Nonlinear Analysis 78 (2013) 168–182

Contents lists available at SciVerse ScienceDirect

Nonlinear Analysis

journal homepage: www.elsevier.com/locate/na

Partial regularity of the Landau–de Gennes energy model for liquid crystals

Dan Liu *

Department of Mathematics, East China Normal University, 200241, PR China
Center for Partial Differential Equations, East China Normal University, Shanghai 200241, PR China

ARTICLE INFO

Article history:
Received 18 June 2012
Accepted 3 October 2012
Communicated by Enzo Mitidieri

MSC:
82D55
35B25
35B40
35Q55

Keywords:
Partial regularity
Landau–de Gennes model
Smectic liquid crystals
Minimizers
Energy decay

ABSTRACT

We discuss the partial regularity of non-trivial minimizers for the Landau–de Gennes energy functional in a bounded domain of $\mathbb{R}^3$. Off some relatively closed subset $\mathcal{Z}$, whose 1-dimensional Hausdorff measure is zero, we prove that the minimizers are analytic.

1. Introduction

In this article, we are interested in the partial regularity of non-trivial minimizers for the Landau–de Gennes model, which describes phase transitions of liquid crystals. Based on the de Gennes theory, the state of liquid crystals can be described by $(\Psi, \mathbf{n})$. They are the minimizers of the Landau–de Gennes energy functional

$$\begin{aligned}\mathcal{LG}[\Psi,\mathbf{n}] &= \int_\Omega \Bigg\{|\nabla_{q\mathbf{n}}\Psi|^2-\kappa^2|\Psi|^2+\frac{\kappa^2}{2}|\Psi|^4+K_1|\mathrm{div}\,\mathbf{n}|^2+K_2|\mathbf{n}\cdot\mathrm{curl}\,\mathbf{n}+\tau|^2\\ &\quad +K_3|\mathbf{n}\times\mathrm{curl}\,\mathbf{n}|^2+(K_2+K_4)[\mathrm{tr}(\nabla\mathbf{n})^2-(\mathrm{div}\,\mathbf{n})^2]\Bigg\}\mathrm{d}x\\ &= \int_\Omega\{|\nabla_{q\mathbf{n}}\Psi|^2+\mathcal{F}(|\Psi|)+\mathcal{W}(\mathbf{n},\nabla\mathbf{n})\}\mathrm{d}x, \end{aligned}\qquad (1.1)$$

where $\nabla_{q\mathbf{n}}\Psi=\nabla\Psi-iq\mathbf{n}\Psi$, Ω is a bounded, smooth, simply-connected domain in $\mathbb{R}^3$ with the smoothness of boundary and boundary data. We call $\mathcal{F}(|\Psi|)$ and $\mathcal{W}(\mathbf{n},\nabla\mathbf{n})$ the smectic energy density and the nematic Oseen–Frank energy density respectively.

* Correspondence to: Department of Mathematics, East China Normal University, 200241, PR China.
E-mail address: dl1567@nyu.edu.

0362-546X/$ – see front matter
doi:10.1016/j.na.2012.10.003

The complex-valued function Ψ is called the order parameter. When $\Psi = 0$, it denotes the nematic phase, and $\Psi \not\equiv 0$ the smectic phase correspondingly. We call that a minimizer $(\Psi, \mathbf{n})$ is nontrivial, if $\Psi \not\equiv 0$. The unit vector field $\mathbf{n}$ is called the director field. The constant τ is called the chiral constant. The real number K_4 and the positive numbers K_1, K_2, K_3 are elastic coefficients. We call κ the Ginzburg–Landau parameter of the liquid crystal. The real number q is called the wave number.

The effect of the wave number q on the behavior of the minimizers has been investigated in [1]. The author studies the nucleation of a nontrivial minimizer from a trivial one, which can be regarded as the phase transition from a nematic phase to a smectic phase. The critical wave number of the q, called Q_{c_3}, is introduced for the first time by X.B. Pan in this paper. And the author also gives a precise description of Q_{c_3}, which is an important indicator to distinguish the smectic and the nematic phase.

There have been some results on the partial regularity for the trivial minimizer $(0, \mathbf{n})$. First, taking a special case $K_1 = K_2 = K_3, K_4 = 0$ and $\Psi = 0$ in functional (1.1), then $\mathbf{n}$ is a minimizing harmonic map from Ω to $\mathbb{S}^2$. In [2,3], R. Schoen and K. Uhlenbeck establish the partial regularity results interior the domain Ω and near the boundary $\partial\Omega$ under the Dirichlet boundary condition for harmonic maps. Moreover, they also show that the closed set $\mathcal{Z}$ consists of finite points. Second, R. Gulliver and B. White [4] prove the asymptotic behavior result on the rate of the convergence of a minimizer near a point of $\mathcal{Z}$. For more precise feature of the subset $\mathcal{Z}$, H. Brezis et al. [5] study some related topics on harmonic maps with defects, where the geometric structure of the defects is a finite number of points or "holes". For some other topics on harmonic maps, see also surveys of Y.M. Chu [6], G.J. Liao [7], X.G. Liu [8], L. Simon [9], C.Y. Wang [10] etc. Third, the existence and partial regularity for the minimizers of the nematic Oseen–Frank energy model have been well discussed by R. Hardt, D. Kinderlehrer and F.H. Lin in [11]. They prove that a minimizer $\mathbf{n}$ is real analytic on $\Omega \setminus \mathcal{Z}$ for some relatively closed subset $\mathcal{Z}$ whose one dimensional Hausdorff measure is zero. For the existence of the minimizers, we note that the Oseen–Frank functional may not be coercive in space $W^{1,2}(\Omega, \mathbb{S}^2)$. Therefore, some constraints on the elastic coefficients are needed in [11]. Actually, X.B. Pan [1] points out that, using the idea of Hardt–Kinderlehrer–Lin, this difficulty can be overcome by considering an equivalent functional which is coercive in $W^{1,2}(\Omega, \mathbb{R}^3)$.

Our motivation is derived from the article of Hardt–Kinderlehrer–Lin (see [11]) on the partial regularity of minimizers for the Oseen–Frank energy model. However, for smectic liquid crystals, the Landau–de Gennes energy model (1.2) involves the smectic energy density term and the $|\nabla_{q\mathbf{n}}\Psi|^2$ term, i.e.,

$$\int_\Omega \left\{ |\nabla_{q\mathbf{n}}\Psi|^2 - \kappa^2|\Psi|^2 + \frac{\kappa^2}{2}|\Psi|^4 \right\} dx.$$

Moreover, the order parameter Ψ is regarded as an independent variable of $\mathbf{n}$. Therefore, we cannot apply the result of partial regularity for the Oseen–Frank energy model to our case. A modification argument is necessary.

In our paper, we will consider the following form of the Landau–de Gennes energy functional in Ω occupied by the liquid crystal

$$\mathcal{E}[\Psi, \mathbf{n}] = \int_\Omega \left\{ |\nabla_{q\mathbf{n}}\Psi|^2 - \kappa^2|\Psi|^2 + \frac{\kappa^2}{2}|\Psi|^4 + K_1|\operatorname{div}\mathbf{n}|^2 + K_2|\operatorname{curl}\mathbf{n} + \tau\mathbf{n}|^2 \right\} dx, \tag{1.2}$$

with Dirichlet boundary condition for $\mathbf{n}$ and Neumann boundary condition for Ψ:

$$\mathbf{n} = \mathbf{n}_0, \quad \nabla_{q\mathbf{n}}\Psi \cdot \nu = 0, \quad \text{on } \partial\Omega \tag{1.3}$$

where $\mathbf{n}_0$ is a smooth unit vector field on $\partial\Omega$ and ν is an outward unit normal vector of Ω.

In [11], it is showed that the last term $\int_\Omega \{\operatorname{tr}(\nabla\mathbf{n})^2 - (\operatorname{div}\mathbf{n})^2\} dx$ in (1.1) is a surface energy term under the Dirichlet boundary condition of $\mathbf{n}$, which only depends on the boundary data $\mathbf{n}_0$. Therefore, by letting $K_2 = K_3$, dropping the surface energy $\int_\Omega \{\operatorname{tr}(\nabla\mathbf{n})^2 - (\operatorname{div}\mathbf{n})^2\} dx$ and making some scalings, we obtain the simplified functional (1.2) from (1.1). Compared with (1.1), the simplified form (1.2) will keep the main feature and the most difficulties of the full Oseen–Frank model. For details see [1].

In order to discuss the partial regularity of non-trivial minimizers $(\Psi, \mathbf{n})$ with $\Psi \neq 0$, the first problem we need to solve is the existence of non-trivial minimizers. This part of work has been studied by X.B. Pan in [1]. First, since the parameter τ is not important to the study of the existence for the minimizers, in [1] the author assumes that $\tau = 0$. It is showed that under the assumption on the smoothness of the domain and the boundary data $\mathbf{n}_0$, for any positive numbers K_1, K_2, κ and for any real number q, the minimizers of the variational problem (1.2) with $\tau = 0$ exist in the space $W^{1,2}(\Omega, \mathbb{C}) \times W^{1,2}(\Omega, \mathbb{S}^2, \mathbf{n}_0)$, where

$$W^{1,2}(\Omega, \mathbb{S}^2, \mathbf{n}_0) = \left\{ \mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2) : \mathbf{n} = \mathbf{n}_0 \text{ on } \partial\Omega \right\}.$$

Next, we want to know if the minimizers are non-trivial. In Theorem 5.4 [1], the sufficient conditions under which the minimizers are non-trivial are proved. It also gives an asymptotic analysis on the behavior of the minimizers when K_1 or K_2 is large. Based on the statements (1i) and (2i) of Theorem 5.4 in [1], throughout this paper we will assume that κ is large enough and positive number q is sufficiently small to ensure the existence of the nontrivial minimizers $(\Psi, \mathbf{n})$.