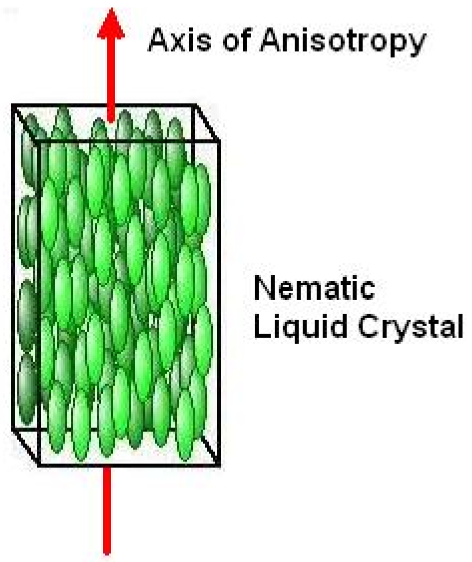
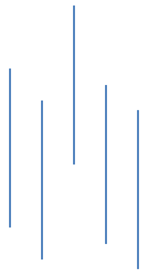
Regularity and Eigenvalue Properties for Minimizers of a Constrained Q-Tensor Energy in Liquid Crystals

P. Bauman and Daniel Phillips
Purdue University

Introduction

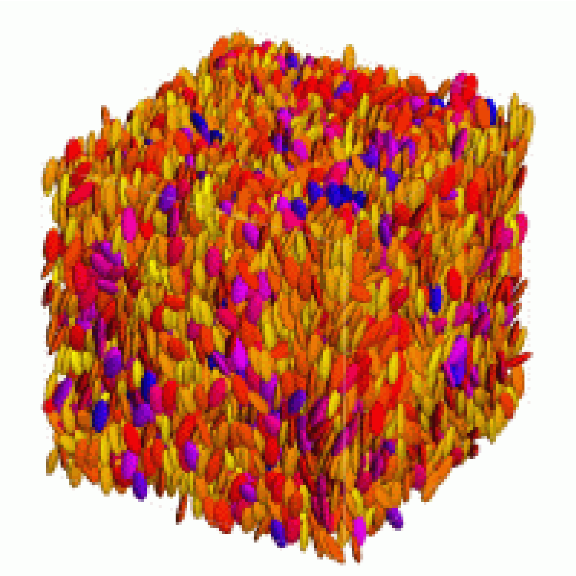
Nematic liquid crystals are states of matter between a liquid and a solid. Their molecules tend to align.





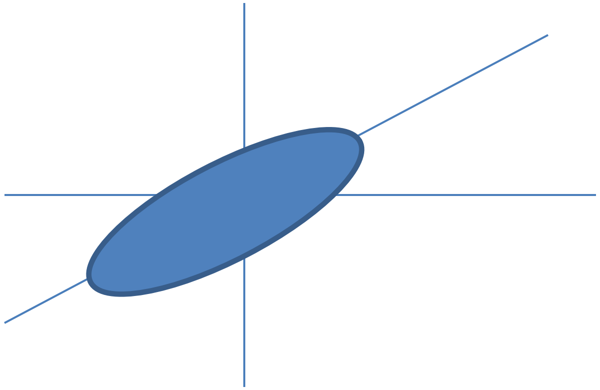
The Frank energy models nematic liquid crystals using a vector field $\mathbf{n}(\mathbf{x})$

$$
\begin{aligned}
G(n, \nabla n) &= \int_\Omega [K_1(\text{div }\mathbf{n})^2 + K_2(\mathbf{n}\cdot \text{curl }\mathbf{n})^2 \\
&+ K_3|\mathbf{n}\times \text{curl }\mathbf{n}|^2 + K_4(\text{tr }(\nabla \mathbf{n})^2 - (\text{div }\mathbf{n})^2)]
\end{aligned}
$$



De Gennes modeled nematic liquid crystals using Q tensors:

$$Q(\mathbf{x}) \in \mathcal{S}_0 := \{Q \in \mathbb{R}^{3\times 3} \colon Q = Q^t \text{ and } tr\ Q = 0\}.$$



- If Q in $\mathcal{S}_0$ has eigenvectors $\mathbf{u}_1, \mathbf{u}_2, \mathbf{u}_3$ with eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3, \quad \lambda_1 + \lambda_2 + \lambda_3 = 0.$

- $\{\mathbf{u}_3, -\mathbf{u}_3\}$ is the most probable line of alignment.

- $\{\mathbf{u}_1, -\mathbf{u}_1\}$ is the least probable line of alignment.

- Q is isotropic if and only if $\lambda_3 = \lambda_2 = \lambda_1$ and this holds if and only if the $\lambda_i = 0$ $(Q = 0)$.
- Q is uniaxial if exactly two eigenvalues are equal.
- Q is biaxial if all eigenvalues are distinct.

The Landau-de Gennes energy has the form:

$$\mathcal{F}(Q) = \int_{\Omega} [f_e(Q(\mathbf{x}), \nabla Q(\mathbf{x})) + f_b(Q(\mathbf{x}))] d\mathbf{x}$$

for $\Omega \subset \mathbb{R}^2$ or $\mathbb{R}^3$ and Q in $H^1(\Omega)$ with values in $\mathcal{S}_0 := \{Q \in \mathbb{R}^{3\times 3} \colon Q = Q^t \text{ and } tr\ Q = 0\}$.

This energy can have minimizers with defects

For the bulk energy density in

$$\mathcal{F}(Q) = \int_\Omega [f_e(Q(\mathbf{x}), \nabla Q(\mathbf{x})) + f_b(Q(\mathbf{x}))] d\mathbf{x}.$$

we assume

- $f_b(Q) \geq 0$
- $f_b(RQR^t) = f_b(Q)$ for all $R \in O(3)$
- Typically $f_b(Q) = 0$ only at a set of uniaxial states.
- An example is:

$$f_b(Q) = a\ tr(Q^2) - \frac{2b}{3}\ tr(Q^3) + \frac{c}{2}(tr(Q^2))^2 + d$$

for certain constants a,b,c,d.

In this case

$$f_b(Q) = f_b^0(Q) = \mathfrak{a}\, tr(Q^2) - \frac{2\mathfrak{b}}{3}\, tr(Q^3) + \frac{\mathfrak{c}}{2}(tr(Q^2))^2 + \mathfrak{d}$$
$$= \mathfrak{a}(\sum_{i=1}^{3} \lambda_i^2) - \frac{2\mathfrak{b}}{3}(\sum_{i=1}^{3} \lambda_i^3) + \frac{\mathfrak{c}}{2}(\sum_{i=1}^{3} \lambda_i^2)^2 + \mathfrak{d}.$$

Indeed, taking $\mathfrak{b}, \mathfrak{c} > 0$, $\mathfrak{a} < \frac{\mathfrak{b}^2}{27\mathfrak{c}}$, and an appropriate choice of $\mathfrak{d}$, we have $f_b^0 \geq 0$

and $f_b^0(Q) = 0$ if and only if $Q \in \Lambda_s$ where $s = \frac{1}{4\mathfrak{c}}(\mathfrak{b} + \sqrt{\mathfrak{b}^2 - 24\mathfrak{a}\mathfrak{c}})$.

Here

$$\Lambda_s = \{Q \in \mathscr{S} : \; Q = s(\mathbf{m} \otimes \mathbf{m} - \tfrac{1}{3}I) \text{ for some } \mathbf{m} \in \mathbb{S}^2$$

A typical elastic energy density f_e is:

$$\begin{aligned} \underline{f_{ld}^{(1)}(\nabla Q)} &= L_1 Q_{ij,x_\ell} Q_{ij,x_\ell} + L_2 Q_{ij,x_j} Q_{ik,x_k} \\ &+ L_3 Q_{ij,x_k} Q_{ik,x_j} \end{aligned}$$

with

$$L_1 + \frac{5}{3} L_2 + \frac{1}{6} L_3 > 0,\ L_1 - \frac{1}{2} L_3 > 0,\ L_1 + L_3 > 0$$

or

$$\begin{aligned} \underline{f_{ld}^{(2)}(Q, \nabla Q)} &= f_{ld}^{(1)}(\nabla Q) + L_4 \varepsilon_{lkj} Q_{li} Q_{ki,x_j} \\ &+ L_5 Q_{lk} Q_{ij,x_l} Q_{ij,x_k} \end{aligned}$$

where $\varepsilon_{\ell kj}$ is the Levi–Civita tensor.

Limitations of the Landau-de Gennes energy:

- Connection between Q and the statistics of local orientational order is suggestive.

- $\mathcal{F}$ is well posed for a limited class of $f_e(Q, \nabla Q)$: Ball and Majumdar have shown that if $L_5 \neq 0$, minimizers for the Dirichlet problem do not exist, since the Landau-de Gennes energy among admissible functions is not bounded below.

  But minimizers do exist if we replace the bulk energy term with a singular Maier-Saupe potential.

- This is the problem we study here.

Maier-Saupe Theory and Constrained Minimizers

- Consider $Q \in \mathcal{S}_0$ of the form

$$Q = \int_{\mathbb{S}^2} (\mathbf{p} \otimes \mathbf{p} - \frac{1}{3}\ I)\rho(\mathbf{p}) d\mathbf{p} \tag{1}$$

where

$$\rho \in L^1(\mathbb{S}^2; \mathbb{R}) : \rho \geq 0, \rho(\mathbf{p}) = \rho(-\mathbf{p}), \int_{\mathbb{S}^2} \rho(\mathbf{p})\ d\mathbf{p} = 1.$$

- Note only certain Q can be written this way, since (1) implies

$$-\frac{1}{3} \leq \xi^t Q \xi \leq \frac{2}{3} \text{ for } \xi \in \mathbb{S}^2$$

so that $-\frac{1}{3} \leq \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \frac{2}{3}$

$$(1) \quad Q = \int_{\mathbb{S}^2} (\mathbf{p} \otimes \mathbf{p} - \frac{1}{3} I) \rho(\mathbf{p}) d\mathbf{p}$$

For $Q \in \mathcal{S}_0$ let $\lambda_1(Q) \leq \lambda_2(Q) \leq \lambda_3(Q)$ denote its eigenvalues.

Let $\mathcal{M} = \{Q \in \mathcal{S}_0 : \lambda_i \in (-\frac{1}{3}, \frac{2}{3})$ for $1 \leq i \leq 3\}$.

Then $\mathcal{M}$ is an open, bounded, and convex subset of $\mathcal{S}_0$.

One can show:

If $Q \in \mathcal{M}$ then it can be represented as in (1).

If $Q \in \partial\mathcal{M}$ a representation requires a singular measure.

If $Q \in \mathcal{S}_0 \setminus \overline{\mathcal{M}}$ then there is no representation.

The Maier-Saupe (bulk) potential f_{ms} is defined as:

$$f_{ms}(Q) \begin{cases} = f(Q) - \kappa|Q|^2 + b_0 \text{ for } Q \in \mathcal{M}, \\ = +\infty \text{ for } Q \in \mathcal{S}_0 \backslash \mathcal{M} \end{cases}$$

$$\text{where } f(Q) := \inf_{\rho \in A_Q} \int_{\mathbb{S}^2} \rho(\mathbf{p}) \ln(\rho(\mathbf{p})) d\mathbf{p}.$$

$$\text{and } A_Q := \{ \quad \rho \in L^1(\mathbb{S}^2; \mathbb{R}) : \rho \geq 0, \int_{\mathbb{S}^2} \rho(\mathbf{p}) \, d\mathbf{p} = 1,$$

$$Q = \int_{\mathbb{S}^2} (\mathbf{p} \otimes \mathbf{p} - \frac{1}{3} \, I) \rho(\mathbf{p}) d\mathbf{p} \}$$

This was studied by: Katriel,Kventsel, Luckhurst, and Sluckin; Ball and Majumdar. They proved that f is well defined and has the properties:

$$f \text{ is convex and } \lim_{Q \to \partial \mathcal{M}} f(Q) = +\infty.$$

Zarnescu proved that $f \in C^\infty(\mathcal{M})$.

We assume without loss of generality that

$$b_0 = -\min_{Q \in \mathcal{M}} \{f(Q) - \kappa |Q|^2\} \text{ and hence } \min f_{ms} = 0.$$

Minimizers of Landau-de Gennes energies with Maier-Saupe-type bulk term

For the Maier-Saupe bulk energy f_b as above, consider minimizers of

$$\mathcal{F}(Q) = \int_{\Omega} [f_e(Q(\mathbf{x}), \nabla Q(\mathbf{x})) + f_b(Q(\mathbf{x}))] d\mathbf{x}$$

$$\text{for } Q \in \mathcal{A}_0 = \{Q \in H^1(\Omega; \overline{\mathcal{M}}) : Q = Q_0 \text{ on } \partial\Omega\}$$

- Assume that $\mathcal{F}(\tilde{Q}) < \infty$ for some $\tilde{Q} \in \mathcal{A}_0$.
- Note that since $\lim_{Q \to \partial\mathcal{M}} f_b(Q) = +\infty$ the energy distinguishes"nonphysical" states $Q(\mathbf{x}) \in \partial\mathcal{M}$.

Prior Results [for Minimizers in $\mathcal{A}_0$]:

$$\mathcal{F}(Q) = \int_\Omega [f_e(Q(\mathbf{x}), \nabla Q(\mathbf{x})) + f_b(Q(\mathbf{x}))]d\mathbf{x}$$

$$\text{for } Q \in \mathcal{A}_0 = \{Q \in H^1(\Omega; \overline{\mathcal{M}}) : Q = Q_0 \text{ on } \partial\Omega\}$$

For $\Omega \subset \mathbb{R}^3$, Ball and Majumdar (2010) showed:

- For f_e satisfying appropriate coercivity conditions (including the $L_5 \neq 0$), minimizers exist.
- Physicality result: If $f_e(Q, \nabla Q) = K|\nabla Q|^2$, and if Q_0 is smooth a valued in a compact subset of $\mathcal{M}$, then minimizers are smooth $\mathcal{M}$–valued. In particular Q satisfies its equilibrium equation thro out Ω.

For $\Omega \subset \mathbb{R}^n$, $n \geq 2$, Evans, Knuess, and Tran (2016) showed:

- If $\mathcal{F} = \int_\Omega [f_e(Q(\mathbf{x}), \nabla Q(\mathbf{x})) + f_b(Q(\mathbf{x}))] d\mathbf{x}$ is quasi–convex then minimizers have partial regularity and are $\mathcal{M}$–valued except in a closed set Ω_0 of measure zero.

- If $f_e = f_e(\nabla Q)$, convex, and f_b satisfies a growth condition then $\mathcal{H}^p(\Omega_0) = 0$ for $p > n - 2$.

Our Main Results:

Consider the energy with "Maier-Saupe-type" bulk term

$$\mathcal{F}(Q) = \int_\Omega [f_e(Q(\mathbf{x}), \nabla Q(\mathbf{x})) + f_b(Q(\mathbf{x}))] d\mathbf{x}$$

with $\Omega \subset \mathbb{R}^2$.

Assume that $f_e(Q, D)$ is continuous on $\overline{\mathcal{M}} \times \mathcal{D}$ and there are constants $0 < \alpha_1 \leq \alpha_2 < \infty$, $0 \leq M_1 \leq M_2 < \infty$ so that

$$(*) \quad \alpha_1 |D|^2 - M_1 \leq f_e(Q, D) \leq \alpha_2 |D|^2 + M_2$$

and

$$f_b(Q) = f(Q) - \kappa |Q|^2 + b_0 \text{ for } Q \in \mathcal{M}$$

with $\kappa \geq 0$,

and f is convex and smooth on $\mathcal{M}$ with $f(Q) \to \infty$ as $Q \to \partial\mathcal{M}$.

We take boundary conditions:

$$Q = Q_0 \in C^{0,1}(\partial\Omega; \overline{\mathcal{M}}) \text{ such that } \int_{\partial\Omega} f_b(Q_0)\,ds < \infty.$$

Recall

$$\mathcal{A}_0 = \{Q \in H^1(\Omega; \overline{\mathcal{M}}) \colon Q = Q_0 \text{ on } \partial\Omega\}.$$

One can show that there exists $Q \in \mathcal{A}_0$ so that $\mathcal{F}(Q) < \infty$.

Under these assumptions we prove:

Theorem 1. Let Q be a minimizer for $\mathcal{F}$ in $\mathcal{A}_0$. Then $Q \in C^\sigma(\overline{\Omega})$ for some $\sigma > 0$.

This result applies to a large class of examples in which the elastic energy f_e is a "Landau-de Gennes elastic energy."

In Maier–Saupe theory the set

$$\begin{aligned}\Lambda(Q) &= \{\mathbf{x} \in \overline{\Omega} \colon Q(\mathbf{x}) \in \partial\mathcal{M}\} \\ &\equiv \{\mathbf{x} \in \overline{\Omega} \colon \lambda_j(Q(\mathbf{x})) \in [-\frac{1}{3}, \frac{2}{3}] \text{ for } 1 \leq j \leq 3 \text{ and} \\ &\quad \lambda_i(Q(\mathbf{x})) \in \{-\frac{1}{3}, \frac{2}{3}\} \text{ for some } i \in \{1,2,3\}\}\end{aligned}$$

corresponds to locations where perfect nematic order occurs and this is interpreted as not physical.

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corresponds to locations where perfect nematic order occurs and this is interpreted as not physical.

Corollary 1. Let Q be a minimizer for $\mathcal{F}$ in $\mathcal{A}_0$. Since Q is Holder continuous in $\overline{\Omega}$, $\Lambda(Q)$ is a closed subset of measure zero.

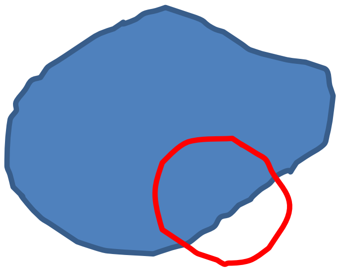
From our proof of Theorem 1 (local estimates) we have:

Corollary 2. *Assume $f_e = f_{ld}(Q, D)$ and f_{ld} satisfies our assumptions. Then:*

> *If B is a disk contained in Ω, a finite energy local minimizer $Q \in H^1(B; \overline{\mathcal{M}})$ for $\mathcal{F}$ satisfies $Q \in C^\infty(B \setminus \Lambda(Q))$.*

Remark. We can also prove that if B is a ball centered at a boundary point of Ω such that $B \cap \Lambda(Q) = \emptyset$, then Q is as smooth in $B_r(\mathbf{o}) \cap \overline{\Omega}$ as $\partial\Omega$ and Q_0 allows.

In particular, if $B \cap \partial\Omega$ is of class $C^{k,\alpha}$ and $Q_0 \in C^{k,\alpha}(B \cap \partial\Omega)$ for some $k \geq 2$ and $0 < \alpha < 1$, then $Q \in C^{k,\alpha}(B_r(\mathbf{o}) \cap \overline{\Omega})$.



Applications to Landau-de Gennes Elastic Energies

Let $f_e(Q,D) = f_{\ell d}(Q,D)$ where $f_{\ell d}$ is a polynomial in Q_{ij} and D_{ijk} that is $SO(3)$ invariant.

Example 1. $f_e = f_{\ell d}(Q,D) \equiv f^{(1)}_{\ell d}(D)$ satisfying

$$(*) \quad \alpha_1 |D|^2 - M_1 \leq f_e(Q,D) \leq \alpha_2 |D|^2 + M_2.$$

In this case recall

$$\begin{aligned} f^{(1)}_{ld}(\nabla Q) &= L_1 Q_{ij,x_\ell} Q_{ij,x_\ell} + L_2 Q_{ij,x_j} Q_{ik,x_k} \\ &+ L_3 Q_{ij,x_k} Q_{ik,x_j}. \end{aligned}$$

Longa showed (*) holds iff the elasticity constants satisfy

$$L_1 + \frac{5}{3} L_2 + \frac{1}{6} L_3 > 0,\ L_1 - \frac{1}{2} L_3 > 0,\ L_1 + L_3 > 0.$$

Remark: If $f_e = f_{\ell d}$ and $(*)$ holds then there exist minimizers for $\mathcal{F}$ in A_0.
[Ball-Majumdar].

Example 2:

$$f_{\ell d}^{(2)}(Q, \nabla Q) = f_{\ell d}^{(1)}(\nabla Q) + L_4 \epsilon_{lkj} Q_{li} Q_{ki,x_j} + L_5 Q_{lk} Q_{ij,x_l} Q_{ij,x_k}$$

where ϵ_{lkj} is the Levi-Civita tensor. There are conditions on $L_1, ..., L_5$ so that $(*)$ holds as well.

We also prove the following physicality result.

Theorem 3 Let Q be a finite energy local minimizer for $\mathcal{F}(\cdot; B)$ for a ball $B \subset \Omega$ where

$$
\begin{aligned}
f_e(Q, \nabla Q) &= L_1 |\nabla Q|^2 + L_4 \varepsilon_{lkj} Q_{\ell i}, Q_{ki,x_j} \\
&+ L_5\, Q_{lk}\, Q_{ij,x_l}\, Q_{ij,x_k}.
\end{aligned}
$$

and

$$
\left.
\begin{aligned}
L_1 - \frac{L_5}{3} > 0 &\qquad \text{if } L_5 \geq 0, \\
L_1 + \frac{2L_5}{3} > 0 &\qquad \text{if } L_5 < 0.
\end{aligned}
\right\} \quad (*)
$$

Then $\Lambda(Q) \cap B = \emptyset$ and we have $Q \in C^\infty(B)$.

Theorem 3 generalizes the physicality result of Ball and Majumdar for Ω a domain in $\mathbb{R}^3$, $f_e(\nabla Q) = L_1 \left|\nabla Q\right|^2$, and Q_0 valued in a compact subset of $\mathcal{M}$, stating that in this case, minimizers Q in $\mathcal{A}_0$ are in $C^\infty(\Omega)$ and have $\Lambda(Q) = \emptyset$.

Why include L_5?

Consider the example:

$$f^{(3)}_{\ell d}(Q, \nabla Q) = f^{(1)}_{\ell d}(\nabla Q) + L_5 Q_{lk} Q_{ij,x_l} Q_{ij,x_k}$$

For constants $L_1, ..., L_5$ so that $(*)$ holds.

Consider

$$\mathcal{F}(Q) = \int_\Omega [f_{\ell d}^{(3)}(Q(\mathbf{x}), \nabla Q(\mathbf{x})) + \frac{1}{\varepsilon^2} f_b(Q(\mathbf{x}))] d\mathbf{x}$$

where $f_b(Q) = f_{ms}(Q) - \kappa |Q|^2 + b_0$ for $Q \in \mathcal{M}$.

- For κ large enough Fatkullin and Slastikov showed: $\{f_b(Q) = 0\} = W_s := \{Q = s(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I)$ for some $\mathbf{n} \in \mathbb{S}^2\}$ for some $s > 0$.
- Suppose that $Q_0 \subset W_s$. Then for $0 < \varepsilon << 1$, away from defects, minimizers $Q(\mathbf{x})$ should be close to W_s.

If locally $Q(\mathbf{x}) = s(\mathbf{n}(\mathbf{x}) \otimes \mathbf{n}(\mathbf{x}) - \frac{1}{3}I)$, then

$$\begin{aligned} f_{\ell d}^{(3)}(Q, \nabla Q) &= K_1(\text{div } \mathbf{n})^2 + K_2(\mathbf{n} \cdot \text{curl } \mathbf{n})^2 \\ &+ K_3|\mathbf{n} \times \text{curl } \mathbf{n}|^2 + (K_2 + K_4)(\text{tr } (\nabla \mathbf{n})^2 - (\text{div } \mathbf{n})^2) \end{aligned}$$

where

$$\begin{aligned} L_1 &= \frac{1}{6s^2}(K_3 - K_1 + 3K_2), \\ L_2 &= \frac{1}{s^2}(K_1 - K_2 - K_4), \\ L_3 &= \frac{1}{s^2}K_4, \\ L_5 &= \frac{1}{2s^3}(K_3 - K_1). \end{aligned}$$

Need $L_5 \neq 0$ to have $K_3 \neq K_1$.

Results in Three-Dimensional Domains

Using some of our methods of proof in 2 dimensions, we extend Ball and Majumdar's results to minimizers and local minimizers defined on a domain $\Omega \subset \mathbb{R}^n$.

We prove:

Let $\mathcal{K} \subset \mathbb{R}^m$ be an open, bounded, convex set where $m \geq 1$.
Consider $\tilde{f} : \mathcal{K} \to \mathbb{R}$ given as $\tilde{f}(\mathbf{p}) = f(\mathbf{p}) - \kappa|\mathbf{p}|^2$ where $\kappa \geq 0$, $f \geq 0$, $f \in C^\infty(\mathcal{K})$ and convex such that $\lim_{\mathbf{p} \to \partial\mathcal{K}} f(\mathbf{p}) = \infty$.

Theorem 4 *Let Ω be a domain in $\mathbb{R}^n$ for $n \geq 1$, $\gamma > 0$, and let $u(\mathbf{x}) \in H^1(\Omega; \overline{\mathcal{K}})$ be a local minimizer for*

$$\mathcal{F}_1(w) = \int_\Omega [\gamma|\nabla w|^2 + \tilde{f}(w)]\, d\mathbf{x}$$

such that $\mathcal{F}_1(u) < \infty$. Then $u(\Omega) \subset \mathcal{K}$, $u \in C^\infty(\Omega)$, and u is a solution to

$$2\gamma \Delta u(\mathbf{x}) = D_u \tilde{f}(u(\mathbf{x})) \text{ in } \Omega.$$

Furthermore if $\partial\Omega$ is of class $C^{2,\sigma}$ for some $0 < \sigma < 1$ and u takes on boundary values $u = u_0 \in C^\sigma(\partial\Omega; \mathcal{K})$, then $u(\Omega) \subset\subset \mathcal{K}$ and it follows that $u \in C^\sigma(\overline{\Omega}; \mathcal{K})$.

Corollary 3. *Let D be a bounded domain in $\mathbb{R}^3$ and let $Q \in H^1(D; \overline{\mathcal{M}})$ be a local minimizer for $\mathcal{F}(V; D) = \int_D [L_1 |\nabla V|^2 + f_b(V)] d\mathbf{x}$ such that $\mathcal{F}(Q; D) < \infty$. Then $Q \in C^\infty(D)$, $Q(\mathbf{x}) \in \mathcal{M}$ for each $\mathbf{x} \in D$ and*

$$2L_1 \Delta Q(\mathbf{x}) = [D_Q f_b(Q(\mathbf{x}))]^{tr} \text{ in } D.$$

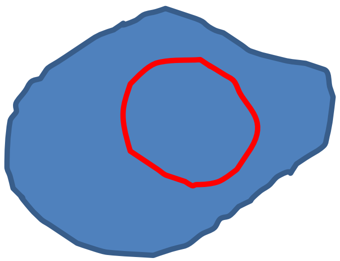
Corollary 4. *Assume $D \subset \mathbb{R}^3$ is a bounded domain with a $C^{2,\sigma}$ boundary and $Q_0 \in H^{1/2}(\partial D; \mathcal{M}) \bigcap C^{\sigma}(\partial D; \mathcal{M})$ for some $0 < \sigma < 1$. If Q is a minimizer for $\mathcal{F}(V; D) = \int_D [L_1 |\nabla V|^2 + f_b(V)] d\mathbf{x}$ in $H^1(D; \overline{\mathcal{M}})$ subject to $Q = Q_0$ on ∂D then $Q(D) \subset\subset \mathcal{M}$ and $Q \in C^{\sigma}(\overline{D}; \mathcal{M})$.*

Remarks on our methods of proof:

Remarks on the proof of Theorem 1:

Let Q be a minimizer for $\mathcal{F}$ in $\mathcal{A}_0$. Then $Q \in C^\sigma(\overline{\Omega})$ for some $\sigma > 0$.

Idea of proof: Given Q we need comparison functions in $\mathcal{S}_0$ valued in $\overline{\mathcal{M}}$. Fix $B_r(\mathbf{x}_0) \subset \Omega$. Let $Q^r \in H^1(\Omega; \mathcal{S}_0)$ so that



$$
\begin{aligned}
Q^r &= Q \text{ in } \Omega \setminus B_r, \\
\Delta Q^r_{ij} &= 0 \text{ in } B_r \text{ for each } i, j
\end{aligned}
$$

Note that by the maximum principle

$$Q^r = Q^{rt}, \text{and } \mathrm{tr}\, Q^r = 0, \text{ so } Q^r \in \mathcal{S}_0.$$

since these hold in $\Omega \setminus B_r$.

Next

$$\lambda_1(Q) = \min_{\xi \in \mathbb{S}^2} \xi^t Q \xi, \lambda_3(Q) = \max_{\xi \in \mathbb{S}^2} \xi^t Q \xi,$$

For each ξ these are linear expressions for the Q_{ij},

$$\sum_{i,j} \xi_i \xi_j Q_{ij}(\mathbf{x})$$

Thus by the maximum principle

$$\inf_{\mathbf{y} \in \partial B_r} \lambda_1(Q(\mathbf{y})) \leq \inf_{\mathbf{y} \in B_r} \lambda_1(Q^r(\mathbf{y})),$$

$$\sup_{\mathbf{y} \in B_r} \lambda_3(Q^r(\mathbf{y})) \leq \sup_{\mathbf{y} \in \partial B_r} \lambda_3(Q(\mathbf{y})),$$

implying $Q^r(\mathbf{x}) \in \overline{\mathcal{M}}$.

We can compare Q and Q_r on B_r.

$$\mathcal{F}(Q; B_r) \leq \mathcal{F}(Q_r; B_r)$$

Thus

$$\int_{B_r} |[\nabla Q|^2 + f(Q)] \leq C \int_{B_r} |[\nabla Q_r|^2 + f(Q_r)] + Br^2$$

f is convex and Q_r is harmonic. Thus $f(Q_r)$ is subharmonic. So

$$\int_{B_r} f(Q_r) \leq \frac{r}{2} \int_{\partial B_r} f(Q_r) = \frac{r}{2} \int_{\partial B_r} f(Q).$$

From elliptic estimates

$$\int_{B_r} |\nabla Q_r|^2 \leq C||Q||^2_{H^{1/2}(\partial B_r)}$$

This means we can estimate

$$\int_{B_r} [|\nabla Q_r|^2 + f(Q_r)] \leq C(||Q||^2_{H^{1/2}(\partial B_r)} + \frac{r}{2} \int_{\partial B_r} f(Q))$$

This means we can estimate

$$\int_{B_r} [|\nabla Q_r|^2 + f(Q_r)] \leq C(||Q||^2_{H^{1/2}(\partial B_r)} + \frac{r}{2} \int_{\partial B_r} f(Q))$$

Given $\frac{s}{2} \leq r \leq \frac{3s}{4}$ these estimates imply that

$$\begin{aligned} \int_{B_{s/2}} [|\nabla Q|^2 + f_b(Q)] \leq & \quad C \int_{B_s \setminus B_{s/2}} [|\nabla Q|^2 + f_b(Q)] \\ + & \quad C_1 s^2 \end{aligned}$$

Next we fill the hole:

$$
\begin{aligned}
(1+C)\int_{B_{s/2}}[|\nabla Q|^2+f_b(Q)] &\leq C\int_{B_s}[|\nabla Q|^2+f_b(Q)] \\
&+ C_1 s^2
\end{aligned}
$$

This leads to

$$
\begin{aligned}
\int_{B_{s/2}}[|\nabla Q|^2+f_b(Q)] &\leq \mu\int_{B_s}[|\nabla Q|^2+f_b(Q)] \\
&+ C_1' s^2
\end{aligned}
$$

where

$$
\mu = \frac{C}{C+1} < 1
$$

Iterating this we find

$$\int_{B_\rho} [|\nabla Q|^2 + f_b(Q)] \le C_2 \rho^{2\sigma}$$

for some $0 < \sigma < 1$.

This implies

$$||Q||_{C^\sigma(K)} \le C_3 \text{ for } K \subset\subset \Omega$$

Ideas in proof of Theorem 3: If $f_e = f_{\ell d}^{(4)}$ then $\Lambda(Q) \bigcap \Omega = \emptyset$.

where

$$f_{\ell d}^{(4)}(Q, \nabla Q) = L_1 |\nabla Q|^2 + L_5 \; Q_{lk} \; Q_{ij,x_l} \; Q_{ij,x_k}.$$

where

$$L_1 - \frac{L_5}{3} > 0 \qquad \text{if } L_5 \geq 0,$$
$$L_1 + \frac{2L_5}{3} > 0 \qquad \text{if } L_5 < 0.$$

Suppose that $\mathbf{x}_0 \in \partial\mathcal{M} \bigcap \Omega$. We know

$$\int_{B_\rho(\mathbf{x}_0)} [|\nabla Q|^2 + f_b(Q)] \le C_2 \rho^{2\sigma}$$

for some $0 < \sigma < 1$.

Here our elastic energy density has the form

$$f_{\ell d}^{(4)} = (L_1 \delta_{lk} + L_4 Q_{lk}) Q_{ij,x_l}\, Q_{ij,x_k}.$$

Because of this we can use elliptic replacements rather than just harmonic replacements to get finer estimates and prove the estimate above for any $\sigma < 1$.

This leads to

$$-\mu r^{3\sigma} \leq -\int_{B_r(\mathbf{x}_0)} f_b(Q) d\mathbf{x} + r(\frac{1}{2} + Mr^{\sigma}) \int_{\partial B_r(\mathbf{x}_0)} f_b(Q) d\mathbf{s}$$

.

Setting $\sigma = \frac{3}{4}$ we get

$$-\mu_1 r^{-\frac{3}{4}} \leq \left(r^{-2}(1 + 2Mr^{3/4})^{8/3} \int_{B_r(\mathbf{x}_0)} f_b(Q) d\mathbf{x} \right)'.$$

Thus

$$r^{-2} \int_{B_r(\mathbf{x}_0)} f_b(Q) d\mathbf{x} \leq C \quad \text{for } 0 < r < r'.$$

Since $\lim_{\mathbf{x} \to \mathbf{x}_0} f_b(Q(\mathbf{x})) = \infty$ this is a contradiction.

The 3-d result follows by showing:

Let $\mathcal{K} \subset \mathbb{R}^m$ be an open, bounded, convex set where $m \geq 1$.

Consider $\tilde{f} : \mathcal{K} \to \mathbb{R}$ given as $\tilde{f}(\mathbf{p}) = f(\mathbf{p}) - \kappa |\mathbf{p}|^2$ where $\kappa \geq 0$, $f \geq 0$, $f \in C^\infty(\mathcal{K})$ and convex such that $\lim_{\mathbf{p} \to \partial\mathcal{K}} f(\mathbf{p}) = \infty$.

Theorem 4 *Let Ω be a domain in $\mathbb{R}^n$ for $n \geq 1$, $\gamma > 0$, and let $u(\mathbf{x}) \in H^1(\Omega; \overline{\mathcal{K}})$ be a local minimizer for*

$$\mathcal{F}_1(w) = \int_\Omega [\gamma |\nabla w|^2 + \tilde{f}(w)] \, d\mathbf{x}$$

such that $\mathcal{F}_1(u) < \infty$. Then $u(\Omega) \subset \mathcal{K}$, $u \in C^\infty(\Omega)$, and u is a solution to

$$2\gamma \Delta u(\mathbf{x}) = D_u \tilde{f}(u(\mathbf{x})) \text{ in } \Omega.$$

Furthermore if $\partial\Omega$ is of class $C^{2,\sigma}$ for some $0 < \sigma < 1$ and u takes on boundary values $u = u_0 \in C^\sigma(\partial\Omega; \mathcal{K})$, then $u(\Omega) \subset\subset \mathcal{K}$ and it follows that $u \in C^\sigma(\overline{\Omega}; \mathcal{K})$.

Corollary 4. *Assume* $D \subset \mathbb{R}^3$ *is a bounded domain with a* $C^{2,\sigma}$ *boundary and* $Q_0 \in H^{1/2}(\partial D; \mathcal{M}) \bigcap C^{\sigma}(\partial D; \mathcal{M})$ *for some* $0 < \sigma < 1$. *If* Q *is a minimizer for* $\mathcal{F}(V; D) = \int_D [L_1 |\nabla V|^2 + f_b(V)] d\mathbf{x}$ *in* $H^1(D; \overline{\mathcal{M}})$ *subject to* $Q = Q_0$ *on* ∂D *then* $Q(D) \subset\subset \mathcal{M}$ *and* $Q \in C^{\sigma}(\overline{D}; \mathcal{M})$.