Local minimizer and De Giorgi's type conjecture for the isotropic-nematic interface

Zhifei Zhang

School of Mathematical Sciences, Peking University

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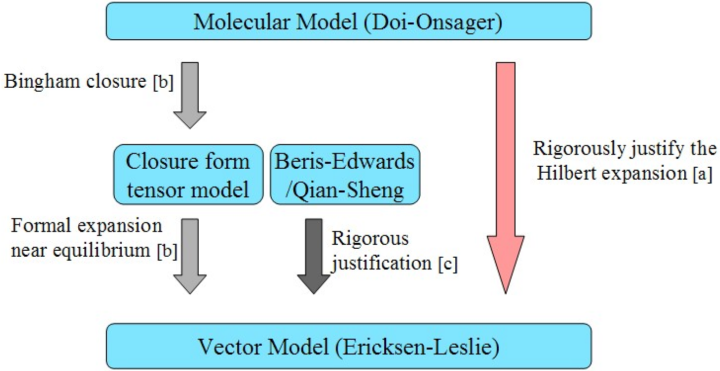
There are three different kinds of theories to model the nematic liquid crystal:

- **Onsager molecular theory**: use a distribution function $f(\mathbf{x}, \mathbf{m})$ to represent the number density for the number of molecules whose orientation is parallel to $\mathbf{m}$ at point $\mathbf{x}$.
- **Landau-de Gennes Q-tensor theory**: use a symmetric traceless tensor $Q(\mathbf{x})$ to describe the orientation of molecules:

$$Q(\mathbf{x}) = \int_{\mathbb{S}^2} f(\mathbf{x}, \mathbf{m})\big(\mathbf{m}\mathbf{m} - \frac{1}{3}\mathbf{I}\big)\mathrm{d}\mathbf{m}.$$

- **Oseen-Frank vector theory**: use a direction field $\mathbf{n}(\mathbf{x})$ to describe the average alignment direction of the molecules at $\mathbf{x}$.

Consistency between the dynamical models



[a] W. Wang, P. Zhang, Z. Zhang, *The small Deborah number limit of the Doi-Onsager equation to the Ericksen-Leslie equation*, CPAM 2015

[b] J. Han, Y. Luo, W. Wang, P. Zhang, Z. Zhang, *From microscopic theory to macroscopic theory: a systematic study on modeling for liquid crystals*, ARMA 2015.

[c] W. Wang, P. Zhang, Z. Zhang, *Rigorous derivation from Landau-de Gennes theory to Ericksen-Leslie theory* , SIAM JMA 2015

[d] W. Wang, P. Zhang, Z. Zhang, *Well-posedness of the Ericksen-Leslie system*, ARMA 2013.

Main ingredients of the proof

To prove the consistency between Doi-Onsager model and Ericksen-Lesile model, the main ingredients are as follows:

- Hilbert expansion:

$$f^{\varepsilon}(\mathbf{x},\mathbf{m},t)=\sum_{k=0}^{3}\varepsilon^{k}f_k(\mathbf{x},\mathbf{m},t)+\varepsilon^{3}f_R^{\varepsilon}(\mathbf{x},\mathbf{m},t),$$

$$v^{\varepsilon}(\mathbf{x},t)=\sum_{k=0}^{2}\varepsilon^{k}v_k(\mathbf{x},t)+\varepsilon^{3}v_R^{\varepsilon}(\mathbf{x},t).$$

- The equilibrium $f_0=f_0(\mathbf{n}\cdot\mathbf{m})$(Liu-Zhang-Zhang, CMS 2005):

$$A[f]=\int_{\mathbb{S}^2}\Big(f(\mathbf{m})\ln f(\mathbf{m})+\frac{1}{2}f(\mathbf{m})\mathcal{U}f(\mathbf{m})\Big)\mathrm{d}\mathbf{m}.$$

- The spectral analysis of the linearized operator around f_0.
- Uniform estimates of (f_R, v_R).

Remark. $(v_0,\mathbf{n})$ satisfies the Ericksen-Lesile system.

- Use a symmetric traceless tensor $Q(\mathbf{x})$ to describe the orientation of molecules:
  - Q=0: $\Rightarrow$ isotropic;
  - Q has two equal eigenvalues: $Q = s\big(\mathbf{nn} - \frac{1}{3}\mathbf{I}\big)$, $\mathbf{n} \in \mathbb{S}^2$. $\Rightarrow$ uniaxial;
  - Q has three different eigenvalues:

$$Q = s\big(\mathbf{nn} - \frac{1}{3}\mathbf{I}\big) + \lambda(\mathbf{n}'\mathbf{n}' - \frac{1}{3}\mathbf{I}), \quad \mathbf{n}, \mathbf{n}' \in \mathbb{S}^2, \quad \mathbf{n} \cdot \mathbf{n}' = 0.$$

  $\Rightarrow$biaxial;

- The Landau-de Gennes energy:

$$F^{(LG)}[Q] = \int_\Omega \underbrace{\left(\frac{a}{2}\mathrm{tr}(Q^2) - \frac{b}{3}\mathrm{tr}(Q^3) + \frac{c}{4}(\mathrm{tr}Q^2)^2\right)}_{F_{bulk}} \mathrm{d}\mathbf{x}$$
$$+ \frac{1}{2}\int_\Omega \underbrace{\left(L_1|\nabla Q|^2 + L_2 Q_{ij,j}Q_{ik,k} + L_3 Q_{ik,j}Q_{ij,k} + L_4 Q_{lk}Q_{ij,k}Q_{ij,l}\right)}_{F_{elastic}} \mathrm{d}\mathbf{x}.$$

Take $L_4 = 0$ to ensure that the energy has a lower bound(Ball-Majumdar, 2010). The L_2 term and L_3 term differ from only a boundary term, so we take $L_3 = 0$.

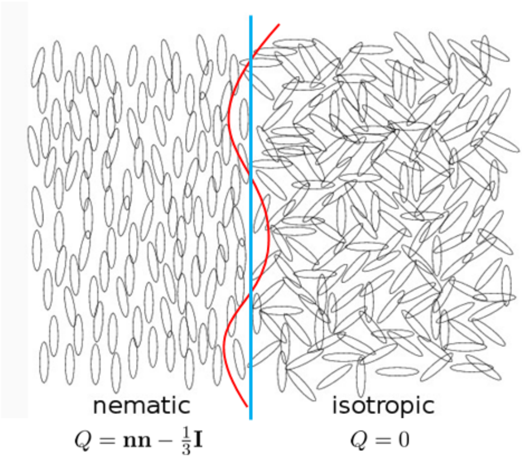
- Critical points of F_{bulk}:

$$Q = 0 \quad \text{or} \quad Q = s^{\pm}(\mathbf{nn} - \frac{1}{3}\mathbf{I}),$$

where $s^{\pm}$ are the solutions of $3a - bs + 2cs^2 = 0$, i.e.,

$$s^{\pm} = \frac{b \pm \sqrt{b^2 - 24ac}}{4c}.$$

- Stability of critical point: if $0 < a < \frac{b^2}{24c}$, then $Q = 0$ and $Q = s^{+}(\mathbf{nn} - \frac{1}{3}\mathbf{I})$ are stable, while $Q = s^{-}(\mathbf{nn} - \frac{1}{3}\mathbf{I})$ is unstable.
- We impose $b^2 = 27ac$ so that the bulk energy of two stable phases are equal. After a scaling if necessary, we may choose $a = 1/3, b = 3, c = 1$ so that $s^{+} = 1$ and $s^{-} = \frac{1}{2}$.



I-N interface problem: study the configuration in which the two phases $Q = 0$ and $Q = \mathbf{nn} - \frac{1}{3}\mathbf{I}$ coexist?

The elastic energy will prevent instantaneous jump from one phase to another one. The transition between two phases appears in a thin region of the width $\sqrt{L_1}$. Thus, we introduce $Q(x) = \widetilde{Q}(x/\sqrt{L_1})$. Letting $L_1 \to 0$, the limiting energy functional takes

$$\mathcal{F}(Q) = \int_{\mathbb{R}^3} \Big(\frac{1}{6}\mathrm{tr}(Q^2) - \mathrm{tr}(Q^3) + \frac{1}{4}(\mathrm{tr}Q^2)^2 + \frac{1}{6}|\nabla Q|^2 + \frac{L}{4} Q_{ij,j} Q_{ik,k} \Big) \mathrm{d}\mathbf{x}.$$

Minimization problem:

$$\min_Q \mathcal{F}(\mathcal{Q})$$

among all symmetric traceless tensor Q satisfying the boundary condition:

$$Q(x_1, x_2, -\infty) = 0, \quad Q(x_1, x_2, +\infty) = \mathbf{nn} - \frac{1}{3}\mathbf{I}. \tag{1}$$

The Euler-Lagrange equation($L = 0$) takes

$$-\Delta\mathbf{Q} + \mathbf{Q} - 9\mathbf{Q}^2 + 3|\mathbf{Q}|^2\mathbf{Q} + 3|\mathbf{Q}|^2\mathbf{I} = 0. \tag{2}$$

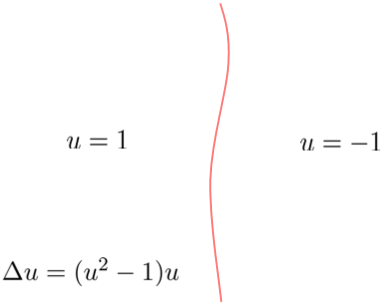
Allen-Cahn equation

Energy functional:

$$E_\varepsilon(v_\varepsilon) = \int_\Omega \frac{\varepsilon}{2}|\nabla v_\varepsilon|^2 + \frac{1}{4\varepsilon}(1 - v_\varepsilon^2)^2 dx.$$

The constant functions $v = \pm 1$ minimize the functional E_ε.

Phase transition problem: study the configurations in which the two phases ± 1 coexist?



- $N = 1$: the function $w(t) = \tanh\left(\frac{t}{\sqrt{2}}\right)$ solves (AC) with the boundary condition $w(\pm\infty) = \pm 1$.
- for any $y, e \in \mathbf{R}^N$, the family

$$u(x) = w((x - y) \cdot e)$$

  solves (AC).
- In 1978, De Giorgi made the following conjecture:

  Let u be a bounded solution of the Allen-Cahn equation, which is monotone in one direction. Then, at least when $N \leq 8$, there exists $y, e \in \mathbf{R}^N$ so that

$$u(x) = w((x - y) \cdot e).$$

  Equivalently, all level sets of u must be hyperplanes.

This conjecture was solved by Ghoussoub and Gu($N = 2$), Ambrosio-Cabré($N = 3$), and Savin($4 \leq N \leq 8$).

We write

$$Q(z) = \lambda_1 \mathbf{n}_1\mathbf{n}_1 + \lambda_2 \mathbf{n}_2\mathbf{n}_2 + \lambda_3 \mathbf{n}_3\mathbf{n}_3, \quad \text{where } \mathbf{n}_i(z)\cdot\mathbf{n}_j(z) = \delta^i_j,$$

with $\lambda_1 + \lambda_2 + \lambda_3 = 0$. Then

$$\mathcal{F}(Q) \geq F(diag\{\lambda_1, \lambda_2, \lambda_3\}).$$

Thus, we may assume

$$Q = diag\Big\{ -\frac{S+T}{3}, -\frac{S-T}{3}, \frac{2S}{3}\Big\}.$$

The energy $\mathcal{F}(Q)$ reduces to

$$\begin{aligned}\mathcal{F}(S,T) =& \frac{2}{9}\int \Big(\frac{1}{6}\big[3(S')^2 + (T')^2\big] \\ &+ \frac{1}{6}(3S^2 + T^2) - S(S^2 - T^2) + \frac{1}{18}(3S^2 + T^2)^2\Big)\mathrm{d}z,\end{aligned}$$

with $S(-\infty) = T(\pm\infty) = 0, S(+\infty) = 1.$

Euler-Lagrange equations:

$$-S'' + S - 3S^2 + T^2 + 2S(3S^2 + T^2)/3 = 0,$$
$$-T'' + T + 6ST + 2T(3S^2 + T^2)/3 = 0.$$

Explicit (uniaxial) solution:

$$S(x) = 1 - (1 + \exp(x - t))^{-1}, \quad T(x) = 0.$$

Theorem (Park-Wang-Zhang-Z, CVPDE 2017)

The global minimizer of $\mathcal{F}(Q)$ must take the form

$$Q(s) = \frac{1}{2}(1 + \tanh\frac{1}{2}(s - t))(\mathbf{nn} - \frac{1}{3}\mathbf{I}), \tag{3}$$

where t is an arbitrary parameter.

Question: Is the uniaxial solution the only solution of all the local minimizers?

Theorem (Chen-Zhang-Z 2017)

All the local minimizers of $\mathcal{F}(Q)$ must take the form (3). In fact, (3) gives all solutions of (2)-(1) in 1-D.

Difficulty: For the global minimizer, one can reduce Q to a diagonal form. For the local minimizer, we have to consider the general form:

$$Q = \lambda_1 \mathbf{n}_1\mathbf{n}_1 + \lambda_2 \mathbf{n}_2\mathbf{n}_2 + \lambda_3 \mathbf{n}_3\mathbf{n}_3,$$

where $\mathbf{n}_i(z) \cdot \mathbf{n}_j(z) = \delta_j^i$.

Key ingredients of the proof:

- Introduce two quantities: $A(x) = |Q(x)|^2$ and $B(x) = |Q'(x)|^2$

$$A'' = -A + 5B + \frac{3}{2}A^2, \quad B(\pm\infty) = 0, \quad A(-\infty) = 0, \quad A(+\infty) = \frac{2}{3}.$$

- $B \geq A - \sqrt{6}A^{3/2} + \frac{3}{2}A^2$ and the equality holds if and only if $\lambda_i = 2a$ and $\lambda_j = -a$ for $j \neq i$.
- $0 < A < \frac{2}{3}$ and $A'(x) > 0$.
- $A''(x) = 4A - 5\sqrt{6}A^{3/2} + 9A^2$, which implies that

$$B = A - \sqrt{6}A^{3/2} + \frac{3}{2}A^2.$$

- Assume that $\lambda_1 = \lambda_2 = -\frac{S(x)}{3}$ and $\lambda_3 = \frac{2S(x)}{3}$. Then we prove that $\mathbf{n}_3(x)$ is a constant vector $\mathbf{n}$.

For the case of $L \neq 0$, the problem becomes more complex. In this case, the direction vector $\mathbf{n}$ on the anchoring condition at $+\infty$ could make a significant effect on the behavior for the minimizers. There are three different types of the alignment director $\mathbf{n}$ on the boundary as below:

1. Homeotropic anchoring: $\mathbf{n} \cdot (0,0,1) = 1$;
2. Planar anchoring: $\mathbf{n} \cdot (0,0,1) = 0$;
3. Tilt anchoring: $0 < \mathbf{n} \cdot (0,0,1) < 1$.

For simplicity, we will first seek minimizers of the diagonal form

$$Q = \begin{pmatrix} -\frac{1}{3}(S+T) & 0 & 0 \\ 0 & -\frac{1}{3}(S-T) & 0 \\ 0 & 0 & \frac{2}{3}S \end{pmatrix}, \tag{4}$$

which is meaningful due to the rotation invariant of the bulk energy.

In 1-D, the energy functional is reduced to

$$\mathcal{F}_L(S,T) = \frac{2}{9}\int_{\mathbb{R}}\Big(\frac{1+L}{2}(S')^2 + \frac{1}{6}(T')^2 + \frac{1}{6}(3S^2+T^2) - S(S^2-T^2) + \frac{1}{18}(3S^2+T^2)^2\Big)\mathrm{d}s.$$

The associated Euler-Lagrange equation takes

$$\begin{cases} -\frac{1+L}{2}S'' + \frac{S}{2} - \frac{3S^2}{2} + \frac{T^2}{2} + \frac{S(3S^2+T^2)}{3} = 0, \\ -\frac{1}{6}T'' + \frac{T}{6} + ST + \frac{T(3S^2+T^2)}{9} = 0. \end{cases} \tag{5}$$

Here we consider the homeotropic anchoring condition, which leads to the following boundary conditions for (S,T):

$$S(+\infty) = 1, \quad T(+\infty) = S(-\infty) = T(-\infty) = 0. \tag{6}$$

It is obvious that (5)-(6) has a uniaxial solution with $T = 0$ and $S(s)$ solving

$$-(1+L)S'' + S - 3S^2 + 2S^3 = 0.$$

That is, an uniaxial equilibrium state takes

$$\mathbf{Q}_0(s) = S(s)\mathrm{diag}\Big\{-\frac{1}{3}, -\frac{1}{3}, \frac{2}{3}\Big\}, \quad S(s) = S^*(s/\sqrt{1+L}),$$

where S^* solves

$$-S'' + S - 3S^2 + 2S^3 = 0, \quad S(-\infty) = 0, \ S(+\infty) = 1. \tag{7}$$

Theorem (Park-Wang-Zhang-Z, CVPDE 2017)

The uniaxial equilibrium state $\mathbf{Q}_0$ *is stable for the energy functional* $\mathcal{F}(Q)$ *when* $L \leq 0$ *and unstable when* $L > 0$.

Conclusion: the stable solution subject to the homeotropic anchoring must be biaxial when $L > 0$.

Questions:

- When $L < 0$, is there any other solution?
- When $L > 0$, the profile of the stable (biaxial) solution?

Partial progress:

Theorem (Chen-Zhang-Z 2017)

For all $L > -1$, the ODE system (5)-(6) *has only one solution*

$$T(x) \equiv 0, \quad S(x) = S^*(\frac{x}{\sqrt{1+L}}),$$

where S^* solves (7).

Conclusion: the stable solution subject to the homeotropic anchoring can not be of the diagonal form (4) when $L > 0$.

Motivated by De Giorgi's conjecture, we propose the following **generalized De Giorgi's conjecture(GDC)**:

Let $\mathbf{Q}$ *be symmetric, traceless and a bounded solution of* (2)-(1)*. Let* λ_3 *be the largest eigenvalue of* Q*. If* $\partial_{x_3}\lambda_3 > 0$*, then all level sets* $\{x \in \mathbf{R}^3 : Q_{ij}(x) = s\}$ *must be hyperplanes.*

Remark.

- Compared with the Allen-Cahn equation, this conjecture seems more difficult, since (2) is a system with five independent components.
- When $L \neq 0$, it remains unclear what is the right version of De Giorgi's conjecture?

Under the assumption that the eigenvector of Q corresponding to the largest eigenvalue is a constant vector, we can give an affirmative answer to GDC.

Theorem (Chen-Zhang-Z 2017)

The level set of global solutions of (2)-(1) *satisfying* $\mathbf{n}_3(x_1, x_2, x_3) \equiv \mathbf{n}$ *and* $\partial_{x_3}\lambda_3 > 0$ *are hyperplanes in* $\mathbf{R}^3$. *Moreover,*

$$\mathbf{Q}(x_1, x_2, x_3) = S(x_3)(\mathbf{nn} - \frac{1}{3}\mathbf{I}).$$

Key point: In this case, we can reduce the system to a PDE system of the form:

$$\Delta S = S - 3S^2 + T^2 + \frac{2S(3S^2 + T^2)}{3},$$
$$\Delta T = 4|\mathbf{n}_1 \cdot \nabla \mathbf{n}_2|^2 \cdot T + T + 6ST + \frac{2T(3S^2 + T^2)}{3}.$$

Key lemma: If $0 \leq S \leq M$ for some $M > 0$, then $T \equiv 0$.

The gradient flow of Landau-de Gennes energy:

$$Q_t^\varepsilon = -\frac{1}{\varepsilon^2} f(Q^\varepsilon) + \mathcal{L}Q^\varepsilon,$$

where

$$f(Q) = aQ - bQ^2 + c|Q|^2 Q + \frac{b}{3}|Q|^2 \mathbf{I},$$

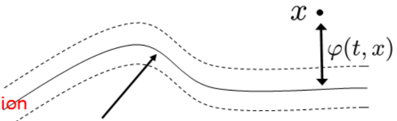
and

$$(\mathcal{L}Q)_{kl} = L_1 \Delta Q_{kl} + \frac{1}{2}(L_2 + L_3)\big(Q_{km,ml} + Q_{lm,mk} - \frac{2}{3}\delta_{kl} Q_{ij,ij}\big).$$

Goal: study the behaviour of the solution Q^ε as $\varepsilon \to 0$.

Outer expansion in isotropic region

$$\mathbf{Q}(t,x)=\mathbf{Q}_-^{(0)}(t,x)+\varepsilon\mathbf{Q}_-^{(1)}+\cdots$$



$$z=\frac{\varphi(t,x)}{\varepsilon}$$

Inner expansion in transition region

$$\widetilde{\mathbf{Q}}(t,x,z)=\widetilde{\mathbf{Q}}^{(0)}(t,x,z)+\varepsilon\widetilde{\mathbf{Q}}^{(1)}(t,x,z)+\cdots$$

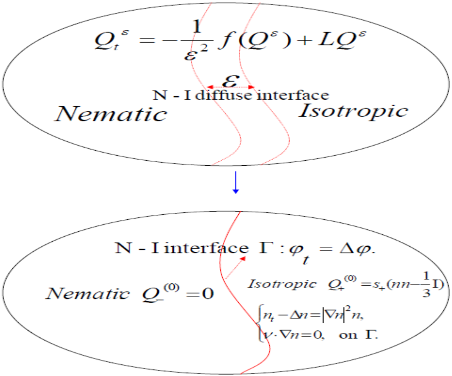
Outer expansion in nematic region

$$\mathbf{Q}(t,x)=\mathbf{Q}_+^{(0)}(t,x)+\varepsilon\mathbf{Q}_+^{(1)}+\cdots$$

Inner-Outer Matching Condition

$$\widetilde{\mathbf{Q}}(t,x,z)=\mathbf{Q}_\pm^{(0)}(t,x),\quad \text{as } z\to\pm\infty.$$

In the case when $L_1 = 1, L_2 = L_3 = 0$, as $\varepsilon \to 0$,



M. Fei, W. Wang, P. Zhang, Z. Zhang, SIAM J. Appl. Math., 75(2015), 1700-1724.

Let $Q_R^\varepsilon = Q^\varepsilon - Q_A^\varepsilon$. Then we have

$$\frac{1}{2}\partial_t \int_\Omega |Q_R^\varepsilon|^2 dx + \int_\Omega \Big(|\nabla Q_R^\varepsilon|^2 + \varepsilon^{-2}\big(f'(Q_A^\varepsilon)Q_R^\varepsilon : Q_R^\varepsilon\big)\Big) dx$$
$$= -\frac{1}{2}\varepsilon^{-2}\int_\Omega (f''(Q_A^\varepsilon + \theta Q_R^\varepsilon) Q_R^{\varepsilon\,2} : Q_R^\varepsilon) dx - \int_\Omega (Q_B^\varepsilon : Q_R^\varepsilon) dx.$$

The key ingredient is to establish the spectral lower bound:

Theorem

There exists a positive constant C independent of ε so that

$$\int_\Omega \big(|\nabla Q|^2 + \varepsilon^{-2}(f'(Q_A^\varepsilon)Q : Q)\big) dx \geq -C \int_\Omega |Q|^2 dx$$

for any traceless and symmetric 3×3 matrix Q.

M. Fei, W. Wang, P. Zhang, Z. Zhang, preprint 2017.

- 1-D problem with $L = 0$: all local minimizers must take the form

$$Q(s) = \frac{1}{2}(1 + \tanh\frac{1}{2}(s - t))(\mathbf{nn} - \frac{1}{3}\mathbf{I}).$$

- 1-D problem with $L \leq 0$ and homeotropic anchoring: the uniaxial equilibrium state $\mathbf{Q}_0 = S(s)\mathrm{diag}\Big\{ -\frac{1}{3}, -\frac{1}{3}, \frac{2}{3}\Big\}$ is stable.
- 1-D problem with $L > 0$ and homeotropic anchoring: the stable solution can not be of the diagonal form.
- 3-D problem with $L = 0$: we propose the generalized De Giorgi's conjecture, and gave a positive answer when the eigenvector of Q corresponding to the largest eigenvalue is a constant vector.
- Sharp interface model without hydrodynamics.

Open problems

- Which profile is stable for 1-D problem with $L \leq 0$ and planar (or tilt) anchoring?
- Which profile is stable for 1-D problem with $L > 0$ and homeotropic (or planar, tilt) anchoring?
- Generalized De Giorgi's conjecture when $L = 0$?
- What is the right version of De Giorgi's conjecture when $L \neq 0$?
- Sharp interface model with hydrodynamics and $L \neq 0$.

Thanks for Your Attention!