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A NOTE ON MINIMIZERS FOR THE OSEEN-FRANK ENERGY WITH APPLIED FIELDS

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Abstract. In this paper, we consider existence of minimizers for the Oseen-Frank energy with applied electric fields with subject to a mixed boundary conditions.

1. Introduction

Liquid crystal is a state of matter between fluid and solid crystalline which has been widely used in displays, optic switches etc. Due to its beautiful and complex structures, it has fascinated many scientists in many different areas and becomes one of the most important topics in the interdisciplinary research area. Mathematically, it brings a challenging problem that requires new theories to be developed[2]. In this paper, we consider a system of a liquid crystal occupying in a bounded domain with an electric field. Let $\rho_x \in L^1(\mathbb{S}^2)$ be the probability density function of molecular direction at x in domain $\Omega \subseteq \mathbb{R}^3$, that is

$$\rho_x : \mathbb{S}^2 \longrightarrow [0, \infty)$$

such that $\displaystyle\int_{\mathbb{S}^2} \rho_x(\mathbf{n}) ds(\mathbf{n}) = 1$ and $\rho_x(\mathbf{n}) = \rho_x(-\mathbf{n})$ for all $\mathbf{n} \in \mathbb{S}^2$

We consider the second moment of ρ_x which is

$$M = \int_{\mathbb{S}^2} (\mathbf{n} \otimes \mathbf{n}) \rho_x(\mathbf{n}) ds(\mathbf{n})$$

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where $\mathbf{v} \otimes \mathbf{w} = \mathbf{v}\mathbf{w}^T$. Then $M = M^T$ and $tr(M) = 1$. In a fluid, the orientation of molecules is equally distributed, that is the probability density $\rho_0(x) = \frac{1}{4\pi}$. The corresponding second moment becomes $\frac{1}{3}I$.

We define 3×3 matrix $Q = M - M_0$. Then $Q^T = Q,\ tr(Q) = 0$ and

$$Q = \int_{\mathbb{S}^2} (\rho_x(\mathbf{n}) - \frac{1}{4\pi})(\mathbf{n} \otimes \mathbf{n}) ds(\mathbf{n}).$$

Since Q is symmetric and traceless, Q can be written as

$$Q = S_1 \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I \right) + S_2 \left(\mathbf{m} \otimes \mathbf{m} - \frac{1}{3} I \right),$$

where $S_1, S_2 : \Omega \longrightarrow \mathbb{R}$ are scalar functions. It is easy to see that $\dfrac{2S_1 - S_2}{3}$, $\dfrac{-S_1 + 2S_2}{3}$, $\dfrac{-S_1 - S_2}{3}$ are three eigenvalues of Q. If two eigenvalues of Q are equal, then we say that molecules are *uniaxial.* We say that molecules are *biaxial* when all three eigenvalues are distinct.

When Q is uniaxial, it can be written by

$$Q = S \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} I \right).$$

Let Ω an open bounded domain and occupied with the liquid crystals. The governing energy functional[5] is given by

$$E(Q) = \int_\Omega [f_{elastic}(Q) + f_{bulk}(Q)]\, dx$$

where

$$f_{elastic}(Q) = L_1 Q_{ij,j} Q_{ik,k} + L_2 Q_{ij,k} Q_{ik,j} + L_3 Q_{ij,k} Q_{ij,k}$$

with $Q_{ij,k} = \frac{\partial Q_{ij}}{\partial x_k}$, and L_1, L_2, L_3 are a constant.

$$f_{bulk}(Q) = \frac{a}{2} tr(Q^2) - \frac{b}{3} tr(Q^3) + \frac{c}{4} tr(Q^2)^2,$$

where a, b, c are temperature dependent constant.

If $Q = S\left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3}I\right)$ with S being constant, $E(Q)$ becomes the Oseen-Frank energy functional

$$E(\mathbf{n}) = \int_\Omega F_{OF}(\mathbf{n}, \nabla \mathbf{n}) dx$$

where

$$\begin{aligned} F_{OF}(\mathbf{n}, \nabla \mathbf{n}) = \frac{1}{2} K_1 (\nabla \cdot \mathbf{n})^2 + \frac{1}{2} K_2 (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + \frac{1}{2} K_3 |\mathbf{n} \times \nabla \times \mathbf{n}|^2 \\ + (K_2 + K_4) \left(tr(\nabla \mathbf{n})^2 - (\nabla \cdot \mathbf{n})^2 \right) \end{aligned}$$

where $K_1,\ K_2,\ K_3,\ K_4$ are constants associated with splay, twist, bending. For more information on the Landau de Gennes energy functional, we refer the reader to [1, 3] and references therein.

2. Existence of Minimizer

From now on, we let Ω be a bounded open subset in $\mathbb{R}^3$ whose boundary is Lipschitz continuous and Γ_1 and Γ_2 be closed subsets of $\partial\Omega$. We will also assume that $\mathbf{n}_0 \in H^{\frac{1}{2}}\left(\Gamma_1, \mathbb{S}^2\right),\ \phi_0 \in H^{\frac{1}{2}}\left(\Gamma_2, \mathbb{R}\right)$.
We consider the problem $(\mathcal{P})$

$$(\mathcal{P})\left\{\begin{array}{c}\text{Minimize } \int_\Omega \tilde{W}(\nabla\mathbf{n}, \mathbf{n}, \nabla\phi)d\mathbf{x} \\ \text{subject to} \\ \mathbf{n} = \mathbf{n}_0 \text{ on } \Gamma_1, \phi = \phi_0 \text{ on } \Gamma_2\end{array}\right\}$$

where

$$\tilde{W}(\nabla\mathbf{n}, \mathbf{n}, \nabla\phi) = W(\nabla\mathbf{n}, \mathbf{n}) + A(\mathbf{n}, \nabla\phi), \tag{2.1}$$

$$\begin{aligned} W(\nabla\mathbf{n}, \mathbf{n}) =& K_1|\nabla\cdot\mathbf{n}|^2 + K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 + K_3|\mathbf{n}\times(\nabla\times\mathbf{n})|^2 \\ &+ (K_2+K_4)\left[tr(\nabla\mathbf{n})^2 - (\nabla\cdot\mathbf{n})^2\right] \end{aligned} \tag{2.2}$$

and

$$A(\mathbf{n}, \nabla\phi) = -\frac{1}{8\pi}\left(\nabla\phi\cdot\left(\varepsilon_\perp I + \varepsilon_a \mathbf{n}\otimes\mathbf{n}\right)\nabla\phi\right) \tag{2.3}$$

We note that $W(\nabla\mathbf{n}, \mathbf{n})$ in (2.1) is the classical Ossen-Frack energy integrand and (2.3) is an interaction between the director vector $\mathbf{n}$ and electric field $\mathbf{E} = -\nabla\phi$. In the case of $\Gamma_1 = \Gamma_2 = \partial\Omega$, the existence and some regularity results of minimizers to the problem to the problem $\mathcal{P}$ were studied by Hardt, Kinderlehrer and Lin [8].

We consider two admissible sets:

$$\begin{aligned}\mathcal{A}\left(\mathbf{n}_0\right) &= \left\{\mathbf{n}\in W^{1,2}\left(\Omega, \mathbb{S}^2\right) : \mathbf{n} = \mathbf{n}_0 \text{ on } \Gamma_1\right\}, \\ \mathcal{B}\left(\phi_0\right) &= \left\{\phi\in W^{1,2}(\Omega) : \phi = \phi_0 \text{ on } \Gamma_2\right\}\end{aligned}.$$

We first invoke a standard lemma stated below.

LEMMA 1. *Let Γ be a closed subset in $\mathbb{R}^n$. There exists a continuous linear operator from $Lip_r(\Gamma)$ into $Lip_r(\mathbb{R}^n)$, where $0 < r \leq 1$ and $Lip_r(\Gamma)$ is the space of continuous functions equipped with the norm*

$$\|\phi\| = \sup_{x\in\Gamma} |\phi(x)| + \sup_{x\neq y\in\Gamma} \frac{|\phi(x)-\phi(y)|}{|x-y|^r}.$$

For $\mathcal{A}(\mathbf{n}_0) \neq \emptyset$, it does not follow directly from the previous lemma because $|\mathbf{n}(\mathbf{x})| = 1$, for all $\mathbf{x} \in \Omega$. In order to prove that $\mathcal{A}(\mathbf{n}_0) \neq \emptyset$, we need one more extension lemma which can be found in [6].

LEMMA 2. *Let Ω be a bounded domain in $\mathbb{R}^n$ and let Γ be a closed subset of $\partial\Omega$. For any $\mathbf{u} \in W^{1,2}(\Omega, \mathbb{R}^3)$ with $|\mathbf{u}| = 1$ on Γ, there exist a function $\mathbf{n} \in W^{1,2}(\Omega, \mathbb{S}^2)$ such that $\mathbf{n} = \mathbf{u}$ on Γ and $\|\nabla\mathbf{n}\|_{L^2(\Omega)} \leq C\|\nabla\mathbf{u}\|_{L^2(\Omega)}$ for some C, independent of $\mathbf{u}$ and Ω.*

Proof. For any $|\alpha| < 1$, define $\mathbf{u}_\alpha$ as follows:

$$\mathbf{u}_\alpha = \frac{\mathbf{u}(x)-\alpha}{|\mathbf{u}(x)-\alpha|}, \mathbf{x} \in \Omega$$

It is possible to choose $\alpha_0, |\alpha_0| < \frac{1}{2}$ so that

$$\int_\Omega |D\mathbf{u}_{\alpha_0}|^2 \, d\mathbf{x} \leq C \int_\Omega |D\mathbf{u}|^2 d\mathbf{x}$$

for some constant $C > 0$. Since the map $\pi_\alpha : y \in \mathbb{S}^2 \to \frac{y-\alpha}{|y-\alpha|} \in \mathbb{S}^2$ is a bi-Lipschitz homeaomorphism of $\mathbb{S}^2$ into itself with bounded Lipschitz constants(independent of α) of $\pi_\alpha, \pi_\alpha^{-1}$. We complete the proof by taking $\mathbf{n} = \pi_{\alpha_0}^{-1} \circ \mathbf{u}_{\alpha_0}$. □

By combining lemma 1 with lemma 2, we conclude that

THEOREM 3. *The admissible sets $\mathcal{A}(\mathbf{n}_0)$ and $\mathcal{B}(\phi_0)$ are not empty.*

Next we will show existence of minimizers. We first assume that $K_1 - K_2 - K_4 \geq 0$, $K_3 - K_2 - K_4 \geq 0$, $K_4 \leq 0$, and $K_2 + K_4 > 0$. We let $\mathcal{E}(\mathbf{n}, \phi)$ denote the functional $\int_\Omega \tilde{W}(\nabla\mathbf{n}, \mathbf{n}, \nabla\phi)d\mathbf{x}$.

We note that the energy functional $\mathcal{E}$ may not be bounded below in $\mathcal{A}(\mathbf{n}_0) \times \mathcal{B}(\phi_0)$. From second order elliptic theory, for each given $\mathbf{n}$, there exists a unique solution $\phi := \Phi(\mathbf{n})$ to the equation

$$\left\{ \begin{array}{c} \nabla \cdot (\varepsilon_\perp I + \varepsilon_a \mathbf{n} \otimes \mathbf{n}) \nabla\phi = 0 \text{ in } \Omega, \\ \phi = \phi_0 \text{ on } \Gamma_2, \\ (\varepsilon_\perp I + \varepsilon_a \mathbf{n} \otimes \mathbf{n}) \nabla\phi) \cdot \nu = 0 \text{ on } \partial\Omega - \Gamma_2. \end{array} \right\} \tag{2.4}$$

In fact, $\Phi(\mathbf{n})$ is the minimizer of $\int_\Omega \nabla\phi \cdot (\varepsilon_\perp I + \varepsilon_a \mathbf{n}\otimes\mathbf{n}) \nabla\phi) d\mathbf{x}$ in $\mathcal{B}(\phi_0)$. We then define a new energy functional as

$$\mathcal{E}^*(\mathbf{n}) := \mathcal{E}(\mathbf{n}, \Phi(\mathbf{n})).$$

THEOREM 4. *There exists a minimizer* $\mathbf{n}$ *of* $\mathcal{E}^*$ *on* $\mathcal{A}(\mathbf{n}_0)$, *that is,*

$$\mathcal{E}^*(\mathbf{n}) = \inf_{\mathbf{m}\in\mathcal{A}(\mathbf{n}_0)} \mathcal{E}^*(\mathbf{m}).$$

Proof. Note that

$$\operatorname{tr}(\nabla\mathbf{n})^2 = |\nabla\mathbf{n}|^2 - (\mathbf{n}\cdot\nabla\times\mathbf{n})^2 - |\mathbf{n}\times\nabla\times\mathbf{n}|^2.$$

Using the identity, we get

$$\begin{aligned}\int_\Omega W(\mathbf{n}, \nabla\mathbf{n}) d\mathbf{x} = \int_\Omega \big\{ &(K_1 - K_2 - K_4)(\nabla\cdot\mathbf{n})^2 \\ &+ (K_3 - K_2 - K_4)|\mathbf{n}\times\nabla\times\mathbf{n}|^2 \\ &- K_4(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 + (K_2 + K_4)|\nabla\mathbf{n}|^2 \} d\mathbf{x}\end{aligned}$$

From the theory of elliptic PDEs, we also have

$$\left| \int_\Omega A(\mathbf{n}, \Phi(\mathbf{n})) d\mathbf{x} \right| \le C |\mathbf{n}_0|^2_{\frac{1}{2},\Gamma_2}.$$

The coercivity of the functional follows from the previous two inequalities. We know that $|\tilde{W}(\nabla\mathbf{n}, \mathbf{n}, \Phi(\mathbf{n}))| \le C\left(\|\nabla\mathbf{n}\|^2 + 1\right)$ for some constant $C > 0$. We prove the weakly lower semicontinuity of energy functional and it has a minimizer. □

If $g(r) = \alpha\left(1 - \omega r^2\right)$ for all $r \in [-1, 1], 0 < \omega < 1$, then g is continuous. Thus, for any sequence $(\mathbf{n}_i)$ which converges weakly to a function $\mathbf{n}$ in $W^{1,2}\left(\Omega, \mathbb{S}^2\right)$ we have

$$\lim_{i\to\infty} \int_{\partial\Omega} g(\mathbf{n}_i \cdot \nu) ds = \int_{\partial\Omega} g(\mathbf{n}\cdot\nu) ds$$

where ν is the unit normal vector to $\partial\Omega$. Therefore, we have

COROLLARY 5. *The energy functional* $\mathcal{E}^*(\mathbf{n}) + \int_{\partial\Omega} g(\mathbf{n}\cdot\nu) ds$ *has a minimizer on* $W^{1,2}\left(\Omega, \mathbb{S}^2\right)$

With taking $\Gamma_1 = \Gamma_2 = \Gamma$, we calculate the corresponding Euler-Lagrange equations as follows

(2.5)
$$\left\{\begin{array}{c}\tilde{K}_1\nabla(\nabla\cdot\mathbf{n})+\tilde{K}_2\Delta\mathbf{n}-\tilde{K}_3\nabla\times(\mathbf{n}\cdot\nabla\times\mathbf{n})\mathbf{n})\\ -\tilde{K}_3(\mathbf{n}\cdot\nabla\times\mathbf{n})\nabla\times\mathbf{n}-\tilde{K}_4\nabla\times\Big((\mathbf{n}\times\nabla\times\mathbf{n})\times\mathbf{n}\Big)\\ -\tilde{K}_4(\nabla\times\mathbf{n})\times(\mathbf{n}\times\nabla\times\mathbf{n})+\frac{1}{4\pi}\varepsilon_a(\mathbf{n}\cdot\nabla\phi)\nabla\phi+\lambda\mathbf{n}=0,\\ \nabla\cdot(\varepsilon_\perp I+\varepsilon_a\mathbf{n}\otimes\mathbf{n})\nabla\phi=0,\end{array}\right\}\text{ in }\Omega$$

with the boundary conditions

$$\left\{\begin{array}{c}(\varepsilon_\perp I+\varepsilon_a\mathbf{n}\otimes\mathbf{n})\nabla\phi\cdot\nu=0\\ \tilde{K}_1(\nabla\cdot\mathbf{n})\nu+\tilde{K}_2\frac{\partial n}{\partial\nu}+\tilde{K}_3(\mathbf{n}\cdot\nabla\times\mathbf{n})\mathbf{n}\times\nu\\ +\tilde{K}_4((\mathbf{n}\times\nabla\times\mathbf{n})\times\mathbf{n})\times\nu=0,\end{array}\right\}\text{ on }\partial\Omega-\Gamma \tag{2.6}$$

where $\tilde{K}_1=K_1-K_2-K_4, \tilde{K}_2=K_2+K_4, \tilde{K}_3=-K_4$ and $\tilde{K}_4=K_3-K_2-K_4$.

Corollary 6. *The corresponding Euler-Lagrange equations for minimizing problem $\mathcal{P}$ reads*

$$\left\{\begin{array}{c}\textit{For given data } \mathbf{n}_0\in H^{\frac{1}{2}}\left(\Gamma,\mathbb{S}^2\right),\phi_0\in H^{\frac{1}{2}}(\Gamma,\mathbb{R})\\ \textit{and } \mathbf{g}\in H^{\frac{1}{2}}(\Sigma,\mathbb{R}),\ \textit{find}(\mathbf{n},\phi)\in W^{1,2}\left(\Omega,\mathbb{S}^2\right)\times W^{1,2}(\Omega,\mathbb{R})\\ \textit{which satisfies}\\ \left(\tilde{K}_1-\tilde{K}_4\right)\Big[\nabla(\nabla\cdot\mathbf{n})-(\nabla(\nabla\cdot\mathbf{n})\cdot\mathbf{n})\mathbf{n}\Big]\\ +\left(\tilde{K}_2+\tilde{K}_4\right)\Big[\Delta\mathbf{n}-(\triangle\mathbf{n}\cdot\mathbf{n})\mathbf{n}\Big]\\ +2\left(\tilde{K}_4-\tilde{K}_3\right)\Big[(\mathbf{n}\cdot\nabla\times\mathbf{n})\nabla\times\mathbf{n}-(\mathbf{n}\cdot\nabla\times\mathbf{n})^2\mathbf{n}\Big]\\ -\left(\tilde{K}_3+\tilde{K}_4\right)\nabla(\mathbf{n}\cdot\nabla\times\mathbf{n})\times\mathbf{n}\\ +\frac{1}{4\pi}\Big[\varepsilon_a(\mathbf{n}\cdot\nabla\phi)\nabla\phi-\varepsilon_a(\mathbf{n}\cdot\nabla\phi)^2\mathbf{n}\Big]=0,\ \textit{in } \Omega,\\ \nabla\cdot\Big((\varepsilon_\perp I+\varepsilon_a\mathbf{n}\otimes\mathbf{n})\nabla\phi\Big)=0,\ \textit{in } \Omega\end{array}\right\} \tag{2.7}$$

with the boundary conditions

$$\left\{\begin{array}{c}\phi=\phi_0,\quad \mathbf{n}=\mathbf{n}_0,\ \textit{on } \Gamma,\\ ((\varepsilon_\perp I+\varepsilon_a\mathbf{n}\otimes\mathbf{n})\nabla\phi)\cdot\nu=0,\ \textit{on } \Sigma,\\ \frac{\partial\mathbf{n}}{\partial\nu}=\mathbf{g}\ \textit{on } \Sigma,\\ (\nabla\cdot\mathbf{n})=-\frac{\tilde{K}_2}{\tilde{K}_1}(\mathbf{g}\cdot\nu),\ \textit{on } \Sigma,\\ (\mathbf{n}\times\nabla\times\mathbf{n})\cdot\nu=\frac{\tilde{K}_2}{\tilde{K}_4}(\mathrm{g}\cdot\nu)(1+\mathbf{n}\cdot\nu),\ \textit{on } \Sigma.\end{array}\right\} \tag{2.8}$$

Proof. After some tedious calculations using vector analysis, we can easily reduce (2.5) to (2.7). For the boundary conditions, since $\frac{\partial\mathbf{n}}{\partial\nu}=\mathbf{g}$ on Σ, we have

$$\tilde{K}_1(\nabla\cdot\mathbf{n})\nu+\Big(\tilde{K}_3(\mathbf{n}\cdot\nabla\times\mathbf{n})\mathbf{n}+\tilde{K}_4(\mathbf{n}\times\nabla\times\mathbf{n})\times\mathbf{n}\Big)\times\nu=-\tilde{K}_2\mathbf{g}\text{ on }\Sigma.$$

Since the two vectors on the left hand side of the above equation are orthogonal,

$$\tilde{K}_1(\nabla\cdot\mathbf{n})\nu=-\tilde{K}_2(\mathbf{g}\cdot\nu)\nu,$$

and

$$\Big(\tilde{K}_3(\mathbf{n}\cdot\nabla\times\mathbf{n})\mathbf{n}+\tilde{K}_4(\mathbf{n}\times\nabla\times\mathbf{n})\times\mathbf{n}\Big)\times\nu=-\tilde{K}_2\mathbf{g}+\tilde{K}_2(\mathbf{g}\cdot\nu)\nu.$$

Since $(\mathbf{n}\times\nabla\times\mathbf{n})\times\mathbf{n}=(\mathbf{n}\cdot\mathbf{n})\nabla\mathbf{n}-(\mathbf{n}\cdot\nabla\mathbf{n})\mathbf{n}$,

$$\Big((\tilde{K}_3-\tilde{K}_4)(\mathbf{n}\cdot\nabla\times\mathbf{n})\mathbf{n}+\tilde{K}_4(\nabla\times\mathbf{n})\Big)\times\nu=-\tilde{K}_2\mathbf{g}+\tilde{K}_2(\mathbf{g}\cdot\nu)\nu.$$

Taking the dot product of the above equation with $\mathbf{n}$, we have

$$\tilde{K}_4((\nabla\times\mathbf{n})\times\nu)\cdot\mathbf{n}=-\tilde{K}_2\mathbf{g}\cdot\mathbf{n}+\tilde{K}_2(\mathbf{g}\cdot\nu)(\nu\cdot\mathbf{n}).$$

Since $\mathbf{g}\cdot\mathbf{n}=\frac{\partial\mathbf{n}}{\partial\nu}\cdot\mathbf{n}=0$ and $(\nabla\times\mathbf{n})\times\nu)\cdot\mathbf{n}=(\mathbf{n}\times\nabla\times\mathbf{n})\cdot\nu$,

$$(\mathbf{n}\times\nabla\times\mathbf{n})\cdot\nu=\frac{\tilde{K}_2}{\tilde{K}_4}(\mathbf{g}\cdot\nu)(1+\nu\cdot\mathbf{n}).$$

Therefore if $\mathbf{n}$ is a minimizer, then it satisfies that

$$\left\{\begin{array}{c}(\nabla\cdot\mathbf{n})(\nu\cdot\mathbf{n})=\frac{\tilde{K}_2}{\tilde{K}_1}(\mathbf{g}\cdot\nu)(\nu\cdot\mathbf{n})\\(\mathbf{n}\times\nabla\times\mathbf{n})\cdot\nu=\frac{\tilde{K}_2}{\tilde{K}_4}(\mathbf{g}\cdot\nu)(1+\nu\cdot\mathbf{n})\end{array}\right\}\text{ on }\Sigma$$

□

COROLLARY 7. *The null-Lagrangian*

$$\int_\Omega\left\{tr(\nabla\mathbf{n})^2-(div\mathbf{n})^2\right\}d\mathbf{x}$$

is a fixed constant for critical points on the space

$$\mathcal{A}^*(\mathbf{n}_0)=\left\{\mathbf{n}\in W^{1,2}\left(\Omega,\mathbf{S}^2\right):\mathbf{n}=\mathbf{n}_0\ on\ \Gamma,\frac{\partial\mathbf{n}}{\partial\nu}\cdot\nu=0\ on\ \partial\Omega-\Gamma\right\}.$$

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