Uniform profile near the point defect of Landau-de Gennes model in the vanishing elasticity limit

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Oseen Frank Model

In the Oseen-Frank model, the state of nematic liquid crystals is described by a unit vector field $n(x)$ which represents the mean local orientation of molecule's optical axis.

Suppose $\Omega \in \mathbb{R}^3$ is the region occupied by the liquid crystals, the total free energy is given by

$$\begin{aligned} E_{OF}(n) = \int_\Omega \Big\{ & k_1(\mathrm{div}\, n)^2 + k_2(n \cdot \mathrm{curl}\, n)^2 + k_3|n \times \mathrm{curl}\, n|^2 \\ & + (k_2 + k_4)\left(\mathrm{tr}(\nabla n)^2 - (\mathrm{div}\, n)^2\right) \Big\}\, dx, \end{aligned} \tag{0.1}$$

Note that when $k_1 = k_2 = k_3 = 1$ and $k_4 = 0$, the energy functional (0.1) reduces to

$$E_{OF}(n) = \int_\Omega |\nabla n|^2\, dx.$$

Singular set of minimizing harmonic maps

Let $n : \Omega \subset \mathbb{R}^3 \to \mathbb{S}^2$ be a minimizing harmonic map with the singular set $\mathcal{S}(n)$.

- (Schoen-Uhlenbeck, 1982) $\mathcal{S}(n)$ contains finitely many points.
- (Brezis-Coron-Lieb, 1986) Near $x_0 \in \mathcal{S}(n)$, n behaves like the "hedgehog" map $T\frac{x-x_0}{|x-x_0|}$ with some $T \in O(3)$.
- (Simon, 1985) The convergence rate can be controlled by

$$\left| n(x_0+x) - T\frac{x}{|x|} \right| \leq C|x|^{\alpha}, \quad \forall |x| < r_0, \text{ for some } \alpha \in (0,1).$$

Landau-de Gennes model

In the Landau-de Gennes model, the order parameter is a 3×3 symmetric traceless matrix Q (the so-called Q-tensors).

$$\mathcal{Q}_0 := \{Q \in \mathcal{M}^{3\times 3},\ Q = Q^T,\ \mathrm{tr}(Q) = 0\}.$$

Total free energy = elastic energy + bulk potential,

$$I_\varepsilon(Q,\Omega) = \int_\Omega \left[\frac{1}{2}|\nabla Q|^2 + \frac{1}{\varepsilon^2} f_b(Q)\right] dx, \quad Q \in H^1(\Omega, \mathcal{Q}_0), \tag{0.2}$$

with $Q = Q_b$ on $\partial\Omega$.

$$f_b(Q) = -\frac{a^2}{2}\mathrm{tr}(Q^2) - \frac{b^2}{3}\mathrm{tr}(Q^3) + \frac{c^2}{4}[\mathrm{tr}(Q^2)]^2 + C. \tag{0.3}$$

where ε, a, b, c are material dependent constants, C is a constant that ensures $\inf_{Q\in\mathcal{Q}_0} f_b(Q) = 0$.

f_b takes its minimum value on a sub-manifold defined by

$$\mathcal{N} = \{Q = s_+(n \otimes n - \frac{1}{3}\mathrm{Id}),\ n \in \mathbb{S}^2\}, \quad s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}. \quad (0.4)$$

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When $\varepsilon \to 0$, we focus on the asymptotic behavior of Q_ε, which minimizes the energy $I_\varepsilon(\cdot, \Omega)$ with the fixed boundary condition $Q = Q_b \in H^{1/2}(\partial\Omega, \mathcal{N})$ on $\partial\Omega$.

f_b obtains minimal value $\Rightarrow$ uniaxial constraint $Q = s_+(n \times n - \frac{1}{3}\mathrm{Id}) \Rightarrow$ Oseen-Frank model.

Vanishing elasticity limit

Theorem (Majumdar-Zarnescu(2010), Nguyen-Zarnescu(2013))

Fix the domain $\Omega \in \mathbb{R}^3$ *and boundary condition* $Q_b = s_+(n_b \times n_b - \frac{1}{3}\mathrm{Id})$, $n_b \in H^{1/2}(\partial\Omega, \mathbb{S}^2)$. *For any sequence* $\varepsilon_k \to 0$, *there exists a subsequence, still denoted by* ε_k, *such that* Q_{ε_k} *converges strongly in* H^1*-norm to* $Q_* = s_+(n_* \times n_* - \frac{1}{3}\mathrm{Id})$, *where* $n_* \in H^1(\Omega, \mathbb{S}^2)$ *is a minimizing harmonic map. Let* $\mathcal{S}(n_*)$ *denote the singular set of* n_*, *then*

$$Q_{\varepsilon_k} \to Q_* \text{ in } C^j_{loc}(\Omega \backslash \mathcal{S}(Q_*), \mathcal{Q}_0), \quad \forall j \geq 1.$$

- Similar limiting problems: Bauman-Park-Phillips(2012), Golovaty -Montero(2014), Canevari(2015, 2017), Contreras-Lamy-Rodiac(2018)... under various settings.
- Influenced by similar analyses of the Ginzburg-Landau model, see Bethuel-Brezis-Hélein(94).

Main result

Fix $x_0 \in \mathcal{S}(n_*)$. Question: What is the behavior of Q_ε in the small neighborhood of x_0?

Blow-up Idea: study the blow-up profile of $Q_\varepsilon(x_0 + \varepsilon x)$.

Theorem (G-Zarnescu, 2022)

There exists a subsequence of Q_{ε_n} and a sequence $x_n \to x_0$ such that the following holds

- $Q_{\varepsilon_n}(x_n + \varepsilon_n x) \to Q(x)$ *in* $C^2_{loc}(\mathbb{R}^3)$ *and* $Q(x)$ *is a local minimizer of the functional* $I(Q) = \int \{\frac{1}{2}|\nabla Q|^2 + f_b(Q)\}\, dx$.
- $Q(x) \to s_+(n(x) \times n(x) - \frac{1}{3}\mathrm{Id})$ *as* $|x| \to \infty$, *where* $n(x) = T(\frac{x}{|x|})$.
- *Let* $B_r(x_0) \cap \mathcal{S}(n_*) = \{x_0\}$. *Then for any sequence* $R_n \uparrow \infty$ *and satisfying* $R_n\varepsilon_n < r$, *there holds*

$$\lim_{n\to\infty} \left(\sup_{R_n\varepsilon_n \le |x| \le r} |Q_{\varepsilon_n}(x_n + x) - Q_*(x_0 + x)| \right) = 0.$$

Analog in 3-D Ginzburg-Landau problem

Theorem (Millot-Pisante, 2010)

Let $u \in H^1_{loc}(\mathbb{R}^3, \mathbb{R}^3)$ *be a nonconstant local minimizer of* $E(u,\Omega) = \int \left(\frac{1}{2}|\nabla u|^2 + \frac{1}{4}(1-|u|^2)^2\right)\, dx$ *and satisfy*

$$\sup_{R>0} \frac{1}{R} E(u, B_R) < +\infty.$$

Then up to a translation on the domain and an orthogonal transformation on the image,

$$u = \frac{x}{|x|} f(|x|)$$

for some function f *such that*

$$f(0) = 0,\ f'(x) > 0,\ f(x) = 1 + O(|x|^{-2}) \text{ as } |x| \to \infty.$$

Proof of the main result

1st Part: Assume $\mathcal{S}(n_*) = \{0\}$ and $n_*(x) \sim \frac{x}{|x|}$ near 0. Define $\Phi(x) := s_+(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}\mathrm{Id})$. By the previous convergence results, we can find a subsequence $\varepsilon_n \downarrow 0$ and $r_n \downarrow 0$ such that, as $n \to \infty$

1. $\frac{r_n}{\varepsilon_n} \to \infty$;
2. $\|Q_{\varepsilon_n}(x) - Q_*(x)\|_{C^2(\Omega \setminus B_{r_n})} \to 0$
3. $\|Q_{\varepsilon_n}(r_n x) - \Phi(x)\|_{C^2(B_2 \setminus B_1)} \to 0$.

Let $D_\delta^n := \{x \in B_{r_n} : \mathrm{dist}(Q_{\varepsilon_n}(x), \mathcal{N}) \geq \delta\}$

Key lemma

For any $\delta > 0$, there exists a constant C_δ,

$$\sup\{|x|, x \in D_\delta^n\} = o(r_n) \quad \text{as } n \to \infty, \tag{0.5}$$

$$\mathrm{diam}(D_\delta^n) \leq C_\delta \varepsilon_n \text{ for } n \text{ large enough.} \tag{0.6}$$

- Take $x_n \in B_{r_n}$ such that

$$\delta_0 \leq \operatorname{dist}(Q_{\varepsilon_n}(x_n), \mathcal{N}) = \sup_{x \in B_{r_n}} \operatorname{dist}(Q_{\varepsilon_n}(x), \mathcal{N}).$$

  Key Lemma $\Rightarrow \frac{|x_n|}{r_n} \to 0$.

- Define

$$Q_n(x) := Q_{\varepsilon_n}(x_n + \varepsilon_n x), \text{ for } |x| \leq \frac{r_n - |x_n|}{\varepsilon_n}.$$

  Key lemma $\Rightarrow \forall \delta > 0$, $\exists c_\delta > 0$, such that $\operatorname{dist}(Q_n(x), \mathcal{N}) < \delta$, $\forall n$ and $|x| > c_\delta$.

- $Q_n \to Q$ in $C^2_{loc}(\mathbb{R}^3, \mathcal{Q}_0)$, Q locally minimizes the functional $I(\cdot)$,

$$\operatorname{dist}(Q(x), \mathcal{N}) \to 0 \text{ as } |x| \to \infty, \ \deg_\infty(Q) = 1,$$

$$\lim_{R \to \infty} \frac{1}{R} I(Q, B_R) = 8 s_+^2 \pi.$$

Tangent map at infinity

2nd Part. Blow-down analysis: study the weak H^1_{loc} limit of $Q_{R_n}(x) := Q(R_n x)$ for some $R_n \to \infty$. Tangent map of Q at infinity.

- Suppose $Q_{R_n}(x) \rightharpoonup \Psi$ weakly in $H^1_{loc}(\mathbb{R}^3, \mathcal{Q}_0)$. Then $Q_{R_n}(x) \to \Psi(x)$ strongly in H^1_{loc} and $\Psi(x) = s_+(n(x) \otimes n(x) - \frac{1}{3}\mathrm{Id})$, where $n(x) = T\frac{x}{|x|}$ for $T \in O(3)$.

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- The tangent map of Q at infinity is unique. i.e.

$$\lim_{R\to\infty} \|Q_R|_{\mathbb{S}^2} - \Psi|_{\mathbb{S}^2}\|_{C^k(\mathbb{S}^2)} = 0, \quad \forall k \in \mathbb{N}^+$$

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- The tangent map at infinity Ψ coincides with the map Φ which is the asymptotic profile of n_* near the singularity.
  Key: estimate of radial derivative: $\exists C > 0$ such that for any n and $R \le \frac{r_n}{2\varepsilon_n}$,

$$R^4 \int_{\{R\varepsilon_n \le |x| \le 2R\varepsilon_n\}} \frac{1}{r} \left| \frac{\partial Q_{\varepsilon_n}(x+x_n)}{\partial r} \right|^2 dx \le C.$$

3rd Part. Let $B_r(x_0) \cap \mathcal{S}(n_*) = \{x_0\}$. Then for any sequence $R_n \uparrow \infty$ and satisfying $R_n \varepsilon_n < r$, there holds

$$\lim_{n\to\infty} \left(\sup_{R_n\varepsilon_n \le |x| \le r} |Q_{\varepsilon_n}(x_n + x) - Q_*(x_0 + x)| \right) = 0.$$

Sketch of proof. Argue by contradiction, suppose $\exists \{\varepsilon_n\}$, $\{y_n\}$ such that

$$\lim_{n\to\infty} \frac{|y_n|}{\varepsilon_n} = \infty, \quad |Q_{\varepsilon_n}(y_n + x_n) - Q_*(y_n)| \ge \delta > 0.$$

On the one hand,

$$\lim_{n\to\infty} |Q_*(y_n) - \Phi(y_n)| = 0, \quad \Phi(y_n) = s_+(\frac{y_n}{|y_n|} \otimes \frac{y_n}{|y_n|} - \frac{1}{3}\mathrm{Id})$$

On the other hand, we define $Z_n := Q_{\varepsilon_n}(|y_n|x + x_n)$, then $Z_n(x) \to \Phi(x)$ strongly in $H^1(B_2) \cap C^2(B_2 \setminus B_{1/2})$ and therefore

$$\lim_{n\to\infty} |Q_{\varepsilon_n}(y_n + x_n) - \Phi(y_n)| = 0,$$

which yields a contradiction.

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- Typical biaxial core structures: the half-degree ring disclination and the split-core solution. see e.g. Yu(2020), Dipasquale-Millot-Pisante(2020,2021), Tai-Yu(2021).

Thank You!