Eigenvalue Constraints and Regularity of Q-tensor Navier-Stokes Dynamics

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Motivation: Eigenvalue Constraints on Q

Suppose $f : \mathbb{S}^2 \to [0,1]$ is a probability density with antipodal symmetry: $f(-\omega) = f(\omega)$ for all $\omega \in \mathbb{S}^2$. The associated de Gennes Q-tensor Q is defined by

$$Q := \int_{\mathbb{S}^2} \left(\omega \otimes \omega - \frac{1}{3} I\right) f(\omega)\, d\omega = \sum_{j=1}^{3} \lambda_j e_j \otimes e_j.$$

Multiplying this equality with a *fixed* eigenvector e_i on the left and taking inner products throughout the result with the same e_i yields

$$\lambda_i = \int_{\mathbb{S}^2} (\omega \cdot e_i)^2 f(\omega)\, d\omega - \frac{1}{3}.$$

From this identity, using the fact that f is a probability density function, one may deduce

$$-\frac{1}{3} \leq \lambda_i \leq \frac{2}{3}.$$

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Motivation: Eigenvalue Constraints on Q

Definition. For dimension $d = 2$ or 3, a matrix belonging to the set

$$\mathrm{Sym}_0(d) := \left\{ Q \in \mathbb{R}^{d\times d} \,:\, Q^T = Q \;\text{ and }\; \mathrm{tr}(Q) = 0 \right\}$$

is said to be a **physical Q-tensor** if and only if its eigenvalues $\{\lambda_j(Q)\}_{j=1}^d$ satisfy the strict inequalities

$$-\frac{1}{d} < \lambda_i(Q) < 1 - \frac{1}{d}$$

for $i = 1, ..., d$.

Motivation:
Physical Predictions of the Static Theory

Consider the whole family of minimisation problems parametrised by the elastic constant $L > 0$:

$$\min_{Q\in\mathcal{X}} \int_{\Omega} \left(\frac{L}{2}|\nabla Q|^2 + \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\mathrm{tr}\left(Q^2\right)^2 \right) \, dx,$$

where $\mathcal{X}$ is the class of all $W^{1,2}(\Omega)$ maps whose trace on the boundary is of the shape

$$Q^{(L)}\Big|_{\partial\Omega} = s_+(\vartheta)\left(\overline{n}\otimes\overline{n} - \frac{1}{3}I\right) \quad \text{for some } \; \overline{n}\in C^{\infty}(\partial\Omega, \mathbb{S}^2),$$

and the important material- and temperature-dependent constant $s_+(\vartheta)$ is given by

$$s_+(\vartheta) := \frac{b + \sqrt{b^2 - 24a(\vartheta)c}}{4c},$$

where $a(\vartheta) := \alpha(\vartheta - \vartheta_*)$, and $\alpha, b, c, \vartheta_* > 0$.

Motivation:
Physical Predictions of the Static Theory

One can infer from the work of Majumdar and Zarnescu **[MZ]** that global minimisers $Q^{(L_j)}$ of the Landau-de Gennes theory can be unphysical in the sense that

$$|Q^{(L_j)}(y)| > \sqrt{\frac{2}{3}}$$

for all $y \in K \subset\subset \Omega$ when the values of the elastic constant $L_j > 0$ are sufficiently small.

N.B. Eigenvalues of $Q^{(L_j)}(x)$ physical $\Longrightarrow |Q^{(L_j)}(x)| < \sqrt{2/3}$.

Consider the 'four elastic constant' Landau de Gennes theory

$$E_{\mathrm{LdG}}[Q] := \int_{\Omega} \left(w(\nabla Q, Q) + \frac{a(\vartheta)}{2}\mathrm{tr}\left(Q^2\right) - \frac{b}{3}\mathrm{tr}\left(Q^3\right) + \frac{c}{4}\mathrm{tr}\left(Q^2\right)^2 \right) dx,$$

where

$$w(\nabla Q, Q) := L_1 |\nabla Q|^2 + L_2 Q_{ik,j} Q_{ij,k} + L_3 Q_{ij,j} Q_{ik,k} + L_4 Q_{\ell k} Q_{ij,k} Q_{ik,\ell},$$

and $L_4 \neq 0$.

A construction of Ball and Majumdar [BM] shows that for any smooth boundary conditions $\overline{Q} : \partial\Omega \to \mathrm{Sym}_0(3)$, there exists a sequence of maps $\{Q_j\}_{j=1}^{\infty}$ in the set of admissible maps

$$\mathcal{A}_{\overline{Q}} := \left\{ Q \in W^{1,2}(\Omega) \, : \, Q|_{\partial\Omega} = \overline{Q} \right\}$$

for which

$$E_{\mathrm{LdG}}[Q_j] < -j \quad \text{for each} \quad j = 1, 2, 3, \ldots .$$

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Motivation: Analytical Issues: Statics

To help address these issues, Ball and Majumdar [BM] construct a competitor to the quartic Landau-de Gennes theory:

$$E[Q] := \int_\Omega \left(w(\nabla Q, Q) + \vartheta\, \psi(Q) - \frac{\kappa}{2}|Q|^2 \right)\, dx,$$

where

$$\psi(Q) := \begin{cases} \inf_{\rho \in \mathcal{A}(Q)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega & \text{if } -\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}, \\ \infty & \text{otherwise,} \end{cases}$$

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$$\mathcal{A}(Q) := \left\{ \rho : \mathbb{S}^2 \to [0,1] \,:\, \int_{\mathbb{S}^2} \rho = 1 \;\text{ and }\; \int_{\mathbb{S}^2} \left(\omega \otimes \omega - \frac{1}{3} I \right) \rho(\omega)\, d\omega = Q \right\}.$$

In their theory, global minimisers respect physicality of eigenvalues **and** the theory, when $L_4 \neq 0$, is well posed.

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Motivation: Analytical Issues: Dynamics

Consider the L^2-gradient flow of the 'one elastic constant' Landau de-Gennes energy,

$$\frac{\partial Q}{\partial t} = L\Delta Q - a(\vartheta)Q + b\left(Q^2 - \frac{1}{3}\mathrm{tr}(Q^2)I\right) - c\,\mathrm{tr}(Q^2)Q. \qquad (1)$$

According to Iyer, Xu and Zarnescu **[IXZ-preprint]**, techniques from convex analysis and explicit estimates on the evolution of eigenvalues under the associated ODE flow enable one to show that, if $|a(\vartheta)| < b^2/3c$,

$$-\frac{1}{3}s_+(\vartheta) < \lambda_i(Q(x,t)) < \frac{2}{3}s_+(\vartheta) \qquad \text{for} \quad i = 1, 2, 3,$$

provided that the initial data Q_0 satisfy the same inequality.

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The Ball-Majumdar Singular Potential ψ

Let us look once again at the definition of ψ:

$$\psi(Q) := \begin{cases} \inf_{\rho \in \mathcal{A}(Q)} \int_{\mathbb{S}^2} \rho(\omega) \log \rho(\omega)\, d\omega & \text{if } -\frac{1}{3} < \lambda_i(Q) < \frac{2}{3}, \\ \infty & \text{otherwise,} \end{cases}$$

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This map ψ is both convex and classically smooth on $\mathrm{D}(\psi) := \{Q \in \mathrm{Sym}_0(d) : \psi(Q) < \infty\}$; moreover, $\psi(Q)$ exhibits logarithmic blow-up as $Q \to \partial\mathrm{D}(\psi)$ from the interior.

The construction of ψ can be generalised to two dimensions, i.e. when ρ is a density on $\mathbb{S}^1$.

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'Physicality' and 'Strict Physicality'

Let $\mathbb{T}^d$ denote the d-dimensional torus, $d = 2$ or 3.

Definition. A Q-tensor field $Q : \mathbb{T}^d \to \mathrm{Sym}_0(d)$ is said to be physical if and only if

$$-\frac{1}{d} < \lambda_i(Q(x)) < 1 - \frac{1}{d} \qquad (2)$$

for almost every $x \in \mathbb{T}^d$.

Definition. We shall call Q strictly physical on $\mathbb{T}^d$ if and only if there exists $\delta > 0$ (sufficiently small) such that

$$-\frac{1}{d} + \delta \leq \lambda_i(Q(x)) \leq 1 - \frac{1}{d} - \delta \qquad (3)$$

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In particular,

$$\psi(Q) \in L^1 \Longrightarrow (2) \quad \text{and} \quad \psi(Q) \in L^\infty \Longleftrightarrow (3).$$

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The Modified Beris-Edwards Model

For given constants $\Gamma, L, \vartheta, \kappa, \nu > 0$, we aim to construct solutions to the following system on the d-dimensional torus $\mathbb{T}^d$:

$$
\text{(S)} \begin{cases} \dfrac{\partial Q}{\partial t} + (u\cdot\nabla)Q - S(Q,\nabla u) = -\Gamma \dfrac{\delta E}{\delta Q}(Q) \\ \dfrac{\partial u}{\partial t} + (u\cdot\nabla)u + \nabla p = \nu\Delta u + \mathrm{Div}\,(\tau(Q)+\sigma(Q)) \\ \nabla\cdot u = 0 \end{cases}
$$

where

$$
E[Q] := \int_{\mathbb{T}^d} \left(\frac{L}{2}|\nabla Q|^2 + \vartheta\,\psi(Q) - \frac{\kappa}{2}|Q|^2\right)\,dx
$$

replaces the usual Landau-de Gennes contribution

$$
E_{\mathrm{LdG}}[Q] := \int_{\mathbb{T}^d} \left(\frac{L}{2}|\nabla Q|^2 + \frac{a(\vartheta)}{2}\mathrm{tr}(Q^2) - \frac{b}{3}\mathrm{tr}(Q^3) + \frac{c}{4}\mathrm{tr}(Q^2)^2\right)\,dx.
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\end{aligned}
\right.
$$

Justification for replacement:

- Both $\vartheta\,\psi(Q) - \kappa\,|Q|^2/2$ and the quartic Landau-de Gennes density f_B are smooth on their domains of definition;
- The expansion of $\vartheta\,\psi(Q) - \kappa\,|Q|^2/2$ near 0 agrees with f_B;
- The singular density also predicts an isotropic-to-nematic phase transition.

Results I: Existence and Strict Physicality

Theorem (W., 2012)

Let $d = 2$ *or* 3. *For initial data* $(Q_0, u_0) \in H^1 \times L^2_{\mathrm{div}}$ *such that* Q_0 *is physical, i.e.*

$$\psi(Q_0) \in L^1,$$

there exist maps

$$Q \in L^\infty_{\mathrm{loc}}(0, \infty; H^1) \cap L^2_{\mathrm{loc}}(0, \infty; H^2)$$

and

$$u \in L^\infty_{\mathrm{loc}}(0, \infty; L^2_{\mathrm{div}}) \cap L^2_{\mathrm{loc}}(0, \infty; H^1_{\mathrm{div}})$$

which satisfy system (S) in the sense of distributions.

Moreover, in the co-rotational case when $\xi = 0$, *the map* Q *is also strictly physical for positive time, i.e.*

$$\psi(Q(\cdot, t)) \in L^\infty \quad \text{for} \quad t > 0.$$

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Results II: Higher Regularity

Corollary (W., 2012)

(Dimension $d = 2$, $\xi = 0$) Given $T > 0$ and initial data $(Q_0, u_0) \in H^2 \times H^1_{\mathrm{div}}$ with Q_0 satisfying the strict physicality condition

$$\psi(Q_0) \in L^\infty,$$

there exist maps

$$Q \in L^\infty(0, T; H^2) \cap L^2(0, T; H^3)$$

$$(\textit{compared with} \ \ L^\infty(0, T; H^1) \cap L^2(0, T; H^2) \ \ \textit{previously})$$

and

$$u \in L^\infty(0, T; H^1_{\mathrm{div}}) \cap L^2(0, T; H^2_{\mathrm{div}})$$

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Regularisation of the Map ψ

We regularise the singular map ψ in two stages.

(i) Extension of Domain. For each $J = 1, 2, 3, ...$, we define $\psi_J : \mathrm{Sym}_0(d) \to \mathbb{R}$ to be the Yosida-Moreau regularisation of ψ, namely

$$\psi_J(Q) := \min_{A \in \mathrm{Sym}_0(d)} \Big(J|A - Q|^2 + \psi(A) \Big) \quad \text{for all} \quad Q \in \mathrm{Sym}_0(d).$$

(ii) Mollification. Given a fixed J, for any $K = 1, 2, 3, \ldots$ we define $\psi_{J,K}$ to be the standard mollification of the map ψ_J,

$$\psi_{J,K}(Q) := K^{d^2} \int_{\mathbb{R}^{d \times d}} \psi_J(K(Q - R))\Phi(R)\, dR,$$

where $\Phi \in C_c^\infty(\mathbb{R}^{d \times d}, \mathbb{R}_+)$ is of unit mass, i.e. $\int_{\mathbb{R}^{d \times d}} \Phi = 1$.

Finally, we define the regularisation $\psi_N := \psi_{N,N}$ for each $N \geq 1$.

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Energy Structure of the Model

Firstly, we take matrix products throughout the Q-tensor equation

$$\frac{\partial Q}{\partial t} + (u \cdot \nabla) Q - S(Q, \nabla u) = -\Gamma \frac{\delta E}{\delta Q}(Q) \quad \text{with the element} \quad \frac{\delta E}{\delta Q}(Q)$$

and then take vector products throughout the Navier-Stokes equation

$$\frac{\partial u}{\partial t} + (u \cdot \nabla) u + \nabla p = \nu \Delta u + \mathrm{Div}\left(\tau(Q) + \sigma(Q)\right) \quad \text{with} \quad u.$$

Now, integrating over the torus, adding both contributions together and noticing certain cancellations in the higher-order derivative terms yields the identity

$$\frac{d}{dt}\left(E[Q(\cdot, t)] + \frac{1}{2}\|u(\cdot, t)\|_2^2\right) = -\Gamma \left\| \left\langle \frac{\delta E}{\delta Q}(Q(\cdot, t)) \right\rangle \right\|_2^2 - \nu \|\nabla u(\cdot, t)\|_2^2 \qquad (4)$$

Energy Structure of the Model

Remark (of John Ball). It is curious that no term which is pre-multiplied by the parameter ξ should contribute to the energy equation

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A Comparison Principle for $\psi(Q)$

Recall:

Theorem ($\xi = 0$ and $d = 2, 3$)

If weak solutions (Q, u) of system (S) start from initial data $(Q_0, u_0) \in H^1 \times L^2_{\mathrm{div}}$ with

$$\psi(Q_0) \in L^1 \qquad \textit{(physical initial data)}$$

then

$$\psi(Q(\cdot, t)) \in L^\infty \quad \textit{for} \quad t > 0 \qquad \textit{(strictly physical solutions)}$$

Issue: Weak solutions are not regular enough for a maximum principle to be applied.

The main idea is to find a way to apply maximum principle arguments for approximate solutions, and then carry information through to the weak limit.

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A Comparison Principle for $\psi(Q)$

Roughly speaking,

1. $\{Q^{M,N}\}_{M,N=1}^{\infty}$ and $\{u^{M,N}\}_{M,N=1}^{\infty}$ are approximate solutions which evolve under (S) when:
   (i) ψ is replaced by ψ_N
   (ii) we take the Galerkin projection of the Navier-Stokes equations onto an M-dimensional subspace of L^2_{div};

2. $\{Q^{M}\}_{M=1}^{\infty}$ and $\{u^{M}\}_{M=1}^{\infty}$ evolve under (S) when:

   (i) ψ is recovered from ψ_N in the limit $N \to \infty$
   (ii) we take the Galerkin projection of the Navier-Stokes equations onto an M-dimensional subspace of L^2_{div}.

A Comparison Principle for $\psi(Q)$

We emphasise that $\xi = 0$ at this point! Multiplying throughout the evolution equation for the approximate solution $Q^{M,N}$

$$\frac{\partial Q^{M,N}}{\partial t} + \left(u^{N,M} \cdot \nabla\right) Q^{M,N} - S(Q^{M,N}, \nabla u^{M,N})$$
$$= \Gamma \left(L\Delta Q^{M,N} - \vartheta \left\langle \frac{\partial \psi_N}{\partial Q}(Q^{M,N}) \right\rangle + \kappa\, Q^{M,N} \right)$$

by $\langle \partial_Q \psi_N(Q^{M,N}) \rangle$ and using the convexity of ψ_N, we discover

$$\left(\frac{\partial}{\partial t} + u^{M,N} \cdot \nabla - \Gamma L \Delta \right) \psi_N(Q^{M,N}) \leq \frac{\Gamma \kappa^2}{2\vartheta} \left| Q^{M,N} \right|^2.$$

By choosing suitable comparison functions, we hope to demonstrate

$$\psi(Q^M(x,t)) \leq \text{constant independent of } M \text{ for } t > 0.$$

If we can show $Q^M \to Q$ in 'good' senses, we may infer $\psi(Q(\cdot,t)) \in L^\infty$ for $t > 0$.

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$$\left(\frac{\partial}{\partial t} + u^{M,N} \cdot \nabla - \Gamma L \Delta\right) \psi_N(Q^{M,N}) \leq C \left(|\xi| \left|\nabla u^{M,N}\right|^2 + \left|Q^{M,N}\right|^2\right).$$

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A Comparison Principle for $\psi(Q)$

Our choice of comparison function has two pieces:

I. Homogeneous problem with mean-zero initial datum: $G = G^{M,N}$

$$(\mathrm{P}^1_{M,N}) \begin{cases} \partial_t G + \left(u^{M,N} \cdot \nabla\right) G - \Gamma L \Delta G = 0, \\ G(\cdot, 0) = \psi_N(Q_0) - \dfrac{1}{|\mathbb{T}^d|} \displaystyle\int_{\mathbb{T}^d} \psi_N(Q_0). \end{cases}$$

II. Inhomogeneous problem with constant initial datum: $H = H^{M,N}$

$$(\mathrm{P}^2_{M,N}) \begin{cases} \partial_t H + \left(u^{M,N} \cdot \nabla\right) H - \Gamma L \Delta H = \dfrac{\Gamma \kappa^2}{2\vartheta} \left| Q^{M,N} \right|^2, \\ H(\cdot, 0) = \dfrac{1}{|\mathbb{T}^d|} \displaystyle\int_{\mathbb{T}^d} \psi_N(Q_0). \end{cases}$$

Let $K^{M,N} := \psi_N(Q^{M,N}) - G^{M,N} - H^{M,N}$. One can show by the classical maximum principle that $K^{M,N} \leq 0$ on $[0, T] \times \mathbb{T}^d$, whence

$$\psi_N(Q^{M,N}) \leq G^{M,N} + H^{M,N} \quad \text{on} \quad [0, T] \times \mathbb{T}^d. \tag{5}$$

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Regarding the analysis of $(\mathrm{P}^1_{M,N})$, we appeal to the following estimate of Constantin, Kiselev, Rhyzhik and Zlatoš **[CKRZ]**:

Proposition

Let v be a smooth, spatially-periodic divergence-free velocity field, and suppose $\gamma > 0$. If φ evolves under the associated advection-diffusion equation on $\mathbb{T}^d$:

$$\begin{cases} \partial_t \varphi + (v \cdot \nabla)\,\varphi - \Delta\varphi = 0, \\ \varphi(\cdot, 0) = \varphi_0 \in L^1(\mathbb{T}^d), \end{cases}$$

where $\int_{\mathbb{T}^d} \varphi_0 = 0$, then there exists $C = C(\gamma) > 0$ which is independent of v such that

$$\|\varphi(\cdot, t)\|_\infty \leq \frac{C}{t^{\frac{d}{2}+\gamma}} \|\varphi_0\|_1 \qquad (6)$$

for $t > 0$.

A Comparison Principle for $\psi(Q)$

Applying estimate (6) to solutions of $(\mathrm{P}^1_{M,N})$, we obtain

$$\left|G^{M,N}(x,t)\right| \leq \frac{C}{t^{\frac{d}{2}+\gamma}}\|\psi_N(Q_0)\|_1 \leq \frac{C}{t^{\frac{d}{2}+\gamma}}\|\psi(Q_0)\|_1. \tag{7}$$

To treat solutions of $(\mathrm{P}^2_{M,N})$, we compare their behaviour with solutions of the following family of problems:

$$(\mathrm{P}^2_M)\begin{cases} \partial_t H^M + \left(u^M\cdot\nabla\right)H^M - \Gamma L\Delta H^M = \dfrac{\Gamma\kappa^2}{2\vartheta}\left|Q^M\right|^2, \\ H^M(\cdot,0) = \dfrac{1}{|\mathbb{T}^d|}\displaystyle\int_{\mathbb{T}^d}\psi(Q_0). \end{cases}$$

Happily, one can show

$$\lim_{N\to\infty}\left\|H^{M,N}(\cdot,t) - H^M(\cdot,t)\right\|_2 = 0,$$

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Using the fact that $Q^M(x,t) \in \mathsf{D}(\psi)$ almost everywhere (and so $|Q^M(x,t)| \leq \sqrt{2/3}$), one may show that

$$\left\| H^M(\cdot,t) \right\|_\infty \leq \left| \int_{\mathbb{T}^d} \psi(Q_0) \right| e^T + \frac{\Gamma\kappa^2 e^T}{2\vartheta} \quad \text{for every} \quad M \geq 1. \tag{8}$$

Finally, using estimates (7) and (8), we deduce that

$$\psi(Q^M(x,t)) = \lim_{N\to\infty} \psi_N(Q^{M,N}(x,t)) \leq \frac{C}{t^{\frac{d}{2}+\gamma}} \|\psi(Q_0)\|_1 + \left| \int_{\mathbb{T}^d} \psi(Q_0) \right| e^T + \frac{\Gamma\kappa^2 e^T}{2\vartheta}$$

almost everywhere on $[0,T] \times \mathbb{T}^d$. Finally, 'good' convergence of Q^M to Q implies that $\psi(Q(\cdot,t)) \in L^\infty$ for $t > 0$, whence strict physicality of weak solutions.

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Higher Regularity of Weak Solutions

If we assume $(Q_0, u_0) \in H^2 \times H^1_{\text{div}}$ with $\psi(Q_0) \in L^\infty$, by adapting the maximum principle argument one can show that there exists a compact subset of matrices $K \subset \mathsf{D}(\psi)$ such that

$$\text{range}\left(Q^M\right) \quad \text{and} \quad \text{range}\left(Q\right) \quad \text{lie essentially in} \quad K \quad \text{for all} \quad M \geq 1.$$

Knowing this, we need not worry about possible blow-up phenomena near the boundary of the effective domain $\mathsf{D}(\psi)$. In particular, this allows us to infer that

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are as distributionally-differentiable as Q^M and Q are, respectively.

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Points of Interest for the Future

1. Can we obtain strict physicality of weak solutions in the non co-rotational case $\xi \neq 0$?
2. It would be interesting to develop an analogous existence theory where the gradient of the energy

$$E[Q] = \int_{\mathbb{T}^d} \left(\frac{L}{2} |\nabla Q|^2 + \vartheta \, \psi(Q) - \frac{\kappa}{2} |Q|^2 \right) \, dx$$

on the RHS of the Beris-Edwards model is replaced by that of the more general 'four elastic constants' theory

$$E[Q] = \int_{\mathbb{T}^d} \left(w(\nabla Q, Q) + \vartheta \, \psi(Q) - \frac{\kappa}{2} |Q|^2 \right) \, dx,$$

where

$$w(\nabla Q, Q) := L_1 |\nabla Q|^2 + L_2 \, Q_{ik,j} \, Q_{ij,k} + L_3 \, Q_{ij,j} \, Q_{ik,k} + L_4 \, Q_{\ell k} \, Q_{ij,k} \, Q_{ik,\ell}.$$

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Thank you for your attention!

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