Landau-de Gennes model with sextic potentials: asymptotics of minimizers and defects

Wei Wang [1] Zhifei Zhang [1]

[1]School of Mathematical Sciences, Peking University, Beijing, 100871, China

Model of Liquid crystal

Liquid crystals are basically anisotropic fluids, where the anisotropy arises from the directional nature of the molecular geometry, physical, or chemical properties. To characterize this anisotropy, mathematical models are introduced to describe the orientation of the molecules. These models are referred to as order parameters in physics. Depending on the choice of order parameter, existing mathematical models for liquid crystals can be broadly classified into three models. The first is to use a probability distribution function, denoted as $f(x, \mathbf{m})$, to represent the probability of the liquid crystal molecules at a fluid point x being oriented in the direction $\mathbf{m}$. This model was initially established by Onsager. The second model, referred to as the vector model or the Oseen-Frank model, uses a unit vector field denoted as $\mathbf{n}(x)$ to characterize the average orientation of liquid crystal molecules at each point x. The third one, known as the Landau-de Gennes model, describes the local configurations of the medium using $\mathbf{Q}$-tensors, which are traceless 3×3 matrices

$$\mathbb{S}_0 := \{\mathbf{Q}\in\mathbb{M}^{3\times 3} : \mathbf{Q}^{\mathrm{T}} = \mathbf{Q},\ \operatorname{tr}\mathbf{Q} = 0\}.$$

Each of these models has its own advantages and disadvantages in practical applications, stemming from their different starting points.

Background

We study a class of Landau-de Gennes energy functionals with a sextic bulk energy density in a three-dimensional domain. Our main focus is to analyze the asymptotic behavior of minimizers under the condition of small elastic constants. We examine the properties of uniformly bounded minimizers in two distinct scenarios: one where their energy remains uniformly bounded, and another where it logarithmically diverges as a function of the elastic constant. In the first case, we provide a proof demonstrating that up to a subsequence, the minimizers converge to a locally minimizing harmonic map. This convergence is in both the H^1_{loc} and C^j_{loc} norms, where $j\in\mathbb{Z}_+$, within compact subsets that are distant from the singularities of the limit. For the second case, we establish the existence of a closed set denoted as $\mathcal{S}_{\mathrm{line}}$. This set has finite length and consists finite segments of lines locally such that the energy of minimizers are locally uniformly bounded away from it.

Our findings provide a resolution to an open question raised by G. Canevari, specifically concerning point and line defects in the Landau-de Gennes model with sextic potentials.

Introduction

In the Landau-de Gennes theory, local configurations of the medium are characterized by $\mathbf{Q}$-tensors, which are traceless 3×3 matrices represented by

$$\mathbb{S}_0 := \{\mathbf{Q}\in\mathbb{M}^{3\times 3} : \mathbf{Q}^{\mathrm{T}} = \mathbf{Q},\ \operatorname{tr}\mathbf{Q} = 0\}.$$

Let $\Omega\subset\mathbb{R}^3$ be a bounded domain. There has been extensive study of the asymptotic behavior of the minimizers for the energy functional

$$E^{(4)}_\varepsilon(\mathbf{Q}) = \int_\Omega \left(\frac12|\nabla\mathbf{Q}|^2 + \frac{1}{\varepsilon^2}\left(a_1 - \frac{a_2}{2}\operatorname{tr}\mathbf{Q}^2 + \frac{a_3}{3}\operatorname{tr}\mathbf{Q}^3 + \frac{a_3}{4}(\operatorname{tr}\mathbf{Q}^2)^2\right)\right)\mathrm{d}x, \tag{1}$$

for $a_2, a_3, a_4 > 0$. In [3, 4] the authors considered minimizers of (1) with uniform bounded energy and in [1], the author focused on the case that the energies blow up logarithmically as $\varepsilon\to 0^+$. Canevari posed the following open question in [1].

[Question] Can the results on the model (1) be generalized to models with a sextic bulk energy density of the form

$$\mathcal{F}^{(6)}_b(\mathbf{Q}) = a_1 - \frac{a_2}{2}\operatorname{tr}\mathbf{Q}^2 + \frac{a_3}{3}\operatorname{tr}\mathbf{Q}^3 + \frac{a_4}{4}(\operatorname{tr}\mathbf{Q}^2)^2 + \frac{a_5}{5}(\operatorname{tr}\mathbf{Q}^2)(\operatorname{tr}\mathbf{Q}^3) + \frac{a_6}{6}(\operatorname{tr}\mathbf{Q}^2)^3 + \frac{a_6'}{6}(\operatorname{tr}\mathbf{Q}^3)^2?$$

Without loss of generality, we study the energy functional

$$E_\varepsilon(\mathbf{Q},\Omega) = \int_\Omega\left(\frac12|\nabla\mathbf{Q}|^2 + \frac{1}{\varepsilon^2}f_b(\mathbf{Q})\right)\mathrm{d}x, \tag{2}$$

where f_b represents a sextic bulk energy density defined as

$$f_b(\mathbf{Q}) := a_1 - \frac{a_2}{2}\operatorname{tr}\mathbf{Q}^2 + \frac{a_4}{4}(\operatorname{tr}\mathbf{Q}^2)^2 + \frac{a_6}{6}(\operatorname{tr}\mathbf{Q}^2)^3 + \frac{a_6'}{6}(\operatorname{tr}\mathbf{Q}^3)^2$$

with $a_2, a_4, a_6, a_6' > 0$. We generalize all the results in [1, 3, 4] to such model.

Theorem (Minimizers with uniform bounded energy)

Let $\Omega\subset\mathbb{R}^3$ be a bounded domain. Assume that $\{\mathbf{Q}_\varepsilon\}_{0<\varepsilon<1}$ is a sequence of local minimizers of (2), satisfying

$$E_\varepsilon(\mathbf{Q}_\varepsilon,\Omega)\le M, \qquad \|\mathbf{Q}_\varepsilon\|_{L^\infty(\Omega)}\le M,$$

for some $M>0$. There exist a subsequence $\varepsilon_n\to 0^+$ and $\mathbf{Q}_0\in H^1(\Omega,\mathcal{N})$ such that the following properties hold.

1. *$\mathbf{Q}_{\varepsilon_n}\to\mathbf{Q}_0$ strongly in $H^1_{\mathrm{loc}}(\Omega,\mathbb{S}_0)$ and $\varepsilon_n^{-2}f_b(\mathbf{Q}_{\varepsilon_n})\to 0$ in $L^1_{\mathrm{loc}}(\Omega)$.*
2. *$\mathbf{Q}_0$ is locally minimizing harmonic in Ω, that is, for every ball $B\subset\subset\Omega$ and any $\mathbf{P}\in H^1(B,\mathcal{N})$ with $\mathbf{P}=\mathbf{Q}_0$ on ∂B, there holds*
$$\frac12\int_B|\nabla\mathbf{Q}_0|^2\mathrm{d}x\le\frac12\int_B|\nabla\mathbf{P}|^2\mathrm{d}x.$$
3. *There exists a locally finite set $\mathcal{S}_{\mathrm{pts}}\subset\Omega$, such that $\mathbf{Q}_0$ is smooth in $\Omega\backslash\mathcal{S}_{\mathrm{pts}}$.*
4. *For any $j\in\mathbb{Z}_{\ge 0}$, $\mathbf{Q}_{\varepsilon_n}\to\mathbf{Q}_0$ in $C^j_{\mathrm{loc}}(\Omega\backslash\mathcal{S}_{\mathrm{pts}},\mathbb{S}_0)$. In particular, for any $B_r(x_0)\subset\subset\Omega\backslash\mathcal{S}_{\mathrm{pts}}$, with $r>0$, $\mathbf{Q}_{\varepsilon_n}$ is a classical solution for*
$$\Delta\mathbf{Q}_{\varepsilon_n} = -\frac{1}{2r_*^2}|\nabla\mathbf{Q}_{\varepsilon_n}|^2\mathbf{Q}_{\varepsilon_n} - \frac{3}{r_*^4}\operatorname{tr}(\nabla\mathbf{Q}_{\varepsilon_n}\nabla\mathbf{Q}_{\varepsilon_n}\mathbf{Q}_{\varepsilon_n})\left(\mathbf{Q}^2_{\varepsilon_n} - \frac{2r_*^2}{3}\mathbf{I}\right) + \mathbf{R}_n.$$
in $B_{r/2}(x_0)$. Here, $\mathbf{R}_n$ is a remainder satisfying the estimate
$$\|D^j\mathbf{R}_n\|_{L^\infty(B_{r/2}(x_0))}\le C\varepsilon_n^2 r^{-j-2},$$
where $C>0$ depends only on $\mathcal{A}$ and M.

Some remarks I

- This theorem provides a generalization of the H^1 and uniform convergence results presented in [3], as well as the C^j convergence result discussed in [4]. In our specific context, where we consider local minimizers, the H^1 convergence can be established using a Luckhaus-type lemma. Furthermore, we provide detailed estimates for the remainder terms in the Euler-Lagrange equation. These results heavily rely on the specific structure of the Euler-Lagrange equation and necessitate the use of bootstrap arguments.
- Furthermore, when considering global minimizers in a smooth domain with prescribed boundary values that are sufficiently smooth themselves, we can obtain stronger regularity properties for the map $\mathbf{Q}_\varepsilon$.

Theorem (Minimizers with logarithmical energy bound)

Let $\Omega\subset\mathbb{R}^3$ be a bounded Lipschitz domain. Assume that $\{\mathbf{Q}_\varepsilon\}_{0<\varepsilon<1}$ is a sequence of local minimizers of (2), satisfying

$$E_\varepsilon(\mathbf{Q}_\varepsilon,\Omega)\le M(|\log\varepsilon|+1), \qquad \|\mathbf{Q}_\varepsilon\|_{L^\infty(\Omega)}\le M,$$

for some $M>0$. There exist a subsequence $\varepsilon_n\to 0^+$ and a closed set $\mathcal{S}_{\mathrm{line}}\subset\overline{\Omega}$ such that

$$\left(\frac12|\nabla\mathbf{Q}_{\varepsilon_n}|^2 + \frac{1}{\varepsilon_n^2}f_b(\mathbf{Q}_{\varepsilon_n})\right)\frac{\mathrm{d}x}{\log\frac{1}{\varepsilon_n}} \rightharpoonup^* \mu_0 \text{ in } (C(\overline{\Omega}))'$$

as $n\to+\infty$ and the following properties hold.

1. *$\operatorname{supp}(\mu_0) = \mathcal{S}_{\mathrm{line}}$.*
2. *$\Omega\cap\mathcal{S}_{\mathrm{line}}$ is a countably $\mathcal{H}^1$-rectifiable set, and $\mathcal{H}^1(\Omega\cap\mathcal{S}_{\mathrm{line}})<+\infty$.*
3. *If a subdomain U of Ω satisfies $U\subset\subset\Omega\backslash\mathcal{S}_{\mathrm{line}}$, then*
$$E_{\varepsilon_n}(\mathbf{Q}_{\varepsilon_n},U)\le C,$$
where $C>0$ depends only on $\mathcal{A}$, M and U. In such U, one can apply Theorem 0.1 to get further results.
4. *For $\mathcal{H}^1$-a.e. $x\in\mathcal{S}_{\mathrm{line}}\cap\Omega$,*
$$\lim_{r\to 0^+}\frac{\mu_0(B_r(x))}{2r}\in\{\kappa_*, 2\kappa_*\},$$
where $\kappa_* = \pi r_*^2/2$.
5. *$\mu_0\llcorner\Omega$ is associated with a 1-dimensional stationary varifold.*
6. *For any open set $K\subset\subset\Omega$, there holds*
$$\mathcal{S}_{\mathrm{line}}\cap\overline{K} = \{L_1, L_2, \dots, L_p\},\ \ p\in\mathbb{Z}_+,$$
where $\{L_i\}_{i=1}^p$ are closed straight line segments such that for $i\ne j$, L_i and L_j are disjoint or they intersect at a common endpoint. Moreover, the assertions as follows are true.
    1. *If $\overline{B^2_r(x)}\subset K$ satisfies $B^2_r(x)\cap\mathcal{S}_{\mathrm{line}} = \{x\}$, and x is not an endpoint for any L_i, then the free homotopy class (see Definition **??**) of $\mathbf{Q}_0|_{\partial B^2_r(x_0)}$ is non-trivial.*
    2. *If $x\in K$ is an endpoint of exactly q segments $L_{i_1},\dots,L_{i_q}$, then $q\ne 1$. If $q=2$, the angle of L_{i_1} and L_{i_2} is π. If $q=3$, L_{i_1}, L_{i_2}, and L_{i_2} are in the same plane and the angles of them are all $2\pi/3$.*

Some remarks II

- This result generalizes Theorem 1 and Proposition 2 from [1] to our specific model. The proof of this theorem relies on the monotonicity formula, which is derived from the Pohozaev identity. Notably, the proof of the sixth property is based on well-established findings regarding 1-dimensional stationary varifolds.
- It is important to emphasize that in [1], the author demonstrated that the endpoints of straight line segments in $\mathcal{S}_{\mathrm{line}}$ must be even. However, in our model, obtaining such a result is not possible due to the differing topological structure of the vacuum manifold. Instead, for our model, we investigate the endpoints of segments with a maximum of three elements and provide their corresponding structure.

When are the assumptions on minimizers are true?

Let $\Omega\subset\mathbb{R}^3$ be a bounded smooth domain. Assume that $\{\mathbf{Q}_\varepsilon\}_{0<\varepsilon<1}$ are global minimizers of (2) in the space $H^1(\Omega,\mathbb{S}_0;\mathbf{Q}_{b,\varepsilon})$ with $\mathbf{Q}_{b,\varepsilon}\in H^{1/2}(\partial\Omega,\mathcal{N})$. The following properties hold.

1. If $\sup_{0<\varepsilon<1}\|\mathbf{Q}_{b,\varepsilon}\|_{H^{1/2}(\partial\Omega,\mathcal{N})}\le C_0$ for some $C_0>0$, then there exists $C>0$ depending only on $\mathcal{A}$, C_0, and Ω such that
$$E_\varepsilon(\mathbf{Q}_\varepsilon,\Omega)\le C(|\log\varepsilon|+1).$$
2. If $\mathbf{Q}_{b,\varepsilon} = \mathbf{Q}_b\in H^{1/2}(\partial\Omega,\mathcal{N})$ for any $0<\varepsilon<1$, then $E_\varepsilon(\mathbf{Q}_\varepsilon,\Omega)\le C$, where $C>0$ depends only on $\mathcal{A},\Omega$, and $\mathbf{Q}_b$.

Highlights

While similar frameworks are used as in previous works, the mathematical analysis is significantly more challenging due to the different nematic phase structure of this model. Specifically, the nematic phase of this model lies in the manifold

$$\mathcal{N} = \{r_*(\mathbf{n}^{\otimes 2} - \mathbf{m}^{\otimes 2}) : (\mathbf{n},\mathbf{m})\in\mathbb{S}^2\times\mathbb{S}^2, \mathbf{n}\cdot\mathbf{m} = 0\},$$

which exhibits a more complicated structure compared to the uniaxial phase whose manifold is isometric to $\mathbb{RP}^2$. The distinct tangent and normal space structures of $\mathcal{N}$ compared to the uniaxial case require employing different quantitative tools when studying higher-order convergence of the minimizers. Additionally, the topological characterization of $\mathcal{N}$ differs substantially from the uniaxial setting. Indeed, we will prove that $\mathcal{N} = \mathbb{S}^3/Q_8$, where Q_8 denotes the quaternion group. When establishing estimates of Jerrard-Sandier type for our model, the functions used for the uniaxial case are no longer applicable. Hence, we must develop more refined quantitative estimates.

Main steps of the proof

1. We introduce quantities associated with the minimal polynomial of matrices in $\mathcal{N}$ and present new iterative arguments to obtain a priori estimates for the solutions of the Euler-Lagrange equation related to the minimizing problem. These calculations heavily rely on the characterization of the tangent and normal spaces of $\mathcal{N}$.
2. We examine the free homotopy class on the manifold $\mathcal{N}$ and use a direct approach to characterize the topological properties of loops on $\mathcal{N}$.
3. Building upon the definitions provided in [1], we introduce new functions to evaluate the differences in eigenvalues for symmetric traceless matrices. Additionally, we emphasize that these functions require higher regularity. By utilizing these functions and the results of Step 2, we establish a new Jerrard-Sandier type estimate.
4. By combining the results obtained from the first three steps, we use the well-known Luckhaus arguments (see [2]) to prove the main theorems outlined in this paper.

References

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