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NONLOCAL EFFECT IN LIQUID CRYSTALS

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Abstract. In this paper, we investigate the role of nonlocal interaction energy on nucleations of periodic solutions in a one-dimensional problem arising in smectic liquid crystals.

1. Introduction

In this article, we analyze the structure of ferroelectric liquid crystals with long-range interactions of polarizations. We assume that the liquid crystals are of smectic type, possess spontaneous polarization.

The vast majority of the nematogens are polar compounds but the absence of nematic ferroelectric behavior indicates that there is equal probability of the dipoles pointing in either direction. Because of this it is generally assumed that the permanent dipolar contribution to the orientational order is small enough to be negligible. However, it has been known that the interaction between neighboring dipoles is significant compared with dispersion forces. It is possible to construct a model that accounts for permanent dipoles but it is still consistent with the non-polar character of the medium. When dealing with such type of interactions, the concept of near-neighbors becomes relevant. We start with the spin-1/2 Ising model with interaction Hamiltonian

$$\mathcal{H} = -J \sum_{<ij>} s_i s_j - H \sum_i s_i, \quad s_i = \pm 1,$$

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where $< ij >$ denotes the chosen interactive neighborhood. We propose a continuum version with free energy

$$W(p) = \int_\Omega \int_\Omega J(\mathbf{x}-\mathbf{y})(p(\mathbf{x})-p(\mathbf{y}))^2 \, d\mathbf{x} \, d\mathbf{y},$$

where Ω is a domain in $\mathbf{R}^3$. The field p is an order parameter corresponding to the dipole moment (either electric or geometric). The antiferro-ordering (i.e., the tendency of immediate neighbors to be of opposite polarization) corresponds to taking $J < 0$, and the case with $J > 0$ gives the ferro-ordering.

In the studies of ferromagnetic materials, R. C. Rogers [9] proposed this type of nonlocal exchange energy. Mathematical advantage of using such a nonlocal energy is to model the highly oscillatory domain structures which are observed in ferromagnetic materials. In [1], the authors studied a discrete model for Ising-like phase transitions and introduced

$$\sum_{r,r' \in \Gamma} \mathcal{J}(r-r')(p(r)-p(r'))^2 + \sum_{r \in \Gamma} W(u(r)),$$

where Γ is a lattice whose sites are occupied by blocks, and W has minima at $u = \pm 1$. The corresponding continuum energy term becomes

$$\int_\Omega \int_\Omega J(x-y)(p(x)-p(y))^2 \, dx \, dy + \int_\Omega W(p(x)) \, dx$$

which is derived in [1]. This can also be written as

$$-2 \int_\Omega \int_\Omega J(x-y) p(x) p(y) \, dx \, dy + \int_\Omega \tilde{W}(p(x)) \, dx$$

for some function $\tilde{W}$. In smectic C* liquid crystals, Cladis et al [3] adopted this type of a term in the total energy in order to study an effective internal field model for the antiferroelectric to field induced ferroelectric transition in smectics. The energy can be considered as interaction between smectic layers.

Throughout this paper, we consider a simplified energy functional for smectic liquid crystals [8]

$$\begin{aligned} \mathcal{E} = \int_\Omega \{ & K|\nabla \mathbf{n}|^2 + \frac{1}{\eta^2}\Big|\mathbf{k}\times\mathbf{n}|\mathbf{P} - |\mathbf{P}|\mathbf{k}\times\mathbf{n}\Big|^2 \\ & + \mu^2 |\nabla \mathbf{P}|^2 + \frac{1}{4\varepsilon}(|\mathbf{P}|^2-1)^2 + \mathcal{K}_\gamma \mathbf{P}\cdot\mathbf{P}\} \, d\mathbf{x}, \end{aligned} \tag{1.1}$$

where $K_i > 0 (i = 1, 2, 3), \mu^2 > 0$, $\mathbf{k} = (0, 0, 1)$, $\varepsilon > 0, \eta \neq 0$, and $\mathcal{K}_\gamma$ is a kernel operator defined by

$$\mathcal{K}_\gamma \mathbf{P}(\mathbf{x}) = \int_\Omega \mathcal{K}(\mathbf{x},\mathbf{y})\mathbf{P}(\mathbf{y})\,d\mathbf{y}.$$

The choice of a kernel function $\mathcal{K}$ depends on material structures. In ferro and antiferroelectric liquid crystals, polarization vector tends to be $\pm\mathbf{P}_0$ between smectic layers, where $|\mathbf{P}_0| = 1$. In this paper, we take $\mathcal{K}$ to be a fundamental solution of $-\Delta + \delta$. Since we are interested in the role of nonlocal energy term in the structure, we further assume that

$$\nabla\omega = \mathbf{k},\ \ \mathbf{P} = \mathbf{P}(z),\ \ \mathbf{n} = (a_1\cos\Phi(z), a_1\sin\Phi(z), b_1),$$
$$\mathbf{P} = p(z)\frac{\mathbf{k}\times\mathbf{n}}{|\mathbf{k}\times\mathbf{n}|},\ \ a_1^2 + b_1^2 = 1,\ \ a_1 > 0,\ \ b_1 > 0,$$

where $p(z)$ is a scalar function and $\Phi(z) = \frac{\pi}{2}$ or $\frac{3\pi}{2}$.

Then the energy functional (1.1) reads

$$\mathcal{E} = \int_{-\infty}^{\infty}\{\frac{1}{2}\mu^2 p_z^2 + \frac{1}{4\epsilon}(p^2-1)^2\}\,dz + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\mathcal{K}(z,w)p(z)p(w)\,dw\,dz,$$

where $\mathcal{K} = -\delta G$ and G is a fundamental solution of $\eta q'' = -p + q$, $q'(\pm\infty) = 0$.

The corresponding Euler-Lagrange equations are

$$\text{(1.2)}\qquad \begin{cases} \mu^2 p'' = -\frac{4}{\varepsilon}p + \delta q + \frac{4}{\varepsilon}p^3, \\ \eta q'' = -p + q. \end{cases}$$

2. Nucleations of periodic solutions

In this section, we study the role of the nonlocal energy to model one dimensional periodic configurations of polarization. We prove that existence of periodic solutions which nucleate from $p = 0$.

Setting $p' = u, q' = v, \eta = \gamma^2$, (1.2) becomes

$$\text{(2.1)}\qquad \begin{pmatrix} p \\ q \\ u \\ v \end{pmatrix}' = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \frac{-4}{\mu^2\varepsilon} & \frac{\delta}{\mu^2} & 0 & 0 \\ -\frac{1}{\gamma^2} & \frac{1}{\gamma^2} & 0 & 0 \end{pmatrix}\begin{pmatrix} p \\ q \\ u \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ \frac{4}{\mu^2\varepsilon}p^3 \\ 0 \end{pmatrix}.$$

Let $a = -\frac{4}{\mu^2\varepsilon}$, $b = \frac{\delta}{\mu^2}$, $c = \frac{1}{\gamma^2}$. Then the characteristic equation, $\det(A - \lambda I) = 0$ becomes

$$\lambda^4 - (a+c)\lambda^2 + c(a+b) = 0$$

where A is the 4×4 matrix appearing in (2.1). Then

$$\lambda^2 = \frac{a + c \pm \sqrt{(a+c)^2 - 4c(a+b)}}{2}.$$

There are several types of eigenvalues of A. In case that $a + b = 0$, A has double zero eigenvalue. By the theory of center manifold, we can reduce the dimension of the problem. We refer the reader to [2, 7] for more study. In our study, we are interested in the case that A has pairs of purely imaginary eigenvalues. From now on, we assume that μ, ε, γ, and δ satisfy

$$a + c < 0 < (a + b) \tag{2.2}$$

so that $(a + c)^2 - 4c(a + b) > 0$.

2.1. Case I: ε is not small.

Without loss of generality, we may assume that

$$-\frac{4}{\mu^2\varepsilon} + \frac{1}{\gamma^2} = -3, \quad -\frac{4}{\mu^2\varepsilon} + \frac{\delta}{\mu^2} = 2\gamma^2.$$

so that eigenvalues of A are $\pm i, \pm\sqrt{2}i$. In fact, other cases can be treated in a similar fashion. Let

$$P = \begin{pmatrix} 1 & 0 & 1 & 0 \\ -\frac{a+1}{b} & 0 & -\frac{a+2}{b} & 0 \\ 0 & 1 & 0 & \sqrt{2} \\ 0 & -\frac{\alpha_1(a+1)}{b} & 0 & -\frac{\sqrt{2}(a+2)}{b} \end{pmatrix}.$$

Use changes of variables $(x, y, z, w) \to P^{-1}(x, y, z, w)^T$ and let $z_1 = y + xi$, $z_2 = y - xi$,$z_3 = w + zi$ $z_4 = w - zi$ to obtain

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix}' = \begin{pmatrix} -i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & -\sqrt{2}i & 0 \\ 0 & 0 & 0 & \sqrt{2}i \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix} + l(z_1, z_2, z_3, z_4) \begin{pmatrix} -(a+2) \\ -(a+2) \\ \frac{a+1}{\sqrt{2}} \\ \frac{a+1}{\sqrt{2}} \end{pmatrix}$$

where $l(z_1, z_2, z_3, z_4) = \frac{a(z_1+z_2+z_3+z_4)^3}{8}$.

Then the basis for $\mathrm{Ker}(L_A^3)$ [2] is

$$\{z_1^2 z_2 \mathbf{e}_1, z_1 z_3 z_4 \mathbf{e}_1, z_1 z_2^2 \mathbf{e}_2, z_2 z_3 z_4 \mathbf{e}_2, z_3^2 z_4 \mathbf{e}_3, z_1 z_2 z_3 \mathbf{e}_3, z_3 z_4^2 \mathbf{e}_4, z_1 z_2 z_3 \mathbf{e}_4\}.$$

We also know that a miniversal deformation of the diagonal matrix with entries $\pm i, \pm\sqrt{2}i$ is

$$\begin{pmatrix} \lambda_1 - i & 0 & 0 & 0 \\ 0 & \bar{\lambda}_1 + i & 0 & 0 \\ 0 & 0 & \lambda_2 - \sqrt{2}i & 0 \\ 0 & 0 & 0 & \bar{\lambda}_2 + \sqrt{2}i \end{pmatrix}$$

for some $\lambda_1, \lambda_2 \in \mathbb{C}$.

Therefore we obtain the following

$$\text{(2.3)} \quad \begin{cases} \dot{z}_1 &= (\lambda_1 + i)z_1 - \frac{a(a+2)}{8}(3|z_1|^2 z_1 + 6|z_3|^2 z_1), \\ \dot{z}_3 &= (\lambda_2 + \sqrt{2}i)z_3 + \frac{a(a+1)}{8\sqrt{2}}(6|z_1|^2 z_3 + 3|z_3|^2 z_3). \end{cases}$$

The equations for z_2, z_4 are obtained by taking conjugates of equations for z_1, z_3 respectively.

Let $z_1 = r_1 e^{i\theta_1}, z_3 = r_2 e^{i\theta_2}$. Then (2.3) becomes

$$\begin{cases} \dot{r}_1 &= \varepsilon_1 r_1 - \frac{a(a+2)}{8} r_1(3r_1^2 + 6r_2^2), \\ \dot{r}_2 &= \varepsilon_2 r_1 + + \frac{a(a+1)}{8\sqrt{2}} r_2(6r_1^2 + 3r_2^2), \end{cases}$$

where $\varepsilon_i, i = 1, 2$ are real parameters and equations for $\theta_i, i = 1, 2$ are determined by r_1, r_2.

Let $\eta_1 = \frac{3a(a+2)}{8}$ and $\eta_2 = \frac{3a(a+1)}{8\sqrt{2}}$. Then

$$\text{(2.4)} \quad \begin{cases} \dot{r}_1 &= \varepsilon_1 r_1 - \eta_1 r_1(r_1^2 + 2r_2^2), \\ \dot{r}_2 &= \varepsilon_2 r_2 + \eta_2 r_2(2r_1^2 + r_2^2). \end{cases}$$

We assume that $\eta_i \neq 0, i = 1, 2$. Take α, β satisfying

$$\frac{\alpha + 1}{\beta} = \frac{2\eta_2}{\eta_1}, \frac{\alpha}{\beta + 1} = \frac{\eta_2}{2\eta_1}.$$

By scalings as in [2]

$$\frac{r_1^2}{|\eta_1|} \to r_1, \frac{r_1^2}{2|\eta_1|} \to r_2, -\frac{\mathrm{sgn}\eta_1}{2} t \to t,$$

the system (2.4) takes the form

$$\begin{cases} \dot{r}_1 &= r_1(\mu_1 + \sigma r_1 - r_2), \\ \dot{r}_2 &= r_2(\mu_2 - \frac{\alpha+1}{\beta} r_1 + \frac{\alpha}{\beta+1} r_2), \end{cases}$$

where $\mu_i, i = 1, 2$ are real parameters, $\sigma = 1$ if $\eta_1\eta_2 > 0$ and $\sigma = -1$ if $\eta_1\eta_2 < 0$. By the change of variables

$$\mu_1 = \xi\delta, \mu_2 = -\xi\frac{\alpha}{\beta}\delta - \gamma\delta^2, r_1 \to \delta r_1, r_2 \to \delta r_2, dt \to \frac{r_1^{\alpha-1} r_2^{\beta-1}}{\delta} dt,$$

we obtain a new system of equations

$$\begin{cases} \dot{r_1} &= r_1^{\alpha} r_2^{\beta-1}(\xi + \sigma r_1 - r_2), \\ \dot{r_2} &= r_1^{\alpha-1} r_2^{\beta}\Big(-\xi\frac{\alpha}{\beta} - \frac{\alpha+1}{\beta}\sigma r_1 + \frac{\alpha}{\beta+1} r_2\Big). \end{cases} \tag{2.5}$$

Notice that the system (2.5) is a Hamiltonian system with a first integral

$$H(r_1, r_2) = r_1^{\alpha} r_2^{\beta}\Big(\frac{\xi + \sigma r_1}{\beta} - \frac{r_2}{\beta+1}\Big). \tag{2.6}$$

We have the following theorem [2]

THEOREM 2.1. *Let*

$$\begin{aligned} r_1^* &= \frac{\beta(\beta+1)\sigma}{\alpha+\beta+1}(\frac{\alpha}{\beta+1}\mu_1 + \mu_2), \\ r_2^* &= \frac{\beta(\beta+1)\sigma}{\alpha+\beta+1}(\frac{\alpha+1}{\beta}\mu_1 + \mu_2), \end{aligned}$$

and $h_1^* = H(r_1^*, r_2^*)$. *Consider the following three cases*

(1) $\sigma = -1,\ \ \xi = 1,\ \ \alpha > 0, \beta > 0,$
(2) $\sigma = 1,\ \ \xi = 1,\ \ -1 < \alpha + \beta < 0,$
(3) $\sigma = 1,\ \ \xi = -1,\ \ \alpha + \beta < -1.$

Then for any h *either in* $(0, h^*)$ *for case* (1) *and* (3) *or* $(h^*, 0)$ *for case* (2), *the level curve* $\{(r_1, r_2) : H(r_1, r_2) = h\}$ *is a closed curve.*

If $0 < \frac{4}{\eta^2\varepsilon} < 1$, then we can take $\alpha = -2,\ \beta = \frac{1}{7}$. This corresponds to the case (3) in the previous theorem (2.1).

COROLLARY 2.2. *Suppose that*

$$-\frac{4}{\mu^2\varepsilon} + \frac{1}{\gamma^2} = -3, \quad -\frac{4}{\mu^2\varepsilon} + \frac{\delta}{\mu^2} = 2\gamma^2, \quad 0 < \frac{4}{\eta^2\varepsilon} < 1.$$

Then level curves $\{(r_1, r_2) : H(r_1, r_2) = h\}$*of the first integral* H *for* (2.5) *are closed for small* h.

We notice that this method does not give us information about closed integral curves when ε is small. We discuss this case in the following.

2.2. Case II: ε is small.

Let

$$\frac{\delta}{\mu^2} = \tilde{\delta}, \quad \varepsilon\mu^2 = \tilde{\varepsilon}, \quad \gamma = \frac{1}{\eta}. \tag{2.7}$$

After dropping the tilde, we get

(2.8) $$\begin{cases} p'' = -\frac{4}{\varepsilon}p + \delta q + \frac{4}{\varepsilon}p^3, \\ q'' = -\gamma p + \gamma q \end{cases}$$

Let $\tilde{q} = -\frac{q}{\lambda}$. Then,

$$\begin{cases} p'' = \frac{4}{\varepsilon}(p^3 - p) + \delta\lambda_0\tilde{q}, \\ \tilde{q}'' = -\frac{\gamma}{\lambda_0}p + \gamma\tilde{q}. \end{cases}$$

Choose λ_0 so that $\lambda_0^2 = -\frac{\gamma}{\delta}$. Again, dropping the tilde symbol, we have

(2.9) $$\begin{cases} p'' = \frac{4}{\varepsilon}(p^3 - p) + \delta\lambda_0 q, \\ q'' = \delta\lambda_0 p + \gamma q. \end{cases}$$

For convenience, we introduce notations:

$$\mathbf{p} = (p_1, p_2)^T, \quad \mathbf{q} = (q_1, q_2)^T,$$
$$p_1 = p, \quad p_2 = q, \quad q_1 = p_1', \quad q_2 = p_2'.$$

In terms of the new notation, the system (2.9) becomes

(2.10) $$\begin{cases} \frac{d\mathbf{p}}{dx} = \mathbf{q}, \\ \frac{d\mathbf{q}}{dx} = (\frac{4}{\varepsilon}(p_1^3 - p_1) + \delta\lambda p_2, \delta\lambda p_1 + \gamma p_2)^T. \end{cases}$$

Let

$$H(\mathbf{p}, \mathbf{q}) = \frac{1}{2}|\mathbf{q}|^2 - \frac{\gamma}{2}p_2^2 - \delta\lambda_0 p_1 p_2 - \frac{1}{\varepsilon}(p_1^2 - 1)^2.$$

We rewrite (2.10) as

(2.11) $$\frac{dU}{dx} = \mathcal{J}\nabla_U H(U),$$

where $U = (\mathbf{p}, \mathbf{q})^T$ and $\mathcal{J} = \begin{pmatrix} O & I \\ -I & O \end{pmatrix}$. We calculate

$$\mathcal{A}_0 := \mathcal{J}\nabla_U H(\mathbf{0}) = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\frac{4}{\varepsilon} & \delta\lambda_0 & 0 & 0 \\ \delta\lambda_0 & \gamma & 0 & 0 \end{pmatrix},$$

and

$$\det(\mathcal{A}_0 - \lambda\mathbf{I}) = \lambda^4 - (\gamma - \frac{4}{\varepsilon})\lambda^2 - \delta^2\lambda_0^2 - \frac{4\gamma}{\varepsilon} = 0.$$

With physically realistic assumptions on the parameters of the problem, we obtain the theorem.

Theorem 2.3. *Assume that* $\gamma < 0$ *and* $\delta\varepsilon < 1$. *Then there exist a* $\sigma > 0$ *and a continuously differentiable surface* $\{(U(r,\kappa), s(r,\kappa)) : r \in (-\sigma,\sigma),\ \kappa \in (\kappa_0-\sigma, \kappa_0+\sigma)\}$ *of nontrivial (real),* $\frac{2\pi}{\kappa}$*−periodic solutions of* (2.11) *through* $(U(0,\kappa), s(0,\kappa)) = (\mathbf{0}, s(0,\kappa))$, *with* $s(0,\kappa_0) = 0$ *in* $C^1_{\frac{2\pi}{\kappa}}(\mathbf{R},\mathbf{R}^4) \times \mathbf{R}$. *Furthermore,* $U(-r,s)$ *is obtained from* $U(r,s)$ *by a phase shift of half the period* $\frac{\pi}{\kappa}$.

Proof. Denote

$$\gamma_1 = \frac{6}{\varepsilon} - \sqrt{\frac{20}{\varepsilon^2} - \delta^2\lambda_0^2},$$
$$\gamma_2 = \frac{6}{\varepsilon} + \sqrt{\frac{20}{\varepsilon^2} - \delta^2\lambda_0^2},$$
$$s = \Big(\gamma - \frac{4}{\varepsilon}\Big)^2 + 4\big(\frac{4\gamma}{\varepsilon} + \delta^2\lambda_0^2\big).$$

We take s as the bifurcation parameter of the problem. If $\gamma_2 > \gamma > \gamma_1$, then $s < 0$ and $\mathcal{A}_0$ has fully complex eigenvalues, i.e., neither the real nor the imaginary parts is zero. If $\gamma < \gamma_1$, then $s > 0$ and $\mathcal{A}_0$ has two pairs of purely imaginary eigenvalues. In the case that $\gamma = \gamma_1$, $s = 0$, $\mathcal{A}_0$ has double purely imaginary eigenvalues $\pm i\kappa_0$, where

$$\kappa_0 = \sqrt{\Big|\frac{2}{\varepsilon} - \sqrt{\frac{20}{\varepsilon^2} - \delta^2\lambda_0^2}\Big|}.$$

Equation (2.11) can be written as

$$\frac{dU}{dx} = \mathcal{J}\nabla_U H(U,s).$$

Let ϕ_0 be an eigenvector of $\mathcal{A}_0$ corresponding to $i\kappa_0$. It has the form

$$\phi_0 = \Big(1, \frac{1}{\delta_2\lambda_0}\big(\frac{4}{\varepsilon} - \kappa_0^2\big), i\kappa_0, \frac{i\kappa_0}{\delta_2\lambda_0}\big(\frac{4}{\varepsilon} - \kappa_0^2\big)\Big)^T.$$

We now calculate,

$$\frac{d}{ds}\Big|_{s=0}\nabla_U^2 H(0,s) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -\gamma'(0) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Hence,

$$< \frac{d}{ds}\Big|_{s=0}\nabla_U^2 H(0,s)\phi_0, \bar{\phi_0} >= -\frac{\gamma'(0)}{\delta^2\lambda^2}\Big(\frac{4}{\varepsilon} - \kappa_0^2\Big)^2 \neq 0,$$

since

$$\gamma'(0) = \frac{1}{2\gamma_1 + \frac{8}{\varepsilon}} \neq 0.$$

By the Hamiltonian Hopf bifurcation theorem [6] (p. 61), we complete the proof. □

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