] = 0 \end{aligned}$$

$$\begin{aligned} \delta^2\tilde{\mathcal{F}}[\mathbf{n}_0](\mathbf{v}, \mathbf{v}) &= \delta_{\mathbf{nn}}^2\mathcal{F}[\mathbf{n}_0, T(\mathbf{n}_0)](\mathbf{v}, \mathbf{v}) + \delta_{\mathbf{n}\varphi}^2\mathcal{F}[\mathbf{n}_0, T(\mathbf{n}_0)](\mathbf{v}, DT(\mathbf{n}_0)\mathbf{v}) \\ &= \delta_{\mathbf{nn}}^2\mathcal{F}[\mathbf{n}_0, T(\mathbf{n}_0)](\mathbf{v}, \mathbf{v}) + \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{n}_0)\nabla\psi \cdot \nabla\psi, \quad \psi = DT(\mathbf{n}_0)\mathbf{v} \end{aligned}$$

using

$$\delta_{\mathbf{n}\varphi}^2\mathcal{F}[\mathbf{n}_0, \varphi_0](\mathbf{v}, \psi) = \int_{\Omega} \mathbf{d}_0 \cdot \nabla\psi$$

and

$$\psi = DT(\mathbf{n}_0)\mathbf{v} \Rightarrow \int_{\Omega} \mathbf{d}_0 \cdot \nabla\psi = \int_{\Omega} \boldsymbol{\varepsilon}(\mathbf{n}_0)\nabla\psi \cdot \nabla\psi$$

Conclusion (in terms of \mathcal{F}): $(\mathbf{n}_0, \varphi_0) \in \mathcal{N}_b \times \Phi_b$ locally stable equilibrium pair \Rightarrow

$$\delta_{nn}^2 \mathcal{F}[\mathbf{n}_0, \varphi_0](\mathbf{u}, \mathbf{u}) + \int_{\Omega} \varepsilon(\mathbf{n}_0) \nabla \psi \cdot \nabla \psi - \int_{\Omega} \lambda_0 |\mathbf{u}|^2 - \int_{\Gamma_1} \mu_0 |\mathbf{u}|^2 \geq 0,$$

$$\forall \mathbf{u} \in \mathcal{U}_0, \text{ with } \psi = DT(\mathbf{n}_0)\mathbf{u}$$

Alternately:

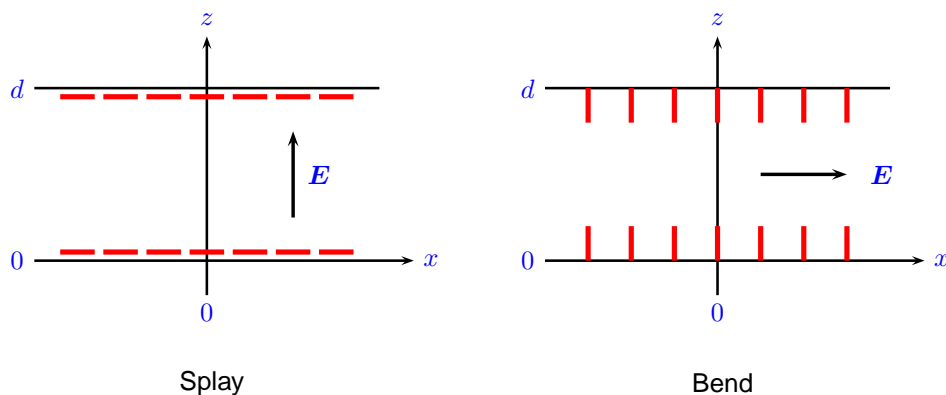
$$\max_{\psi \in \Phi_0} \delta^2 \mathcal{F}[\mathbf{n}_0, \varphi_0](\mathbf{u}, \psi), (\mathbf{u}, \psi) - \int_{\Omega} \lambda_0 |\mathbf{u}|^2 - \int_{\Gamma_1} \mu_0 |\mathbf{u}|^2 \geq 0, \quad \forall \mathbf{u} \in \mathcal{U}_0$$

Points: recall strong form ψ : $\boxed{\operatorname{div}(\varepsilon(\mathbf{n}_0)\nabla\psi) = \operatorname{div} \mathbf{d}_0 \text{ in } \Omega, \quad \psi = 0 \text{ on } \partial\Omega}$

1. $\operatorname{div} \mathbf{d}_0 = 0 \Rightarrow \psi = 0 \Rightarrow$ coupling has *no effect* on local stability of an equilibrium phase.
2. $\operatorname{div} \mathbf{d}_0 \neq 0 \Rightarrow \psi \neq 0 \Rightarrow$ coupling is *stabilizing* (e.g., can only *elevate* an instability threshold).
3. The φ_0 variation ψ is slaved to the \mathbf{n}_0 variation \mathbf{u} , just as φ_0 is slaved to \mathbf{n}_0 .

Application

Electric-Field Fréedericksz Transitions: “splay geometry” vs “bend geometry”



Splay: references: Deuling (MCLC, 1972); Iain Stewart book (2004)

$$\mathbf{n}_0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \Rightarrow \mathbf{u} = \begin{bmatrix} 0 \\ 0 \\ w(z) \end{bmatrix}, \quad \mathbf{E}_0 = \begin{bmatrix} 0 \\ 0 \\ E_0 \end{bmatrix}$$

$$\Rightarrow \mathbf{d}_0 = \varepsilon_0 \varepsilon_a (\mathbf{n}_0 \otimes \mathbf{u} + \mathbf{u} \otimes \mathbf{n}_0) \mathbf{E}_0 = \varepsilon_0 \varepsilon_a E_0 \begin{bmatrix} w(z) \\ 0 \\ 0 \end{bmatrix}$$

$$\Rightarrow \operatorname{div} \mathbf{d}_0 = 0 \Rightarrow \text{no effect on stability}$$

threshold: $E_c^2 = \frac{K_1}{\varepsilon_0 \varepsilon_a} \frac{\pi^2}{d^2}$ vs magnetic-field case $H_c^2 = \frac{K_1}{\mu_0 \Delta \chi} \frac{\pi^2}{d^2}$

Bend:

$$\mathbf{n}_0 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \Rightarrow \mathbf{u} = \begin{bmatrix} u(z) \\ 0 \\ 0 \end{bmatrix}, \quad \mathbf{E}_0 = \begin{bmatrix} E_0 \\ 0 \\ 0 \end{bmatrix}$$

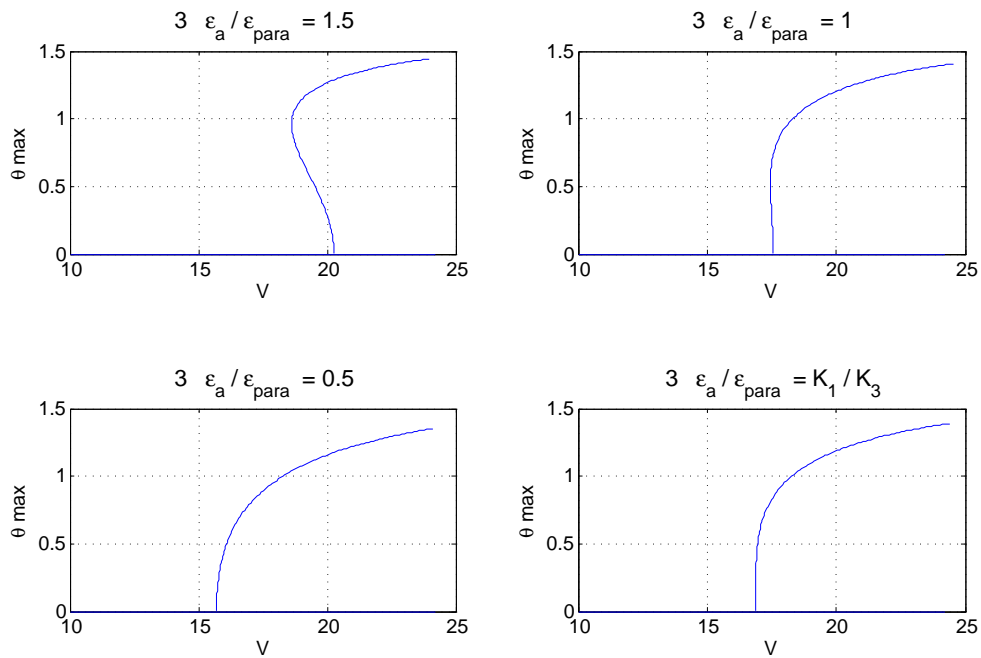
$$\Rightarrow \mathbf{d}_0 = \varepsilon_0 \varepsilon_a E_0 \begin{bmatrix} 0 \\ 0 \\ u(z) \end{bmatrix} \Rightarrow \operatorname{div} \mathbf{d}_0 = \varepsilon_0 \varepsilon_a E_0 u'(z) \neq 0$$

elevated threshold:

$$E_c^2(\text{ignore coupling}) = \frac{K_3}{\varepsilon_0 \varepsilon_a} \frac{\pi^2}{d^2} \quad \text{vs} \quad E_c^2(\text{with coupling}) = \frac{\varepsilon_{\parallel}}{\varepsilon_{\perp}} \frac{K_3}{\varepsilon_0 \varepsilon_a} \frac{\pi^2}{d^2}$$

Remarks:

1. Effect is *not* small: for 5CB, $\varepsilon_{\parallel} = 18.5$, $\varepsilon_{\perp} = 7 \Rightarrow 63\%$ higher voltage!
2. Transition can be *1st order*: $K_1/K_3 < 3\varepsilon_a/\varepsilon_{\parallel} \approx 1.86$, for 5CB
3. Reference: Arakelyan, Karayan, and Chilingaryan, Dokl. Akad. Nauk SSSR, 1984.



Reference: Gregory P. Richards, Masters Thesis, Kent State University, 2006
 ($K_1/K_3 = 3.6/4.3 \doteq 0.84$)

Comparison with Experiment

??? MAKE A FIGURE HERE WITH FRISKEN-PALFFY DATA VS BIFURCATION
 DIAGRAM FOR THOSE MATERIAL PARAMETERS (JOHN BALL QUESTION) ???

Reference: Frisken and Palffy-Muhoray, *Electric-field-induced twist and bend
 Fréedericksz transitions in nematic liquid crystals*, PRA **39** (1989).

Conclusions

- Local stability assessment complicated by pointwise constraint and minimax nature.
- One-sided nature of the coupling: can only *elevate* an instability threshold.
- Instability threshold elevation: $\delta\varphi_0 = O(|\delta\mathbf{n}_0|)$ vs $O(|\delta\mathbf{n}_0|^2)$?
- Similar effects in ferroelectrics, flexoelectric polarization terms, ...
- Numerical implementation: $\lambda_{\min}(Z^T(A + DC^{-1}D^T)Z) \geq 0$
- Additional references:
 - Rosso, Virga, and Kralj, *Local elastic stability for nematic liquid crystals*, PRE **70** (2004).
 - Bevilacqua and Napoli, *Re-examination of the Helfrich-Hurault effect in smectic-A liquid crystals*, PRE **72** (2005).