The Beris-Edwards system for nematic liquid crystal flows

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The University of Queensland

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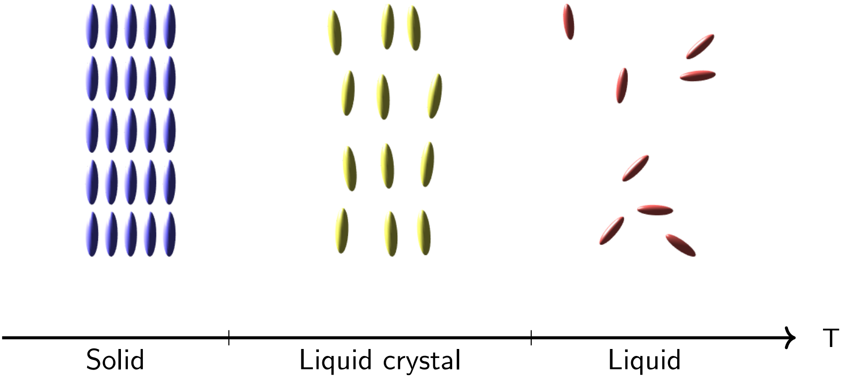

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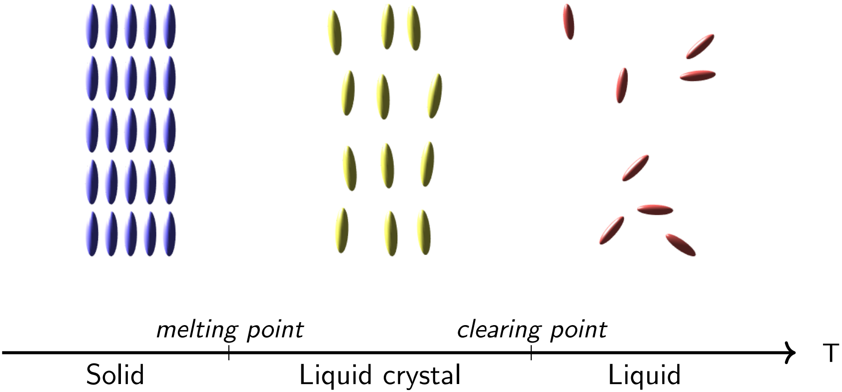

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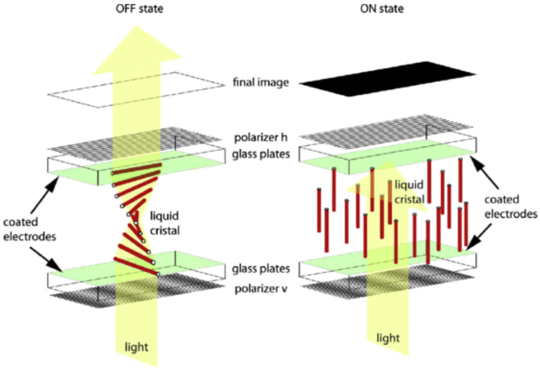

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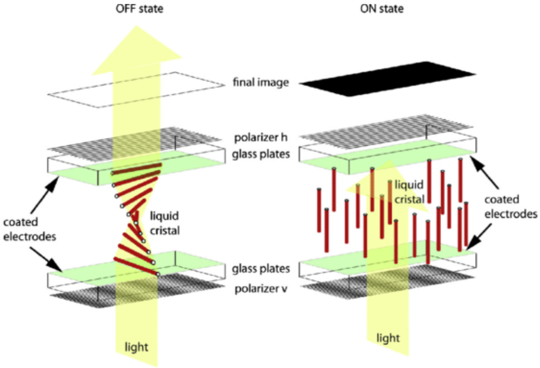

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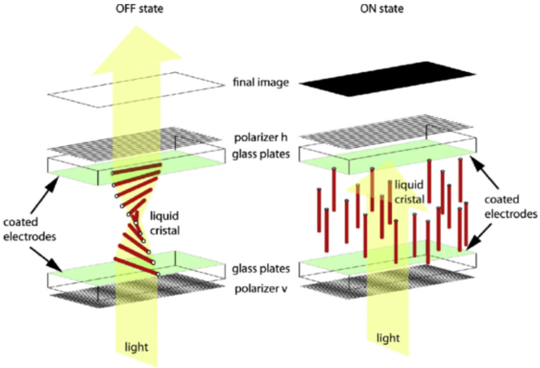

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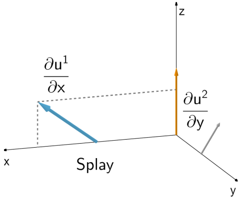

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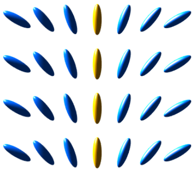

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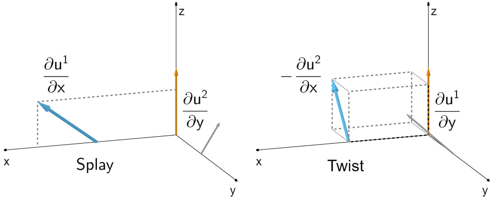

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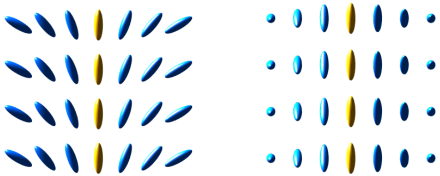

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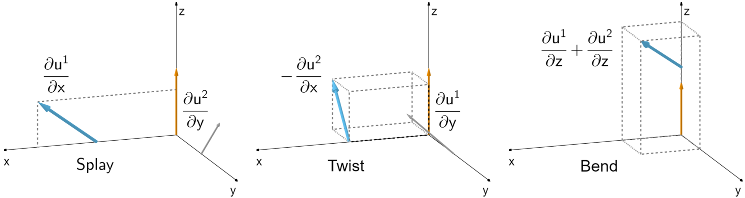

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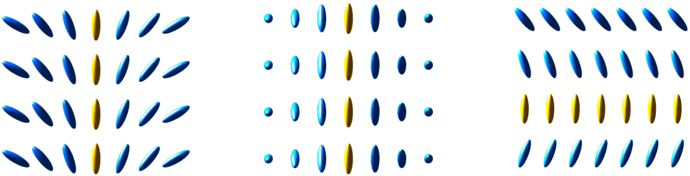

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- The energy is frame-indifference and rotational invariant.
- For $u = (0, 0, 1)$ at the origin, we have a vector notation on the molecular orientations, for instance,

$$\text{the splay type:} \quad \frac{\partial u^1}{\partial x} + \frac{\partial u^2}{\partial y} = \operatorname{div} u.$$

The Oseen–Frank energy

- For $u \in H^1(\Omega; S^2), \Omega \in \mathbb{R}^3$, the associated energy is

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- The coordinate free form of the energy density is

$$\begin{aligned} W(u, \nabla u) = k_1(\operatorname{div} u)^2 + k_2(u \cdot \operatorname{curl} u)^2 \\ + k_3|u \times \operatorname{curl} u|^2 + (k_2 + k_4)[\operatorname{tr}(\nabla u)^2 - (\operatorname{div} u)^2] \end{aligned}$$

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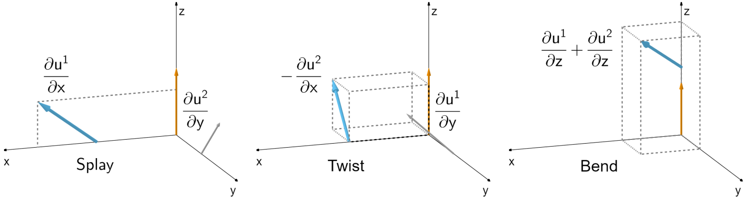
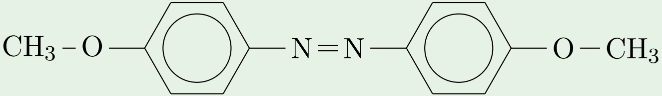
$$+ k_3 \overbrace{|u \times \operatorname{curl} u|^2}^{\textit{Bend}} + (k_2 + k_4) \overbrace{[\operatorname{tr}(\nabla u)^2 - (\operatorname{div} u)^2]}^{\textit{Surface energy}}$$



Lab measurements for the Frank constant

PPA (4,4′-dimethoxyazoxybenzene):



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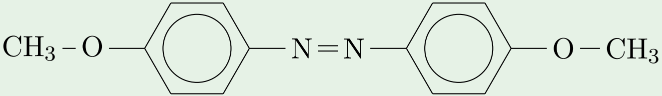

at 125 degrees Celsius has

$$k_1 = 9, \quad k_2 = 5.8 \quad \text{and} \quad k_3 = 19 \text{ (unit: } 10^{-12} \text{ Newtons)}$$

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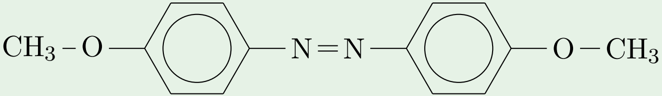

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Hardt–Kinderlehrer–Lin (CMP, '86) proved that a minimizer u of the energy $E(u)$ is smooth away from a closed set $\Sigma \subset \Omega$ which has Hausdorff dimension strictly less than one (the set Σ may not be finite).

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The Ericksen–Leslie system (ELS)

$$\partial_t v^i + v^j \nabla_j v^i + \nabla_i P - \Delta v = \nabla_j {\sigma^E}_{ij}$$
$$\nabla_j v^j = 0$$
$$\partial_t u^i + v^j \nabla_j u^i = (\delta_{ik} - u^i u^k)(\nabla_j W_{p_j^k}(u, \nabla u) - W_{u^k}(u, \nabla u))$$

where $p_j^i := \nabla_j u^i$, σ^E is the Ericksen tensor.

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- Physics background for ELS: conservation laws for linear momentum, mass and angular momentum respectively.

The Dirichlet energy

The one-constant model (OCM): $W(u, \nabla u) \equiv |\nabla u|^2$.

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- Such method was initially appeared in the study the phase transition in superconductivity in the 50's.

- The main idea is to relax the constrain

$$u \in S^2 \quad \Rightarrow \quad u_\varepsilon \in \mathbb{R}^3,$$

at the cost of a penalized energy

$$E(u) = \int_\Omega |\nabla u|^2 \, dx \quad \Rightarrow \quad E(u_\varepsilon) = \int_\Omega |\nabla u_\varepsilon|^2 + \frac{(1 - |u_\varepsilon|^2)^2}{2\varepsilon^2} \, dx.$$

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The Ginzburg–Landau system (OCM case)

$$\partial_t v_\varepsilon^i + v_\varepsilon^j \nabla_j v_\varepsilon^i + \nabla_i P_\varepsilon = \nabla v_\varepsilon^i - \nabla_j (\nabla_i u_\varepsilon^k \nabla_j u_\varepsilon^k)$$
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The Lin–Liu problem

Does $(u_\varepsilon, v_\varepsilon)$ converge to functions that solve ELS as $\varepsilon \to 0$?

Significant research and study have been dedicated to the topic of convergence:

- Lin-Liu (ARMA '00)
- Hong (CVPDE '10)
- Hong-Xin (Adv Math '12)
- Hong-Li-Xin (CPDE '14)
- F.-Hong-Mei (SIAM Math Anal '20)

This problem provides further motivation for the generalisation of the ELS, which is known as the Beris-Edwards system.

Some background for the Beris-Edwards system

The most general elastic theory for nematics, which describes all reorientation types, is

the Landau-de Gennes theory.

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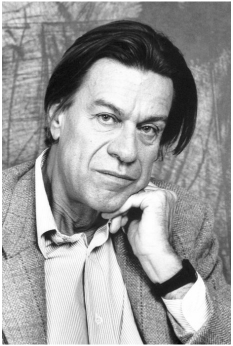

Photo from the Nobel Foundation archive

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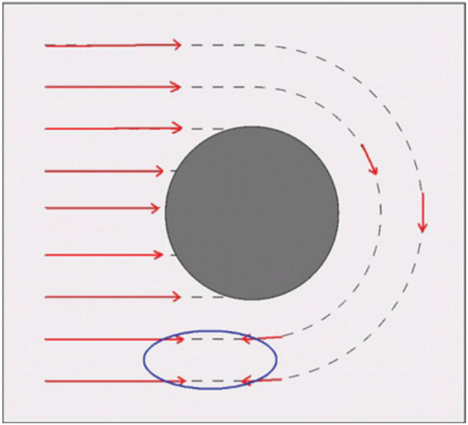
Pierre-Gilles de Gennes was awarded a Nobel prize for physics in 1991 for his work on liquid crystals and polymers.

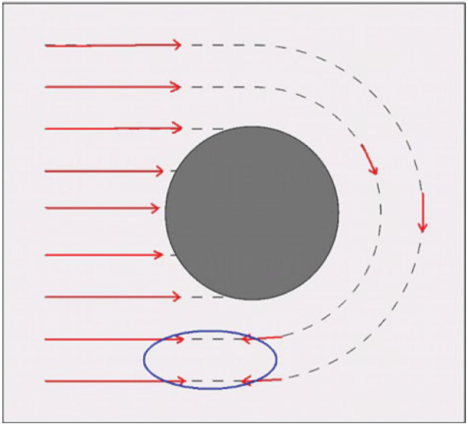
A problem for vector representation in S^2



Non-simply-connected domains (Ball '17)

A problem for vector representation in S^2

The Landau-de Gennes model is a tensor representation.
(isomorphic to the projective plane $\mathbb{R}P2$ up to a scaling)



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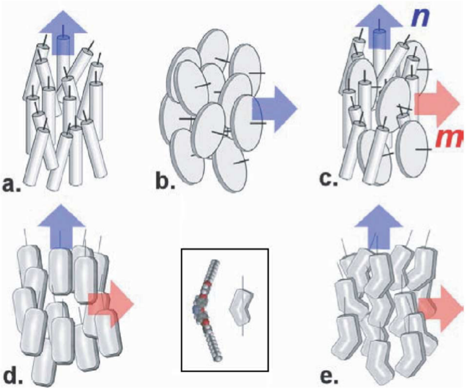

Madsen el al. '04.

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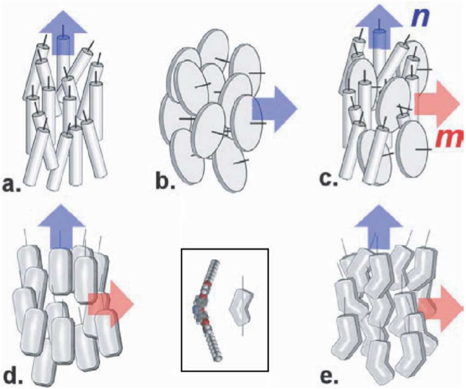
The Landau-de Gennes model works for both uniaxials and biaxials.



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- Landau's expansion for phase transitions

$$f_B(Q) = -\frac{a}{2}\mathrm{tr}(Q^2) - \frac{b}{3}\mathrm{tr}(Q^3) + \frac{c}{4}\left[\mathrm{tr}(Q^2)\right]^2, \quad a,b,c > 0.$$

Extension to the Landau-de Gennes energy density

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An example from Ball-Majumdar '10

$$Q(x) = \eta(|x|)\left(\frac{x}{|x|}\otimes\frac{x}{|x|} - \frac{1}{3}I\right), \eta(1) = 0, x \in B(0,1).$$

$$\eta(r) = \begin{cases} \eta_0(2+\sin(kr)), & 0 < r < \frac{1}{2} \\ 2\eta_0(2+\sin(\frac{k}{2}))(1-r), & \frac{1}{2} \le r < 1. \end{cases}$$

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- Longa et al. '87, Ball-Majumdar '10 and Golovaty et al. '20 pointed out the L_4 term is problematic.

An example from Ball-Majumdar '10

The energy density can be arbitrarily large and negative.

$$Q(x) = \eta(|x|)\left(\frac{x}{|x|}\otimes\frac{x}{|x|} - \frac{1}{3}I\right), \eta(1) = 0, x \in B(0,1).$$

$$\eta(r) = \begin{cases} \eta_0(2+\sin(kr)), & 0 < r < \frac{1}{2} \\ 2\eta_0(2+\sin(\frac{k}{2}))(1-r), & \frac{1}{2} \le r < 1. \end{cases}$$

- Existence of minimizers cannot be guaranteed.

For uniaxial Q-tensors

$$Q \in S_* = \{Q \in S_0 : Q_{ij} = s_+(u_i u_j - \frac{1}{3}\delta_{ij}),\ u \in S^2\},$$

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We suggest a new representation

F.-Hong (CVPDE '22)

$$f_E(Q, \nabla Q) = \left(\frac{L_1}{2} - \frac{s_+ L_4}{3} \right) |\nabla Q|^2 + \frac{L_2}{2} \frac{\partial Q_{ij}}{\partial x_j} \frac{\partial Q_{ik}}{\partial x_k} + \frac{L_3}{2} \frac{\partial Q_{ik}}{\partial x_j} \frac{\partial Q_{ij}}{\partial x_k} + \frac{3L_4}{2s_+} Q_{ln} Q_{kn} \frac{\partial Q_{ij}}{\partial x_l} \frac{\partial Q_{ij}}{\partial x_k}.$$

Existence of minimizers through scaling analysis

In the case $L_2 = L_3 = L_4 = 0$, Majumdar-Zarnescu (ARMA '10) introduced a rescaled energy:

$$\int_\Omega \frac{1}{2}|\nabla Q_L|^2 + \frac{\tilde{f}_B(Q_L)}{L}\, dx,$$

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Let $Q^* \in S_*$ be a global minimizer of the Dirichlet energy. They proved that $Q_L \to Q^*$ in $W^{1,2}$ up to a subsequence as $L \to 0$. Nguyen-Zarnescu (CVPDE '13) proved local smooth convergence of minimizers Q_L away from the singular set of Q_*.

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Relevance in Physics: the constant L is small $\sim 10^{-11} J \backslash M$.

The limit $L \to 0$ is analogous to the Ginzburg–Landau functional.

In the spirit of Majumdar-Zarnescu's work, we suggest a rescaled Landau-de Gennes energy:

$$E_L(Q;\Omega) = \int_\Omega f_E(Q_L, \nabla Q_L) + \frac{\tilde{f}_B(Q_L)}{L}\,\mathrm{d}x.$$

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The case of $L_2 = L_3 = L_4 = 0$:

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The hydrodynamic flow for liquid crystals

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\nabla \cdot v =& 0, \\
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- $H(Q, \nabla Q)$ is the first variation for $Q \in S_*$
- σ is a distortion stress tensor
- $[\cdot, \cdot]$ is the Lie bracket

A scaling analysis

- Recall the rescaled Landau-de Gennes energy

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- Gartland (MMA '18): This scaling analysis is analogous to
- "London limit" in the Ginzburg-Landau theory of superconductivity
- "large-body limit" in the Landau-Lifshitz theory of ferromagnetism

F.-Hong-Mei (arXiv:2112.04074)

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$$f_E(Q,\nabla Q) = \left(\frac{L_1}{2} - \frac{s_+ L_4}{3}\right)|\nabla Q|^2 + \frac{L_2}{2}\frac{\partial Q_{ij}}{\partial x_j}\frac{\partial Q_{ik}}{\partial x_k} + \frac{L_3}{2}\frac{\partial Q_{ik}}{\partial x_j}\frac{\partial Q_{ij}}{\partial x_k} + \frac{3L_4}{2s_+}Q_{ln}Q_{kn}\frac{\partial Q_{ij}}{\partial x_l}\frac{\partial Q_{ij}}{\partial x_k}.$$

- For the initial condition

$$(Q_0, v_0) \in H^2_{Q_e}(\mathbb{R}^3; S_*) \times H^1(\mathbb{R}^3; \mathbb{R}^3), \text{ div } v_0 = 0,$$

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  in the limit of (Q_L, v_L), we prove the existence of a unique strong solution (Q, v) to the Beris-Edwards system for uniaxials up to some maximal time T^*.
- Moreover, for any $T < T^*$, we prove that

$$(\nabla Q_L, v_L) \to (\nabla Q, v) \text{ in } C^\infty(\tau, T; C^\infty_{loc}(\mathbb{R}^3)) \text{ for any } \tau > 0.$$

Ideas from ELS

- Recall the first variation in ELS:

$$\nabla_\alpha W_{p^i_\alpha}(u_\varepsilon, \nabla u_\varepsilon) - W_{u^i}(u_\varepsilon, \nabla u_\varepsilon) + \frac{u^i_\varepsilon(1-|u_\varepsilon|^2)}{\varepsilon^2}.$$

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- Hong-Li-Xin '14: To obtain $\|\nabla^2 u_\varepsilon\|^2_{L^2}$ type estimate (uniform in ε), we multiply the equation by $-\Delta u_\varepsilon$ and have

$$\begin{aligned}
&- \int_{\mathbb{R}^3} \Delta u^i_\varepsilon \frac{u^i_\varepsilon(1-|u_\varepsilon|^2)}{\varepsilon^2}\, dx \\
&\leq \int_{\mathbb{R}^3} C|\nabla u_\varepsilon|^2 \frac{(1-|u_\varepsilon|^2)}{\varepsilon^2} - \frac{1}{4}\frac{|\nabla(|u_\varepsilon|^2)|^2}{\varepsilon^2}\, dx \\
&\leq \int_{\mathbb{R}^3} -\frac{1}{4}\frac{|\nabla(|u_\varepsilon|^2)|^2}{\varepsilon^2} + \eta \frac{|1-|u_\varepsilon|^2|^2}{\varepsilon^4} + C(\eta)|\nabla u_\varepsilon|^4\, dx
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- The first variation in BES:

$$\mathcal{H}(Q_L, \nabla Q_L) + \frac{1}{L} g_B(Q_L), \quad g_B(Q_L) := \frac{\delta f_B(Q_L)}{\delta Q_L}$$

with $f_B(Q_L) = -\frac{a}{2}\operatorname{tr}(Q_L^2) - \frac{b}{3}\operatorname{tr}(Q_L^3) + \frac{c}{4}\left[\operatorname{tr}(Q_L^2)\right]^2.$

Ideas for the proof

- The substitution technique does not apply for

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$$S_\delta := \{ Q \in S_0 : \quad dist(Q; S_*) \le \delta \} .$$

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- A new idea for uniform in L estimates: define a set 'close to' S_*

$$S_\delta := \{Q \in S_0 : \quad dist(Q; S_*) \le \delta\}.$$

- For each smooth $Q \in S_\delta$, the nearest point projection $\pi(Q) \in S_*$ has a constant number of distinct eigenvalues, so there exists a smooth rotation $R_Q := R(\pi(Q)) \in SO(3)$ (Nomizu '73) such that

- $$R_Q^T \pi(Q) R_Q = \begin{pmatrix} \frac{-s_+}{3} & 0 & 0 \\ 0 & \frac{-s_+}{3} & 0 \\ 0 & 0 & \frac{2s_+}{3} \end{pmatrix} =: Q^+.$$

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- Nguyen-Zarnescu '13: $\pi(Q)$ commutes with Q for any $Q \in S_\delta$. Then we find

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- F.-Hong-Mei: The Hessian of the bulk density f_B satisfies

$$\lambda |\xi|^2 \leq \partial^2_{\tilde{Q}_{ij}\tilde{Q}_{kl}} f_B(Q^+) \xi_{ij} \xi_{kl}, \text{ for some } \lambda > 0.$$

- For any $Q_L \in S_\delta$, we derive

$$\left\langle \frac{1}{L}\nabla g_B(\tilde{Q}_L), \nabla \tilde{Q}_L \right\rangle$$
$$\geq \frac{\lambda}{2}\frac{|\nabla(Q_L - \pi(Q_L))|^2}{L} - C|\nabla Q_L|^2 \frac{|Q_L - \pi(Q_L)|^2}{L}.$$

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- Similarly, we prove the high-order estimate of the kind

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- A local L^3 criteria

$$\sup_{t, x_0} \int_{B_{R_0}(x_0)} |\nabla Q|^3 + \left| \frac{Q - \pi(Q)}{L^{\frac{1}{2}}} \right|^3 dx \leq \varepsilon_0^3.$$

- Assume that (Q_{L,T_0}, v_{L,T_0}) satisfies

$$\|Q_{L,T_0}\|^2_{H^2_{Q_e}(\mathbb{R}^3)} + \|v_{L,T_0}\|^2_{H^1(\mathbb{R}^3)} + \frac{\|Q_{L,T_0} - \pi(Q_{L,T_0})\|^2_{H^1(\mathbb{R}^3)}}{L} \leq M.$$

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- The Gagliardo–Nirenberg interpolation:

$$\begin{aligned}&\|Q_L - \pi(Q_L)\|_{L^\infty(\mathbb{R}^3)}\\ \leq& C\|Q_L - \pi(Q_L)\|^{\frac{1}{4}}_{L^2(\mathbb{R}^3)}\|\nabla^2(Q_L - \pi(Q_L))\|^{\frac{3}{4}}_{L^2(\mathbb{R}^3)} \leq \frac{\delta}{2},\end{aligned}$$

and

$$\begin{aligned}&\sup_{t,x_0}\int_{B_{R_0}(x_0)} |\nabla Q_L|^3\,dx \leq C\sup_{t,x_0}\left(\frac{1}{R_0}\int_{B_{R_0}(x_0)} |\nabla Q_L|^2\,dx\right)^{3/2}\\ &+ C\sup_{t,x_0}\left(R_0\int_{B_{R_0}(x_0)} |\nabla^2 Q_L|^2\,dx\right)^{3/2} \leq \frac{\varepsilon_0^3}{2}\end{aligned}$$

for sufficiently small L and some uniform constants T, R_0 in L.

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- Prove the convergence up to a uniform short time T_M and extend the result to maximal time T^*.