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Asymptotic Behavior of Nematic States in the Theory of Liquid Crystals under Applied Magnetic Fields

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Abstract

We consider the asymptotic behavior of nematic states of liquid crystals under applied magnetic fields. We treat the Landau-de Gennes functional with the Dirichlet boundary condition for the director field. We show that under some conditions, strong field does not bring the pure nematic state that is a very different responce with superconductors.

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1 Introduction

In this paper, we consider the nematic state of liquid crystals under applied magnetic fields. Let $\mathcal{F}_N(\boldsymbol{n}, \nabla \boldsymbol{n})$ be the classical Oseen-Frank density of nematic liquid crystals. Then for the applied field $\boldsymbol{H}$, we must add a density $-\chi(\boldsymbol{H}\cdot\boldsymbol{n})^2$ to $\mathcal{F}_N(\boldsymbol{n}, \nabla \boldsymbol{n})$, and consider an energy functional:

$$\int_\Omega \{\mathcal{F}_N(\boldsymbol{n}, \nabla \boldsymbol{n}) - \chi(\boldsymbol{H}\cdot\boldsymbol{n})^2\}dx.$$

Here χ is a positive parameter and $\boldsymbol{n} : \overline{\Omega} \to \mathbb{S}^2$ is a director field of the nematic crystals. See de Gennes and Prost [6, p. 287]. Though there are many article on liquid crystals without magnetic field (for example, Aramaki [2], [3], Bauman et al. [4], Hardt et al. [9], Pan [11], [14]), there are few references which treat applied fields. See Lin and Pan [10] and Pan [12], [13], Aramaki [1].

According to the Landau-de Gennes theory, phase transitions of nematic states to smectic states can be described by the minimizer $(\psi, \boldsymbol{n})$ of the Landau-de Gennes functional:

$$\mathcal{E}[\psi, \boldsymbol{n}] = \int_\Omega \Big\{ |\nabla_{q\boldsymbol{n}}\psi|^2 + \frac{\kappa^2}{2}(1-|\psi|^2)^2 + K_1|\operatorname{div}\boldsymbol{n}|^2 + K_2|\boldsymbol{n}\cdot\operatorname{curl}\boldsymbol{n}|^2 + K_3|\boldsymbol{n}\times\operatorname{curl}\boldsymbol{n}|^2 + (K_2+K_4)[\operatorname{tr}(\nabla\boldsymbol{n})^2 - |\operatorname{div}\boldsymbol{n}|^2] - \chi(\boldsymbol{H}\cdot\boldsymbol{n})^2 \Big\} dx \tag{1.1}$$

where κ, K_1, K_2, K_3 and χ are positive constants, K_4 is a constant, and q is a real number. Here we denoted $\nabla_{q\boldsymbol{n}}\psi = \nabla\psi - iq\boldsymbol{n}\psi$. Without loss of generality, we may assume that $q \ge 0$.

We consider the functional $\mathcal{E}$ under the strong anchoring condition, mathematically, the Dirichlet boundary condition $\boldsymbol{n} = \boldsymbol{u}_0$ on $\partial\Omega$ for the director field $\boldsymbol{n}$ where $\boldsymbol{u}_0$ is a given smooth boundary data. We note that under this anchoring condition, we can drop the divergence term $\operatorname{tr}(\nabla\boldsymbol{n})^2 - |\operatorname{div}\boldsymbol{n}|^2$ in (1.1) (cf. [9]). We consider the functional $\mathcal{E}$ on the space $W^{1,2}(\Omega,\mathbb{C}) \times W^{1,2}(\Omega,\mathbb{S}^2,\boldsymbol{u}_0)$ where $W^{1,2}(\Omega,\mathbb{C})$ is the usual Sobelev space of complex-valued functions and

$$W^{1,2}(\Omega,\mathbb{S}^2,\boldsymbol{u}_0) = \{\boldsymbol{n}\in W^{1,2}(\Omega,\mathbb{R}^3); |\boldsymbol{n}(x)| = 1 \text{ a.e. in } \Omega, \boldsymbol{n} = \boldsymbol{u}_0 \text{ on } \partial\Omega\}.$$

Here and from now, for some Euclidean space $E\,(=\mathbb{R}, \mathbb{C}$ or $\mathbb{R}^3)$, $W^{1,2}(\Omega, E)$ denotes the usual Sobolev space with values in E.

Throughout this paper, we only consider the case where $K_1 = K_2 = K_3 = K$, Ω is simply connected domain in $\mathbb{R}^3$ with smooth boundary $\Gamma = \partial\Omega$, and assume that the applied magnetic field $\boldsymbol{H}$ and the boundary data $\boldsymbol{u}_0$ are constant vectors with angle θ. Thus we assume that

$$\boldsymbol{H} = \sigma\boldsymbol{h}, \quad \boldsymbol{h}\cdot\boldsymbol{e} = \cos\theta \tag{1.2}$$

where $\boldsymbol{h}$ and $\boldsymbol{u}_0 = \boldsymbol{e}$ are constant unit vectors and $\sigma \ge 0$ denotes the intensity of the applied magnetic field.

If we replace $\boldsymbol{h}$ by $-\boldsymbol{h}$, we can assume that $0 < \theta \le \pi/2$. When $\theta = \pi/2$, [10] considered the magnetic field-induced instability in great detail. Therefore we assume that

$$0 < \theta < \frac{\pi}{2}. \tag{1.3}$$

The states of liquid crystals are described by the minimizers $(\psi, \boldsymbol{n})$ of $\mathcal{E}$. If $\psi = 0$, the minimizers correspond to the nematic states, and if $\psi \ne 0$, the minimizers correspond to the smectic states. Compared with the theory of superconductivity, the nematic states look like normal states and the smectic states look like superconducting states.

For brevity, we write

$$\mathcal{E}[\psi, \boldsymbol{n}] = \mathcal{G}[\psi, \boldsymbol{n}] + \mathcal{F}[\boldsymbol{n}] - \int_\Omega \chi(\boldsymbol{H} \cdot \boldsymbol{n})^2 dx \tag{1.4}$$

where

$$\mathcal{F}[\boldsymbol{n}] = \int_\Omega \{K\{|\operatorname{div} \boldsymbol{n}|^2 + |\operatorname{curl} \boldsymbol{n}|^2\} dx \tag{1.5}$$

is the simplified Oseen-Frank energy for nematics and

$$\mathcal{G}[\psi, \boldsymbol{n}] = \int_\Omega \left\{ |\nabla_{q\boldsymbol{n}}\psi|^2 + \frac{\kappa^2}{2}(1 - |\psi|^2)^2 \right\} dx \tag{1.6}$$

is the Ginzburg-Landau energy for smectics. Moreover, we write

$$\mathcal{F}_{\sigma \boldsymbol{h}}[\boldsymbol{n}] = \mathcal{F}[\boldsymbol{n}] - \chi\sigma^2 \int_\Omega (\boldsymbol{h} \cdot \boldsymbol{n})^2 dx. \tag{1.7}$$

Then the energy functional $\mathcal{E}$ has a trivial critical point

$$\psi = 0, \quad \boldsymbol{n} = \boldsymbol{n}_\sigma$$

where $\boldsymbol{n}_\sigma$ is a global minimizer of $\mathcal{F}_{\sigma \boldsymbol{h}}$ on $W^{1,2}(\Omega, \mathbb{S}^2, \boldsymbol{e})$, and we call $(\psi, \boldsymbol{n}) = (0, \boldsymbol{n}_\sigma)$ the pure nematic state. However, as we will see in Section 2, for any $\psi \in W^{1,2}(\Omega, \mathbb{C})$, $(\psi, \boldsymbol{e})$ is not a critical point of $\mathcal{E}$ under the assumption (1.3). Thus there is no pure smectic states in the sense of [10].

In the supeconductivity theory, it is well known that the superconductivity is destroyed for the strong magnetic field. But we can show that in the theory of liquid crystals, if σ is sufficiently large, the pure nematic states are not global minimizer of $\mathcal{E}$ when $K_1 = K_2 = K_3 = K$.

Theorem 1.1. *Fix $q, \kappa, K, \boldsymbol{h}$ and $\boldsymbol{e}$. When σ is sufficiently large, the pure nematic states $(0, \boldsymbol{n}_\sigma)$ are not global minimizers of $\mathcal{E}$. We can also show that*

$$\boldsymbol{h} \cdot \boldsymbol{n}_\sigma(x) \to 1 \quad \text{in } L^2(\Omega) \quad \text{as } \sigma \to \infty.$$

Remark 1.2. *This theorem implies that when σ is large enough, the states are not pure nematic, and moreover that $\boldsymbol{n}_\sigma$ tends to the direction of $\boldsymbol{h}$ as $\sigma \to \infty$.*

2 Preliminaries

In this section, we give preliminaries for the proof of Theorem 1.1.

In general, we call $(\psi_0, \boldsymbol{n}_0) \in W^{1,2}(\Omega, \mathbb{C}) \times W^{1,2}(\Omega, \mathbb{S}^2, \boldsymbol{u}_0)$ a critical point of $\mathcal{E}$, if for any $\phi \in W^{1,2}(\Omega, \mathbb{C})$ and $\boldsymbol{v} \in W_0^{1,2}(\Omega, \mathbb{R}^3) \cap L^\infty(\Omega, \mathbb{R}^3)$,

$$\frac{d}{dt}\bigg|_{t=0} \mathcal{E}[\psi_t, \boldsymbol{n}_t] = 0$$

where

$$\psi_t = \psi_0 + t\phi, \quad \boldsymbol{n}_t = \frac{\boldsymbol{n}_0 + t\boldsymbol{v}}{|\boldsymbol{n}_0 + t\boldsymbol{v}|}.$$

Here we note that we can write

$$\boldsymbol{n}_t = \boldsymbol{n}_0 + t\boldsymbol{n}_1 + O(t^2)$$

where $\boldsymbol{n}_1 = \boldsymbol{v} - (\boldsymbol{v} \cdot \boldsymbol{n}_0)\boldsymbol{n}_0$. By a simple computation shows that $(\psi_0, \boldsymbol{n}_0) \in W^{1,2}(\Omega, \mathbb{C}) \times W^{1,2}(\Omega, \mathbb{S}^2, \boldsymbol{u}_0)$ is a critical point of $\mathcal{E}$ if and only if

$$\mathcal{A}(\psi_0, \boldsymbol{n}_0; \phi, \boldsymbol{v}) - \chi\sigma^2 \int_\Omega (\boldsymbol{h} \cdot \boldsymbol{n}_0)(\boldsymbol{h} \cdot \boldsymbol{n}_1) dx = 0 \tag{2.1}$$

where

$$\begin{aligned}\mathcal{A}(\psi_0, \boldsymbol{n}_0; \phi, \boldsymbol{v}) = \int_\Omega \Big\{ & \Re[\nabla_{q\boldsymbol{n}_0}\psi_0 \cdot \overline{\nabla_{q\boldsymbol{n}_0}\phi} - \kappa^2(1 - |\psi_0|^2)\psi_0\overline{\phi}] \\ & - q\boldsymbol{n}_1 \cdot \Im(\overline{\psi_0}\nabla_{q\boldsymbol{n}_0}\psi_0) + K\{(\operatorname{div} \boldsymbol{n}_0)(\operatorname{div} \boldsymbol{n}_1) + \operatorname{curl} \boldsymbol{n}_0 \cdot \operatorname{curl} \boldsymbol{n}_1\} \Big\} dx.\end{aligned}$$

Therefore, if $(\psi_0, \boldsymbol{n}_0) \in W^{1,2}(\Omega, \mathbb{C}) \times W^{1,2}(\Omega, \mathbb{S}^2, \boldsymbol{u}_0)$ is a critical point of $\mathcal{E}$, then ψ_0 satisfies

$$\begin{cases} -\nabla_{q\boldsymbol{n}}^2\psi_0 = \kappa^2(1 - |\psi_0|^2)\psi_0 & \text{in } \Omega, \\ \nabla_{q\boldsymbol{n}}\psi_0 \cdot \boldsymbol{\nu} = 0 & \text{on } \partial\Omega \end{cases} \tag{2.2}$$

where $\boldsymbol{\nu}$ denotes the outer unit normal vector field to $\partial\Omega$.

Remark 2.1. *We note that for any $\psi_0 \in W^{1,2}(\Omega, \mathbb{C})$, $(\psi_0, \boldsymbol{e})$ is not a critical point of $\mathcal{E}$.*

In fact, let $(\psi_0, \boldsymbol{e})$ be a critical point of $\mathcal{E}$. Since ψ_0 satisfies the equation (2.2), then for any $\phi \in W^{1,2}(\Omega, \mathbb{C})$, if we multiply $\overline{\phi}$ with the first line of (2.2) and using the second line of (2.2), integrate over Ω, we see that

$$\mathcal{A}(\psi_0, \boldsymbol{e}; \phi, \boldsymbol{v}) = -\int_\Omega q\boldsymbol{n}_1 \cdot \Im(\overline{\psi_0}\nabla_{q\boldsymbol{e}}\psi_0) dx.$$

Thus (2.1) becomes

$$\int_\Omega \{q\Im(\overline{\psi_0}\nabla_{q\boldsymbol{e}}\psi_0)\cdot \boldsymbol{n}_1 + \chi\sigma^2(\boldsymbol{h}\cdot\boldsymbol{e})(\boldsymbol{h}\cdot\boldsymbol{n}_1)\}dx = 0$$

for any $\boldsymbol{v} \in W_0^{1,2}(\Omega,\mathbb{R}^3)\cap L^\infty(\Omega,\mathbb{R}^3)$. Since $W_0^{1,2}(\Omega,\mathbb{R}^3)\cap L^\infty(\Omega,\mathbb{R}^3)$ is dense in $W_0^{1,2}(\Omega,\mathbb{R}^3)$, we have

$$q\{\Im(\overline{\psi_0}\nabla_{q\boldsymbol{e}}\psi_0) - (\Im(\overline{\psi_0}\nabla_{q\boldsymbol{e}}\psi_0)\cdot\boldsymbol{e})\boldsymbol{e}\} + \chi\sigma^2\{(\boldsymbol{h}\cdot\boldsymbol{e})\boldsymbol{h} - (\boldsymbol{h}\cdot\boldsymbol{e})^2\boldsymbol{e}\} = 0.$$

Since Γ is smooth, there exists $x_0\in\Gamma$ such that $\boldsymbol{\nu}(x_0) = \boldsymbol{e}^\perp$ where $\boldsymbol{e}^\perp$ is a unit vector which is orthogonal to $\boldsymbol{e}$ and $\boldsymbol{h}\cdot\boldsymbol{e}^\perp\neq 0$. Using the second line of (2.2), we have

$$\begin{aligned}\chi\sigma^2(\boldsymbol{h}\cdot\boldsymbol{e})\boldsymbol{h}\cdot\boldsymbol{\nu}(x_0) &= \chi\sigma^2(\boldsymbol{h}\cdot\boldsymbol{e})^2\boldsymbol{e}\cdot\boldsymbol{\nu}(x_0)\\ &\quad + q(\Im(\overline{\psi(x_0)}\nabla_{q\boldsymbol{e}}\psi_0(x_0))\cdot\boldsymbol{e})\boldsymbol{e}\cdot\boldsymbol{\nu}(x_0) = 0.\end{aligned}$$

From this equality, we get $\chi\sigma^2(\boldsymbol{h}\cdot\boldsymbol{e})\boldsymbol{h}\cdot\boldsymbol{e}^\perp = 0$. Since $\boldsymbol{h}\cdot\boldsymbol{e} = \cos\theta > 0$, if $\sigma > 0$, we have $\boldsymbol{h}\cdot\boldsymbol{e}^\perp = 0$. This leads to a contradiction. Thus there is no pure smectic state in the sense of [10].

Define

$$C(\sigma) = C(\sigma, K, \boldsymbol{h}, \boldsymbol{e}) = \inf_{\boldsymbol{n}\in W^{1,2}(\Omega,\mathbb{S}^2,\boldsymbol{e})} \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}]. \tag{2.3}$$

Then we have

Lemma 2.2. *For any $\sigma, K > 0$, and $\boldsymbol{h}, \boldsymbol{e}$ satisfying (1.3), $C(\sigma)$ is achieved in $W^{1,2}(\Omega,\mathbb{S}^2,\boldsymbol{e})$.*

Proof. For any $\boldsymbol{n}\in W^{1,2}(\Omega,\mathbb{S}^2,\boldsymbol{e})$, it is easily seen that

$$\mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}] = \mathcal{F}[\boldsymbol{n}] - \chi\sigma^2\int_\Omega(\boldsymbol{h}\cdot\boldsymbol{n})^2dx \geq -\chi\sigma^2|\Omega|.$$

On the other hand, we see that

$$C(\sigma) \leq \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{e}] = -\chi\sigma^2(\cos\theta)^2|\Omega|.$$

Thus we have

$$-\chi\sigma^2|\Omega| \leq C(\sigma) \leq -\chi\sigma^2(\cos\theta)^2|\Omega|.$$

Let $\{\boldsymbol{n}_j\}\subset W^{1,2}(\Omega,\mathbb{S}^2,\boldsymbol{e})$ be a minimizing sequence of $C(\sigma)$. Then

$$\mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}_j] = \mathcal{F}[\boldsymbol{n}_j] - \chi\sigma^2\int_\Omega(\boldsymbol{h}\cdot\boldsymbol{n}_j)^2dx = C(\sigma) + o(1)$$

as $j \to \infty$. From this equality, we have

$$K\int_\Omega \{|\mathrm{div}\, \boldsymbol{n}_j|^2 + |\mathrm{curl}\, \boldsymbol{n}_j|^2\}dx \leq \chi\sigma^2 \int_\Omega |\boldsymbol{h}\cdot\boldsymbol{n}_j|^2 dx + C(\sigma) + 1 \leq \chi\sigma^2|\Omega| + C(\sigma) + 1.$$

Therefore, $\{\mathrm{div}\, \boldsymbol{n}_j\}$ is bounded in $L^2(\Omega)$ and $\{\mathrm{curl}\, \boldsymbol{n}_j\}$ is bounded in $L^2(\Omega, \mathbb{R}^3)$. Since $|\boldsymbol{n}_j| = 1$ a.e. in Ω and $\boldsymbol{n}_j|_\Gamma = \boldsymbol{e}$, it follows from Dautray and Lions [5] that $\{\boldsymbol{n}_j\}$ is bounded in $W^{1,2}(\Omega, \mathbb{R}^3)$. Passing to a subsequence, we may assume that $\boldsymbol{n}_j \to \boldsymbol{n}_0$ weakly in $W^{1,2}(\Omega, \mathbb{R}^3)$, strongly in $L^4(\Omega, \mathbb{R}^3)$ and a.e. in Ω. Thus we have $|\boldsymbol{n}_0| = 1$ a.e. in Ω and $\boldsymbol{n}_0|_\Gamma = \boldsymbol{e}$, so $\boldsymbol{n}_0 \in W^{1,2}(\Omega, \mathbb{S}^2, \boldsymbol{e})$. We note that $\mathrm{div}\, \boldsymbol{n}_j \to \mathrm{div}\, \boldsymbol{n}_0$ weakly in $L^2(\Omega)$ and $\mathrm{curl}\, \boldsymbol{n}_j \to \mathrm{curl}\, \boldsymbol{n}_0$ weakly in $L^2(\Omega, \mathbb{R}^3)$. We have

$$\begin{aligned} &\left|\int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n}_j)^2 dx - \int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n}_0)^2 dx\right| \\ &\quad = \left|\int_\Omega (\boldsymbol{h}\cdot(\boldsymbol{n}_j - \boldsymbol{n}_0) + \boldsymbol{h}\cdot\boldsymbol{n}_0)^2 dx - \int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n}_0)^2 dx\right| \\ &\quad \leq \left|\int_\Omega (\boldsymbol{h}\cdot(\boldsymbol{n}_j - \boldsymbol{n}_0))^2 dx\right| + \left|\int_\Omega 2(\boldsymbol{h}\cdot(\boldsymbol{n}_j - \boldsymbol{n}_0))(\boldsymbol{h}\cdot\boldsymbol{n}_0) dx\right| \\ &\quad \leq C\|\boldsymbol{n}_j - \boldsymbol{n}_0\|^2_{L^2(\Omega,\mathbb{R}^3)} \to 0 \end{aligned}$$

as $j \to \infty$. Hence we have

$$\lim_{j\to\infty} \int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n}_j)^2 dx = \int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n}_0)^2 dx.$$

Therefore, we have

$$\begin{aligned} \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}_0] &= \mathcal{F}[\boldsymbol{n}_0] - \chi\sigma^2 \int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n}_0)^2 dx \\ &\leq \liminf_{j\to\infty} \left[\mathcal{F}[\boldsymbol{n}_j] - \chi\sigma^2 \int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n}_j)^2 dx\right] = C(\sigma). \end{aligned}$$

Thus $\boldsymbol{n}_0$ is a minimizer of $\mathcal{F}_{\sigma\boldsymbol{h}}$. □

When $\boldsymbol{n}$ is a minimizer of $\mathcal{F}_{\sigma\boldsymbol{h}}$, we look for the Euler-Lagrange equation for $\boldsymbol{n}$. For any $\boldsymbol{v} \in W_0^{1,2}(\Omega, \mathbb{R}^3)$, we compute the following equation

$$\left.\frac{d}{dt}\right|_{t=0} \left\{\mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n} + t\boldsymbol{v}] - \int_\Omega \lambda(|\boldsymbol{n} + t\boldsymbol{v}|^2 - 1) dx\right\} = 0$$

where λ is the Lagrange multiplier which depends on x. Note that $\mathrm{curl}^2\boldsymbol{n} = -\Delta\boldsymbol{n} + \nabla\mathrm{div}\, \boldsymbol{n}$ and $-\Delta\boldsymbol{n}\cdot\boldsymbol{n} = |\nabla\boldsymbol{n}|^2$ which is easily followed from $\boldsymbol{n}\cdot\boldsymbol{n} = 1$. By the standard arguments, we get the Euler-Lagrange equation for $\boldsymbol{n}$:

$$\begin{cases} -K\Delta\boldsymbol{n} = K|\nabla\boldsymbol{n}|^2\boldsymbol{n} + \chi\sigma^2\big((\boldsymbol{h}\cdot\boldsymbol{n})\boldsymbol{h} - (\boldsymbol{h}\cdot\boldsymbol{n})^2\boldsymbol{n}\big) & \text{in } \Omega, \\ \boldsymbol{n} = \boldsymbol{e} & \text{on } \Gamma. \end{cases} \tag{2.4}$$

Since $\boldsymbol{h} \cdot \boldsymbol{e} = \cos\theta > 0$, we note that $\boldsymbol{e}$ is not a critical point of $\mathcal{F}_{\sigma \boldsymbol{h}}$ for any $\sigma > 0$.

Define

$$\mathcal{M}(\sigma) = \mathcal{M}(\sigma, K, \boldsymbol{h}, \boldsymbol{e}) = \{\boldsymbol{n} \in W^{1,2}(\Omega, \mathbb{S}^2, \boldsymbol{e}); \mathcal{F}_{\sigma \boldsymbol{h}}[\boldsymbol{n}] = C(\sigma)\}. \tag{2.5}$$

We note that $(0, \boldsymbol{n})$ is a critical point of $\mathcal{E}$ if and only if $\boldsymbol{n}$ is a critical point of $\mathcal{F}_{\sigma \boldsymbol{h}}$, and if $\boldsymbol{n} \in \mathcal{M}(\sigma)$, then $(0, \boldsymbol{n})$ is a critical point of $\mathcal{E}$.

Let $\mu = \mu(q\boldsymbol{n})$ be the lowest eigenvalue of the following magnetic Neumann problem

$$\begin{cases} -\nabla_{q\boldsymbol{n}}^2 \phi = \mu\phi & \text{in } \Omega, \\ \nabla_{q\boldsymbol{n}}\phi \cdot \boldsymbol{\nu} = 0 & \text{on } \Gamma \end{cases} \tag{2.6}$$

where $\boldsymbol{\nu}$ denotes the unit outer normal vector field on Γ. That is to say,

$$\mu(q\boldsymbol{n}) = \inf_{0 \neq \phi \in W^{1,2}(\Omega, \mathbb{C})} \frac{\|\nabla_{q\boldsymbol{n}}\phi\|^2_{L^2(\Omega)}}{\|\phi\|_{L^2(\Omega)}}. \tag{2.7}$$

Define

$$\mu_*(q, \sigma) = \inf_{\boldsymbol{n} \in \mathcal{M}(\sigma)} \mu(q\boldsymbol{n}). \tag{2.8}$$

Then we have

Lemma 2.3 ([10]). *(i) If $(\psi, \boldsymbol{n})$ is a global minimizer of $\mathcal{E}$ which is not a pure nematic state, then $\mu(q\boldsymbol{n}) < \kappa^2$.*

(ii) If $\mu_*(q, \sigma) < \kappa^2$, then the pure nematic states are not global minimizers of $\mathcal{E}$.

Proof. (i) Let $(\psi, \boldsymbol{n})$ be a global minimizer of $\mathcal{E}$. If $\psi = 0$, then $\boldsymbol{n} \in \mathcal{M}(\sigma)$. Therefore, $(\psi, \boldsymbol{n}) = (0, \boldsymbol{n})$ is a pure nematic state. Thus if $(\psi, \boldsymbol{n})$ is not a pure nematic state, then $\psi \neq 0$. Choose $\boldsymbol{n}_\sigma \in \mathcal{M}(\sigma)$. Then

$$\mathcal{E}[\psi, \boldsymbol{n}] = \mathcal{G}[\psi, \boldsymbol{n}] + \mathcal{F}_{\sigma \boldsymbol{h}}[\boldsymbol{n}] \leq \mathcal{G}[0, \boldsymbol{n}_\sigma] + \mathcal{F}_{\sigma \boldsymbol{h}}[\boldsymbol{n}_\sigma] = \frac{\kappa^2}{2}|\Omega| + \mathcal{F}_{\sigma \boldsymbol{h}}[\boldsymbol{n}_\sigma].$$

From this inequality, we get

$$\int_\Omega \{|\nabla_{q\boldsymbol{n}}\psi|^2 - \kappa^2|\psi|^2 + \frac{\kappa^2}{2}|\psi|^4\} dx = \mathcal{G}[\psi, \boldsymbol{n}] - \frac{\kappa^2}{2}|\Omega| \leq \mathcal{F}_{\sigma \boldsymbol{h}}[\boldsymbol{n}_\sigma] - \mathcal{F}[\boldsymbol{n}] \leq 0.$$

Therefore, we have

$$\int_\Omega \{|\nabla_{q\boldsymbol{n}}\psi|^2 - \kappa^2|\psi|^2\} dx \leq -\frac{\kappa^2}{2} \int_\Omega |\psi|^4 dx < 0.$$

Hence we get

$$\mu(q\boldsymbol{n}) \leq \frac{\|\nabla_{q\boldsymbol{n}}\psi\|^2_{L^2(\Omega,\mathbb{C}^3)}}{\|\psi\|^2_{L^2(\Omega,\mathbb{C})}} < \kappa^2.$$

(ii) Let $(0, \boldsymbol{n}_\sigma)$ be a pure nematic state of $\mathcal{E}$. Then

$$\mathcal{E}[0, \boldsymbol{n}_\sigma] = \frac{\kappa^2}{2}|\Omega| + \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}_\sigma] = \frac{\kappa^2}{2}|\Omega| + C(\sigma).$$

If $\mu_*(q,\sigma) < \kappa^2$, choose $\boldsymbol{n} \in \mathcal{M}(\sigma)$ such that $\mu(q\boldsymbol{n}) < \kappa^2$. Let ϕ be an eigenfunction of (2.6) associated with $\mu(q\boldsymbol{n})$. Then for any $t \in \mathbb{R}$,

$$\begin{aligned}
\mathcal{E}[t\phi, \boldsymbol{n}] &= \int_\Omega \{t^2(|\nabla_{q\boldsymbol{n}}\phi|^2 - \kappa^2|\phi|^2) + \frac{\kappa^2}{2}t^4|\phi|^4\}dx + \frac{\kappa^2}{2}|\Omega| + \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}] \\
&= (\mu(q\boldsymbol{n}) - \kappa^2)t^2\int_\Omega |\phi|^2 dx + \frac{\kappa^2}{2}t^4\int_\Omega |\phi|^4 dx + \frac{\kappa^2}{2}|\Omega| + \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}] \\
&< \frac{\kappa^2}{2}|\Omega| + C(\sigma) = \mathcal{E}[0, \boldsymbol{n}_\sigma]
\end{aligned}$$

for small $t > 0$. Thus $(0, \boldsymbol{n}_\sigma)$ is not a global minimizer of $\mathcal{E}$. □

Lemma 2.4. *Assume that Ω is simply connected and $\sigma > 0$. If $\boldsymbol{n}$ is a minimizer of $\mathcal{F}_{\sigma\boldsymbol{h}}$, then $\mathcal{F}[\boldsymbol{n}] > 0$ and*

$$\int_\Omega \{(\boldsymbol{h}\cdot\boldsymbol{n})^2 - (\cos\theta)^2\}dx > 0.$$

Proof. We have

$$\begin{aligned}
-\chi\sigma^2\int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n})^2 dx &\leq \mathcal{F}[\boldsymbol{n}] - \chi\sigma^2\int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n})^2 dx \\
&= \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}] \\
&\leq \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{e}] = -\chi\sigma^2(\cos\theta)^2|\Omega|.
\end{aligned}$$

Here we claim that $\mathcal{F}[\boldsymbol{n}] > 0$. In fact, if $\mathcal{F}[\boldsymbol{n}] = 0$, we see that $\operatorname{div}\boldsymbol{n} = 0, \operatorname{curl}\boldsymbol{n} = 0, |\boldsymbol{n}| = 1$ a.e. in Ω. Since Ω is simply connected, $\boldsymbol{n}$ is a constant vector (cf. [11]). Since $\boldsymbol{n}|_\Gamma = \boldsymbol{e}$, we have $\boldsymbol{n} = \boldsymbol{e}$ in Ω. However, since $\boldsymbol{e}$ does not satisfy (2.4), $\boldsymbol{e}$ is not a global minimizer of $\mathcal{F}_{\sigma\boldsymbol{h}}$. Thus for $\sigma > 0$, we have

$$\int_\Omega \{(\boldsymbol{h}\cdot\boldsymbol{n})^2 - (\cos\theta)^2\}dx > 0.$$

□

3 Proof of the Main Theorem

In this section we shall prove the main theorem 1.1. In order to do so, we need a lemma.

Lemma 3.1. *(i) For large σ, $C(\sigma) \le -\chi\sigma^2|\Omega| + C_1\sigma$ where $C_1 > 0$ depends only on $K, \boldsymbol{h}, \boldsymbol{e}$ and Ω.*

(ii) Let $\boldsymbol{n}_\sigma$ be a global minimizer of $\mathcal{F}_{\sigma\boldsymbol{h}}$. Then $|\boldsymbol{h}\cdot\boldsymbol{n}_\sigma| \to 1$ in $L^2(\Omega)$ as $\sigma \to +\infty$.

(iii) Moreover, we see that $\boldsymbol{h}\cdot\boldsymbol{n}_\sigma \to 1$ in $L^2(\Omega)$ as $\sigma \to +\infty$.

Proof. After rotating the coodinate system, we may assume that $\boldsymbol{h} = \boldsymbol{e}_3$ and $\boldsymbol{e} = (\sin\theta, 0, \cos\theta)$. Choose a test field $\boldsymbol{n} = (n_1, n_2, n_3) = (\cos\phi, 0, \sin\phi)$ where ϕ is a smooth function on $\overline{\Omega}$ and $\phi = (\pi/2) - \theta$ on Γ. Since $\boldsymbol{n}|_\Gamma = \boldsymbol{e}$, we note that $\boldsymbol{n} \in W^{1,2}(\Omega, \mathbb{S}^2, \boldsymbol{e})$.

Since

$$\begin{aligned}
\operatorname{div}\boldsymbol{n} &= -\sin\phi\,\partial_1\phi + \cos\phi\,\partial_3\phi,\\
\operatorname{curl}\boldsymbol{n} &= (\cos\phi\,\partial_2\phi, -\sin\phi\,\partial_3\phi - \cos\phi\,\partial_1\phi, -\sin\phi\,\partial_2\phi),
\end{aligned}$$

we see that $|\operatorname{div}\boldsymbol{n}|^2 + |\operatorname{curl}\boldsymbol{n}|^2 \le C(|\nabla\phi|^2 + 1)$. Thus if we write $\mathcal{F}_\sigma[\boldsymbol{n}] = \int_\Omega f_{\sigma,\boldsymbol{h}}(\phi)dx$ where

$$f_{\sigma,\boldsymbol{h}}(\phi) = K(|\operatorname{div}\boldsymbol{n}|^2 + |\operatorname{curl}\boldsymbol{n}|^2) - \chi\sigma^2(\boldsymbol{h}\cdot\boldsymbol{n})^2,$$

we have

$$|f_{\sigma,\boldsymbol{n}}(\phi)| \le CK(|\nabla\phi|^2 + 1) + \chi\sigma(\cos\phi)^2.$$

For any $\varepsilon > 0$, define $\Omega_\varepsilon = \{x \in \Omega; d(x, \partial\Omega) < \varepsilon\}$ and $\Omega^\varepsilon = \{x \in \Omega; d(x.\partial\Omega) \ge \varepsilon\}$, and decompose $\mathcal{F}_\sigma[\boldsymbol{n}]$ as follows: $\mathcal{F}_\sigma[\boldsymbol{n}] = \mathcal{F}_{\sigma,1}[\boldsymbol{n}] + \mathcal{F}_{\sigma,2}[\boldsymbol{n}]$ where

$$\mathcal{F}_{\sigma,1}[\boldsymbol{n}] = \int_{\Omega_\varepsilon} f_{\sigma,\boldsymbol{h}}(\phi)dx, \quad \mathcal{F}_{\sigma,2}[\boldsymbol{n}] = \int_{\Omega^\varepsilon} f_{\sigma,\boldsymbol{h}}(\phi)dx.$$

Choose ϕ such that

$$\phi = \begin{cases} \pi/2 & \text{in } \Omega^\varepsilon,\\ (\pi/2) - \theta & \text{on } \partial\Omega,\\ |\nabla\phi| \le C_2/\varepsilon & \text{in } \Omega. \end{cases}$$

Then $\mathcal{F}_{\sigma,2}[\boldsymbol{n}] \le CK$ and

$$\begin{aligned}
\mathcal{F}_{\sigma,1}[\boldsymbol{n}] &\le \int_{\Omega_\varepsilon} \{CK(|\nabla\phi|^2 + 1) + \chi\sigma(\cos\phi)^2\}dx\\
&\le \big[CK\big(\frac{C_2^2}{\varepsilon^2} + 1\big) + \chi\sigma^2\big]|\Omega_\varepsilon|.
\end{aligned}$$

Since $\partial\Omega$ is smooth, there exists $C_0 > 0$ depending only on $\partial\Omega$ such that $|\Omega_\varepsilon| \le C_0\varepsilon$ for any small $\varepsilon > 0$. For large σ, choose $\varepsilon > 0$ so that

$$\varepsilon = \frac{C_2}{\sigma}\sqrt{\frac{CK}{CK+\chi}}.$$

Then we have $\mathcal{F}_{\sigma,1}[\boldsymbol{n}] \le C_3\sigma$. Therefore, we have

$$C(\sigma) \le \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}] \le -\chi\sigma^2|\Omega| + C_3\sigma + C_4.$$

Thus (i) holds.

Proof of (ii). From (i), we see that

$$\mathcal{F}_\sigma[\boldsymbol{n}_\sigma] = \mathcal{F}[\boldsymbol{n}_\sigma] + \chi\sigma^2\int_\Omega (n_1^2+n_2^2)dx \le C_1\sigma.$$

This implies that

$$\int_\Omega (n_1^2+n_2^2)dx \le \frac{C_1}{\chi\sigma} \to 0$$

as $\sigma \to +\infty$. Thus $\int_\Omega (1-|n_3|^2)dx \to 0$ as $\sigma \to +\infty$. Since $|n_3| \le 1$, for any $1 < p < +\infty$,

$$\int_\Omega (1-|n_3|)^p dx \le 2^{p-1}\int_\Omega (1-|n_3|)dx \to 0.$$

Since $\boldsymbol{h}\cdot\boldsymbol{n}_\sigma = n_3$, we see that $|\boldsymbol{h}\cdot\boldsymbol{n}_\sigma| \to 1$ in $L^2(\Omega)$ as $\sigma \to +\infty$.

Proof of (iii). We shall show that $\boldsymbol{n}_\sigma = (n_{\sigma,1}, n_{\sigma,2}, n_{\sigma,3})$ has the following propertiy: $n_{\sigma,3} > 0$ in Ω or $n_{\sigma,3} \equiv 0$ in Ω.

In fact, $\boldsymbol{n}_\sigma$ satisfies the Euler-Lagrange equation (2.4). That is to say, if we write $\boldsymbol{n}_\sigma = \boldsymbol{n} = (n_1, n_2, n_3)$ for brevity,

$$\begin{cases} -\Delta\boldsymbol{n} = |\nabla\boldsymbol{n}|^2\boldsymbol{n} + b^2\sigma^2((\boldsymbol{h}\cdot\boldsymbol{n})\boldsymbol{h} - (\boldsymbol{h}\cdot\boldsymbol{n})^2\boldsymbol{n}) & \text{in } \Omega, \\ \boldsymbol{n} = \boldsymbol{e} = (\sin\theta, 0, \cos\theta) & \text{on } \Gamma \end{cases}$$

where $b^2 = \chi/K$. We claim that $\boldsymbol{u} = (n_1, n_2, |n_3|)$ is also a minimizer of $\mathcal{F}_{\sigma\boldsymbol{h}}$. In fact, for any $\boldsymbol{n} \in W^{1,2}(\Omega, \mathbb{S}^2)$, the following equality holds (cf. [4]):

$$|\operatorname{div}\boldsymbol{n}|^2 + |\operatorname{curl}\boldsymbol{n}|^2 = |\nabla\boldsymbol{n}|^2 - [\operatorname{tr}(\nabla\boldsymbol{n})^2 - |\operatorname{div}\boldsymbol{n}|^2].$$

Moreover, it follows from [9] that

$$\mathcal{S}(\boldsymbol{n}|_\Gamma) = \int_\Omega [\operatorname{tr}(\nabla\boldsymbol{n})^2 - |\operatorname{div}\boldsymbol{n}|^2]dx$$

depends only on $\boldsymbol{n}|_\Gamma = \boldsymbol{e}$. Therefore, we can write

$$\mathcal{F}_{\sigma \boldsymbol{h}}[\boldsymbol{n}] = \int_\Omega K|\nabla \boldsymbol{n}|^2 dx + \mathcal{S}(\boldsymbol{e}) - \chi\sigma^2 \int_\Omega (\boldsymbol{h}\cdot\boldsymbol{n})^2 dx.$$

Since $\boldsymbol{n} \in W^{1,2}(\Omega, \mathbb{S}^2)$, it follows that $|\nabla|n_3|| = |\nabla n_3|$ a.e. in Ω. Since $n_3|_\Gamma = \cos\theta > 0$ on Γ, $|n_3||_\Gamma = \cos\theta$. Thus $\mathcal{S}(\boldsymbol{u}|_\Gamma) = \mathcal{S}(\boldsymbol{n}|_\Gamma)$. Thus we have $\mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{n}] = \mathcal{F}_{\sigma\boldsymbol{h}}[\boldsymbol{u}]$. Hence $\boldsymbol{u}$ also satisfies the Euler-Lagrange equation. In particular,

$$\begin{cases} -\Delta u_3 = |\nabla \boldsymbol{n}|^2 u_3 + b^2\sigma^2(u_3 - u_3^3) \geq 0 & \text{in } \Omega, \\ u_3 = \cos\theta & \text{on } \Gamma. \end{cases}$$

That is to say,

$$\begin{cases} \Delta(u_3 - \cos\theta) \leq 0 & \text{in } \Omega, \\ u_3 - \cos\theta = 0 & \text{on } \Gamma. \end{cases}$$

By the weak Harnack inequality for supersolution (cf. Gilbarg and Trudinger [7, Theorem 8.18], for $B_{4R}(y) \subset \Omega$,

$$\|u_3 - \cos\theta\|_{L^p(B_{2R}(y))} \leq C(R) \inf_{B_R(y)} (u_3 - \cos\theta)$$

for some $p > 0$. From this inequality and the fact that Ω is connected, if $u_3 \not\equiv \cos\theta$ in Ω, we have $u_3 - \cos\theta > 0$ in Ω. Since from (ii), $u_3 = |n_3| \to 1 \neq \cos\theta$ in $L^2(\Omega)$, we see that $u_3 \not\equiv \cos\theta$ for large σ. Therefore, $u_3 = |n_3| > \cos\theta > 0$ in Ω. Since $n_3|_\Gamma = \cos\theta > 0$, we have $n_3 > 0$ in Ω. Therefore, $n_3 \to 1$ in $L^2(\Omega)$ as $\sigma \to \infty$. That is to say, $\boldsymbol{n}_\sigma \to \boldsymbol{h}$ in $L^2(\Omega, \mathbb{R}^3)$ as $\sigma \to \infty$. □

Proof of the main Theorem 1.1

Let $(0, \boldsymbol{n}_\sigma)$ be a pure nematic state, that is to say, $\boldsymbol{n}_\sigma$ is a global minimizer of $\mathcal{F}_{\sigma\boldsymbol{h}}$. By Lemma 3.1, we may assume that $\boldsymbol{n}_\sigma \to \boldsymbol{h} = \boldsymbol{e}_3$ strongly in $L^2(\Omega, \mathbb{R}^3)$. If we take $\phi(x) = e^{iqx_3}$, then $\nabla_{q\boldsymbol{n}_\sigma}\phi = iq(\boldsymbol{e}_3 - \boldsymbol{n}_\sigma)e^{iqx_3}$. Therefore, we have

$$\int_\Omega |\nabla_{q\boldsymbol{n}_\sigma}\phi|^2 dx = q^2 \int_\Omega |\boldsymbol{e}_3 - \boldsymbol{n}_\sigma|^2 dx \to 0$$

as $\sigma \to +\infty$. Hence

$$\begin{aligned} \mu(q\boldsymbol{n}_\sigma) &\leq \frac{\|\nabla_{q\boldsymbol{n}_\sigma}\phi\|^2_{L^2(\Omega,\mathbb{C}^3)}}{\|\phi\|^2_{L^2(\Omega,\mathbb{C})}} \\ &= \frac{q^2\|\boldsymbol{e}_3 - \boldsymbol{n}_\sigma\|^2_{L^2(\Omega,\mathbb{R}^3)}}{|\Omega|} \to 0 \end{aligned}$$

as $\sigma \to +\infty$. Thus for any $\kappa > 0$, there exists $\widehat{\sigma} > 0$ such that $\mu(q\boldsymbol{n}_\sigma) < \kappa^2$ for $\sigma > \widehat{\sigma}$. Thus from Lemma 2.3 (ii), we see that pure nematic states are not global minimizers of $\mathcal{E}$.

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