New Scaling Properties of Liquid Crystal Flow

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Overview I

Liquid crystals are soft matter systems consisting of rigid, rod-like molecules that tend to align themselves along preferred directions. A main issue in their application is the ability to control macroscopic size regions of uniform molecular alignment. In display devices, control is achieved by means of electromagnetic fields.

Control in material processes is achieved by flow. The Ericksen-Leslie equations are central to the study of nematic liquid crystal flow. The analytic difficulties related with singularities and constraints in the model prompted research on relaxed and approximate forms, pioneered by Liu and Lin (1995). Since then, relaxed models of variable length director have received a lot of attention.

Overview II

We examine some of the physical inconsistencies of the variable director models and use additional information to resolve them. Molecular theory and rheological data applied to the Leslie coefficients provide the missing ingredients. Here, we point out the crucial research role of the polymeric industry. This brings out the multiscale nature of the system which allows us to establish a key maximum principle. Another requirement is ensuring a consistency between the free energy and the rate of energy dissipation near the isotropic state. This also turns out to be a key ingredient in predicting formation of defects in flow.
This information is used to 'reorganize terms' in the rate of energy dissipation function. From that point on, all results found in the literature hold, with some modifications.

Outline

1. The Leslie-Ericksen equations
2. Models of *variable length director*
3. Ericksen's model of liquid crystals with variable degree of orientation
4. Proposal of a variable director model
5. Well-posedness
6. Conclusions

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Distortion energy of nematic

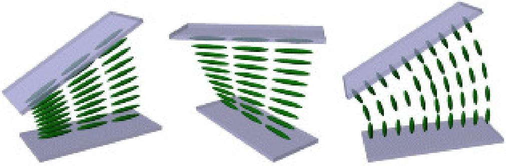


Figure: spaly, twist and bend distortions

The energy density $\mathcal{W}_{\text{OF}}$ corresponds to the Oseen and Zocher (1920's) established by Frank (1958),

$$\begin{aligned}\mathcal{W}_{\text{OF}} =& \frac{1}{2}K_1(\nabla\cdot\boldsymbol{n})^2 + \frac{1}{2}K_2(\boldsymbol{n}\cdot\nabla\times\boldsymbol{n})^2 + \frac{1}{2}K_3|\boldsymbol{n}\times\nabla\times\boldsymbol{n}|^2 \\ &+\frac{1}{2}(K_2+K_4)[(\boldsymbol{n}\cdot\nabla)\boldsymbol{n} - (\nabla\cdot\boldsymbol{n})\boldsymbol{n})], \quad |\boldsymbol{n}| = 1.\end{aligned}$$

Invariant under rotations with $\boldsymbol{n}$-axis; invariant under inversion $\boldsymbol{n}\to-\boldsymbol{n}$.

The Leslie-Ericksen Equations for $\{\boldsymbol{v}, \boldsymbol{n}, p\}$

Balance of Linear Momentum:

$$\rho \dot{\boldsymbol{v}} - \nabla \cdot (-pI + T_{\text{v}} + T_{\text{e}}) = \rho \boldsymbol{f}$$

Balance of Angular Momentum:

$$-\chi \ddot{\boldsymbol{n}} + \mathbf{g}_{\text{e}} + \mathbf{g}_{\text{v}} + \lambda \boldsymbol{n} = \rho \boldsymbol{g}$$

Constraints: $\boldsymbol{n} \cdot \boldsymbol{n} = 1, \quad \nabla \cdot \boldsymbol{v} = 0$

- $T_{\text{e}} = -(\nabla \boldsymbol{n})^T \frac{\partial \mathcal{W}_{\text{OF}}}{\partial \nabla \boldsymbol{n}}$, elastic stress tensor;
- T_{v}, viscous stress tensor
- $\mathbf{g}_{\text{e}} = -\nabla \cdot (\frac{\partial \mathcal{W}_{\text{OF}}}{\partial \nabla \boldsymbol{n}}) + \frac{\partial \mathcal{W}_{\text{OF}}}{\partial \boldsymbol{n}}$, elastic molecular force
- $\mathbf{g}_{\text{v}}$, viscous molecular force
- λ, Lagrange multiplier
- $\dot{\boldsymbol{n}} = \frac{\partial \boldsymbol{n}}{\partial t} + \boldsymbol{v} \cdot \nabla \boldsymbol{n}$, material time derivative.

Neglect rotational inertia, $\chi = 0$.

Viscous stress and molecular force

Invariant time rate quantities:

$$D(\boldsymbol{v}) = \frac{1}{2}(\nabla \boldsymbol{v} + \nabla \boldsymbol{v}^T), \quad W(\boldsymbol{v}) = \frac{1}{2}(\nabla \boldsymbol{v} - \nabla \boldsymbol{v}^T)$$

$$\mathbf{N} = \dot{\boldsymbol{n}} - W(\boldsymbol{v})\boldsymbol{n} : \text{ Lie derivative}$$

Experiments of Miesowicz (1936) and Zwetkoff (1939) suggested that T_{v} and $\mathbf{g}_{\text{v}}$ have linear dependence on $D(\boldsymbol{v})$ and $\mathbf{N}$:

$$T_{ij} = \mathcal{A}_{ij} + \mathcal{B}_{ijk}(\boldsymbol{n})N_k + \mathcal{C}_{ijkp}D_{kp}(\boldsymbol{v})$$

Smith and Rivlin (1957) proved that these can be expressed explicitly. Accounting for nematic symmetries, Leslie (1966) found

$$\begin{aligned} T_{\text{v}} = \quad & \alpha_1(\boldsymbol{n}\cdot D(\boldsymbol{v})\boldsymbol{n})\boldsymbol{n}\otimes\boldsymbol{n} + \alpha_2\mathbf{N}\otimes\boldsymbol{n} + \alpha_3\boldsymbol{n}\otimes\mathbf{N} \\ & \alpha_4 D(\boldsymbol{v}) + \alpha_5 D(\boldsymbol{v})\boldsymbol{n}\otimes\boldsymbol{n} + \alpha_6\boldsymbol{n}\otimes D(\boldsymbol{v})\boldsymbol{n} \\ \mathbf{g}_{\text{v}} = \quad & \gamma_2 D(\boldsymbol{v})\boldsymbol{n} + \gamma_1\mathbf{N}. \end{aligned}$$

α_i are viscosity coefficients measured in experiments.

$\gamma_1 = \alpha_3 - \alpha_2, \quad \gamma_2 = \alpha_6 - \alpha_5.$

Energy law and rate of dissipation

Suppose that $\{\boldsymbol{n}, \boldsymbol{v}, p\}$ are smooth solutions of the governing equations. Then, they satisfy energy law

$$\frac{d}{dt}\int_V \left(\frac{1}{2}\rho|\boldsymbol{v}|^2 + \frac{1}{2}\chi|\dot{\boldsymbol{n}}|^2 + \mathcal{W}_{\text{OF}}\right) + \int_V \mathcal{R}_{\text{EL}} = \int_V \boldsymbol{f}\cdot\boldsymbol{v} + \boldsymbol{g}\cdot\dot{\boldsymbol{n}} + \int_{\partial V} (\boldsymbol{t}\cdot\boldsymbol{v} + \mathbf{l}\cdot\dot{\boldsymbol{n}})$$

for every subdomain $V \subseteq \Omega$ with the smooth boundary ∂V.

Rate of energy dissipation:

$$\begin{aligned} 2\mathcal{R}_{\text{EL}} &= (T_{\text{v}}, \nabla\boldsymbol{v}) + (\mathbf{g}_{\text{v}}, \dot{\boldsymbol{n}}) \\ &= \alpha_1(\boldsymbol{n}^T D(\boldsymbol{v})\boldsymbol{n})^2 + \gamma_1|\mathbf{N}|^2 + (\alpha_5+\alpha_6)|D(\boldsymbol{v})\boldsymbol{n}|^2 \\ &+ (\alpha_3+\alpha_2+\gamma_2)\mathbf{N}^T D(\boldsymbol{v})\boldsymbol{n} + \alpha_4|D(\boldsymbol{v})|^2 \end{aligned}$$

Assume that Parodi's relation holds:

$$\alpha_6 - \alpha_5 = \alpha_2 + \alpha_3,$$

Projection operator on planes perpendicular to $\boldsymbol{n}$

Let us consider the projection operator (Ericksen, 1991),

$$P = I - \boldsymbol{n} \otimes \boldsymbol{n}, \quad |\boldsymbol{n}| = 1.$$

Denoting $A = D(\boldsymbol{v})$, which has the property $\operatorname{tr} A = 0$, we let

$$\begin{aligned} B =& A + \frac{1}{2}\boldsymbol{n} \cdot A\boldsymbol{n} I - \boldsymbol{n} \otimes PA\boldsymbol{n} - PA\boldsymbol{n} \otimes \boldsymbol{n} - \frac{3}{2}(\boldsymbol{n} \cdot A\boldsymbol{n})\boldsymbol{n} \otimes \boldsymbol{n}, \\ B =& B^T, \ B\boldsymbol{n} = 0, \ \operatorname{tr} B = 0, \\ & \operatorname{tr} A^2 = \operatorname{tr} B^2 + \frac{3}{2}(\boldsymbol{n} \cdot A\boldsymbol{n})^2 + 2|PA\boldsymbol{n}|^2. \end{aligned}$$

Hence,

$$2\mathcal{R}_{\mathrm{EL}} = \eta_1 \operatorname{tr}(B^2) + \eta_2(\boldsymbol{n} \cdot A\boldsymbol{n})^2 + \eta_3|PA\boldsymbol{n}|^2 + \gamma_1\left|\mathbf{N} + \frac{\gamma_2}{\gamma_1}PA\boldsymbol{n}\right|^2.$$

Miesowitz viscosities:

$$\begin{aligned} \eta_1 =& \alpha_4, \\ \eta_2 =& \alpha_1 + \frac{3}{2}\alpha_4 + \alpha_5 + \alpha_6, \\ \eta_3 =& 2\alpha_4 + \alpha_5 + \alpha_6 - \gamma_2^2\gamma_1{}^{-1}. \end{aligned}$$

Second Law of Thermodynamics and Leslie inequalities

Second Law of Thermodynamics requires

$$\mathcal{R}_{\mathrm{EL}} \geq 0.$$

$\mathcal{R}_{\mathrm{EL}} \geq 0$ (strictly) if and only if the following inequalities hold:

$$\begin{aligned}
&\gamma_1 = \alpha_3 - \alpha_2 \geq 0, \\
&\eta_1 := \alpha_4 \geq 0, \\
&\eta_2 \geq 0 \iff 4\gamma_1(2\alpha_4 + \alpha_5 + \alpha_6) \geq (\alpha_2 + \alpha_3 + \gamma_2)^2, \\
&\eta_3 := 2\alpha_1 + 3\alpha_4 + 2\alpha_5 + 2\alpha_6 \geq 0.
\end{aligned}$$

Parodi's relation yields

$$T_{\mathrm{v}} = \frac{\partial \mathcal{R}_{\mathrm{EL}}}{\partial(\nabla \boldsymbol{v})} \text{ and } \mathbf{g}_{\mathrm{v}} = \frac{\partial \mathcal{R}_{\mathrm{EL}}}{\partial \dot{\boldsymbol{n}}}.$$

Summary of the Ericksen-Leslie equations

$$\rho\dot{\boldsymbol{v}} = -\nabla p - \nabla\cdot\left(\frac{\partial\mathcal{W}_{\mathrm{OF}}}{\partial\nabla\boldsymbol{n}}\right) + \nabla\cdot T_{\mathrm{v}} + \boldsymbol{f}$$

$$\nabla\cdot\boldsymbol{v} = 0$$

$$\begin{aligned}\gamma_1\dot{\boldsymbol{n}} =& \nabla\cdot\left(\frac{\partial\mathcal{W}_{\mathrm{OF}}}{\partial\nabla\boldsymbol{n}}\right) - \frac{\partial\mathcal{W}_{\mathrm{OF}}}{\partial\boldsymbol{n}} - \gamma_2 D(\boldsymbol{v})\boldsymbol{n} \\ &+\gamma_1 W(\boldsymbol{v})\boldsymbol{n} - \lambda\boldsymbol{n} + \boldsymbol{g}\end{aligned}$$

$$\boldsymbol{n}\cdot\boldsymbol{n} = 1$$

Well-posedness of Leslie Ericksen system: some references

Relaxation of constraint $|\boldsymbol{n}| = 1$ by adding energy penalty

- Lin and Liu (1995, 1998), Liu and Walkington (2002) studied well-posedness of reduced model and discretizations
- Walkington (2011), full LE-system and discretizations
- Wu, Zhang, Zhang (2013) well posedness of the approx Leslie Ericksen system, plus stability and bifurcation results
- Du, Guo and Chen (2007). Spectral methods for LE-equations
- Emmrich and Lazerzick (2016).

With constraint $|bn| = 1$:

- Lin, Lin and Wang (2010), Lin and Wang (2010), Lin and Wang (2015) study well-posedness of reduced model
- Wang, Zhang and Zhang (2012), well-posedness in $\mathbb{R}^3$ of a family of approximate models.

Order tensor model: DeAnna and Zarnescu.

Variable length director model and energy penalty

In this approach, the unit director $\boldsymbol{n}$ is replaced with a variable length director $\mathbf{d}$,

$$\mathbf{d} = |\mathbf{d}|\boldsymbol{n}, \quad |\mathbf{d}| \neq 1.$$

An additional term in the energy, as in Ginzburg-Landau model, penalizes departure from $|\mathbf{d}| = 1$. New energy density:

$$\mathcal{W} = \mathcal{W}_{\text{OF}}(\mathbf{d}, \nabla\mathbf{d}) + \frac{1}{\epsilon^2}(1 - |\mathbf{d}|^2)^2$$

$\epsilon > 0$ arbitrarily small but fixed.
The rest of the model remains unchanged.

With the new director, the transition to $\mathbf{d} = 0$ at defect locations may occur continuously from $|\mathbf{d}| > 0$, instead of the discontinuous, singular, transition from unit $\boldsymbol{n}$ to $\boldsymbol{n} = 0$.

Questions on the consistency of the new model

- Addition of a new unknown field $|\mathbf{d}|$
- Constitutive equations, $\mathcal{W}$, $\alpha_i, \dots,$ may now depend on $|\mathbf{d}|$.
- Introduction of new scales in the model

The new stress tensor becomes

$$\begin{aligned}\tilde{T}_{\mathrm{v}} = \quad & \alpha_1 |\mathbf{d}|^4 (\boldsymbol{n} \cdot D(\boldsymbol{v})\boldsymbol{n})\boldsymbol{n} \otimes \boldsymbol{n} + \alpha_2 |\mathbf{d}|^2 \mathbf{N} \otimes \boldsymbol{n} + \alpha_3 |\mathbf{d}|^2 \boldsymbol{n} \otimes \mathbf{N} \\ & \alpha_4 D(\boldsymbol{v}) + \alpha_5 |\mathbf{d}|^2 D(\boldsymbol{v})\boldsymbol{n} \otimes \boldsymbol{n} + \alpha_6 |\mathbf{d}|^2 \boldsymbol{n} \otimes D(\boldsymbol{v})\boldsymbol{n}\end{aligned}$$

Note the different scales of the terms α_1 and α_4

Modified Leslie's inequalities

$$\gamma_1 = \alpha_3 - \alpha_2 \geq 0, \quad \alpha_4 \geq 0,$$
$$2\alpha_4 + |\mathbf{d}|^2(\alpha_5 + \alpha_6) \geq 0,$$
$$4\gamma_1(2\alpha_4 + |\mathbf{d}|^2(\alpha_5 + \alpha_6)) \geq |\mathbf{d}|^2(\alpha_2 + \alpha_3 + \gamma_2)^2,$$
$$2\alpha_1|\mathbf{d}|^4 + 3\alpha_4 + 2|\mathbf{d}|^2(\alpha_5 + \alpha_6) \geq 0$$

Whereas these inequalities might be satisfied for special values of $|\mathbf{d}|$, they can break down for other values. Let us focus on last inequality and rewrite it as

$$\alpha_1|\mathbf{d}|^4 + [2\alpha_4 + |\mathbf{d}|^2(\alpha_5 + \alpha_6)] \geq \frac{\alpha_4}{2}$$

Note that it may break down for $\alpha_1 < 0$ (satisfied by standard liquid crystals).

There is no sufficient information in the equations to control $|\mathbf{d}|$.

Restricted inequalites in contradiction with data

Sufficient conditions on α_i giving $\mathcal{R} \geq 0$, in full viscosity models:

$$\gamma_1 = \alpha_3 - \alpha_2 \geq 0, \quad \alpha_4 \geq 0, \ \alpha_1 > 0,$$

$$\alpha_5 + \alpha_6 - \frac{\alpha_6 - \alpha_5}{\alpha_3 - \alpha_2}(\alpha_3 + \alpha_2) > 0,$$

$$4[(\alpha_5 + \alpha_6)(\alpha_3 - \alpha_2) - (\alpha_6 - \alpha_5)(\alpha_3 + \alpha_2)]$$

$$\geq (\alpha_3 + \alpha_2 - (\alpha_6 - \alpha_5))^2.$$

Viscosities	5CB	MBBA	PBG
α_1	-11	-18 ± 6	-3660
α_2	-83	-109 ± 2	-6920
α_3	-2	-1 ± 0.2	18
α_4	75	83 ± 2	348
α_5	102	80 ± 15	6610
α_6	-27	-34 ± 2	-292

Kleman and Lavrentovich, *Soft Matter Physics*, 2003.Units 10^{-2} poise.

Can we control $|\mathbf{d}|$ from the equations?

$$\gamma_1 \dot{\mathbf{d}} = \nabla \cdot \left(\frac{\partial \mathcal{W}_{\mathsf{OF}}}{\partial \nabla \mathbf{d}}\right) + \frac{4}{\epsilon^2}(1 - |\mathbf{d}|^2)\mathbf{d} - \gamma_2 D(\boldsymbol{v})\mathbf{d} + \gamma_1 W(\boldsymbol{v})\mathbf{d}$$

Perform inner product with **d** on both sides of eqn to obtain a nonliner parabolic equation for $|\mathbf{d}|^2$:

$$\frac{\gamma_1}{2}\frac{D|\mathbf{d}|^2}{Dt} = \left[\nabla \cdot \left(\frac{\partial \mathcal{W}_{\mathsf{OF}}}{\partial \nabla \mathbf{d}}\right)\right] \cdot \mathbf{d} + \frac{4}{\epsilon^2}(1 - |\mathbf{d}|^2)|\mathbf{d}|^2 - \gamma_2 D(\boldsymbol{v})\mathbf{d} \cdot \mathbf{d}$$

It does not have a maximum principle

Liquid crystals with variable degree of orientation, Ericksen (1991)

The discovery and synthesis of the Kevlar fiber (Dupont, 1978) prompted research on lyotropic polymeric liquid crystals towards generating bulk samples. Processing flows are able to imprint alignment in fibers and thin material layers used in coating reinforcements. However, three dimensional samples present multi-aligned domains leading to material failure.
Work by Kurt Wissbrun (polymer scientist, Celanese Labs; 1981-article) motivated Ericksen (1991) to construct a model able to account for point as well as line and surface defects. It has three main ingredients: Ericksen-Leslie, Landau-de Gennes and Onsager theories. In a main contribution, Doi linked the continuum E-L model with Onsager's.

Governing equations (Ericksen, 1991) $\{\boldsymbol{v}, \boldsymbol{n}, s, p\}$

$$
\begin{aligned}
\rho\dot{\boldsymbol{v}} &= -\nabla p + \nabla\cdot(T_{\mathrm{e}} + T_{\mathrm{v}}) \\
\beta_2(s)\dot{s} &= \nabla\cdot\left(\frac{\partial\mathcal{W}}{\partial\nabla s}\right) - \frac{\partial\mathcal{W}}{\partial s} - \beta_3(s)\boldsymbol{n}\cdot D(\boldsymbol{v})\boldsymbol{n} \\
\gamma_1(s)\dot{\boldsymbol{n}} &= \nabla\cdot\left(\frac{\partial\mathcal{W}}{\partial\nabla\boldsymbol{n}}\right) - \frac{\partial\mathcal{W}}{\partial\boldsymbol{n}} + \gamma_1(s)W(\boldsymbol{v})\boldsymbol{n} - \gamma_2(s)D(\boldsymbol{v})\boldsymbol{n} + \lambda\boldsymbol{n} \\
&\nabla\cdot\boldsymbol{v} = 0, \quad \boldsymbol{n}\cdot\boldsymbol{n} = 1
\end{aligned}
$$

Elastic and viscous stress tensors:

$$
\begin{aligned}
T_{\mathrm{e}} &= -\nabla\boldsymbol{n}^T\frac{\partial\mathcal{W}}{\partial\nabla\boldsymbol{n}} - \nabla s\otimes\frac{\partial\mathcal{W}}{\partial\nabla s} \\
T_{\mathrm{v}} &= \big(\beta_1\dot{s} + \alpha_1\boldsymbol{n}\cdot D(\boldsymbol{v})\boldsymbol{n}\big)\boldsymbol{n}\otimes\boldsymbol{n} + \alpha_2\mathbf{N}\otimes\boldsymbol{n} \\
&\quad + \alpha_3\boldsymbol{n}\otimes\mathbf{N} + \alpha_4 D(\boldsymbol{v}) + \alpha_5 D(\boldsymbol{v})\boldsymbol{n}\otimes\boldsymbol{n} + \alpha_6\boldsymbol{n}\otimes D(\boldsymbol{v})\boldsymbol{n}.
\end{aligned}
$$

The Leslie coefficients α_i and $\beta_i(s)$ are now functions of s,
$\alpha_i = \alpha_i(s), \quad s\in(-\frac{1}{2}, 1)$.

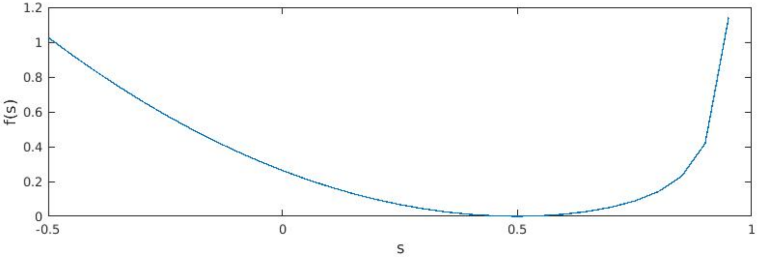
Energy and singular potentials

Simplified energy, with $k_1, k_2 > 0$, related to Frank's constants:

$$\mathcal{W} = k_1|\nabla s|^2 + k_2 s^2 |\nabla \boldsymbol{n}|^2 + f(s)$$

$f(s)$, $s \in (-\frac{1}{2}, 1)$ is a polynomial (Doi, 1983) or a singular, single (or double-well) potential, (Ericksen, 1991)

$$\lim_{s \to \{-\frac{1}{2}, 1\}} f(s) = +\infty.$$



High concentration or low temperature nematic. For the purpose of the s-model to inform the variable director one, we further restrict s to $(0, 1)$.

The viscosity coefficients

For lyotropic liquid crystals, in the 1980's and 90's, a great deal of effort by the rheological community was devoted to determine the functions $\alpha_i(s)$ and $\beta_i(s)$:

- Expressions for $\alpha_i(s)$ near $s = 0$ and concentration studies of double-well potential $f(s)$ (Kuzzuu-Doi, 1983-84). Two approaches: model flow with Smolukowsky equation (1983) or with Ericksen-Leslie (1984).
- Rheological measurements coupled with molecular theory, along the lines of Miesowitz's expermients (Berry, Doi, Marrucci, Larson,. . . 1980-90's). In particular, these provide information on the behavior near $s = 0$, defect locations.
- Ericksen (1991) further explored the compatibility of the above results with the dissipation function emerging from the Landau-deGennes theory.

On the approximation of viscosity coefficients α_i

Developed by Kuzzu-Doi (1983) and based on Onsager's theory of lyotripic liquid crystals, combined with expression of Leslie's viscous stress tensor. Two main assumptions:

- Aligning regime flow
- The order tensor Q takes equilibrium values only.

The α_i coefficients are found to depend on isotropic viscosity η_0, dimensionless concentration C and order parameters

$$S_2 =< P_2(\mathbf{u} \cdot \mathbf{n}) >\equiv s, \quad S_4 =< P_4(\mathbf{u} \cdot \mathbf{n}) >$$

P_2, P_4 are Legendre polynomials of 2nd and 4th degree. $< \cdots >$ denotes the average with respect to the distribution function $f_0(\mathbf{u})$. The function $f_0(\mathbf{u})$ is the minimizer of Onsager's microscopic free energy $\mathcal{A}$.

Approximated Onsager free energy minimization

Approximation schemes to minimize $\mathcal{A}$ developed by Kuzzuu-Doi (1984), Marrucci (1981) and Berry (1988) consisted in expressing

$$\alpha_i(s) = k(p)A_i(s), \quad 1 \leq i \leq 6,\ i \neq 4,$$
$$k(p) = \eta_0(1 - p^2)^2$$

The minimization provides expressions for the dimensionless rational functions $A_i(s)$. p aspect ratio of rod-like molecules. The quantity η_0 depends on concentration, isotropic viscosity and the molecular weight as well the length of the rod.

For a survey of experimental and theoretical work on viscosity coefficients: R. Larson, *The Structure and Rheology of Complex Fluids*, 1999.

The previous methods commonly yield

$$|\frac{\gamma_1}{\gamma_2}(s)| \leq 1, \quad s \in (-\frac{1}{2}, 1),$$

$$\lim_{s \to 0} \frac{\gamma_1}{\gamma_2}(s) = 0, \quad \gamma_1(s) = O(s^2), \quad \gamma_2(s) = O(s)$$

$$\lim_{s \to 1^-} \frac{\gamma_1}{\gamma_2}(s) = -1, \qquad \lim_{s \to -\frac{1}{2}^+} \frac{\gamma_1}{\gamma_2}(s) = 1.$$

These relations proved relevant to study of defects in flow (MCC-Mukherjee; 1996, 1997).

To obtain information on the coefficients β_i, we require consitency between between the *dissipation function*, $\mathcal{R}$, expressed as a quadratic on $\{\dot{s}$, $\mathbf{N}$ and $D(\boldsymbol{v})\}$ and the analogous function written in terms of $D(\boldsymbol{v})$ and the co-rotational time derivative of Q, $\hat{Q} = \dot{Q} - W(\boldsymbol{v})Q + QW(\boldsymbol{v})$. This yields

$$\beta(s) \equiv -\beta_1(s) = -\beta_3(s) > 0, \quad \beta_2(s) = O(1).$$

Marrucci's viscosities

For $k(p) = \eta_0(1-p^2)^2$.
p is the aspect ratio of a rod-like molecule.

$$\alpha_1 = -s^2 k(p), \quad \alpha_2 = -\frac{s(1+2s)}{(2+s)} k(p), \quad \alpha_3 = -\frac{s(1-s)}{(2+s)} k(p),$$

$$\alpha_4 = \frac{(1-s)}{3} k(p), \quad \alpha_5 = s k(p), \quad \alpha_6 = 0.$$

In view of moelcular theory and rheological data, we assume that

$$\begin{aligned}
\alpha_1(s) =& \alpha_1^0 s^2, \\
\alpha_i(s) =& \alpha_i^0 s, \quad i = 2, 3, 5, 6, \\
\alpha_4(s) =& \alpha_4, \\
\gamma_1(s) =& \gamma_1^0 s^2, \quad \gamma_2(s) = \gamma_2^0 s, \\
\beta_1(s) =& \beta_3(s) = \mathrm{const}, \quad \beta_2 = \mathrm{const}.
\end{aligned}$$

From these properties, it follows that s satisfies a nonlinear parabolic equation: it has maximum and comparison principles.

The maximum principle: s bounded away from 1

Suppose that the liquid crystal occupies a 3-dimensional, bounded domain $\Omega \subset \mathbb{R}^3$, with a smooth boundary $\partial\Omega$. Let $s(x,t)$, $\boldsymbol{n}(x,t)$, $v(x,t)$, $p(x,t)$ be a smooth solution of the governing equations corresponding to initial and boundary data $0 < s(x,0) \leq 1-\epsilon$ and $0 < s(x,t) < 1-\epsilon$, $x \in \partial\Omega$. Then $s(x,t) \leq 1-\epsilon$, for all $x \in \Omega$ and $T > t > 0$.

$$s_t + (\boldsymbol{v}\cdot\nabla)s = \Delta s - f'(s) - s|\nabla \mathbf{n}|^2 - \mathbf{n}\cdot D(\boldsymbol{v})\mathbf{n}.$$

We argue by contradiction and suppose that $s(x,t)$ reaches its maximum at a point and time $(x^*, t^*) \in \Omega \times [0,T]$ and such that $s(x^*, t^*)$ is arbitrarily close to $s = 1$:

$$s_t = 0,\ \nabla s = 0,\ \triangle s \leq 0,\ \mathrm{at},\ (x^*, t^*).$$

Since the left-hand side is identically 0 and the right-hand side is strictly negative, we conclude that, either

- Max $s(x,t)$ is bounded away from 1, or
- Max $s(x,t)$ occurs at $t = 0$ or $x \in \partial\Omega$.

The result holds for the full equation since $\boldsymbol{n}\cdot D(\boldsymbol{v})\boldsymbol{n}$ remains bounded as $s \to 1$.

Invariant set $s \geq 0$: a formal result

Let $\epsilon > 0$ be small. Suppose that

$$\lim_{s \to \epsilon^+} f(s) = +\infty, \quad \lim_{s \to \epsilon^+} f'(s) = -\infty.$$

Let $\{s(\mathbf{x}, t), \boldsymbol{n}(\mathbf{x}, t), \boldsymbol{v}(\mathbf{x}, t), p(\mathbf{x}, t)\}$, $\mathbf{x} \in \Omega$, $T > t > 0$ be a smooth solution of the governing equations corresponding to initial and boundary data

$$0 < \epsilon \leq s(\mathbf{x}, 0) < 1, \; 0 < \epsilon \leq s(\mathbf{x}, t) < 1, \; \mathbf{x} \in \partial\Omega, \; t \in (0, T).$$

Then, $s(\mathbf{x}, t) > \epsilon > 0$, for all $\mathbf{x} \in \Omega$ and $T > t > 0$. Indeed, for $0 < s < s^*$,

$$s_t + (\boldsymbol{v} \cdot \nabla)s = \Delta s + |f'(s)| - s|\nabla \mathbf{n}|^2 - s^2 \mathbf{n} \cdot D(\boldsymbol{v})\mathbf{n}.$$

Note that smooth solutions cannot have an interior minimum such that $s > 0$, small. For the purpose of well-posedness of Ericksen's model assumptions on $f(s)$ can be relaxed to a single-well potential at s^*.

Some conclusions

Let us set $\mathbf{d} = \sqrt{s}\boldsymbol{n}$, $s \in (0,1)$ and rewrite Ericksen's equations in terms of $\mathbf{d}$ and s. The new equations do not correspond to a variable director model. Otherwise, the following E-model equation

$$\frac{\gamma_1^0}{2}\frac{d}{dt}|\mathbf{d}|^2 = 2k\Big(\mathbf{d}\cdot\triangle\mathbf{d} + \frac{2}{z}(\nabla\mathbf{d})\nabla z\cdot\mathbf{d}\Big) - \frac{\gamma_2^0}{z^2}\mathbf{d}\cdot D(\boldsymbol{v})\mathbf{d} + \hat{\lambda}|\mathbf{d}|^2$$

would be compatible with the s-eqn

$$\beta_2(s)\dot{s} = \nabla\cdot\Big(\frac{\partial\mathcal{W}}{\partial\nabla s}\Big) - \frac{\partial\mathcal{W}}{\partial s} - f'(s) - \beta_3(s)\boldsymbol{n}\cdot D(\boldsymbol{v})\boldsymbol{n}.$$

However there is no Lagrange multiplier $\hat{\lambda}$ such that both equations are identical (otherwise β_1 and β_3 would take nonphysical values). Ericksen's model serves as guidance in formulating a variable director model. We want to preserve the maximum principle, Leslie's inequalities and the viscous stress tensor.

Proposal of a variable director model

Step 1. Postulate a free energy of the form

$$W = W_0(\mathbf{d}, \nabla \mathbf{d}) + f(|\mathbf{d}|^2), \quad f'(z^*) = 0,\ z^* \in (0,1).$$

where f is a single-well potential, singular at $s = 1$, with $f'(0) < 0$ and W_0 satisfies a Hadamard condition (e.g, it can be obtained as a quadratic form of $M = \mathbf{d} \otimes \mathbf{d}$). Can we take $W_0 = \mathcal{W}_{OF}(\frac{\mathbf{d}}{|\mathbf{d}|})$?

Step 2. Postulate the viscous stress tensor

$$\begin{aligned} T_{\text{v}} =& \alpha_1^0(\mathbf{d} \cdot D(\boldsymbol{v})\mathbf{d})\mathbf{d} \otimes \mathbf{d} + \alpha_2^0 \mathring{\mathbf{d}} \otimes \mathbf{d} + \alpha_3^0 \mathbf{d} \otimes \mathring{\mathbf{d}} + \alpha_4 D(\boldsymbol{v}) \\ &+ \alpha_5^0 D(\boldsymbol{v})\mathbf{d} \otimes \mathbf{d} + \alpha_6^0 \mathbf{d} \otimes D(\boldsymbol{v})\mathbf{d}. \end{aligned}$$

It follows from stress tensor for Ericksen's model $\frac{\gamma_2^0}{2} = \beta_3 = \beta_1$.

Step 3. Keeping up with the scaling leading to T_{v}, take

$$\mathbf{g}_{\text{v}} = \gamma_1^0 \mathring{\mathbf{d}} + \gamma_2^0 D(\boldsymbol{v})\mathbf{d}.$$

Rate of dissipation function and maximum principle

$$2\mathcal{R}_d = T_e \cdot \nabla \boldsymbol{v} + \mathbf{g}_v \cdot \mathring{\mathbf{d}} = \alpha_1^0(\mathbf{d} \cdot D(\boldsymbol{v})\mathbf{d})^2 + 2\gamma_2^0 \mathring{\mathbf{d}} \cdot D(\boldsymbol{v})\mathbf{d}$$
$$+\gamma_1^0|\mathring{\mathbf{d}}|^2 + (\alpha_5^0 + \alpha_6^0)|D(\boldsymbol{v})\mathbf{d}|^2 + \alpha_4|D(\boldsymbol{v})|^2.$$

Evolution equation for $\mathbf{d}$:

$$\gamma_1^0 \mathring{\mathbf{d}} = \nabla \cdot \frac{\partial W_0}{\partial \nabla \mathbf{d}} - \frac{\partial W_0}{\partial \mathbf{d}} - \gamma_2^0 D(\boldsymbol{v})\mathbf{d} - 2f'(|\mathbf{d}|^2)\mathbf{d}.$$

For the one-constant energy, we get

$$\gamma_1^0 \mathring{\mathbf{d}} = 2k\triangle \mathbf{d} - \gamma_2^0 D(\boldsymbol{v})\mathbf{d} - 2f'(|\mathbf{d}|^2)\mathbf{d}.$$

Taking the inner product of the previous equation by $\mathbf{d}$, we get

$$\frac{\gamma_1^0}{2}\frac{d}{dt}(|\mathbf{d}|^2) = 2k(\triangle(|\mathbf{d}|^2) - |\nabla \mathbf{d}|^2)) - \gamma_2^0 D(\boldsymbol{v})\mathbf{d} \cdot \mathbf{d} - 2f'(|\mathbf{d}|^2).$$

Smooth solutions have maximum principle properties which yield bounds on $|\mathbf{d}|$.

Sufficient conditions for $\mathcal{R} \geq 0$

Suppose that $\alpha_1^0 < 0$ *and* $|\mathbf{d}| \neq 0$. *Then the dissipation function satisfies* $\mathcal{R}_d > 0$ *provided* $\alpha_4 > 0$ *and*

$$\alpha_1^0 + \frac{3\bar{\alpha}_4}{2} + \alpha_5^0 + \alpha_6^0 > 0 \quad \textit{and} \quad 2\bar{\alpha}_4 + \alpha_5^0 + \alpha_6^0 - \frac{(\gamma_2^0)^2}{\gamma_1^0} > 0.$$

A simple calculation shows that

$$\begin{aligned} 2\mathcal{R}_d =& \epsilon |D(\boldsymbol{v})|^2 + \bar{\alpha}_4 \operatorname{tr} B^2 + \frac{\eta_3^0}{|\mathbf{d}|^2} |\mathbf{d} \times D(\boldsymbol{v})\mathbf{d}|^2 + \frac{\eta_2^0}{|\mathbf{d}|^2} |D(\boldsymbol{v})\mathbf{d} \cdot \mathbf{d}|^2 \\ &+ \gamma_1^0 |\mathbf{d}|^2 |\mathring{\mathbf{d}} + \frac{\gamma_2^0}{\gamma_1^0 |\mathbf{d}|^2} \mathbf{d} \times D(\boldsymbol{v})\mathbf{d}|^2, \\ \eta_2^0 =& \alpha_1^0 |\mathbf{d}|^2 + \frac{3\bar{\alpha}_4}{2|\mathbf{d}|^2} + \alpha_5^0 + \alpha_6^0, \quad \eta_3^0 = \frac{2\bar{\alpha}_4}{|\mathbf{d}|^2} + \alpha_5^0 + \alpha_6^0 - \frac{(\gamma_2^0)^2}{\gamma_1^0}. \end{aligned}$$

Expressed in terms of $\boldsymbol{n}$, we observe that there are no singularities in the coefficients.

Governing equations

$$\rho \dot{\boldsymbol{v}} = \nabla \cdot \left(\frac{\partial W_0(\mathbf{d}, \nabla \mathbf{d})}{\partial(\nabla \mathbf{d})} \nabla \mathbf{d}^T\right) + \nabla \cdot T_{\mathrm{v}} - \nabla p,$$

$$\nabla \cdot \boldsymbol{v} = 0$$

$$\gamma_1^0 \dot{\mathbf{d}} = \nabla \cdot \frac{\partial W_0}{\partial \nabla \mathbf{d}} - \frac{\gamma_2^0}{|\mathbf{d}|^2} D(\boldsymbol{v})\mathbf{d} + \gamma_1^0 W(\boldsymbol{v})\mathbf{d} - f'(|\mathbf{d}|^2)|\mathbf{d}|^{-2}\mathbf{d}.$$

$$T_{\mathrm{v}} = \alpha_1^0(\mathbf{d} \cdot D(\boldsymbol{v})\mathbf{d})\mathbf{d} \otimes \mathbf{d} + \alpha_2^0 \mathring{\mathbf{d}} \otimes \mathbf{d} + \alpha_3^0 \mathbf{d} \otimes \mathring{\mathbf{d}} + \alpha_4 D(\boldsymbol{v}) + \alpha_5^0 D(\boldsymbol{v})\mathbf{d} \otimes \mathbf{d} + \alpha_6^0 \mathbf{d} \otimes D(\boldsymbol{v})\mathbf{d}.$$

Taking $f(s)$ as a 'narrow' well with minimum at $0 < s* < 1$, the model corresponds to relaxing the constraint $|\mathbf{d}| = \sqrt{s^*}$.

Well posedness of the model

Let $(\boldsymbol{v}, \mathbf{d})$ be a weak solution of the system. Then the following additional regularity properties hold:

$$\mathbf{d} \in W^{1,4/3}(0,T;L^2) \subset \mathcal{AC}([0,T];L^2) \subset \mathcal{C}_w([0,T;H_0^1])$$

$$\boldsymbol{v} \in W^{1,4/3}(0,T;L^2_\sigma) \subset \mathcal{AC}([0,T];L^2_\sigma) \subset \mathcal{C}_w([0,T];H^1_{0,\sigma}).$$

Theorem

Assume that the free energy of the system is as in Step 1. Assume that the viscosity coefficients satisfy inequalities. Suppose that $\mathbf{d}$ *and* $\boldsymbol{v}$ *satisfy prescribed Dirichlet boundary conditions, with* $\boldsymbol{v} = 0$ *on* $\partial\Omega$*. For dimension* $n \leq 3$ *and* $\Omega \subset R^3$*, open, bounded and convex, initial data* $\boldsymbol{v}_0 \in V^{0,2}(\Omega))$ *and* $0 < T < \infty$, $\mathbf{d}_0 \in H^1$, $|\mathbf{d}_0| \leq 1$ *the system has a global weak solution* $(\boldsymbol{v}, \mathbf{d}, p)$ *with the properties*

$$\boldsymbol{v} \in L^2(0,T;V^{1,2}(\Omega)) \cap L^\infty(0,T;V^{0,2}(\Omega)),$$

$$\mathbf{d} - \mathbf{d}_0 \in L^\infty[0,T;L^2(\Omega)] \cap H^1[0,t;L^{\frac{4}{3}}(\Omega)].$$

Proofs analogous to (Emmrich, Lasarovich 2016). All analyses with the assumption $\alpha_1 \geq 0$ hold with the relevant modifications.

Conclusions

- Variable director models are very *coarse* and do not represent the multiscale physics of liquid crystal flow. They are not appropriate to describe defects.
- Their simplifying value diminishes as more information on constitutive functions around $s = 0$ is brought in.
- It provides the necessary ingredients to prove well-posedness of Ericksen's system (ongoing work, in 3d).
- Ericksen's model reduces to Leslie-Ericksen when setting $s > 0$ constant and taking variations with respect to product $\sqrt{s}\mathbf{d}$.
- The results extend to the case $W_0 = \mathcal{W}_{OF}(\frac{\mathbf{d}}{|\mathbf{d}|})$. However, the analysis turns out to be cumbersome and Ericksen's model is a better choice.
- This work allows us to establish well-posedness of the liquid crystal model coupled with electrokinetics and when very small particles are present.

Poisson-Nernst-Planck- Leslie Ericksen equations

$$\frac{\partial c_k}{\partial t} + \nabla \cdot (\boldsymbol{v} c_k) = \nabla \cdot \left(\frac{c_k}{k_B T}\mathcal{D}\nabla \mu_k\right)$$

$$-\varepsilon_0 \nabla \cdot (\epsilon \nabla \Phi) = \sum_{k=1}^{N} q z_k c_k$$

$$\rho \dot{\boldsymbol{v}} - \nabla \cdot (-pI + \mu D(\boldsymbol{v}) + T_{\text{v}} + T_{\text{e}}) - \sum_{k=1}^{N} c_k z_k \nabla \Phi = \rho \boldsymbol{f}$$

$$\mathbf{g}_{\text{v}} - \nabla \cdot \left(\frac{\partial \mathcal{W}}{\partial \nabla \boldsymbol{n}}\right) + \frac{\partial \mathcal{W}}{\partial \boldsymbol{n}} + \epsilon_a (\boldsymbol{n} \cdot \nabla \Phi) \nabla \Phi + \lambda \boldsymbol{n} = \rho \boldsymbol{g}$$

Chemical Potential:

$$\mu_k := \frac{\partial \mathcal{W}}{\partial c_k} = \frac{\partial \mathcal{W}_{\text{ion}}}{\partial c_k} + q z_k \Phi = k_B T(\ln c_k + 1) + q z_k \Phi, \quad k = 1, \ldots N$$

Fields of the problem

- liquid crystal velocity field $\boldsymbol{v}$
- nematic director $\boldsymbol{n}$
- Leslie coefficients α_i and their combinations γ_i, $\hat{\gamma}_i$
- Oseen-Frank energy $\mathcal{W}_{OF}$
- Frank coefficients K_i
- Molecular forces $\mathbf{g}_{\mathrm{e}}$, $\mathbf{g}_{\mathrm{v}}$
- Stress tensor T_{e}, T_{v}

- Electrostatic potential Φ, $\Phi_i := \Phi - \Phi_e$
- Ion concentration variables c_k. Take $\{c_1, c_2\}$
- Balance z_k. Take $z_1 = 1 = -z_2$
- Chemical Potential μ_k
- Ionic energy density $\mathcal{W}_{\mathrm{ion}}$
- Electrostatic energy $\mathcal{W}_{\mathrm{C}}$. Coulombic (ions) + Dielectric (lc's)

$$\mathbf{u}_k - \boldsymbol{v} = \frac{1}{_B T}\mathcal{D}\big(\nabla(\frac{\partial \mathcal{W}_{\text{ion}}}{\partial c_k}) - z_k c_k \nabla\Phi\big), \quad k = 1, \ldots N$$

Dissipation Function:

$$\begin{aligned} \mathcal{R} = & \quad \mathcal{R}_{LC} + \sum_{k=1}^{N} \big(\frac{1}{2} K_B T c_k \mathcal{D}^{-1}(\mathbf{u}_k - \boldsymbol{v}) \cdot (\mathbf{u}_k - \boldsymbol{v}) \\ + & \quad \frac{c_k}{K_B T}\mathcal{D}\nabla\mu_k \cdot \nabla\mu_k\big) \geq c_v\big(\boldsymbol{n}^T D(\boldsymbol{v})\boldsymbol{n})^2 + |\mathbf{N}|^2 \\ + & \quad |D(\boldsymbol{v})\boldsymbol{n}|^2 + c_k(|\mathbf{u}_k - \boldsymbol{v}|^2 + |\nabla\mu_k|^2)\big) \end{aligned}$$

Total Energy Density

:

$$\mathcal{W} = \mathcal{W}_{\mathrm{OF}}(\boldsymbol{n}, \nabla \boldsymbol{n}) + k_B T \sum_{k=1}^{N} c_k \log c_k - \frac{1}{2}(\epsilon \nabla \Phi \cdot \nabla \Phi) + \sum_{k=1}^{N} z_k c_k \Phi$$

Diffusivity Tensor:

$$\mathcal{D} = D_{\perp} I + D_a \boldsymbol{n} \otimes \boldsymbol{n}$$

Dielectric Tensor:

$$\varepsilon = \varepsilon_{\perp} I + \varepsilon_a \boldsymbol{n} \otimes \boldsymbol{n}$$

Energy Relation:

$$\frac{d}{dt} \int_{\Omega} \{ \frac{1}{2} \rho |\boldsymbol{v}|^2 + \mathcal{W} \} + \int_{\Omega} \{ \mu |D(\boldsymbol{v})|^2 + (T_{\mathrm{v}}, \nabla \boldsymbol{v}) + (\mathbf{g}_{\mathrm{v}}, \dot{\boldsymbol{n}}) + \sum_{k=1}^{N} \frac{D_k c_k}{k_B T} (\mathcal{D}_k \nabla \mu_k \cdot \nabla \mu_k) \} = \int_{\Omega} (\rho \boldsymbol{f}, \boldsymbol{v}) + (\rho \boldsymbol{g}, \dot{\boldsymbol{n}})$$