Analysis of topological defects in nematic liquid crystals

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VIASM-IAMP Summer School - Quy Nhon - August 1st-5th, 2023

Abstract

In these lectures, we discuss recent progresses and challenges in the study of defects in mathematical theories of nematic liquid crystals. We will start with a brief survey of topological point defects for vector-valued maps in Oseen-Frank and Ginzburg-Landau theories. We then move on with tensor-valued maps in Landau-de Gennes theory, which have been studied more intensively recently. The lectures will focus on aspects related to minimality, stability, uniqueness, and symmetry of stationary solutions.

1 Lecture 1: Mathematical models for nematic liquid crystals

Liquid crystals are ubiquitous in our daily life, from the displays to even food coloring, and it's a multi-billion industry. Physically, liquid crystals is an intermediate state between fluids and solid: it flows like a fluid but the molecules retain an orientational order. The mathematics of liquid crystals involves a variational functional of the form

$$\int_\Omega f(x, u(x), \nabla u(x))\, dx$$

where u is a vector-valued map, called the order parameter, and $\Omega \subset \mathbb{R}^2$ or $\mathbb{R}^3$ is a domain (container) which is filled with liquid crytals.

Liquid crystals are of many different types, the most popular ones are nematics, cholesterics and smectics. Depending on the types of molecules, their interaction and the temperature, the molecules can arrange themselves into different phases

- isotropic: no orientational order.

- nematic: orientational but no positional order
- smectics: orentational and positional order
- cholesterics: the mean orientational order rotates in a helical manner.

In these lectures, we will only discuss nematics where the molecules are rod-like with length about a couple of nanometers. We will only consider the case of staticity where the fluid velocity is zero.

1.1 Director model

Perhaps the simplest mathematical description of nematics is to reprensent the mean orientation around a position x by a unit vector $n(x)$. A typical variational functional for this model is the one-constant Oseen-Frank functional

$$I^{OF}[n] = \int_\Omega \frac{1}{2}|\nabla n|^2\,dx, \qquad n : \Omega \to \mathbb{S}^2. \tag{1}$$

Critical point of this functional are $\mathbb{S}^2$-valued harmonic maps. These are very well understood. The Euler-Larange equation is

$$\Delta n = -|\nabla n|^2 n.$$

Note however, for most nematics, n is equivalent to $-n$, so a more realistic model is to identify n with $-n$, resulting in line field model.

1.2 Continuum model

Perhaps the most accurate mathematical description of nematics is to associate with each position x and probability measure μ_x on $\mathbb{S}^2$ which gives the distribution of molecular orientation in a small ball around x. To respect the head-to-tail symmetry, we also need that μ_x is even: $\mu_x(E) = \mu_x(-E)$ for any measurable $E \subset \mathbb{S}^2$.

For example, if the molecules around x are perfectly aligned in a direction e, then $\mu_x = \frac{1}{2}(\delta_e + \delta_{-e})$. If the molecules around x has no orientational order, i.e. isotropic, then $\mu_x = \frac{1}{4\pi}dp$ where dp is the standard measure dp on $\mathbb{S}^2$. If μ_x is absolutely continuous with respect to dp, we can write $\mu_x = \rho(p)dp$ with $\rho(p) = \rho(-p)$ and $\int_{\mathbb{S}^2} f(p)\,dp = 1$.

A lot of work has been done, but the analysis on this model remains largely under-developed.

1.3 Q-tensor model

Another model, which is popular with both mathematicians and physicists, is the Landau-de Genners Q-tensor model. In this model, the only information of the sophisticated probability distribution μ_x which is retained is its second moment. Note that the first moment of μ_x is zero by evenness. The second moment is

$$M = \int_{\mathbb{S}^2} p \otimes p d\mu(p).$$

This is a 3×3 symmetric matrix with unit trace.

For example, in isotropy, $\mu_x = \frac{1}{4\pi} dp$ and $M = M_0 = \frac{1}{3} I_3$.

The de Gennes Q-tensor

$$Q = M - M_0$$

measures the deviation of M from isotropy. This tensor Q has the property that it is symmetric and traceless and furthermore

$$-\frac{1}{3} I_3 \leq Q \leq \frac{2}{3} I_3.$$

This last mathematical property is frequently ignored in many physical as well as mathematical treatments of the theory. The nature of this constraint is very similar to the constraint of positive Jacobian in non-linear elasticity or the constraint of incompressibility in fluid mechanics. Some work on this has been done by Ball and co-authors.

There are other intermediate model where one retains only a mean orientational order unit vector n and a mean scalar order parameter s such as in Ericksen-Leslie model, but we will not consider them in these lectures.

Let $\mathscr{S}_0$ denote the 5-dimensional vector space of symmetric traceless 3×3 matrices. The variational functional for this model is typically

$$I_L^{LdG}[Q] = \int_\Omega \left[\frac{1}{2} |\nabla Q|^2 + \frac{1}{L} f_b(Q) \right] dx, \qquad Q : \Omega \to \mathscr{S}_0. \tag{2}$$

Here $|\nabla Q|^2$ is the elastic energy density that penalizes spatial inhomogeneities, f_b is the bulk energy density that accounts for the bulk effects, and L is a positive constant.

This is usually referred to as the one constant Landau-de Gennes model. A more complete treatment (e.g. for cholesterics, smectics) involves five constants in the elastic term.

A popular expression for f_b takes the form

$$f_B(Q) = -\frac{a^2}{2} \mathrm{tr}(Q^2) - \frac{b^2}{3} \mathrm{tr}(Q^3) + \frac{c^2}{4} [\mathrm{tr}(Q^2)]^2, \tag{3}$$

where a^2 is a temperature-dependent constant and b^2 and c^2 are material-dependent and positive constants. It is well-known that this type of bulk energy density is the simplest form that allows multiple local minima and a first order nematic-isotropic phase transition [de Gennes], [Virga]. This is the truncated Taylor (Landau) expansion of the physical bunk energy density around the isotropic state $Q = 0$.

The Euler-Lagrange equation reads

$$L\Delta Q = -a^2\, Q - b^2(Q^2 - \frac{1}{3}|Q|^2\, Id) + c^2|Q|^2\, Q.$$

Here the term $\frac{1}{3}|Q|^2\, Id$ is a Lagrange multiplier term accounting for the tracelessness constraint.

The size of the constant L is relevant. But this notion of size only makes sense after non-dimensionalization. Consider for example a sample of typical size $10^{-4}m$ of $MBBA$ where one has $a^2, b^2, c^2 \approx 10^4 \frac{J}{m^3}$ and $L \approx 10^{-11} \frac{J}{m}$. One first has to measure measure in the unit of the sample, i.e. rescales the domain $x \mapsto \frac{x}{10^{-4}m}$ so that the sample now has size 1 and is non-dimensionalized, and then divide the whole energy density by a constant (namely $10^4 \frac{J}{m^3}$) so that the new a^2, b^2, c^2 are of size 1 and non-dimensionalized. The new constant L is then non-dimensionalised and $\approx 10^{-7}$.

1.4 Existence and regularity of minimizers

This follows from standard theories as f_b has subcritical nonlinearity.

Theorem 1.1. *Let $Q_b \in H^1(\Omega, \mathscr{S}_0)$. For every $L > 0$, there exists a minimizer of I_L^{LdG} in $H^1_{Q_b}(\Omega, \mathscr{S}_0)$ and this minimizer is smooth (analytic).*

Proof. Existence follows from standard direct argument in calculus of variations. Smoothness follows from standard regularity theories. □

1.5 From the Q-tensor model to the director/line field model

We have said above that the constant L is very small. Heuristically speaking, in order to keep energy as small as possible, it's preferable that $f_b(Q)$ be as small as possible, i.e. Q is close to the set

$$\mathscr{S}_* = \{Q : f_b(Q) = \min f_b\}.$$

Lemma 1.2. *Assume $b^2, c^2 > 0$. The set $\mathscr{S}_*$ is given by*

$$\mathscr{S}_* = \{s_+(n \otimes n - \frac{1}{3}Id) : n \in \mathbb{S}^2\}, s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}.$$

Thus, $\mathscr{S}_*$ is a copy of $\mathbb{R}P^2$ in $\mathscr{S}_0$.

Remark 1.3. *When $b = 0$, the minimizing set of f_b is instead a 4-sphere.*

Proof. Note that the function $f_b(Q)$ depends only on the eigenvalues of Q. Since Q is traceless, we can label its eigenvalue as λ_1, λ_2 and $-\lambda_1 - \lambda_2$. Then

$$f_b(Q) = h(\lambda_1, \lambda_2) = -a^2(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2) + b^2\lambda_1\lambda_2(\lambda_1 + \lambda_2) + c^2(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2)^2.$$

We compute

$$\begin{aligned}\partial_{\lambda_1} h &= -a^2(2\lambda_1 + \lambda_2) - b^2(2\lambda_1\lambda_2 + \lambda_2^2) + 2c^2(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2)(2\lambda_1 + \lambda_2)\\ &= (2\lambda_1 + \lambda_2)\Big[-a^2 + b^2\lambda_2 + 2c^2(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2)\Big],\\ \partial_{\lambda_1} h &= (\lambda_1 + 2\lambda_2)\Big[-a^2 + b^2\lambda_1 + 2c^2(\lambda_1^2 + \lambda_2^2 + \lambda_1\lambda_2)\Big].\end{aligned}$$

The critical points of h are thus

- $\lambda_1 = \lambda_2 = 0$,
- $\lambda_2 = -2\lambda_1$, with λ_1 solving $-a^2 + b^2\lambda_1 + 6c^2\lambda_1^2 = 0$, i.e. $\lambda_1 = \frac{-b^2 \pm \sqrt{b^4 + 24a^2c^2}}{12c^2} =: \lambda_\pm$,
- $\lambda_1 = -2\lambda_2$, with $\lambda_2 = \frac{-b^2 \pm \sqrt{b^4 + 24a^2c^2}}{12c^2}$,
- $\lambda_1 = \lambda_2 = \lambda_\pm$.

Note that the last three cases are equivalent at the Q-tensor level: it means that Q has eigenvalues $(\lambda_\pm, \lambda_\pm, -2\lambda_\pm)$ and thus can be written as

$$Q = s_\mp(n \otimes n - \frac{1}{3}I_3), \quad n \in \mathbb{S}^2, s_\mp = \frac{b^2 \mp \sqrt{b^4 + 24a^2c^2}}{4c^2}.$$

As $h(\lambda_1, \lambda_2) \to \infty$ as $|(\lambda_1, \lambda_2)| \to \infty$, we only need to compare $h(0) = 0$ and

$$\begin{aligned}h(\lambda_\pm, \lambda_\pm) &= -3a^2\lambda_\pm^2 - 2b^2\lambda_\pm^3 + 9c^2\lambda_\pm^4\\ &= \lambda_\pm^2[2(-a^2 + b^2\lambda_\pm + 6c^2\lambda_\pm) - a^2 - 12\lambda_\pm^2]\\ &= -\lambda_\pm^2(a^2 + 12\lambda_\pm^2).\end{aligned}$$

As $|\lambda_-| > |\lambda_+|$ we deduce that the mininum value of h is $h(\lambda_-, \lambda_-)$. Returning to Q, this means that $f_b(Q)$ is minimised by $Q = s_+(n \otimes n - \frac{1}{3}I_3)$ with $n \in \mathbb{S}^2$. □

The following results are proven for $\Omega \subset \mathbb{R}^3$.

- Majumdar-Zarnescu '10: Given a smooth boundary data $Q_b : \Omega \to \mathscr{S}_*$, the minimizers Q_L of I_{LdG} on $H^1(\Omega; \mathscr{S}_0)$ converges in H^1 along subsequence to some minimizing harmonic map $Q_* : \Omega \to \mathscr{S}_*$.

- N.-Zarnescu '13: away from the singularity of Q_*, the H^1 convergence of Q_L to Q_* is actually in any C^k.
- Ball-Zarnescu '11: If Ω is simply connected, $Q_* = s_+(n_* \otimes n_* - \frac{1}{3}Id)$ for some minimizing harmonic map $n_* : \Omega \to \mathbb{S}^2$.
- Schoen-Uhlenbeck '82, 83: n_* is smooth away finitely many singularity points.
- Brezis-Coron-Lieb '86: near each singularity, $n_* = \pm\frac{Rx}{|x|}$ where R is a rotation.

Let us prove the statement of Majumdar-Zarnescu.

Proof. For $L > 0$, let Q_L be the minimizer of $I_L^{LdG} = I_L$ in $H^1_{Q_b}(\Omega, \mathscr{S}_0)$. It's more convenient to work with an equivalent functional

$$\tilde{I}_L[Q] = \int_\Omega \Big[\frac{1}{2}|\nabla Q|^2 + \frac{1}{L}(f_b(Q) - \min f_b)\Big]\,dx$$

which has a positive integrand. Clearly, I_L differs from $\tilde{I}_L$ by a constant, so Q_L also minimizes $\tilde{I}_L$.

Taking Q_b as a competitor we have

$$I_L[Q_L] \le I_L[Q_b] = \int_\Omega \frac{1}{2}|\nabla Q_b|^2\,dx =: C.$$

which implies that ∇Q_L is bounded in L^2 and, by Poincare's inequality, Q_L is bounded in H^1.

Passing to a subsequence and using embedding theorems, we can assume that Q_L converges weakly in H^1, strongly in L^2 and pointwise a.e. to a limit map Q_*. By weak lower semi-continuity,

$$\int_\Omega \frac{1}{2}|\nabla Q_*|^2\,dx \le \liminf \int_\Omega \frac{1}{2}|\nabla Q_L|^2\,dx \le \liminf I_L[Q_L].$$

Also, note that

$$\frac{1}{L}\int_\Omega (f_b(Q_L) - \min f_b)\,dx \le I_L[Q_L] \le C.$$

This means that $f_b(Q_L) - \min f_b \to 0$ in L^1. By Fatou's lemma, this implies

$$\int_\Omega (f_b(Q_*) - \min f_b) \le 0.$$

But since the integrand on the left hand side is non-negative, we have $f_b(Q_*) = \min f_b$, i.e. $Q_* \in \mathscr{S}_*$ almost everywhere. Taking Q_* as a competitor, we have

$$I_L[Q_L] \le I_L[Q_*] = \int_\Omega \frac{1}{2}|\nabla Q_*|^2\,dx.$$

Therefore, we must have

$$\int_\Omega \frac{1}{2}|\nabla Q_*|^2\,dx = \liminf \int_\Omega \frac{1}{2}|\nabla Q_L|^2\,dx (= \liminf I_L[Q_L]).$$

This together with the weak convergence in H^1 implies that Q_L converges strongly in H^1 to Q_*.

Finally, if $Q \in H^1(\Omega, \mathscr{S}_*)$, then

$$\int_\Omega \frac{1}{2}|\nabla Q_*|^2\,dx = \liminf I_L[Q_L] \le \liminf I_L[Q] = \int_\Omega \frac{1}{2}|\nabla Q|^2\,dx,$$

i.e. Q_* is a $\mathscr{S}_*$-valued minimizing harmonic map. □

1.6 3D defects

In the the director model defects are defined as discontinuity of the director field. In 3D, by Brezis-Coron-Lieb, each defect looks like $\frac{x}{|x|}$, up to a rotation.

In the Q-tensor model, it's challenging to have a simple mathematical definition of a defect, even though it can be seen with naked eyes. From regularity point of view, it may make sense to define it as discontinuity of eigenvectors (not of Q_L as Q_L is analytic), but this is not wholly accepted. We refers to these as optical defects. Ignoring the issue of the definition, it is valid to ask the question of the structure of Q_L near a singular point (defect) of the limit map Q_* when L is small.

Let us pose the mathematical question we would like to discuss in these lectures: Let $\Omega = B$ be the unit ball and let the boundary map be given by

$$Q_b(x) = s_+(\frac{x}{|x|} \otimes \frac{x}{|x|} - \frac{1}{3}Id) =: s_+\bar{H}(x).$$

The map $\bar{H}$ is called the hedgehog. We aim to study property of minimizers Q_L of I_L subjected to Q_b.

Conjecture 1.4. *Minimizers of the Landau-de Gennes functional I_L subjected to the radially symmetric boundary condition*

$$Q_b(x) = s_+\,\bar{H}(x) \text{ on } \partial B$$

with sufficiently small L are axially symmetric but not radially symmetric.

Closely related to this connection is the following open problem:

Open Problem 1.5. *Classify entire (minimizing) critical points of I_1 on $\Omega = \mathbb{R}^n$ subjected to the boundary condition*

$$\lim_{|x|\to\infty} Q(x) - s_+\bar{H}(x) = 0.$$

State of art:

- There exists a unique radially symmetric critical point of the form $u(|x|)\bar{H}(x)$.
- The radially symmetric critical point is unstable for $a \gg 1$ (Gartland-Mkkadem '99) and stable for $a \ll 1$ (Ignat, N., Slastikov, Zarnescu '14).
- When the radially symmetric critical point is unstable, minimizers are not radially symmetric, but it is not known what symmetry property they have. Some recent results on axially symmetric critical points have been obtained by Yu '20, Dipasquale, Millot and Pisante '20, Pisante '21.
- When the radially symmetric critical point is stable, existence of another critical point is not known.

In the next lectures, I will not discuss these problem. I will instead discuss the analogous question for Ginzburg-Landau theory of superconductivity and the 2D Landau-de Gennes model, where more has been achieved.

2 Lecture 2: Ginzburg-Landau theory of superconductivity

In this lecture, we consider instead a related model in superconductivity which has been studied extensively in the last 30 years.

Consider the Ginzburg-Landau functional

$$E_\varepsilon[u] = \int_{B^N} \left[\frac{1}{2}|\nabla u|^2 + \frac{1}{4\varepsilon^2}(1-|u|^2)^2\right] dx$$

for vector fields $u : B^N \to \mathbb{R}^N$, $N \geq 2$.

As in the previous lecture it can be shown that, as $\varepsilon \to 0$ and under suitable boundary condition, the minimizer of E_ε converges to an $\mathbb{S}^{N-1}$-valued minimizing harmonic maps. In the particular case of boundary value $u(x) = x$ on ∂B^N, the limit map is exactly $\frac{x}{|x|}$.

Theorem 2.1 (Brezis, Coron, Lieb '86, Lin '87, see also Hélein '87)**.** *Let $N \geq 3$. The map $\frac{x}{|x|}$ is the unique minimizing harmonic map from B^N into $\mathbb{S}^{N-1}$ taking on value x at ∂B^N.*

Proof. Let $u : B^N \to \mathbb{S}^{N-1}$. Observe that $u_j \partial_i u_j = 0$ and so $\nabla u : (u \otimes u) = 0$. Here $:$ denotes denote the Frobenius product of matrices. We compute

$$\begin{aligned}|\nabla u|^2 &= \frac{1}{N-1}(\nabla \cdot u)^2 + \left|\nabla u - \frac{1}{N-1}\nabla \cdot u(I_N - u \otimes u)\right|^2 \\ &= \frac{1}{N-1}(\nabla \cdot u)^2 + \frac{1}{4}|\nabla u - (\nabla u)^T|^2 \\ &\quad + \left|\frac{1}{2}(\nabla u + (\nabla u)^T) - \frac{1}{N-1}\nabla \cdot u(I_N - u \otimes u)\right|^2.\end{aligned}$$

Hence

$$\begin{aligned}&(N-1)|\nabla u|^2 - (\nabla \cdot u)^2 - \frac{1}{2}|\nabla u - (\nabla u)^T|^2 \\ &\quad = \frac{N-3}{4}|\nabla u - (\nabla u)^T|^2 + (N-1)\left|\frac{1}{2}(\nabla u + (\nabla u)^T) - \frac{1}{N-1}\nabla \cdot u(I_N - u \otimes u)\right|^2 \\ &\quad \geq 0.\end{aligned}$$

Also, note that

$$|\nabla u|^2 - (\nabla \cdot u)^2 - \frac{1}{2}|\nabla u - (\nabla u)^T|^2 = \sum_{i,j}(\nabla_i u_j \nabla_j u_i - \nabla_i u_i \nabla_j u_j) = \sum_{i,j}\nabla_i(u_j \nabla_j u_i - u_i \nabla_j u_j).$$

We thus have

$$
\begin{aligned}
0 &\le \int_{B^N} \left\{(N-2)|\nabla u|^2 + [|\nabla u|^2 - (\nabla \cdot u)^2 - \frac{1}{2}|\nabla u - (\nabla u)^T|^2]\right\} dx \\
&= \int_{B^N} (N-2)|\nabla u|^2 \, dx + \int_{\partial B^N} \sum_{i,j} x_i(u_j \nabla_j u_i - u_i \nabla_j u_j) \, dS \\
&= \int_{B^N} (N-2)|\nabla u|^2 \, dx - \int_{\partial B^N} \sum_j \nabla_j u_j \, dS.
\end{aligned}
$$

Note that the value of $\nabla \cdot u$ on ∂B^N depends only on the value u on ∂B^N. For example, consider the north pole e_n and parametrized a patch of the sphere there by $(x', f(x') = \sqrt{1 - |x'|^2})$. We then have

$$
u_i(x', f(x')) = x_i \text{ for } 1 \le i \le N-1.
$$

Differentiating in the x_i direction gives and so

$$
1 = \nabla_i u_i(e_n) + \nabla_n u_i \underbrace{\nabla_i f(0)}_{=0} = \nabla_i u_i(e_n).
$$

Also, as $|u| = 1$,

$$
0 = \sum_i u_i \partial_n u_i = u_n \partial_n u_n = \partial_n u_n.
$$

The above gives $\nabla \cdot u = N - 1$ on ∂B^N.

Summarizing, we have shown that

$$
\int_{B^N} |\nabla u|^2 \, dx \ge \frac{1}{N-2} \int_{\partial B^N} \nabla \cdot u \, dS = \frac{N-1}{N-2} |\mathbb{S}^{N-1}|.
$$

On the other hand, the map $n(x) = \frac{x}{|x|}$ has $|\nabla n(x)|^2 = \frac{N-1}{|x|^2}$ and so

$$
\int_{B^N} |\nabla n|^2 \, dx = \int_{B^N} \frac{N-1}{|x|^2} \, dx = \frac{N-1}{N-2} |\mathbb{S}^{N-1}| \le \int_{B^N} |\nabla u|^2 \, dx.
$$

This proves that n is a minimizing harmonic map.

Consider the equality case where we have

$$
\nabla u + (\nabla u)^T = \frac{2}{N-1} \nabla \cdot u (I_3 - u \otimes u). \tag{4}
$$

Multiplying both sides of (4) with u gives

$$
u \cdot \nabla u = 0.
$$

Hence, if we let γ_t be the flow generated by u, i.e.

$$\begin{cases} \frac{d}{dt}\gamma_t(x) = u(\gamma_t(x)), \\ \gamma_0(x) = x, \end{cases}$$

then

$$\frac{d^2}{dt^2}\gamma_t(x) = u(\gamma_t(x)) \cdot \nabla u(\gamma_t(x)) = 0.$$

This means that, for any given x, the integral curve $t \mapsto \gamma_t(x)$ is a straightline. As $u(x) = x$ on ∂B^N, we deduce that $\gamma_t(x) = (1-t)x$ for $x \in \partial B^N$. By semiflow properties, we can determine γ_t inside B^N and see that $u = n$. $\square$

Fact 2.2 (Hervé and Hervé '94)**.** *For $\varepsilon > 0$, $N \geq 2$, There exists a unique radially symmetric critical point of E_ε of the form $u_\varepsilon(x) = f_\varepsilon(|x|)\frac{x}{|x|}$ with boundary value x on ∂B^N. f_ε satisfies*

$$\begin{cases} f_\varepsilon'' + \frac{N-1}{r^2}f_\varepsilon' - \frac{N-1}{r^2}f_\varepsilon = -\frac{1}{\varepsilon^2}(1-f_\varepsilon^2)f_\varepsilon, \\ f_\varepsilon(0) = 0, f_\varepsilon(1) = 1, \end{cases}$$

and f_ε is monotonically increasing.

The following question was raised by Bethuel, Brezis and Hélein '94 in their book on Ginzburg-Landau vortices in dimension $N = 2$ and later by Brezis '99 in higher dimensions.

Open Problem 2.3. *Is it true that u_ε is the unique minimizer for E_ε for every $\varepsilon > 0$ and $N \geq 2$ with boundary value x on ∂B^N.*

State of art

- In any dimension, E_ε is convex for large ε and it is clear that u_ε is the unique critical point (hence minimizer) of E_ε.
- In dimension $N = 2$, Pacard and Rivière '00 showed in their book that the answer is positive for small $\varepsilon > 0$.
- In dimension $N \geq 7$, the answer to this open question has been proved affirmative recently for all $\varepsilon > 0$ in a joint work of myself with Ignat, Slastikov and Zarnescu '18.
- It remains otherwise at large an open problem for dimensions $2 \leq N \leq 6$.

- The issue of local minimality of the vortex solution is fully understood. This was proved in dimension $N = 2$ by Mironescu '95 (see also Lieb and Loss '95), in dimension $N \geq 7$ by the work of Ignat, N., Slastikov and Zarnescu '18 mentioned above, and in dimension $3 \leq N \leq 6$ by a joint work with Ignat '23.

Theorem 2.4 (Ignat, N., Slastikov and Zarnescu '18)**.** *For $N \geq 7$ and ε, u_ε is the unique minimizer of E_ε with the boundary value x on ∂B^N.*

Proof. We compute

$$\begin{aligned}
E_\varepsilon[u] - E_\varepsilon[u_\varepsilon] &= \int_{B^N} \Big\{ \frac{1}{2}[|\nabla u|^2 - |\nabla u_\varepsilon|^2] + \frac{1}{4\varepsilon^2}[(1-|u|^2)^2 - (1-|u_\varepsilon|^2)^2] \Big\}\,dx \\
&= \int_{B^N} \Big\{ \frac{1}{2}[2\nabla u_\varepsilon : \nabla(u-u_\varepsilon) + |\nabla(u-u_\varepsilon)|^2] \\
&\quad + \frac{1}{4\varepsilon^2}[-2(1-|u_\varepsilon|^2)(\underbrace{|u|^2 - |u_\varepsilon|^2}_{=2u_\varepsilon\cdot(u-u_\varepsilon)+|u-u_\varepsilon|^2}) + (|u|^2-|u_\varepsilon|^2)^2] \Big\}\,dx \\
&= \int_{B^N} \Big\{ \nabla u_\varepsilon : \nabla(u-u_\varepsilon) - \frac{1}{\varepsilon^2}(1-|u_\varepsilon|^2)(u-u_\varepsilon) \Big\}\,dx \\
&\quad + \frac{1}{2}\int_{B^N} \Big\{ |\nabla(u-u_\varepsilon)|^2] - \frac{1}{\varepsilon^2}(1-|u_\varepsilon|^2)|u-u_\varepsilon|^2 \Big\}\,dx \\
&\quad + \frac{1}{4\varepsilon^2}\int_{B^N} (|u|^2 - |u_\varepsilon|^2)^2\,dx \\
&=: I_1 + I_2 + I_3.
\end{aligned}$$

I_1 vanishes because $\Delta u_\varepsilon = -\frac{1}{\varepsilon^2}(1-|u_\varepsilon|^2)u_\varepsilon$ and $u - u_\varepsilon = 0$ on ∂B^N. I_3 is clearly non-negative. Thus

$$E_\varepsilon[u] - E_\varepsilon[u_\varepsilon] \geq \frac{1}{2}F_\varepsilon[u-u_\varepsilon] := \int_{B^N} \Big\{ |\nabla(u-u_\varepsilon)|^2] - \frac{1}{\varepsilon^2}(1-|u_\varepsilon|^2)|u-u_\varepsilon|^2 \Big\}\,dx.$$

Thus, we only need to show

$$F_\varepsilon[v] \geq 0 \text{ for } v \in H_0^1(B^N, \mathbb{R}^n) \text{ with equality only if } v \equiv 0. \tag{5}$$

Step 1: Consider $v \in C_c^\infty(B \setminus \{0\}, \mathbb{R}^N)$. We write

$$v = f_\varepsilon w$$

and compute

$$\begin{aligned}
F_\varepsilon[v] &= \int_{B^N} \Big\{ |\nabla(f_\varepsilon w)|^2 + \frac{1}{\varepsilon^2}(1-f_\varepsilon^2)f_\varepsilon^2 w^2 \Big\}\,dx \\
&= \int_{B^N} \Big\{ f_\varepsilon^2|\nabla w|^2 + \nabla f_\varepsilon \cdot \nabla(|w|^2 f_\varepsilon) + \frac{1}{\varepsilon^2}(1-f_\varepsilon^2)f_\varepsilon^2 w^2 \Big\}\,dx.
\end{aligned}$$

Integrating by parts on the middle term and use $\Delta f_\varepsilon - \frac{N-1}{r^2} f_\varepsilon = -\frac{1}{\varepsilon^2}(1-f_\varepsilon^2)$, we get

$$F_\varepsilon[v] = \int_{B^N} f_\varepsilon^2 \Big\{ |\nabla w|^2 - \frac{N-1}{r^2}|w|^2 \Big\}\, dx.$$

Digression: In the limit $\varepsilon \to 0$, $f_\varepsilon \to 1$ and the above becomes

$$\int_{B^N} \Big\{ |\nabla w|^2 - \frac{N-1}{r^2}|w|^2 \Big\}\, dx.$$

Sharp Hardy's inequality state

$$\int_{B^N} |\nabla w|^2\, dx > \frac{(N-2)^2}{4} \int_{B^N} \frac{1}{r^2}|w|^2\, dx \text{ for } w \in H_0^1(B^N).$$

Equality is not attained, and minimizing sequence approaches $r^{-\frac{N-2}{2}}$ (which is not in H^1). We thus expect F_ε to be non-negative when

$$N-1 \le \frac{(N-2)^2}{4} \quad \Leftrightarrow \quad N \ge 7.$$

Let us resume the proof. We write

$$w = \varphi g, \quad \varphi = r^{-\frac{N-2}{2}}.$$

and perform a similar computation:

$$\begin{aligned} F_\varepsilon[v] &= \int_{B^N} f_\varepsilon^2 \Big\{ |\nabla(\varphi g)|^2 - \frac{N-1}{r^2}\varphi^2 |g|^2 \Big\}\, dx \\ &= \int_{B^N} f_\varepsilon^2 \Big\{ \varphi^2 |\nabla g|^2 + \nabla\varphi \cdot \nabla(\varphi |g|^2) - \frac{N-1}{r^2}\varphi^2|g|^2 \Big\}\, dx. \end{aligned}$$

Now, using $\Delta\varphi = -\frac{(N-2)^2}{4} r^{-2}\varphi$, we arrive at

$$\begin{aligned} F_\varepsilon[v] &= \int_{B^N} f_\varepsilon^2 \Big\{ |\nabla(\varphi g)|^2 - \frac{N-1}{r^2}\varphi^2 |g|^2 \Big\}\, dx \\ &= \int_{B^N} f_\varepsilon^2 \Big\{ \varphi^2|\nabla g|^2 - f_\varepsilon^{-2}\varphi|g|^2 \underbrace{\nabla\varphi\cdot\nabla f_\varepsilon}_{=\varphi' f_\varepsilon'} + \Big(\frac{(N-2)^2}{4} - (N-1) \Big) \frac{1}{r^2}\varphi^2 |g|^2 \Big\}\, dx. \end{aligned}$$

As saw above, when $N \ge 7$, the last term is positive. For the middle term, we use $\varphi' < 0$ and $f_\varepsilon' > 0$. We deduce that

$$F_\varepsilon[v] \ge \Big(\frac{(N-2)^2}{4} - (N-1) \Big) \int_{B^N} \frac{1}{r^2}|v|^2\, dx \ge 0.$$

Thus (5) holds for $v \in C_c^\infty(B \setminus \{0\})$.

Step 2: Consider $v \in H_0^1(B^N, \mathbb{R}^N)$. By density, there exists $\{v_m\} \subset C_c^\infty(B \setminus \{0\})$ such that $v_m \to v$ in H^1. We then have

$$F_\varepsilon[v_m] \geq \Big(\frac{(N-2)^2}{4} - (N-1)\Big) \int_{B^N} \frac{1}{r^2}|v_m|^2\,dx.$$

The left side converges to $F_\varepsilon[v]$ as $m \to \infty$. The right hand say may not, but by Fatou's lemma,

$$\int_{B^N} \frac{1}{r^2}|v|^2\,dx \leq \liminf \int_{B^N} \frac{1}{r^2}|v_m|^2\,dx.$$

We thus deduce

$$F_\varepsilon[v] \geq \Big(\frac{(N-2)^2}{4} - (N-1)\Big) \int_{B^N} |v|^2\,dx.$$

This gives the desired (5). □

Exercise 1. *Show that if* $2 \leq N \leq 6$, *there exists* $v \in H_0^1(B^N)$ *such that* $F_\varepsilon[v] < 0$.

3 Lecture 3: Defects in the 2D Landau-de Gennes model

3.1 The energy functional: recap

We work in 2D disk $B_R \subset \mathbb{R}^2$. For maps $Q : B_R \to \mathscr{S}_0$, the set of traceless symmetric 3×3 matrices, we consider

$$I_L[Q] = \int_{B_R} \Big[\frac{1}{2}|\nabla Q|^2 + \frac{1}{L} f_b(Q)\Big]\, dx, \qquad Q \in H^1(B_R, \mathscr{S}_0). \tag{6}$$

When $L = 1$, we write $I = I_1$.

The bulk energy density f_b takes the form

$$f_B(Q) = -\frac{a^2}{2}\mathrm{tr}(Q^2) - \frac{b^2}{3}\mathrm{tr}(Q^3) + \frac{c^2}{4}[\mathrm{tr}(Q^2)]^2, \tag{7}$$

The Euler-Lagrange equation reads

$$\varepsilon \Delta Q = -a^2\, Q - b^2(Q^2 - \frac{1}{3}|Q|^2\, Id) + c^2 |Q|^2\, Q.$$

The appearance of the b^2 term complicates things; most notably the way one uses maximum principle to treat Ginzburg-Landau no longer works.

3.2 The boundary condition

We impose that on ∂B_R, the boundary value Q_b belongs to $\mathscr{S}_*$ with a planar director field n carrying certain topological defect:

$$Q_b(x) = s_+(n(x) \otimes n(x) - \frac{1}{3} Id) \text{ on } \partial B_R,$$

where, for some integer $k \neq 0$,

$$n = n(\varphi) = \big(\cos(\tfrac{k}{2}\varphi), \sin(\tfrac{k}{2}\varphi), 0\big)\,, x = (r\cos\varphi, r\sin\varphi)$$

and, as before,

$$s_+ = \frac{b^2 + \sqrt{b^4 + 24a^2c^2}}{4c^2}.$$

Physicists refers to this as a defect of degree $k/2$: As x winds around the circle ∂B_R once, $n(x)$ winds around the unit circle $k/2$ times. However, note that, when considering Q_b as map from $\partial B_R \approx \mathbb{S}^1$ into $\mathbb{R}P^1$, the degree of Q_b is k.

3.3 Symmetry structure

The functional and the boundary condition respect the following symmetry:

- A map $Q : B_R \subset \mathbb{R}^2 \to \mathscr{S}_0$ is said to be k-radially symmetric if

$$Q(O_2(\psi)x) = O_k(\psi)\, Q(x)\, O_k(\psi)^t$$

  for any x and ψ where $O_k(\psi)$ is a rotation of $\frac{k}{2}\psi$ radiant about the z axis.

The boundary condition has an extra symmetry:

$$Q(x) \text{ admits } e_3 \text{ as an eigenvectors for all } x \in \partial B_R.$$

We also define

- A map $Q : B_R \subset \mathbb{R}^2 \to \mathscr{S}_0$ is said to be coaxially k-radially symmetric if it is k-radially symmetric and it admits e_3 as an eigenvector.

In order to classify k-radially symmetric maps on disks $B_R \subset \mathbb{R}^2$ centered at the origin with $R \in (0, \infty]$ and $k \neq 0$, we introduce some notation. We define $\{e_i\}_{i=1}^3$ to be the standard basis in $\mathbb{R}^3$ and denote, for $\varphi \in [0, 2\pi)$,

$$n = n(\varphi) = \left(\cos(\tfrac{k}{2}\varphi), \sin(\tfrac{k}{2}\varphi), 0\right), \; m = m(\varphi) = \left(-\sin(\tfrac{k}{2}\varphi), \cos(\tfrac{k}{2}\varphi), 0\right).$$

We endow the space $\mathscr{S}_0$ of Q-tensors with the scalar product

$$Q \cdot \tilde{Q} = \mathrm{tr}(Q\tilde{Q})$$

and for any $\varphi \in [0, 2\pi)$, we define the following orthonormal basis in $\mathscr{S}_0$:

$$\begin{aligned}
E_0 &= \sqrt{\frac{3}{2}}\left(e_3 \otimes e_3 - \frac{1}{3}I\right),\\
E_1 &= E_1(\varphi) = \sqrt{2}\left(n \otimes n - \frac{1}{2}I_2\right),\; E_2 = E_2(\varphi) = \frac{1}{\sqrt{2}}\left(n \otimes m + m \otimes n\right),\\
E_3 &= \frac{1}{\sqrt{2}}(n \otimes e_3 + e_3 \otimes n),\; E_4 = \frac{1}{\sqrt{2}}\left(m \otimes e_3 + e_3 \otimes m\right).
\end{aligned}$$

Obviously, only E_1 and E_2 depend on φ and we have

$$\frac{\partial E_1}{\partial \varphi} = kE_2 \quad \text{and} \quad \frac{\partial E_2}{\partial \varphi} = -kE_1. \tag{8}$$

Also, E_3 and E_4 are continuous across $\varphi = 0$ if and only if k is even.

Proposition 1. *Let $R \in (0,\infty)$, $k \neq 0$ and $Q \in H^1(B_R, \mathscr{S}_0)$ be a k-radially symmetric map.*

1. *If k is odd, then*
$$Q = \sum_{i=0}^{2} w_i(r) E_i,$$
where $w_0 \in H^1((0,R); r\,dr)$ and $w_1, w_2 \in H^1((0,R); r\,dr) \cap L^2\left((0,R); \frac{1}{r}\,dr\right)$.

2. *If k is even, then*
$$Q = \sum_{i=0}^{4} w_i(r) E_i,$$
where $w_0 \in H^1((0,R); r\,dr)$ and $\tilde{w}, \hat{w}, w_1, w_2 \in H^1((0,R); r\,dr) \cap L^2\left((0,R); \frac{1}{r}\,dr\right)$.

3. *If Q is co-axial, then $w_3 = w_4 = 0$.*

Proof. Let

$$\tilde{E}_3 = \frac{1}{\sqrt{2}}(e_1 \otimes e_3 + e_3 \otimes e_1),\ \tilde{E}_4 = \frac{1}{\sqrt{2}}(e_2 \otimes e_3 + e_3 \otimes e_2)$$

and

$$w_i(r,\theta) = Q : E_i \text{ for } i = 0,1,2,3,4 \text{ and } \tilde{w}_i(r,\theta) = Q : \tilde{E}_i \text{ for } i = 3,4.$$

Then

$$Q = w_0 E_0 + w_1 E_1 + w_2 E_2 + w_3 E_3 + w_4 E_4 = w_0 E_0 + w_1 E_1 + w_2 E_2 + \tilde{w}_3 \tilde{E}_3 + \tilde{w}_4 \tilde{E}_4.$$

k-radial symmetry then implies

$$\begin{aligned} w_i(r,\varphi+\psi) &= w_i(r,\varphi) \text{ for } i = 0,1,2,3,4,\\ \tilde{w}_3(r,\varphi+\psi) &= \tilde{w}_3(r,\varphi)\cos\frac{k\psi}{2} - \tilde{w}_4(r,\varphi)\sin\frac{k\psi}{2},\\ \tilde{w}_4(r,\theta+\psi) &= \tilde{w}_3(r,\varphi)\sin\frac{k\psi}{2} + \tilde{w}_4(r,\varphi)\cos\frac{k\psi}{2}. \end{aligned}$$

The first line implies that $w_i = w_i(r)$. This gives 1.

The second and third lines implies that

$$\begin{aligned} \tilde{w}_3(r,\psi) &= \tilde{w}_3(r,0)\cos\frac{k\psi}{2} - \tilde{w}_4(r,0)\sin\frac{k\psi}{2},\\ \tilde{w}_4(r,\psi) &= \tilde{w}_3(r,0)\sin\frac{k\psi}{2} + \tilde{w}_4(r,0)\cos\frac{k\psi}{2}. \end{aligned}$$

When k is odd, continuity of Q on almost all ∂B_r implies that $\tilde{w}_3 = \tilde{w}_4 = 0$, and hence $w_3 = w_4 = 0$. This gives 2.

Note that E_0, E_1, E_2 always admits e_3 as an eigenvector, while $w_3 E_3 + w_4 E_4$ admits e_3 as an eigenvector if and only if $w_3 = w_4 = 0$. This gives 3. $\square$

We have the following self-improving property for coaxially k-radially symmetric solution.

Proposition 2. *Let $k \in \mathbb{Z} \setminus \{0\}$ and $R \in (0, \infty]$. If $Q \in H^1_{loc}(B_R, \mathscr{S}_0)$ is a k-radially symmetric solution of the Euler-Lagrange equations of I_L on B_R satisfying the stated boundary condition, then*

$$Q(x) = \sum_{i=0}^{4} w_i(r) E_i,$$

where w_i's satisfy the following system of ODEs in $(0, R)$:

$$\begin{cases} L(w_0'' + \frac{w_0'}{r}) & = P_0(w_0, \dots, w_4), \\ L(w_1'' + \frac{w_1'}{r} - \frac{k^2 w_1}{r^2}) & = P_1(w_0, \dots, w_4) \\ L(w_2'' + \frac{w_2'}{r} - \frac{k^2 w_2}{r^2}) & = P_2(w_0, \dots, w_4), \\ L(w_3'' + \frac{w_3'}{r} - \frac{k^2 w_1}{4r^2}) & = P_3(w_0, \dots, w_4), \\ L(w_4'' + \frac{w_4'}{r} - \frac{k^2 w_2}{4r^2}) & = P_4(w_0, \dots, w_4), \end{cases} \tag{9}$$

or

$$L(w_i'' + \frac{w_i'}{r} - \frac{k_i^2 w_i}{r^2}) = P_i(w_0, \dots, w_4),$$

subject to boundary conditions:

$$\begin{aligned} w_0'(0) = 0, w_1(0) = w_2(0) = w_3(0) = w_4(0) = 0, \\ w_0(R) = -\frac{1}{\sqrt{6}} s_+, w_1(R) = \frac{1}{\sqrt{2}} s_+, w_2(R) = w_3(R) = w_4(R) = 0. \end{aligned} \tag{10}$$

If Q is co-axial, then $w_2 \equiv w_3 \equiv w_4 \equiv 0$.
The converse also holds.

Proof of $w_2 \equiv 0$ when Q is co-axially k-radially symmetric. Let $S_0 = e_1 \otimes e_2 - e_2 \otimes e_1$ so that $\partial_\varphi Q = \frac{k}{2}(S_0 Q - Q S_0)$. Note that $(S_0 Q - Q S_0) : Q^k = 0$ for any k since $\mathrm{tr}(AB) = tr(BA)$. Taking inner product of the Euler-Lagrange equation with $S_0 Q - Q S_0$ gives

$$-L \Delta Q : (S_0 Q - Q S_0) = 0.$$

Integrating over B_r gives

$$\begin{aligned} 0 &= \int_{B_r} \Delta Q : (S_0 Q - Q S_0)\, dx \\ &= -\int_{B_r} \nabla Q : \underbrace{\nabla(S_0 Q - Q S_0)}_{= S_0 \nabla Q - \nabla Q S_0} \, dx + \int_{\partial B_r} \partial_r Q : (S_0 Q - Q S_0)\, dS \\ &= \frac{2}{k} \int_{\partial B_r} \partial_r Q : \partial_\varphi Q \, dS. \end{aligned}$$

Using $Q = \sum_{i=0}^{2} w_i E_i$, this means $w_1' w_2 - w_1 w_2' = 0$. As $w_1(R) = \frac{1}{\sqrt{2}} s_+, w_2(R) = 0$, this implies that $w_1 > 0$ and $w_2 \equiv 0$ in some interval (r_1, R). Local uniqueness of ODE implies that $w_2 \equiv 0$. □

Here are the state of the art:

- Coaxially k-radially symmetric solution exists (di Frata, Robbins, Slastikov and Zarnescu '15).
- For $b^2 = 0$ (i.e. Ginzburg-Landau type) and $R < \infty$, the coaxially radially symmetric solution is unique and is globally minimizing (di Frata, Robbins, Slastikov and Zarnescu '15).
- For $b^2 = 0$ and $R = \infty$, there is no entire radially symmetric solution.
- If $|k| \geq 2$ and $a^2, b^2, c^2 > 0$, entire coaxially k-radially symmetric solutions (exist and) are unstable (Ignat, N., Slastikov, Zarnescu '16). Thus, one expect that for large enough radius, these are also unstable and so the minimizer is non radially symmetric.
- If $|k| = 1$, entire k-radially symmetric solutions with sign invariance (exist and) are stable (Ignat, N., Slastikov, Zarnescu '16).
- For $k \neq 0$, and $b^4 \leq 3a^2c^2$, coaxially k-radially symmetric solutions (on finite balls or the whole space) with sign invariance are unique (Ignat, N., Slastikov, Zarnescu '16).
- For $k \neq 0$ even, minimizers are k-radially symmetric, but is not coaxially k-radially symmetric (Ignat, N., Slastikov, Zarnescu '20).

Note that the above uniqueness result is not sharp, and it requires new idea. In the case $b^4 = 3a^2c^2$, the treatment reduces to that of a scalar ODE, which is already nontrivial, e.g.

Theorem 3.1 (Ignat, N., Slastikov, Zarnescu '14)**.** *Let $R \in (0, \infty]$. Solutions to the ODE*

$$u'' + \frac{u'}{r} - \frac{k^2}{r^2}u = u(-a^2 - \frac{b^2}{3}u + \frac{2c^2}{3}u^2)$$
$$u(0) = 0, u(R) = s_+.$$

is unique.

When $b^2 = 0$, this goes back to Hervé and Hervé (also Chen-Elliott-Qi, Farina and Gueda). But these proofs do not apply to the above.

Sketch for $R = \infty$ and $u > 0$. Suppose u and v are two entire solutions. One use sliding method
Step 1: $u(r) \sim c_u r^k$ as $r \to 0$ with $c_u > 0$. This step is standard for a regular singular point of ODE.
Step 2: $u(r) \sim s_+ - C_{a,b,c}/r^2$ as $r \to \infty$ with $\beta_u > 0$. There is complication as ∞ is an irregular singular point. One needs to construct careful barriers.

(Clearly these two properties also hold for v.)
Step 3: Define

$$u_\theta(r) = u(r/\theta), \quad \theta \in (0, 1).$$

Note that

$$u_\theta'' + \frac{u_\theta'}{r} - \frac{k^2}{r^2}u_\theta \leq u_\theta(-a^2 - \frac{b^2}{3}u_\theta + \frac{2c^2}{3}u_\theta^2).$$

For $\theta \ll 1$, one can have $u_\theta > v$. Let

$$\bar{\theta} = \sup\{\theta \in (0, 1) : u_\theta > v\}.$$

The goal is to show that $\bar{\theta} = 1$, which implies $u \geq v$. Reversing the role of u and v gives $u \leq v$ and hence $u \equiv v$.

Suppose by contradiction that $\bar{\theta} < 1$. Note that if there isn't any $r_0 \in (0, \infty)$ such that $u_{\bar{\theta}}(r_0) = v(r_0)$: If so there is a contradiction to the strong comparison principle. Also, using Step 2, there is $r_1 > 0$ such that

$$u_{\bar{\theta}} > v \text{ in } (r_1, \infty).$$

Therefore the maximality of $\bar{\theta}$ implies

$$\lim_{r \to 0} \frac{u_{\bar{\theta}}}{r^k} = \lim_{r \to 0} \frac{v}{r^k}.$$

One then develop a kind of Hopf lemma to show that this isn't possible. □

The proof of uniqueness for system uses in addition some idea by Alama, Bronsard and Giorgi '99. The idea is to show that all solutions are stable. Now if non-uniqueness holds, then there exists a mountain pass solution which is unstable and gives a contradiction.

4 Lecture 4: Defects in the 2D Landau-de Gennes model (cont.)

In this lecture, we will speak about the case when k is even and on the unit disk B.

Theorem 4.1 (Ignat, N., Slastikov, Zarnescu '20)**.** *Let $a^2 \geq 0$, $b^2, c^2 > 0$ be any fixed constants and $k \in 2\mathbb{Z} \setminus \{0\}$. There exists some $L_0 = L_0(a^2, b^2, c^2) > 0$ such that for all $L < L_0$, there exists exactly two minimizers of I_L subjected to the given boundary condition on ∂B and these minimizers are non-coaxially k-radially symmetric.*

Furthermore, there exists $L_1 \leq L_0$ such that for $L < L_1$, I_L has at least five k-radially symmetric critical points satisfying the given boundary condition on ∂B and at least four of which is non-coaxially symmetric.

Remark 4.2. *A result of Bauman-Park-Phillips '12 asserts the existence of non-symmetric solutions, for both even and odd k.*

Remark 4.3. *For the minimizers, the components w_2 and w_4 are zero but $w_3 \not\equiv 0$.*

Energy levels as $\varepsilon \to 0$

Solution type	Energy
minimizers	O(1)
coaxially k-radially symmetric solutions	$O(k^2 \lvert\ln \varepsilon\rvert)$
non symmetric solutions (Bauman-Park-Phillips)	$O(k \lvert\ln \varepsilon\rvert)$
the other two non-coaxially k-radially symmetric solutions	O(1)

4.1 Sketch of the proof of first part

In the limit $L \to 0$, one obtains the problem

$$\min I_*[Q] = \min \int_B \frac{1}{2} |\nabla Q|^2 \, dx,$$

where Q satisfies the same boundary condition, but Q maps B into the "limit manifold"

$$\mathscr{S}_* = \{s_+(v \otimes v - \frac{1}{3} Id) : v \in \mathbb{S}^2\}, s_+ = s_+(a^2, b^2, c^2) > 0, \text{ i.e. a projective sphere.}$$

$\mathscr{S}_*$ is the set of global minima of f_b.

As B is simply connected, a result of Ball-Zarnescu '11 implies that minimizers Q_* of of the above $\mathscr{S}_*$-harmonic map problem can be written as $Q_* = s_+(n_* \otimes n_* - \frac{1}{3}Id)$ where $n_* : B \to \mathbb{S}^2$ is a minimizing harmonic map with

$$n_* = n = (\cos\frac{k}{2}\varphi, \sin\frac{k}{2}\varphi, 0) \text{ on } \partial B.$$

These minimizers are understood: they are the complex maps $z \mapsto z^{\pm\frac{k}{2}}$ under a stereographic projection:

$$n_*^\pm(r\cos\varphi, r\sin\varphi) = \Big(\frac{2r^{\frac{k}{2}}\cos\frac{k}{2}\varphi}{1+r^k}, \frac{2r^{\frac{k}{2}}\sin\frac{k}{2}\varphi}{1+r^k}, \pm\frac{1-r^k}{1+r^k}\Big).$$

Denote the corresponding Q-tensors as $Q_*^\pm$. Note that $Q_*^\pm$ are non-coaxially k-rotationally symmetric. We can explicitly write $Q_*^\pm$ in terms of basis tensors $\{E_i\}$

$$Q_*^\pm = w_0^*(r)E_0 + w_1^*(r)E_1 \pm w_3^*(r)E_3,$$

where

$$w_0^*(r) = \frac{2(1-r^k)^2 - 4r^k}{\sqrt{6}(1-r^k)^2},\ w_1^*(r) = \frac{4s_+r^k}{\sqrt{2}(1+r^k)^2},\ w_3^*(r) = \frac{4s_+r^{\frac{k}{2}}(1-r^k)}{\sqrt{2}(1+r^k)^2}.$$

We know that, for any sequence of minimizers Q_{L_k} of I_{L_k}, one can extract a subsequence which converges in $C^{1,\alpha}(\bar{D})$ and $C^j_{loc}(D)$ for any $j \geq 2$ to either Q_*^+ or Q_*^- (see Majumdar-Zarnescu, Nguyen-Zarnescu). Then that if $Q_L = \sum_{i=0}^4 w_{i,L}E_i$ is a minimizer of I_L, then $\tilde{Q}_L = \sum_{i=0}^2 w_{i,L}E_i - \sum_{i=3}^4 w_{i,L}E_i$ is also a minimizer of I_L. Thus both $Q_*^\pm$ can appear as limits of minimizers (since if $Q_{L'_k} \to Q_*^+$, then $\tilde{Q}_{L'_k} \to Q_*^-$ and vice versa).

Now, restrict I_L to the set of k-radially symmetric tensors. By the same token, any sequence of minimizers $Q^{rs}_{L_k}$ of I_{L_k} under k-radial symmetry has a subsequence which converges in $C^{1,\alpha}(\bar{D})$ and $C^j_{loc}(D)$ for any $j \geq 2$ to a minimizer of I_* in the set of weakly k-radially symmetric $\mathscr{S}_*$-valued tensors, which must be either Q_*^+ or Q_*^+ as these are weakly k-radially symmetric.

Therefore, to prove the theorem, one possible approach is to show that

> there are "neighborhoods" $N^\pm$ of $Q_*^\pm$ such that when L is small enough I_L admits at most one critical point in each of $N^\pm$. (†)

As $Q_*^\pm$ are equivalent up to an inflection, it suffices to establish (†) for $Q_* = Q_*^+$.

As in many other singularly perturbed problems, the neighborhoods $N^\pm$ are necessarily set up in relatively stronger norms than the energy norm and they are L-dependent. As for the norm, we will choose ad hoc a modified H^2-norm. That $N^\pm$

are L-dependent is more of an issue: there is a competition between the size of the neighborhood where one can prove uniqueness and the rate of convergence to the limit (so that one can squeeze all minimizers into the designed neighborhood).

Observe that, as $L \to 0$,

- the mimimizers Q_L of I_L converges to $Q_*^\pm$,
- the mimimizers Q_L^{rs} of I_L in the subclass of k-radially symmetric tensors also converges to $Q_*^\pm$, as $Q_*^\pm$ respect k-radial symmetry.

We thus show that there exists neighborhoods $N^\pm$ of $Q_*^\pm$ such that in each of these neighborhood, I_L has at most one critical point when L is small enough. Note however that $N^\pm$ is L dependent, so there is a competition: the size of $N^\pm$ where one can get uniqueness and the rate of convergence of Q_L and Q_L^{rs} to $Q_*^\pm$. For example, as known in Ginzburg-Landau context, the part transverse to the limit manifolds of the minimizers converge to zero with different speed in different norms ($O(L)$ in L^2, but slower in e.g. H^2).

4.2 Mountain pass solutions

It will be convenient to work with a modified energy functional

$$\tilde{I}_R[Q] = \int_{B_R} \Big[\frac{1}{2}|\nabla Q|^2 + \tilde{f}_{bulk}(Q)\Big]\,dx, \qquad Q \in H^1(B_R, \mathscr{S}_0).$$

where $\tilde{f}_{bulk} = f_{bulk} - \min f_{bulk}$. Clearly, Q is a critical point/minimizer of $I[\cdot; B_R]$ if and only if it is a critical point/minimizer of $\tilde{I}_R$.

Denote by A_R^{str} and A_R^{rs} respectively the sets of coaxially k-radially symmetric and k-radially symmetric Q tensors satisfying the boundary condition i.e.

$$A_R^{str} = \Big\{Q \in H^1(B_R, \mathscr{S}_0) : Q = s_+(n_k \otimes n_k - \frac{1}{3}I_3) \text{ on } \partial D \\ \text{and } Q \text{ is coaxially } k\text{-radially symmetric}\Big\},$$

$$A_R^{rs} = \Big\{Q \in H^1(B_R, \mathscr{S}_0) : Q = s_+(n_k \otimes n_k - \frac{1}{3}I_3) \text{ on } \partial D \\ \text{and } Q \text{ is } k\text{-radially symmetric}\Big\}.$$

Fact 4.4. *There exists some $\delta > 0$ depending only on a^2, b^2 and c^2 such that, for all $R \in (0, \infty)$ and $k \in \mathbb{Z} \setminus \{0\}$, there holds*

$$\alpha_R := \min_{A_R^{str}} \tilde{I}_R \ge \delta k^2 \,(\ln \frac{R}{k^2} - \frac{1}{\delta}).$$

Remark 4.5. *In Bauman-Park-Philips, it is shown that $\tilde{I}_R$ has critical points whose energies are of order $k \ln R$; and these are not radially symmetric for $k \neq \pm 1$.*

Let us indicate how the above fact is proved. We have

$$\alpha_R = 2\pi \min\Big\{E_R[w_0, w_1] : w_0 \in H^1((0,R); r\,dr), w_1 \in H^1((0,R); r\,dr) \cap L^2((0,R); \frac{1}{r}dr), \\ w_0(R) = -\frac{s_+}{\sqrt{6}}, w_1(R) = \frac{s_+}{\sqrt{2}}\Big\},$$

where

$$E_R[w_0, w_1] = \int_0^R \Big\{\frac{1}{2}[|w_0'|^2 + |w_1'|^2] + \frac{k^2}{2r^2}|w_1|^2 + h(w_0, w_1)\Big\}dx,$$
$$h(x,y) = \big(-\frac{a^2}{2} + \frac{c^2}{4}[|x|^2 + |y|^2]\big)[|x|^2 + |y|^2] - \frac{b^2\sqrt{6}}{18}x(x^2 - 3y^2) - \min f_{bulk}.$$

One see that w_1 wants to be close to $\frac{s_+}{\sqrt{2}}$ for 'a long time'. The term $\frac{k^2}{2r^2}|w_1|^2$ thus contributes $O(k^2 \ln R)$.

In the proof, C will denote some positive constant which will always be independent of R.

By the theorem about 'uniqueness and symmetry' of minimizers, there exists $R_0 > 0$ such that, for $R \geq R_0$, $\tilde{I}_R$ has two distinct minimizers in A_R^{rs} which are non-coaxially k-radially symmetric. Label these minimizers $Q_R^{\pm}$. Then, it can be shown that, for $0 < d < \|Q_R^+ - Q_R^-\|_{H^1(B_R)}$, we have

$$\inf\Big\{\tilde{I}_R[Q] : Q \in H^1(B_R, \mathscr{S}_0), Q \text{ satisfies BC}, \|Q - Q_R^+\|_{H^1(B_R)} = d\Big\} > \tilde{I}_R[Q_R^{\pm}].$$

Now, by the mountain pass theorem, for $R \geq R_0$, $\tilde{I}_R$ has a mountain pass solution connecting $Q_R^{\pm}$, which will be denoted by Q_R^{mp}.

To show that $Q_R^{\mp}$ is not coaxially k-radially symmetric, we shows that there exists some $R_1 > R_0$ such that

$$\tilde{I}_R[Q_R^{mp}] \leq C \text{ for all } R > R_1. \tag{11}$$

To this end, one engineers, for all sufficiently large R, a continuous path $\gamma : [-2, 2] \to A_R^{rs}$ such that $\gamma(\pm 2) = Q_R^{\pm}$, and there exists some C independent of R and t such that

$$\tilde{I}_R[\gamma(t)] \leq C \tag{12}$$

for all $t \in [-2, 2]$.