On the role of the α_1 -viscosity in the Ericksen-Leslie equations with Ginzburg-Landau penalisation and molecular stretching

Francesco De Anna Joint work with H. Wu

University of Würzburg

Analysis of Nematic Liquid Crystals Flows Nonlinear Partial Differential Equations in Fluid Dynamics

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Outline

- The Ericksen-Leslie equations:
 - a quick overview of the model,
 - the Leslie coefficients and the values of α₁,
 - ► Ginzburg-Landau penalisation.
- Established results and contribution:
 - definition of weak solutions,
 - uniqueness,
 - non-triviality of the problem.
- Some details on the result:
 - ► the double-logarithmic inequality,
 - ► frequencies decomposition,
 - ► conclusion.

The Ericksen-Leslie model



The fluid behaviour





The center of mass of each constituent molecule has a freely degree of translation, as a common particle in a liquid.

Widespread formalisms:

- Ericksen-Leslie: Oseen-Frank directors
- Beris-Edwards: De Gennes order tensors

¹⁰. J. DeCamp, G. S. Redner, A. Baskaran, M. F. Hagan, and Z. Dogic, Nat Mater

Molecular alignment



• Privileged direction modeled through a director field

$$n: (0,T) \times \Omega \to \mathbb{S}^2 \subseteq \mathbb{R}^3$$
 (i.e. $|n(t,x)| = 1$).

• **Ericksen-Leslie**: constitutive equations for the director n(t, x) and the velocity field u(t, x).

The Oseen-Frank energy density

The mathematical theory of liquid crystals goes back to the seminal works by Frank (1958) and Oseen (1933). **Distortion free energy density:**

$$w_F(n, \nabla n) := \frac{K_1}{2} |\operatorname{div} n|^2 + \frac{K_2}{2} |n \cdot \operatorname{curl} n|^2 + \frac{K_3}{2} |n \wedge \operatorname{curl} n|^2 + \frac{K_2 + K_4}{2} (\operatorname{tr}(\nabla n)^2 - |\operatorname{div} n|^2)$$



When the resulting equilibrium equations are complicated: one-constant approximation

$$w_F(n, \nabla n) = w_F(\nabla n) = \frac{K}{2} |\nabla n|^2.$$

The Ericksen-Leslie model

The most frequently used form of the equations consist of the **constrain** |n| = 1 together with

Conservation of mass:	$\operatorname{div} u = 0$
Balance of linear momentum:	$\partial_t u + u \cdot \nabla u = \operatorname{div} \mathbb{T}$
Balance of angular momentum:	$n \wedge (g + h) = 0$

- p pressure in \mathbb{R}
- *u* velocity field in \mathbb{R}^d
- n director field

- g kinematic transport
- h molecular field
- T total stress tensor

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$$\sigma^{\mathrm{L}} = \alpha_1(n \cdot \mathbb{D}n)n \otimes n + \alpha_2 \mathscr{N} \otimes n + \alpha_3 n \otimes \mathscr{N} + \alpha_4 \mathbb{D} + \alpha_5 \mathbb{D}n \otimes n + \alpha_6 n \otimes \mathbb{D}n$$

- p pressure in ℝ
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• High powers interacting with the flow.

- p pressure in ℝ
- u velocity field in R^d
- n director field

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• Maximal derivatives.

- p pressure in ℝ
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Balance of angular momentum:	$n \wedge (\mathbf{g} + \mathbf{h}) = 0$

$$g = \lambda_1 \mathscr{N} + \lambda_2 \mathbb{D}n$$

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The most frequently used form of the equations consist of the **constrain** |n| = 1 together with

$$\begin{cases} \operatorname{div} u = 0, \\ \partial_t u + \operatorname{div}(u \otimes u) - \nu \Delta u + \nabla p = -\operatorname{div}(\nabla n \odot \nabla n) + \alpha_1 \operatorname{div}(n \otimes n(n \otimes n : \nabla u)), \\ \partial_t n + u \cdot \nabla n - n \cdot \nabla u = \Delta n + |\nabla n|^2 n. \end{cases}$$

- p pressure in ℝ
- u velocity field in R^d
- n director field

- g kinematic transport
- h molecular field
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Measuring the Leslie coefficients

• Laminar flow under a strong orienting Field [Miesowicz, 1946], the molecules are firmly aligned in one direction by a constant magnetic field.



• When the shear stress $(\sigma_L)_{\alpha\beta}$ is known, one can derive the effective viscosity η

$$\eta = \frac{(\sigma_L)_{\alpha\beta}}{2\mathbb{D}_{\alpha\beta}}$$

Kneppe & Schneider; Stephen & Straley; Stewart;

Quantities	MBBA near 25°	PAA near 122°	5CB near 26°
α_1	-0.0181	0.0043	-0.0060
α_2	-0.1104	-0.0069	-0.0812
α_3	-0.001104	-0.0002	-0.0036
α_4	0.0826	0.0068	0.0652
α_5	0.0779	0.0047	0.0640
α_6	-0.0336	-0.0023	-0.0208

Viscous dissipation and Parodi relation

• The total energy is dissipative along time evolution. Basic energy law

$$\frac{d}{dt} \int_{\Omega} \left(\frac{1}{2} |u|^2 + w_F(n, \nabla n) \right) dx = -\int_{\Omega} \left(\alpha_1 |n \cdot \mathbb{D}n|^2 + (\alpha_2 + \alpha_3 + \lambda_2) \mathcal{N} \cdot \mathbb{D}n + \alpha_4 |\mathbb{D}|^2 + (\alpha_5 + \alpha_6) |\mathbb{D}n|^2 - \lambda_1 |\mathcal{N}|^2 \right) dx$$

• We require

$$\begin{aligned} \alpha_3 - \alpha_2 &\geq 0, \quad \alpha_4 \geq 0, \quad 2\alpha_4 + \alpha_5 + \alpha_6 \geq 0, \\ \alpha_1 + 3\alpha_4 + 2\alpha_5 + 2\alpha_6 \geq 0, \quad -4\lambda_1(2\alpha_4 + \alpha_5 + \alpha_6) \geq (\alpha_2 + \alpha_3 - \lambda_2)^2. \end{aligned}$$

Onsager relations between flows and forces in irreversible thermodynamic systems. Parodi
suggested that the Leslie coefficients shall be further restricted:

$$\lambda_1 = \alpha_2 - \alpha_3, \qquad \lambda_2 = \alpha_5 - \alpha_6, \qquad \alpha_6 - \alpha_5 = \alpha_2 + \alpha_3.$$

Quantities	MBBA near 25°	PAA near 122°	5CB near 26°
$\alpha_2 + \alpha_3$	-0.111504	-0.0071	-0.0848
$\alpha_6 - \alpha_5$	-0.1115	-0.007	-0.0848

Unitary constraint vs Ginzburg-Landau relaxation

• Balance of angular momentum:

$$\partial_t n + u \cdot \nabla n - n \cdot \nabla u - \Delta n = |\nabla n|^2 n.$$

• Relaxing the unitary constraint |n(t, x)| = 1 through

$$\int_{\Omega} \frac{|\nabla n(t,x)|^2}{2} dx \quad \to \quad \int_{\Omega} \frac{|\nabla n(t,x)|^2}{2} dx + \int_{\Omega} \frac{(|n(t,x)|^2 - 1)^2}{4\varepsilon} dx$$

Natural physical interpretations, attributed to the extensibility of liquid crystal molecules.

• Balance of angular momentum:

$$\partial_t n + u \cdot \nabla n - n \cdot \nabla u - \Delta n = -\frac{|n|^2 - 1}{\varepsilon}n.$$

• In general, loss of an uniform bound for |n(t, x)|. Related difficulties on the momentum equation:

$$\ldots \operatorname{div}\left(n\otimes n(n\otimes n:\nabla u)\right)\ldots$$

Questions on the analysis of EL

- Is the Ericksen-Leslie model solvable in two and three dimensions?
- Which type of solutions can we build?
- Under which restrictions on the Leslie viscous coefficients?
- What can we say about uniqueness?

Overview of related literature and contribution



Overview of the literature

- C. Liu & F.-H. Lin (2000): First analysis result on a three dimensional smooth bounded domain subject to Dirichlet boundary conditions. Any initial data with finite total energy generates a global-in-time weak solution. Restriction on the Leslie coefficients, corotational framework (λ₂ = 0) and weak maximum principle.
- D. Coutand & S. Shkoller ('01): First attempt for the general case λ₂ ≠ 0. Local existence and uniqueness of a local-in-time classical solution. Total energy of the system is not dissipative, small-data global existence result even in two dimensions.
- *H. Sun & C. Liu ('09)*: Setting of Leslie coefficients, energy dissipation property is guaranteed (in particular $\alpha_1 = 0$). Existence of global strong solutions provided that the dimension is two or the viscosity $\alpha_4 > 0$ is sufficiently large.
- H. Wu & X. Xu & C. Liu ('13): three dimensional periodic setting, global strong solutions and long-time behavior, under large viscosity α₄; With Parodi's relation, global well-posedness and Lyapunov stability for the system near local energy minimizers.

Overview of the literature

 C. Cavaterra & E. Rocca & H. Wu ('13): Three dimensional bounded domain, natural boundary conditions and suitable requirements on the Leslie coefficients that ensure the energy dissipation. Existence of global-in-time weak solutions, new formulation of weak solutions that took into account the low regularity of those highly nonlinear stress. Double-level Faedo-Galerkin approximation scheme. Uniqueness was still an open problem.

 $\lambda_1 = \alpha_2 - \alpha_3 < 0, \quad \alpha_1 \ge 0, \quad \alpha_4 > 0, \quad \alpha_5 + \alpha_6 \ge 0, \quad \lambda_2 = \alpha_5 - \alpha_6.$

$$\begin{cases} \text{with Parodi:} & \frac{\lambda_2^2}{-\lambda_1} \leq \alpha_5 + \alpha_6, \\ \text{without Parodi:} & |\lambda_2 - \alpha_2 - \alpha_3| < 2\sqrt{-\lambda_1}\sqrt{\alpha_5 + \alpha_6} \end{cases} \end{cases}$$

Life can always be more complicated...

- Unitary constraint: M.-C. Hong ('10), M.-C. Hong & J.-K. Li & Z.-P. Xin ('14), T. Huang & F.-H. Lin & C. Liu & C.-Y. Wang ('16), F.-H. Lin & C.-Y. Wang ('16)...
- Thermal effects: E. Feireisl & M. Frémond & E. Rocca & G. Schimperna ('12), M. Hieber & M. Nesensohn & J. Prüss, K. Schade ('14), M. Hieber & J. Prüss ('16),....
- Inertia: F.D.A & A. Zarnescu ('16), C. Yuan & W. Wei ('20),...
- ...

Weak solutions

A pair (u, n) is called a weak solution to the Ericksen-Leslie system if it is a distributional solution and for any $\zeta, \zeta' \in (0, 1)$:

$$u \in L^{\infty}(0, T; L^{2}(\mathbb{T}^{2})) \cap L^{2}(0, T; \dot{H}^{1}(\mathbb{T}^{2}))$$
$$n \in L^{\infty}(0, T; H^{1}(\mathbb{T}^{2})) \cap L^{2}(0, T; \dot{H}^{2}(\mathbb{T}^{2}))$$
$$n \cdot \mathbb{D}n \in L^{2}((0, T) \times \mathbb{T}^{2}),$$

with
$$\partial_t u \in L^2(0,T; W^{-1,\frac{2}{1+\zeta}}(\mathbb{T}^2)),$$

$$\begin{array}{ll} \text{with} & \partial_t n \in L^2(0,T; L^{\frac{1}{1+\zeta'}}(\mathbb{T}^2)), \\ \text{and} & \mathbb{D}n \in L^2((0,T) \times \mathbb{T}^2). \end{array}$$

With Parodi

$$\mathcal{E}(t) + \int_0^t \int_{\mathbb{T}^2} \alpha_1 |\mathbf{n} \cdot \mathbb{D}\mathbf{n}|^2 + \frac{\alpha_4}{2} |\nabla u|^2 - \frac{1}{\lambda_1} \left| \Delta n - \frac{n^2 - 1}{\varepsilon} n \right|^2 + \left(\alpha_5 + \alpha_6 + \frac{\lambda_2^2}{\lambda_1} \right) |\mathbb{D}n|^2 \le \mathcal{E}(0),$$

Without Parodi

$$\mathcal{E}(t) + \int_0^t \int_{\mathbb{T}^2} \alpha_1 |\mathbf{n} \cdot \mathbb{D}\mathbf{n}|^2 + \frac{\alpha_4}{2} |\nabla u|^2 - \frac{1}{\lambda_1} \Big| \Delta \mathbf{n} - \frac{n^2 - 1}{\varepsilon} \mathbf{n} \Big|^2 + \eta \Big(|\mathbb{D}\mathbf{n}|^2 + |\mathcal{N}|^2 \Big) \le \mathcal{E}(0).$$

Theorem (C. Cavaterra, E. Rocca, H. Wu (2013))

There exists a global-in-time weak solution, satisfying the energy inequality.

Contribution

F. D.A. & H. Wu (2021)

Consider Ericksen Leslie in $(0, T) \times \mathbb{T}^2$. Let (u_1, n_1) and (u_2, n_2) be two global weak solutions, subject to the same initial data $(u_0, n_0) \in L^2(\mathbb{T}^2) \times H^1(\mathbb{T}^2)$. Then we have $(u_1(t), n_1(t)) = (u_2(t), n_2(t))$ for all $t \in (0, T)$ (Uniqueness).

• For the proof, ansatz on the Leslie coefficients:

$$\alpha_1 = 1, \quad \alpha_2 = -1, \quad \alpha_3 = 0, \quad \alpha_4 = 2\nu > 0, \quad \alpha_5 = 3, \quad \alpha_6 = 1,$$

in particular we do not require the Parodi's relation. In general $\alpha_1 \ge 0$.

- To clarify:
 - what we mean with weak solutions,
 - why the problem is not trivial even in two dimension,
 - philosophy behind the proof.

Weak solutions á la Leray

The Ericksen-Leslie model inherits the major challenges of the Navier-Stokes equations:

 $\partial_t u + \operatorname{div}(u \otimes u) - \nu \Delta u + \nabla p = 0, \quad \operatorname{div} u = 0, \quad (t, x) \in (0, T) \times \mathbb{T}^d.$

Leray (1934)

For any initial data $u_0 \in L^2(\mathbb{T}^d)$ with div $u_0 = 0$, there exists a Leray solution on $(0, T) \times \mathbb{T}^d$.

A Leray solution u is a distributional solution, such that

- $u \in L^{\infty}(0,T;L^2(\mathbb{T}^d)),$
- $u \in L^2(0,T;\dot{H}^1(\mathbb{T}^d)),$
- $\lim_{t\to 0} ||u(t) u_0||_{L^2} = 0,$
- Energy inequality: $||u(t)||_{L^2}^2 + 2\int_0^t ||\nabla u(s)||_{L^2}^2 ds \le ||u_0||_{L^2}^2$.

In two dimensions d = 2 one has the energy equality and the uniqueness of these solutions. Why does this result not work for us?

Non triviality of the problem

Navier-Stokes:

- In dimension two the problem is critical. Scaling invariance.
- Energy equality and continuity $u \in C([0,T], L^2(\mathbb{T}^2))$.
- $\partial_t u$ belongs to $L^2(0,T;\dot{H}^{-1}(\mathbb{T}^2))$ since $u \in L^4((0,T) \times \mathbb{T}^2)$ and

$$\partial_t u - \nu \Delta u + \nabla p = -\operatorname{div}\left(\underbrace{u \otimes u}_{\in L^2((0,T) \times \mathbb{T}^2)}\right)$$

Ericksen-Leslie:

• The velocity could lose energy at high modes: $u \notin C([0, T], L^2(\mathbb{T}^2))$:

$$\partial_t u - \nu \Delta u + \nabla p = -\operatorname{div}\left(\underbrace{n \otimes n(n \otimes n : \nabla u)}_{\notin L^2((0,T) \times \mathbb{T}^2)}\right) + \dots$$

• The stretching prevents the director to be bounded $n \notin L^{\infty}((0,T) \times \mathbb{T}^2)$.















Uniqueness for EL - Conclusion

• Controlling the difference $(\delta u, \delta n) = (u_1, n_1) - (u_2, n_2)$ at lower regularities than the energy space:

$$\delta \mathcal{E}(t) = \|\delta u(t)\|_{\dot{H}^{-\frac{1}{2}}}^2 + \|\delta n(t)\|_{\dot{H}^{\frac{1}{2}}}^2.$$

• Approach on frequencies decomposition (paradifferential calculus and Bony's decomposition); double logarithmic inequality

$$\delta \mathcal{E}(t) + \int_0^t \delta \mathfrak{D}(s) ds \leq \int_0^t f(s) \delta \mathcal{E}(s) \Big(-\ln\big(\delta \mathcal{E}(s)\big) \Big) \ln\big(-\ln\big(\delta \mathcal{E}(s)\big) \Big) ds.$$

• Osgood lemma $\delta \mathcal{E} \equiv 0 \Rightarrow$ Uniqueness

Some details on the double logarithmic inequality



A first identity

The contribution of the Leslie tensor $\sigma_L : \nabla u$ is not integrable on $(0, T) \times \mathbb{T}^2$. We need to pass to lower regularities for a first identity:

$$\frac{1}{2} \|\delta u(t)\|_{H^{-\frac{1}{2}}}^{2} + \frac{1}{2} \|\nabla \delta n(t)\|_{H^{-\frac{1}{2}}}^{2} + \int_{0}^{t} \left(\frac{\alpha_{4}}{2} \|\nabla \delta u(s)\|_{H^{-\frac{1}{2}}}^{2} + \frac{\lambda_{2}}{-\lambda_{1}} \|\nabla \delta n(s)\|_{H^{\frac{1}{2}}}^{2}\right) ds$$
$$= -\alpha_{1} \int_{0}^{t} \left\langle (d_{1} \otimes d_{1})(d_{1} \otimes d_{1} : \nabla \delta u), \nabla \delta u \right\rangle_{H^{-\frac{1}{2}}} ds + \dots$$

- Identity holds, since each inner product is well-defined and time integrable.
- Aim: localise any dissipative term and estimate the remaining ones through a modulus of continuity.
- A standard commutator would provide a dissipative contribution; Further analysis is however inconclusive.
- Alternative approach: better for of the dissipation through Fourier analysis and Littlewood-Paley decomposition.

Dyadic decomposition





Dyadic decomposition





Dyadic decomposition





A toolbox of Fourier Analysis

• The
$$H^{-1/2}$$
-inner product $\approx \sum_q 2^{-q} \langle \dot{\Delta}_q f, \dot{\Delta}_q g \rangle_{L^2}$.

- Low-frequencies cut-off: $S_{q-1}f := \sum_{j < q-1} \dot{\Delta}_q f$.
- Bony's paraproduct decomposition:

$$\begin{split} \dot{\Delta}_{q}(fg) &= \sum_{|j-q| \leq 5} \left[\dot{\Delta}_{q}, \dot{\mathbf{S}}_{j-1}f, \right] \dot{\Delta}_{j}g \qquad \overrightarrow{\mathbf{\Box}} \rightarrow \quad \text{commutator inequality} \\ &+ \sum_{|j-q| \leq 5} \left(\dot{\mathbf{S}}_{q-1} - \dot{\mathbf{S}}_{1-1} \right) f \dot{\Delta}_{q} \dot{\Delta}_{j}g \quad \overrightarrow{\mathbf{\Box}} \rightarrow \quad \text{Bernstein inequality} \\ &+ \frac{\mathbf{S}_{q-1}f \dot{\Delta}_{q}g}{+ \sum_{j \geq q+5} \dot{\Delta}_{q} \left(\dot{\Delta}_{j}f, \, \mathbf{S}_{q+2}g \right)} \quad \overrightarrow{\mathbf{\Box}} \rightarrow \quad \text{Young inequality} \end{split}$$

• The third element generates nonlinear challenging terms to control. The structure of the Ericksen-Leslie system cancels them or make them dissipative terms.

A Brezis-Gallouet inequality

• Similar approach as for proving the Brezis-Gallouet inequality:

$$||f||_{L^{\infty}} \leq C ||u||_{H^1} \left\{ 1 + \sqrt{\ln\left(1 + \frac{||u||_{H^2}}{||u||_{H^1}}\right)} \right\}.$$

• We separately control low and high frequencies of the Leslie viscous stress:

$$\alpha_1 \underbrace{\langle (d_2 \cdot (\nabla u_2 d_2)) \delta d \otimes S_N d_1, \nabla \delta u \rangle_{H^{-\frac{1}{2}}}}_{=:\mathcal{I}} + \alpha_1 \underbrace{\langle (d_2 \cdot (\nabla u_2 d_2)) \delta d \otimes (\mathrm{Id} - S_N) d_1, \nabla \delta u \rangle_{H^{-\frac{1}{2}}}}_{=:\mathcal{II}}$$

• The first term increases proportionally to the radius *N*, where the **low frequencies** are localised:

$$\mathcal{I} \leq C \Big(\text{term that is integrable in time} \Big) \|S_N d_1\|_{L^{\infty}}^2 \|\delta d\|_{H^{\frac{1}{2}}}^2 + \text{terms that can be absorbed} \\ \leq C \Big(\text{term that is integrable in time} \Big) \|d_1\|_{H^{\frac{1}{2}}}^2 \|\delta d\|_{H^{\frac{1}{2}}}^2 N + \text{terms that can be absorbed.}$$

• The high frequencies fix the value of $N \approx -\ln \delta \mathcal{E}(t)$ and therefore the logarithmic inequality:

$$\mathcal{II} \leq C \Big(ext{term that is integrable in time} \Big) 2^{-N}$$

The double-logarithmic inequality

• We use the following Sobolev interpolation inequality for a general $\varepsilon \in (0, 1/2]$,

$$\|f\|_{L^{\frac{2}{\varepsilon}}} \leq \frac{C}{\sqrt{\varepsilon}} \|f\|_{L^{2}}^{\varepsilon} \|f\|_{L^{2}}^{\varepsilon}.$$

• Key tool: explicit constant of embedding in terms of ε . We aim at choosing an appropriate value of ε , in order to get a modulus of continuity.

$$\left| \alpha_1 \langle (d_1 \cdot (\nabla \delta u d_2)) d_1 \otimes d_1, \nabla \delta u \rangle_{H^{-\frac{1}{2}}} \right| \leq \\ (\dots) \left(\frac{N}{\varepsilon} \right)^{\frac{1}{1-\varepsilon}} \delta \mathcal{E}(t) + (\dots) 2^{-N} + \text{terms that can be absorbed}$$

• By choosing a fix value ε , such as $\varepsilon = 1/2$, we lose the modulus of continuity:

$$\left(\frac{N}{\varepsilon}\right)^{\frac{1}{1-\varepsilon}} \delta \mathcal{E}(t) \le CN^2 \delta \mathcal{E}(t) \le C\delta \mathcal{E}(t) \ln\left(-\delta \mathcal{E}(t)\right)^2 \qquad \mathbb{X}$$

• Solution: choose $\varepsilon \approx (1 + \ln N)^{-1}$ and $N \approx -\ln \delta \mathcal{E}(t)$:

$$\left(\frac{N}{\varepsilon}\right)^{\frac{1}{1-\varepsilon}} \delta \mathcal{E}(t) \le C \frac{N}{\varepsilon} \delta \mathcal{E}(t) \le C \delta \mathcal{E}(t) \ln\left(-\delta \mathcal{E}(t)\right) \ln\left(\ln\left(-\delta \mathcal{E}(t)\right)\right) \qquad \Box$$

The uniqueness follows by using Osgood theorem.

Conclusion

- Ericksen-Leslie equations.
- The leslie viscous coefficients, in particular the value of α_1 .
- The Ginzbourg-Landau penalisation.
- Model based on assumption $\alpha_1 \ge 0$ (with further conditions to ensure viscous dissipation) admits a unique weak solution.
- Uniqueness follows from suitable frequencies decompositions, leading to a logarithmic inequality of Osgood type.
- For details see: F. D.A. & H. Wu: Uniqueness of weak solutions for the general Ericksen-Leslie system with Ginzburg-Landau penalization in T², arXiv:2107.02101

Thanks for your attention!

