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VARIOUS FERROELECTRIC CONFIGURATIONS IN LIQUID CRYSTALS

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Abstract. In this paper, we study ferroelectric configurations of liquid crystals by nonlocal interaction energy associated with the polarization.

1. Introduction

Let Ω be a bounded domain occupied by a ferroelectric liquid crystal. In a system of ferroelectric liquid crystals, the polarization vector field $\mathbf{p}, |\mathbf{p}| = 1$, plays an important role in the equilibrium states of the system. There are two very distinct types which depend on the net polarization. In this case, several types of local polarization arrangements are possible to produce the total value of the polarization. This explains the observations of multiple periodic phases found in ferroelectric phases of smectic C* [6, 14]. Assume that $\mathbf{p} = (p, 0, 0)$, The energy functional associated with the polarization is given by

$$\tilde{\mathcal{F}} = \int_\Omega W(p)\, d\mathbf{x} + \eta \int_\Omega \int_\Omega k(x-y)(p(x)-p(y))^2\, d\mathbf{y}\, d\mathbf{x},$$

where $W(p) = \frac{a_0}{4}(p^2-1)^2, a_0 > 0, \eta > 0$, and $q(\mathbf{x}) = \int_\Omega k(\mathbf{x}-\mathbf{y})p(\mathbf{y})\, d\mathbf{y}$ satisfies

$$-\alpha\Delta q + q = p \text{ in } \Omega. \tag{1.1}$$

We note that the term $W(p)$ forces p to have values ± 1. With p being ± 1, $q = \pm 1$ are solutions of (1.1). This motivates us to replace $W(p)$ by

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$W(q)$. Then we obtain the modified energy functional to minimize on a suitable subspace of $W^{2,2}(\Omega)$,

$$\mathcal{F}_\alpha(q) = \int_\Omega \{\eta\alpha^2(\Delta q)^2 + \eta\alpha|\nabla q|^2 + \frac{a_0}{4}(q^2-1)^2\}\, d\mathbf{x}. \tag{1.2}$$

In this paper, we shall investigate configurations of the equilibrium states of energy functionals related to the above energy in an appropriate subspace of $W^{2,2}(\Omega)$ and the corresponding limiting energy.

2. The limiting energy

In this section, we first consider Ω to be an open interval $(-1,1)$ and study the behavior of minimizers of $\frac{1}{a_0}\mathcal{F}_\alpha$ as $\alpha \to 0$.

THEOREM 2.1. *Let* $w : \mathbf{R} \to \mathbf{R}$ *be a minimizer of* $\lim_{\alpha\to 0} \frac{1}{a_0}\mathcal{F}_\alpha(q)$ *and let*

$$E = w'w''' - \frac{1}{2}(w'')^2 + \frac{a}{2}(w')^2 + \frac{1}{4}(1-w^2)^2.$$

If $\alpha \to 0^+$ *and* $\eta > 4a_0$, *then* w *belongs to one of the following cases:*

(1) *The three constant solutions:* $w = -1, w = 0, w = 1$.
(2) *Two kink solutions connecting* $w = -1$ *and* $w = 1$ *(modulo shifts).*
(3) *For each* $E \in (0, \frac{1}{4})$ *there exists a unique periodic solution* $w(x,E)$ *that is even with respect to their critical points, odd with respect to their zeros, and*

$$\max\{|w(x,E)| x \in \mathbb{R}\} < \sqrt{1-2\sqrt{E}}.$$

If $\alpha \to 0^-$ *or* $\alpha \to 0^+, 0 < \eta < 4a_0$, *then the corresponding equation for* w *has*

(1) *at least two kink type solutions with small and large oscillations around* 0 *in a finite interval.*
(2) *at least two solutions with small and large pulses in a region and have value* 1 *outside a finite interval. These solutions bifurcate from the increasing kink at* $\eta = 8$.
(3) *infinitely many even and odd periodic solutions with small and large oscillations.*

Proof. We introduce

$$z = \frac{x}{\varepsilon}, \quad \varepsilon = \sqrt[4]{\frac{2\eta\alpha^2}{a_0}}, \quad a = -\mathrm{sign}(\alpha)\sqrt{\frac{2\eta}{a_0}}.$$

Define $u_\varepsilon : (-\frac{1}{\varepsilon}, \frac{1}{\varepsilon}) \to \mathbf{R}$ by

$$u_\varepsilon(z) = q_\alpha(x) \text{ for all } x \in (-1, 1).$$

Then we have

$$\frac{1}{a_0}\mathcal{F}_\alpha(q) = \int_{-1}^{1} \left\{ \frac{1}{2}\varepsilon^4 (q'')^2 - \frac{a}{2}\varepsilon^2 (q')^2 + \frac{1}{4}(q^2-1)^2 \right\} dx.$$

Suppose that $\{q_\alpha\}$ is a minimizing sequence. Since $\varepsilon \to 0$ as $\alpha \to 0$, the function $u(z) = \lim_{\varepsilon\to 0} u_\varepsilon(z)$ is a minimizer of the new energy functional

$$\mathcal{F}_1(w) = \int_{-\infty}^{\infty} \left\{ \frac{1}{2}(w'')^2 - \frac{a}{2}(w')^2 + \frac{1}{4}(w^2-1)^2 \right\} dz.$$

The corresponding Euler-Lagrange equation is given by

$$\frac{d^4 w}{dz^4} + a\frac{d^2 w}{dz^2} + w^3 - w = 0.$$

The rest of the proof follows from previous results done by many authors [7, 10, 11, 12, 13, 4, 2, 3]. □

The equation

$$\frac{d^4 u}{dx^4} + a\frac{d^2 u}{dx^2} + u^3 - u = 0. \tag{2.1}$$

also arises in the study of pattern formations in physics and mechanics. Especially, the equation (2.1) for a negative value a explains the stationary states for the Extended Fisher-Kolmogorov equation proposed by Dee and van Saarloos [1]

$$\frac{\partial v}{\partial t} = -\gamma\frac{\partial^4 v}{\partial x^4} + \frac{\partial^2 v}{\partial x^2} + v - v^3, \tag{2.2}$$

where $\gamma > 0$. It is easy to see that u and v are related as

$$v(x) = u(\frac{x}{\sqrt[4]{\gamma}}), \quad a = -\frac{1}{\sqrt{\gamma}}.$$

For $a < 0$, let u be a solution of (2.1). If we define

$$w(x) = \sqrt{|\kappa-1|}\,u(\sqrt[4]{|\kappa-1|}x), \quad a = \frac{2}{|\kappa-1|},$$

then w becomes a stationary solution of

$$\frac{\partial w}{\partial t} = \kappa w - \Big(1 + \frac{\partial^2}{\partial x^2}\Big)^2 w - w^3.$$

which is known as the Swift-Hohenberg equation. For $a \leq -\sqrt{8}$, it was proved in [3] that solutions of (2.1) behave like solutions to Ginzburg-Landau equation

$$u'' + u - u^3 = 0.$$

For more details about these equations, we refer the reader to [7, 10, 11, 12, 13, 4, 2, 3].

Notice that all these kinds of solutions in Theorem 2.1 exist for any given α. In particular, if $\alpha > 0$, then $a < 0$. This prevents the energy functional from having chaotic critical points. One can expect the minimizers to approach to a function p_0 having values only ± 1 as $\varepsilon \to 0$. The limiting energy may be calculated from the number of jumps. In case that $\alpha > 0, 2\eta = a_0$, we get $a = -1$ and define

$$\mathcal{E}_\varepsilon(q) = \frac{1}{\varepsilon a_0}\mathcal{F}_\alpha(q) = \frac{1}{2}\int_{-1}^{1}[\varepsilon^3(q'')^2 + \varepsilon(q')^2 + \frac{1}{2\varepsilon}(q^2-1)^2]\,dx.$$

Let

$$\mathcal{E}(q) = \frac{1}{2}\int_{\mathbf{R}}[(q'')^2 + (q')^2 + \frac{1}{2}(q^2-1)^2]\,dx,$$

and $\xi_\pm \in C^\infty$ denote fixed functions satisfying both $\xi_\pm(x) = \mp 1$ for all $x \leq -1$ and $\xi_\pm(x) = \pm 1$ for $x \geq 1$.

It was shown in [8] that the functional $\mathcal{E}$ has global minimizers $q_\pm$ on the affine spaces $\xi_\pm + W^{2,2}(\mathbf{R})$. Moreover, if (q_ε) is a sequence of minimizers for $\mathcal{E}_\varepsilon$ on a suitable subspace of $W^{2,2}(-1,1)$, then (q_ε) converges to a function $q(x) \in \{-1, 1\}$ in $L^1[-1,1]$. In particular, if N^+ and N^- are the numbers of jumps from -1 to 1 and from 1 to -1 respectively, then

$$\mathcal{E}_\varepsilon(q_\varepsilon) \to \mathcal{E}_0(q) \text{ as } \varepsilon \to 0,$$

where $\mathcal{E}_0(q) = N^+\mathcal{E}(q_+) + N^-\mathcal{E}(q_-)$.

3. Asymptotics with an application

In this section, we investigate the asymptotic behavior of the energy functional (1.2) when α approaches 0. Suppose that Ω is an open bounded domain in $\mathbf{R}^3$ with Lipschitz boundary and $\alpha > 0$. We consider the admissible space of functions

$$\mathcal{X} = \left\{ q \in W^{2,2}(\Omega); \int_\Omega q\,d\mathbf{x} = m|\Omega| \right\},$$

where $m \in [-1, 1]$.

For each $\alpha > 0$, let q_α be a minimizer of $\mathcal{F}_\alpha$. It follows from the standard arguments in $\Gamma-$convergence and Young measures that the minimizing sequence $\{q_\alpha\}$ generates a Young measure $\{\mu_x\}$, i.e. there exists a subsequence, not relabelled, which converges weakly star to $\bar{q}$ where $\bar{q}(\mathbf{x}) = \mu_{\mathbf{x}} = \frac{1}{2}(1+m)\delta_1 + \frac{1}{2}(1-m)\delta_{-1}$. Here δ_{x_0} denotes the Dirac delta at x_0. It is easy to see that $\inf_{\alpha\to 0}\{\mathcal{F}_\alpha(q) : q \in \mathcal{X}\} = 0$. We now define

$$\mathcal{G}_\alpha(q) = \begin{cases} \frac{1}{\varepsilon a_0}\mathcal{F}_\alpha(q) & \text{if } q \in \mathcal{X}, \\ \infty & \text{if } q \in L^1(\Omega) \setminus \mathcal{X}. \end{cases}$$

If $\varepsilon = \sqrt[4]{\frac{2\eta\alpha^2}{a_0}}$, then $\mathcal{G}_\alpha$ can be written as

$$\mathcal{G}_\alpha(q) = \int_\Omega \{\frac{1}{2}\varepsilon^3|\Delta q|^2 + \varepsilon\sqrt{\frac{\eta}{2a_0}}|\nabla q|^2 + \frac{1}{4\varepsilon}(q^2-1)^2\}\, d\mathbf{x}.$$

Applying Theorem 4.1 in [5], we obtain the following Modica-Mortola type theorem.

Theorem 3.1. *Let Ω be an open bounded domain in $\mathbf{R}^3$ with Lipschitz boundary. Then the sequence $\mathcal{G}_\alpha$ $\Gamma-$converges to $\mathcal{G}_0$ in $L^1(\Omega)$, where*

$$\mathcal{G}_0(u) = \begin{cases} \frac{1}{2}c_1||Du|| & \textit{if } u \in \tilde{\mathcal{X}}, \\ \infty & \textit{otherwise}, \end{cases}$$

where

$\tilde{\mathcal{X}} = \left\{q \in BV(\Omega); \int_\Omega q\, d\mathbf{x} = m|\Omega|, q(\mathbf{x}) \in \{-1,1\}, \text{ for a.e. } x \in \Omega\right\}$,

$c_1 = \min\left\{\int_{\mathbf{R}}\{\frac{1}{2}(w'')^2 + \sqrt{\frac{\eta}{2a_0}}(w')^2 + \frac{1}{4}(w^2-1)^2\}\, dx; w', w'', w^2-1 \in L^2(\mathbf{R})\right\}$,

and $||Du|| = \sup\{\int_\Omega u \text{ div } \varphi\, dx : \varphi \in C_c^1(\Omega, \mathbf{R}^3), ||\varphi||_\infty \le 1\}$.

As an application, we let the molecular director field $\mathbf{n} = (a\cos\phi, a\sin\phi, c)$ and the polarization field $\mathbf{p} = (p, 0, 0)$ in the bookshelf geometry for smectic liquid crystals [9]. After certain scalings, we may assume that the structure of the system is governed by the energy functional

$$\mathcal{G}_\varepsilon(\phi, p) = \int_0^1 \left\{a^2(\phi')^2 - 2acp'\cos\phi + \frac{1}{2}\varepsilon^4(p'')^2 - \frac{a}{2}\varepsilon^2(p')^2 + \frac{1}{4}(p^2-1)^2\right\} dx.$$

The first term in the energy is one constant elastic energy for the Oseen-Frank energy and the second term accounts for interactions of the director field with the polarization [9]. The last remaining parts are terms associated with the polarization field. Let

$$\mathcal{F}_\varepsilon = \int_0^1 \left\{\frac{1}{2}\varepsilon^4(q'')^2 - \frac{a}{2}\varepsilon^2(q')^2 + \frac{1}{4}(q^2-1)^2\right\} dx.$$

Let $(\phi_\varepsilon, p_\varepsilon)$ be a sequence of minimizers of $\mathcal{G}_\varepsilon$ in $\mathcal{Y}$, where

$$\mathcal{Y} = \left\{ (\phi, p) \in W^{1,2}(0,1) \times W^{2,2}(0,1) | \int_0^1 p(x)\, dx = d \right\},$$

with a constant $-1 \leq d \leq 1$. It follows from the previous section that as $\varepsilon \to 0$, the energy $\mathcal{G}_\varepsilon(\phi_\varepsilon, p_\varepsilon)$ behaves like

$$\mathcal{F}_{OF}(\phi_\varepsilon, p_\varepsilon) := \int_0^1 \left\{ a^2 (\phi_\varepsilon')^2 - 2acp_\varepsilon' \cos\phi_\varepsilon \right\} dx.$$

Let $\{p_\varepsilon\}$ converge to $p \in BV((0,1), \{\pm 1\})$. In order to understand the behavior of ϕ_ε as $\varepsilon \to 0$, we let $\{\phi_\varepsilon\}$ converge to a function ϕ as $\varepsilon \to 0$.

Since $p \in BV((0,1), \{\pm 1\})$, we take $0 < z_1 < z_2 <, \cdots, z_N < 1$ the points where p jumps. Then p' would be either

$$\delta_{z_1} - \delta_{z_2} + \delta_{z_3} - ... + (-1)^{N+1} \delta_{z_N}$$

or

$$-(\delta_{z_1} - \delta_{z_2} + \delta_{z_3} - ... + (-1)^{N+1} \delta_{z_N}).$$

Assuming $p' = \delta_{z_1} - \delta_{z_2} + \delta_{z_3} - ... + (-1)^{N+1} \delta_{z_N}$, we obtain that

$$\begin{aligned} &\mathcal{F}_{OF}(\phi, p) \\ &= \int_0^1 a^2 (\phi')^2\, dz \\ &\quad -2ac[\cos\phi(z_1) - \cos\phi(z_2) + \cos\phi(z_3) - \cdots + (-1)^N \cos\phi(z_N)]. \end{aligned}$$

In order for ϕ to minimize $\mathcal{F}_{OF}(\phi, p)$, ϕ must satisfy

$$\cos(\phi(z_1)) = 1, \cos(\phi(z_2)) = -1, \cdots, \cos(\phi(z_N)) = (-1)^{N+1},$$

so that

$$\phi(z_1) = \phi(z_3) = \cdots = 0, \;\; \phi(z_2) = \phi(z_4) = \cdots = \pm\pi.$$

For each interval (z_i, z_{i+1}), ϕ satisfies the equation

$$\begin{gathered} \phi'' = 0, \\ \phi(z_i) = 0(\text{ or } \pm\pi), \phi(z_{i+1}) = \pm\pi \text{ (or 0)}. \end{gathered}$$

Combining them together, we construct a piecewise linear function ϕ independent of ε which minimizes $\mathcal{F}_{OF}(\cdot, p)$. This analysis suggests that bulk part of the total energy forces the molecules to rotate by the angle π when they move from one layer to another.

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