

What an Old Problem Has Still to Say: the Infamous K_{13} Case

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Summary

Splay-Bend Elasticity

Continuum Limit

Surface Order on Nematic Shells

Splay-Bend Elasticity

For a *uniaxial nematic* phase

$$\mathbf{Q} = S \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{I} \right)$$

S scalar order parameter

\mathbf{n} nematic director

Splay-Bend Elasticity

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elastic energy density

Letting $S \equiv 1$, we can write the elastic free-energy per unit volume in the form

$$\begin{aligned} W_e(\mathbf{n}, \nabla \mathbf{n}) &= \frac{1}{2} K_1 (\operatorname{div} \mathbf{n})^2 + \frac{1}{2} K_2 (\mathbf{n} \cdot \operatorname{curl} \mathbf{n})^2 + \frac{1}{2} K_3 |\mathbf{n} \times \operatorname{curl} \mathbf{n}|^2 \\ &+ \frac{1}{2} (K_2 + K_{24}) [\operatorname{tr}(\nabla \mathbf{n})^2 - (\operatorname{div} \mathbf{n})^2] + K_{13} \operatorname{div}[(\operatorname{div} \mathbf{n}) \mathbf{n}] \end{aligned}$$

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K_2 twist constant

K_3 bend constant

K_{24} saddle-splay constant

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one-constant approximation

$$K_1 = K_2 = K_3 = K \quad \& \quad K_{24} = 0 \quad K_{13} = 0 \quad \Rightarrow \quad W_e = \frac{K}{2} |\nabla \mathbf{n}|^2$$

free-energy functional

$$\mathcal{F}_e[\mathbf{n}] = \int_{\mathcal{B}} W_e(\mathbf{n}, \nabla \mathbf{n}) dV$$

\mathcal{B} region in space

V volume measure

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Null Lagrangians

$$\text{tr}(\nabla \mathbf{n})^2 - (\text{div } \mathbf{n})^2 = \text{div}[(\nabla \mathbf{n})\mathbf{n} - (\text{div } \mathbf{n})\mathbf{n}]$$

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$$\int_{\mathcal{B}} [\text{tr}(\nabla \mathbf{n})^2 - (\text{div } \mathbf{n})^2] dV = \int_{\partial \mathcal{B}} [(\nabla_s \mathbf{n})\mathbf{n} - (\text{div}_s \mathbf{n})\mathbf{n}] \cdot \boldsymbol{\nu} dA$$

$\partial \mathcal{B}$ boundary of \mathcal{B}

$\boldsymbol{\nu}$ outer unit normal to $\partial \mathcal{B}$

∇_s surface gradient

div_s surface divergence

A area measure

$$\begin{aligned}\int_{\mathcal{B}} \operatorname{div}[(\operatorname{div} \mathbf{n})\mathbf{n}]dV &= \int_{\partial\mathcal{B}} (\operatorname{div} \mathbf{n})\mathbf{n} \cdot \boldsymbol{\nu}dA \\ &= \int_{\partial\mathcal{B}} (\operatorname{div}_{\boldsymbol{\nu}} \mathbf{n} + \operatorname{div}_{\mathbf{s}} \mathbf{n})\mathbf{n} \cdot \boldsymbol{\nu}dA\end{aligned}$$

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pitfall

In the presence of *strong* boundary conditions, which prescribe the nematic director over the whole $\partial\mathcal{B}$, the derivatives $(\nabla_{\mathbf{s}}\mathbf{n})\mathbf{e}$ of \mathbf{n} in all surface directions \mathbf{e} are prescribed, whereas the normal derivative $(\nabla_{\mathbf{s}}\mathbf{n})\boldsymbol{\nu}$ is completely *free*.

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- OLDANO & BARBERO (1985) found by example that K_{13} makes \mathcal{F}_e *unbounded* from below.

first attempted remedies

- Adding to W_e terms quadratic in the second gradient $\nabla^2 \mathbf{n}$ that comply with both *frame-indifference* and *nematic symmetry*.

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It formally solves the unboundedness of \mathcal{F}_e , but in a rather ad hoc manner.

towards proving that $K_{13} = 0$

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- **YOKOYOMA (1997)** proved that a properly phrased density functional theory requires that $K_{13} = 0$, in accord with the well-posedness of the phenomenological theory, and that $K_{24} \geq \frac{1}{2} (K_1 - K_2)$.

K_{13} cyclic resurrections

Recently, an extension of Nehring & Saupe's theory to a mean-field treatment that would incorporate the effects of molecular anisotropy into the dispersion forces interactions, has reproduced a mutation of K_{13} , though both its sign and its dependence on temperature make it different from the other elastic constants predicted by theory, and so open to suspicion.

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undistorted state (at zero temperature) & homogeneity

$$W_{13} := K_{13} \operatorname{div}[(\operatorname{div} \mathbf{n})\mathbf{n}] = K_{13} [(\operatorname{div} \mathbf{n})^2 + \underbrace{\nabla(\operatorname{div} \mathbf{n}) \cdot \mathbf{n}}_{\text{linear}}]$$

If we assume that the *undistorted* state is attained when \mathbf{n} is *uniform* in space, then in the limit of small distortions the linear component of W_{13} would prevail over all other elastic terms, making the undistorted state unstable, unless $K_{13} = 0$.

(YOKOYAMA 1997)

Ericksen inequalities

$$W_e \geq 0 \quad \Leftrightarrow \quad K_1 \geq \frac{1}{2} (K_2 + K_{24}), \quad K_2 \geq |K_{24}|, \quad K_3 \geq 0 \quad \& \quad K_{13} = 0$$

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illuminating passage

“Even though the two approaches [phenomenological and molecular] lead to nearly the same result, there is a fundamental difference between both ways of treating elastic properties. In the phenomenological method, we regard the *free* energy which is the interesting quantity for the determination of equilibrium structures. The molecular method deals only with the *interaction* energy, which is assumed to be additive, and takes no account of the entropy.”

(NEHRING & SAUPE 1971)

Continuum Limit

Inspired by the work of NEHRING & SAUPE (1971), we consider a simple molecular interaction model as a heuristic, conceptual tool to identify the appropriate *measure* of elastic distortion.

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r inter-molecular distance

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U_{iso} U_{aniso} interaction strengths

σ interaction range

(LUCKHURST & ROMANO (1980))

molecular distortion

We imagine that at *equilibrium* the first neighbors of the spin ℓ at $p \in \mathcal{B}$ lie on a *sphere* of radius r_e .

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$\ell_{\mathbf{u}}$ spin at $p_{\mathbf{u}}$

average distortion energy

$$w_e := -\frac{3}{2}U_{\text{aniso}}\varrho \left(\frac{\sigma}{r_e}\right)^6 \langle (\boldsymbol{\ell} \cdot \boldsymbol{\ell}_u)^2 \rangle_{S^2} \quad \varrho \text{ volume number density}$$

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- The elastic free energy density is a quadratic function of $\nabla \boldsymbol{n}$.

Surface Order on Nematic Shells

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ℓ molecular director

\mathcal{S} closed orientable surface

ν outer unit normal

$$\ell \cdot \nu \equiv 0$$

order tensor

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order bounds

$$0 \leq \lambda \leq \frac{1}{2}$$

Elastic Model

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$$\ell_{\mathbf{u}} = \ell + r_e (\nabla_{\mathbf{s}} \ell) \mathbf{u} + \frac{1}{2} r_e^2 (\nabla_{\mathbf{s}}^2 \ell) \cdot (\mathbf{u} \otimes \mathbf{u}) + o(r_e^2)$$

$\nabla_{\mathbf{s}}$ surface gradient

$\ell_{\mathbf{u}}$ spin at $p_{\mathbf{u}}$

elastic surface energy density

$$w_s := -\frac{3}{2}U_{\text{aniso}}\varrho \left(\frac{\sigma}{r_e}\right)^6 \langle (\boldsymbol{\ell} \cdot \boldsymbol{\ell}_u)^2 \rangle_{\mathbb{S}^1}$$

ϱ surface number density

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ϱ surface number density

Evaluating the average,

$$\langle \mathbf{u} \otimes \mathbf{u} \rangle_{\mathbb{S}^1} = \frac{1}{2} (\mathbf{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}) \quad (\nabla_s \boldsymbol{\ell})^\top \boldsymbol{\ell} = \mathbf{0}$$

$\boldsymbol{\nu}$ outer unit normal to \mathcal{S}

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$$w_s = \frac{k}{2} |\nabla_s \boldsymbol{\ell}|^2 + \text{constant} \quad k := \frac{3}{2} \varrho U_{\text{aniso}} r_e^2 \left(\frac{\sigma}{r_e}\right)^6$$

elastic surface energy density

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A similar conclusion was also arrived at via Monte Carlo simulations on tori by [SELINGER, KONYA, TRAVESSET & SELINGER \(2011\)](#).

continuum limit

Thus $\nabla_s \mathbf{n}$ is the natural measure of local distortion in the continuum limit and W_s should be taken as a quadratic invariant function of the tensor $\nabla_s \mathbf{n}$

$$\begin{aligned} W_s(\mathbf{n}, \nabla_s \mathbf{n}) := & \frac{1}{2} k_1 (\operatorname{div}_s \mathbf{n})^2 + \frac{1}{2} k_2 (\mathbf{n} \cdot \operatorname{curl}_s \mathbf{n})^2 + \frac{1}{2} k_3 |\mathbf{n} \times \operatorname{curl}_s \mathbf{n}|^2 \\ & + \frac{1}{2} (k_2 + k_{24}) [\operatorname{tr}(\nabla_s \mathbf{n})^2 - (\operatorname{div}_s \mathbf{n})^2] \end{aligned}$$

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k 's surface elastic moduli

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k 's surface elastic moduli

undistorted state

$$\mathbf{n} \cdot \boldsymbol{\nu} \equiv 0 \quad \Rightarrow \quad (\nabla_s \mathbf{n})^\top \boldsymbol{\nu} + (\nabla_s \boldsymbol{\nu}) \mathbf{n} \equiv \mathbf{0}$$

$\nabla_s \boldsymbol{\nu}$ curvature tensor

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$\nabla_s \boldsymbol{\nu}$ curvature tensor

$$\nabla_s \mathbf{n} = \mathbf{0} \quad \Rightarrow \quad (\nabla_s \boldsymbol{\nu}) \mathbf{n} = \mathbf{0}$$

W_s is **not** minimized by letting $\nabla_s \mathbf{n} = \mathbf{0}$

director representation

$$\mathbf{n} = \cos \alpha \mathbf{u} + \sin \alpha \mathbf{u}_\perp$$

director representation

$$\mathbf{n} = \cos \alpha \mathbf{u} + \sin \alpha \mathbf{u}_\perp$$

$$\mathbf{u}_\perp := \boldsymbol{\nu} \times \mathbf{u} = \mathbf{N}\mathbf{u}$$

N skew-symmetric tensor associated with $\boldsymbol{\nu}$
 $(\mathbf{u}, \mathbf{u}_\perp, \boldsymbol{\nu})$ local co-ordinate basis

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\mathbf{N} skew-symmetric tensor associated with $\boldsymbol{\nu}$

$(\mathbf{u}, \mathbf{u}_\perp, \boldsymbol{\nu})$ local co-ordinate basis

parallel transport

The unit vector \mathbf{n} is parallel transported along a curve \mathcal{C} whenever it is seen as immobile in a frame $(\mathbf{e}_1, \mathbf{e}_2, \boldsymbol{\nu})$ whose spin $\boldsymbol{\Omega}$ is everywhere *tangential*, $\boldsymbol{\Omega} \cdot \boldsymbol{\nu} \equiv 0$.

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$$\alpha' = \mathbf{w} \cdot \mathbf{t}$$

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$$\alpha' = \mathbf{w} \cdot \mathbf{t}$$

\mathbf{t} unit tangent vector to \mathcal{C}

' arc-length derivative

$$\mathbf{w} := (\nabla_s \mathbf{u}_\perp)^\top \mathbf{u} \quad \text{spin connection}$$

parallel connection

The *undistorted* state is obtained by requiring that a given director \mathbf{n} be parallel transported in all directions:

$$(\nabla_{\mathbf{s}} \mathbf{n})_{\mathbf{u}} := -\boldsymbol{\nu} \otimes (\nabla_{\mathbf{s}} \boldsymbol{\nu}) \mathbf{n}$$

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gradient decomposition

$$\nabla_{\mathbf{s}} \mathbf{n} = \mathbf{n}_{\perp} \otimes (\nabla_{\mathbf{s}} \alpha - \mathbf{w}) - \boldsymbol{\nu} \otimes (\nabla_{\mathbf{s}} \boldsymbol{\nu}) \mathbf{n}$$

$$\mathbf{w} := (\nabla_{\mathbf{s}} \mathbf{u}_{\perp})^{\top} \mathbf{u}.$$

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Equivalently, we can write

$$\nabla_{\mathbf{s}} \mathbf{n} = \mathbf{D} \mathbf{n} - \boldsymbol{\nu} \otimes (\nabla_{\mathbf{s}} \boldsymbol{\nu}) \mathbf{n}$$

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covariant gradient

$$\mathbb{D} \mathbf{n} := (\mathbf{I} - \boldsymbol{\nu} \otimes \boldsymbol{\nu}) \nabla_{\mathbf{s}} \mathbf{n} = \mathbf{n}_{\perp} \otimes (\nabla_{\mathbf{s}} \alpha - \mathbf{w})$$

surface irrotationality

$$\operatorname{curl}_s \nabla_s \alpha = \mathbf{N}(\nabla_s \boldsymbol{\nu}) \nabla_s \alpha$$

surface irrotationality

$$\begin{aligned} \operatorname{curl}_s \nabla_s \alpha &= \mathbf{N}(\nabla_s \boldsymbol{\nu}) \nabla_s \alpha \\ \mathbf{a} \cdot \boldsymbol{\nu} \equiv 0 \quad \mathbf{a} = \nabla_s \alpha &\Leftrightarrow \operatorname{curl}_s \mathbf{a} = \mathbf{N}(\nabla_s \boldsymbol{\nu}) \mathbf{a} \end{aligned}$$

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surface distortion

$$\operatorname{curl}_s \mathbf{w} = K \boldsymbol{\nu} + \mathbf{N}(\nabla_s \boldsymbol{\nu}) \mathbf{w}$$

K Gaussian curvature of \mathcal{S}

surface irrotationality

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surface distortion

$$\operatorname{curl}_s \mathbf{w} = K \boldsymbol{\nu} + \mathbf{N}(\nabla_s \boldsymbol{\nu}) \mathbf{w}$$

K Gaussian curvature of \mathcal{S}

energy splitting

$$|\nabla_s \mathbf{n}|^2 = \underbrace{|\nabla_s \alpha - \mathbf{w}|^2}_{\text{distortion energy}} + \underbrace{\mathbf{n} \cdot (\nabla_s \boldsymbol{\nu})^2 \mathbf{n}}_{\text{curvature field}}$$

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$$K \neq 0 \quad \Rightarrow \quad \mathbf{w} \neq \nabla_s \alpha \quad \Rightarrow \quad \text{distortion energy} \neq 0$$

no saddle-splay analogue

$$\nabla_s \mathbf{n} = D\mathbf{n} - \boldsymbol{\nu} \otimes (\nabla_s \boldsymbol{\nu})\mathbf{n} \quad \Rightarrow \quad \text{tr}(\nabla_s \mathbf{n})^2 - (\text{div}_s \mathbf{n})^2 \equiv 0$$

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curvature field

$$\nabla_s \boldsymbol{\nu} = \sigma_1 \mathbf{e}_1 \otimes \mathbf{e}_1 + \sigma_2 \mathbf{e}_2 \otimes \mathbf{e}_2$$

$\mathbf{e}_1, \mathbf{e}_2$ principal directions of curvature

σ_1, σ_2 principal curvatures

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$\mathbf{e}_1, \mathbf{e}_2$ principal directions of curvature

σ_1, σ_2 principal curvatures

$$\mathbf{n} = \cos \vartheta \mathbf{e}_1 + \sin \vartheta \mathbf{e}_2$$

$$W_s = \frac{1}{2}k_1(\mathbf{n}_\perp \cdot \nabla_s \vartheta)^2 + \frac{1}{2}k_2(\sigma_2 - \sigma_1)^2(\mathbf{n} \cdot \mathbf{e}_1)^2(\mathbf{n} \cdot \mathbf{e}_2)^2 \\ + \frac{1}{2}k_3\{[\sigma_1(\mathbf{n} \cdot \mathbf{e}_1)^2 + \sigma_2(\mathbf{n} \cdot \mathbf{e}_2)^2] + (\mathbf{n} \cdot \nabla_s \vartheta)^2\}$$

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Ericksen inequalities

$$k_1 \geq 0 \quad \& \quad k_3 \geq 0$$

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Ericksen inequalities

$$k_1 \geq 0 \quad \& \quad k_3 \geq 0$$

curvature field equilibria

$$\underbrace{\sin 2\vartheta = 0}_{\text{curvature lines}} \quad \& \quad \underbrace{\cos 2\vartheta = \frac{k_3}{k_2 - k_3} \frac{\sigma_1 + \sigma_2}{\sigma_1 - \sigma_2}}_{\text{spiralling lines}} \in [-1, 1]$$

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Discussion

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