

Pattern Formation for a Planar Layer of Nematic Liquid Crystal

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Abstract

Using equivariant bifurcation theory, and on the basis of symmetry considerations independent of the model, we classify square and hexagonally periodic patterns that typically arise when a homeotropic or planar isotropic nematic state becomes unstable, perhaps as a consequence of an applied magnetic or electric field. We relate this to a Landau – de Gennes model for the free energy, and derive dispersion relations in sufficient generality to illustrate the role of up/down symmetry in determining which patterns can arise as a stable bifurcation branch from either initial state.

1 Introduction

In the Landau theory of phase transitions for a liquid crystal the degree of coherence of alignment of molecules is usually represented by a *tensor order parameter*, a field of symmetric 3×3 tensors $Q(\mathbf{x})$, $\mathbf{x} \in \mathbf{R}^3$ with $\text{tr}(Q) = 0$ [15]. We think of Q as the second moment of a probability distribution for the directional alignment of a rod-like molecule. In a spatially uniform system, Q is independent of $\mathbf{x} \in \mathbf{R}^3$. When $Q = 0$ the system is *isotropic*, with molecules not aligned in any particular direction. If there is a preferred

direction along which the molecules tend to lie (but with no positional constraints) the liquid crystal is in *nematic* phase. There are many other types of phase involving local and global structures, see [15].

In this paper we consider a thin planar layer of nematic liquid crystal where the top and bottom boundary conditions on this layer are identical. In this situation the symmetries of any liquid crystal model will include planar Euclidean symmetries $\mathbf{E}(2)$ as well as up/down reflection symmetry.

A configuration or *state* of a liquid crystal is just a director field that at each point \mathbf{x} in the planar layer indicates the direction $\mathbf{n}(\mathbf{x})$ in \mathbf{R}^3 along which molecules tend to align. We approximate a planar layer by a plane — so our states consist of a 3-dimensional direction field \mathbf{n} defined on \mathbf{R}^2 . In the Landau theory the direction $\mathbf{n}(\mathbf{x})$ is just the eigendirection corresponding to the largest eigenvalue of $Q(\mathbf{x})$ — the direction in which a molecule has the ‘maximum probability’ of aligning. We shall also refer to $Q(\mathbf{x})$ as the *state* of the system.

In our discussion we assume an initial equilibrium state Q_0 that is $\mathbf{E}(2)$ -invariant. Because of translation symmetry such states are spatially uniform and because of rotation symmetry they have the form

$$Q_0 = \eta \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

for some nonzero $\eta \in \mathbf{R}$. For $\eta > 0$ the state Q_0 represents a *homeotropic* phase (the state has constant alignment in the vertical direction), whereas for $\eta < 0$ it represents a planar *isotropic* liquid crystal (a molecule is equally likely to align in any horizontal direction). The state Q_0 is also invariant under up/down reflection, that is conjugacy by the matrix

$$\tau = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

We consider models that are determined internally by a free energy rather than externally by, say, a magnetic field. Thus, the symmetry group for our discussion is

$$\Gamma = \mathbf{E}(2) \times \mathbf{Z}_2(\tau),$$

since these are the symmetries of both the initial state Q_0 and the model.

Our aim in this paper is to study local bifurcation from Q_0 to states that have spatially varying alignment along the plane. Specifically, we consider bifurcation to states exhibiting spatial periodicity with respect to some planar lattice. We use group representation theory (following [11, 10]) to extract information about nonlinear behavior near bifurcation that is independent of the model.

There is a common approach to all lattice bifurcation problems, which we now describe. This discussion, adapted from [2], will be familiar to anyone who has studied pattern formation in Bénard convection models, although there are minor differences due to the change in context. See [11, 10].

Let λ be a bifurcation parameter and assume that the equations have Q_0 as an equilibrium for all λ . Let L denote the equations linearized about Q_0 . In the models, λ is the temperature and bifurcation occurs as λ is decreased.

1. A linear analysis about Q_0 leads to a *dispersion curve*.

Translation symmetry in a given direction implies that (complex) eigenfunctions have a *plane wave factor* $w_{\mathbf{k}}(\mathbf{x}) = e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$ where $\mathbf{k} \in \mathbf{R}^2$. Rotation symmetry implies that the linearized equations have infinite-dimensional eigenspaces; instability occurs simultaneously to all functions $w_{\mathbf{k}}(\mathbf{x})$ with constant $k = |\mathbf{k}|$. The number k is called the *wave number*. Points (k, λ) on the dispersion curve are defined by the maximum values of λ for which an instability of the solution Q_0 to an eigenfunction with wave number k occurs.

2. Often, the dispersion curve has a unique maximum, that is, there is a *critical* wave number k_* at which the first instability of the homogeneous solution occurs as λ is decreased.

Bifurcation analyses near such points are difficult since the kernel of the linearization is infinite-dimensional. This difficulty can be side-stepped by restricting solutions to the class of possible solutions that are doubly periodic with respect to a planar lattice \mathcal{L} .

3. The symmetries of the bifurcation problem restricted to \mathcal{L} change from Euclidean symmetry in two ways.

First, translations act on the restricted problem modulo \mathcal{L} ; that is, translations act as a torus \mathbf{T}^2 . Second, only a finite number of rotations and reflections remain as symmetries. Let the *holohedry* $H_{\mathcal{L}}$ be the group of rotations and reflections that preserve the lattice. The

symmetry group $\Gamma_{\mathcal{L}}$ of the lattice problem is then generated by $H_{\mathcal{L}}$, \mathbf{T}^2 , as well as (in our case) $\mathbf{Z}_2(\tau)$.

4. The restricted bifurcation problem must be further specialized. First, a *lattice type* needs to be chosen (in this paper square or hexagonal). Second, the *size* of the lattice must be chosen so that a plane wave with critical wave number k_* is an eigenfunction in the space $\mathcal{F}_{\mathcal{L}}$ of matrix functions periodic with respect to \mathcal{L} .

Those $\mathbf{k} \in \mathbf{R}^2$ for which the scalar plane wave $e^{2\pi i \mathbf{k} \cdot \mathbf{x}}$ is \mathcal{L} -periodic are called *dual wave vectors*. The set of dual wave vectors is a lattice, called the *dual lattice*, and is denoted by \mathcal{L}^* . In this paper we consider only those lattice sizes where the critical dual wave vectors are vectors of shortest length in \mathcal{L}^* . Therefore, generically, we expect $\ker \mathbf{L} = \mathbf{R}^n$ where n is 4 and 6 on the square and hexagonal lattices, respectively.

5. Since $\ker \mathbf{L}$ is finite-dimensional, we can use Liapunov-Schmidt or center manifold reduction to obtain a system of reduced bifurcation equations on \mathbf{R}^n whose zeros are in 1:1 correspondence with the steady-states of the original equation. Moreover, this reduction can be performed so that the reduced bifurcation equations are $\Gamma_{\mathcal{L}}$ -equivariant.
6. Solving the reduced bifurcation equations is still difficult. A partial solution can be found as follows. A subgroup $\Sigma \subset \Gamma_{\mathcal{L}}$ is *axial* if $\dim \text{Fix}(\Sigma) = 1$ where

$$\text{Fix}(\Sigma) = \{x \in \ker \mathbf{L} : \sigma x = x \quad \forall \sigma \in \Sigma\}.$$

The Equivariant Branching Lemma [11] states that generically there exists a branch of solutions corresponding to each axial subgroup. These solution types are then classified by finding all axial subgroups, up to conjugacy.

On general grounds, when restricting attention to bifurcations corresponding to shortest wave length vectors, we may assume the representation (action) of $\Gamma_{\mathcal{L}}$ to be irreducible: see [11, 7]. In Section 2 we show that there are four distinct types of irreducible representation of $\Gamma_{\mathcal{L}}$ that can occur in bifurcations from Q_0 . These representations are the four combinations of (i) scalar or pseudoscalar (see [1, 2, 10]) and (ii) preserve or break τ symmetry. In Section 2 we also compute the axial subgroups for each of these

representations and draw pictures of each of the relevant planforms on the square and hexagonal lattices. It is an elementary yet curious observation that in Landau models restricted to a planar layer, bifurcations from the homeotropic phase ($\eta > 0$) do not lead to clear new patterns unless τ symmetry is broken: the τ symmetry ‘freezes’ the director field to the vertical. This point is discussed in more detail in Section 2. Therefore we present pictures of the four bifurcations from the isotropic case ($\eta < 0$) and only the two bifurcations when τ acts as -1 in the homeotropic case ($\eta > 0$). The $\tau = +1$ bifurcations in the homeotropic case can lead to patterns in a theory posed on a thickened planar layer. In such a theory, which goes beyond what we present here, the precise form of boundary conditions on the upper and lower boundaries of the layer will determine the pattern types. In the other bifurcations, the contributions to pattern selection of these boundary conditions should be less important.

In fact, the bifurcation theory for each of these four representations of $\Gamma_{\mathcal{L}}$ has been discussed previously in different contexts. It is only the interpretation of eigenfunctions in the context of $Q(\mathbf{x})$ that needs to be computed, along with the pictures of the resulting planforms. More specifically, when τ acts trivially on $\ker \mathbf{L}$ the scalar representation has been used in the study of pattern formation in Rayleigh-Bénard convection by Busse [4] and Buzano and Golubitsky [5], and the pseudoscalar representation has been studied by Bosch-Vivancos, Chossat, and Melbourne [1] and also in the context of geometric visual hallucinations by Bressloff, Cowan, Golubitsky, and Thomas [3, 2]. When τ acts nontrivially the two representations have the same matrix generators and although the planforms are different for these two representations the bifurcation theory is identical. Indeed, this theory is just the one studied for Rayleigh-Bénard convection with a midplane reflection by Golubitsky, Swift, and Knobloch [12].

Perhaps the most interesting patterns that appear from our analysis are the stripes or ‘rolls’ (from convection studies) type patterns that bifurcate from the isotropic state when τ symmetry is not broken, that is $\tau = +1$. The scalar pattern is a ‘martensite’ pattern whereas the pseudoscalar pattern is a ‘chevron’ pattern. See Figure 1. The fact that such patterns do occur in liquid crystal layers is well known: see for example [14], from which the pictures in Figure 2 are taken. Note, however, that these patterns are examples that bifurcate from homeotropy; moreover, they also exhibit finer periodic structures (a characteristic feature in practice) that we do not discuss in this paper.

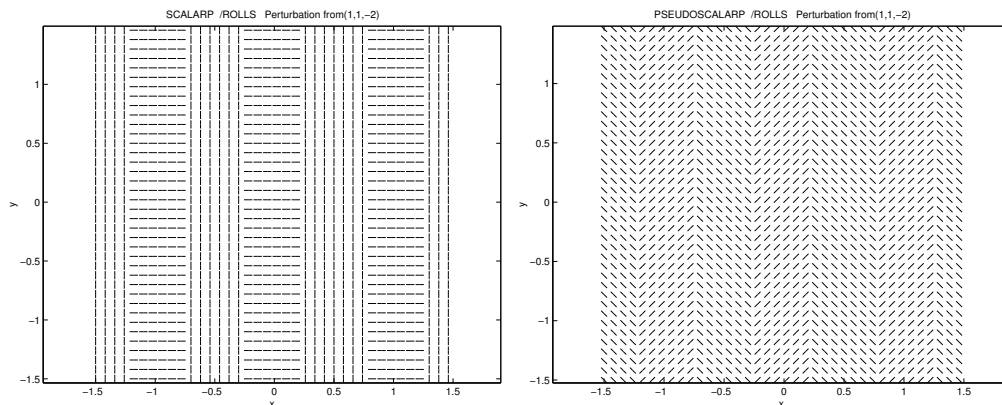


Figure 1: Rolls from isotropic ($\eta < 0$) state with $\tau = +1$ representations: scalar ‘martensite’ (left); pseudoscalar ‘chevron’ (right).

In Section 3 we introduce free energies that illustrate that all four representations can be encountered as λ is decreased, although in our model only two of them can be the first bifurcation from homeotropy while only the other two can be the first bifurcation from isotropy. (It is likely that different models will allow other variations.) It then follows from the Equivariant Branching Lemma that each of the axial equilibrium types that we describe in Section 2 is an equilibrium solution to the nonlinear model equations.

2 Spatially Periodic Equilibrium States

In this section we list the axial subgroups for each of the four representations of $\Gamma_{\mathcal{L}}$ on the square and hexagonal lattices, and then plot the planforms for the associated bifurcating branches from both the isotropic ($\eta < 0$) and homeotropic ($\eta > 0$) states. We emphasize that these results depend only on symmetry and can be obtained independently of any particular model. First, we describe the form of the eigenspaces for each of these four representations. Second, we discuss the group actions and the axial subgroups for each of these representations. Finally, we plot the associated direction fields.

Linear Theory

Let L denote the linearization of the governing system of differential equations at Q_0 (for the free energy model with free energy \mathcal{F} we have $L = d^2F(Q_0)$).

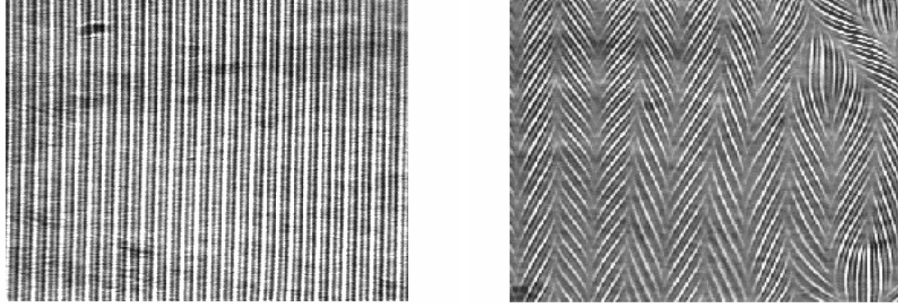


Figure 2: Rolls (left) and chevrons (right) bifurcating from homeotropy. (Pictures courtesy of J.-H. Huh.)

Bifurcation occurs at parameter values where L has nonzero kernel. We prove that generically, at bifurcation to shortest dual wave vectors, $\ker L$ has the form given in Theorem 2.1. Let

$$\begin{aligned}
 Q^{++} &= \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & -a-b \end{bmatrix} & Q^{+-} &= \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix} \\
 Q^{-+} &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} & Q^{--} &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & i & 0 \end{bmatrix}
 \end{aligned} \tag{2.1}$$

In the double superscript on Q , the first \pm refers to scalar or pseudoscalar representation and the second \pm refers to the action of τ . In Table 1 we also fix the generators of the lattice and its dual lattice.

Lattice	ℓ_1	ℓ_2	\mathbf{k}_1	\mathbf{k}_2
Square	$(1, 0)$	$(0, 1)$	$(1, 0)$	$(0, 1)$
Hexagonal	$(1, \frac{1}{\sqrt{3}})$	$(0, \frac{2}{\sqrt{3}})$	$(1, 0)$	$\frac{1}{2}(-1, \sqrt{3})$

Table 1: Generators for the planar lattices and their dual lattices.

Theorem 2.1. *On the square lattice, let ξ be rotation counterclockwise by $\frac{\pi}{2}$. Then, in each irreducible representation, $\ker \mathbf{L}$ is four-dimensional and its elements have the form*

$$z_1 e^{2\pi i \mathbf{k}_1 \cdot \mathbf{x}} Q^{\pm\pm} + z_2 e^{2\pi i \mathbf{k}_2 \cdot \mathbf{x}} \xi \cdot Q^{\pm\pm} + c.c. \quad (2.2)$$

for $z_1, z_2 \in \mathbf{C}$, where $Q^{\pm\pm}$ is the appropriate matrix specified in (2.1), $\xi \cdot Q$ denotes $\xi Q \xi^{-1}$, and *c.c.* denotes complex conjugate.

On the hexagonal lattice, let ξ be rotation counterclockwise by $\frac{\pi}{3}$. Then, in each irreducible representation, $\ker \mathbf{L}$ is six-dimensional and its elements have the form

$$z_1 e^{2\pi i \mathbf{k}_1 \cdot \mathbf{x}} Q^{\pm\pm} + z_2 e^{2\pi i \mathbf{k}_2 \cdot \mathbf{x}} \xi^2 \cdot Q^{\pm\pm} + z_3 e^{2\pi i \mathbf{k}_3 \cdot \mathbf{x}} \xi^4 \cdot Q^{\pm\pm} + c.c. \quad (2.3)$$

for $z_1, z_2, z_3 \in \mathbf{C}$.

Proof. Let V and $V_{\mathbf{C}}$ denote the space of (respectively) real and complex 3×3 symmetric matrices with zero trace. Planar translation symmetry implies that eigenfunctions (nullvectors) of \mathbf{L} are linear combinations of matrices that have the plane wave form

$$e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q + c.c. \quad (2.4)$$

where $Q \in V_{\mathbf{C}}$ is a constant matrix and $\mathbf{k} \in \mathbf{R}^2$ is a wave vector. For fixed \mathbf{k} let

$$W_{\mathbf{k}} = \{e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q + c.c. : Q \in V_{\mathbf{C}}\} \quad (2.5)$$

be the ten-dimensional \mathbf{L} -invariant real linear subspace consisting of such functions.

Rotations and reflections $\gamma \in \mathbf{O}(2) \times \mathbf{Z}_2(\tau) \subset \mathbf{O}(3)$ act on $W_{\mathbf{k}}$ by

$$\gamma(e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q) = e^{2\pi i (\gamma \mathbf{k}) \cdot \mathbf{x}} \gamma Q \gamma^{-1}. \quad (2.6)$$

When looking for nullvectors we can assume, after rotation, that $\mathbf{k} = k(1, 0)$. We can also rescale length so that the dual wave vectors of shortest length have length 1; that is, we can assume that $k = 1$.

Bosch Vivancos, Chossat, and Melbourne [1] observed that reflection symmetries can further decompose $W_{\mathbf{k}}$ into two \mathbf{L} -invariant subspaces. To see why, consider the reflection

$$\kappa(x, y, z) = (x, -y, z).$$

Note that the action (2.6) of κ on $W_{\mathbf{k}}$ (dropping the *+c.c.*) is

$$\kappa(e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q) = e^{2\pi i \kappa(\mathbf{k}) \cdot \mathbf{x}} \kappa Q \kappa^{-1} = e^{2\pi i \mathbf{k} \cdot \mathbf{x}} \kappa Q \kappa^{-1}.$$

Since $\kappa^2 = 1$, the subspace $W_{\mathbf{k}}$ itself decomposes as

$$W_{\mathbf{k}} = W_{\mathbf{k}}^+ \oplus W_{\mathbf{k}}^- \quad (2.7)$$

where κ acts trivially on $W_{\mathbf{k}}^+$ and as minus the identity on $W_{\mathbf{k}}^-$, and each of $W_{\mathbf{k}}^+$ and $W_{\mathbf{k}}^-$ are \mathbf{L} invariant. We call functions in $W_{\mathbf{k}}^+$ *even* and functions in $W_{\mathbf{k}}^-$ *odd*. Bifurcations based on even eigenfunctions are called *scalar* and bifurcations based on odd eigenfunctions are called *pseudoscalar*.

A further simplification in the form of Q can be made. Consider $\rho \in \mathbf{SO}(2) \subset \mathbf{O}(3)$ given by $(x, y, z) \mapsto (-x, -y, z)$. Since (dropping the *+c.c.*)

$$\rho(e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q) = e^{2\pi i \rho \mathbf{k} \cdot \mathbf{x}} \rho Q \rho^{-1} = e^{-2\pi i \mathbf{k} \cdot \mathbf{x}} \rho Q \rho^{-1} = e^{2\pi i \mathbf{k} \cdot \mathbf{x}} \overline{\rho Q \rho^{-1}}$$

the associated action of ρ on $V_{\mathbf{C}}$ is related to the conjugacy action by

$$\rho(Q) = \overline{\rho Q \rho^{-1}}. \quad (2.8)$$

Since \mathbf{L} commutes with ρ and $\rho^2 = 1$, the subspaces of the kernel of \mathbf{L} where $\rho(Q) = Q$ and $\rho(Q) = -Q$ are \mathbf{L} -invariant. Therefore, we can assume that Q is in one of these two subspaces. Note moreover that translation by $\frac{1}{4}\mathbf{k}$ implies that if $e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q$ is an eigenfunction then $ie^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q$ is a (symmetry related) eigenfunction. It follows from (2.8) that if ρ acts as minus the identity on Q , then ρ acts as the identity on iQ . Thus we can assume without loss of generality that up to translational symmetry Q is ρ -invariant, that is Q has the form

$$Q = \begin{bmatrix} a & g & ic \\ g & b & ih \\ ic & ih & -a - b \end{bmatrix}$$

where $a, b, c, g, h \in \mathbf{R}$. Therefore we have proved

Lemma 2.2. *Up to symmetry eigenfunctions in $W_{\mathbf{k}}$ have the form*

$$e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q + c.c.$$

where Q is nonzero, ρ -invariant, and either even or odd.

Lemma 2.2 implies that typically eigenfunctions in $W_{\mathbf{k}}$ lie in one of the 2-dimensional subspaces $V_{\mathbf{k}}^+, V_{\mathbf{k}}^-$ of $W_{\mathbf{k}}^+, W_{\mathbf{k}}^-$ that have the form

$$\begin{aligned} V_{\mathbf{k}}^+ &= \{ze^{2\pi i\mathbf{k}\cdot\mathbf{x}}Q^+ : z \in \mathbf{C}\} \\ V_{\mathbf{k}}^- &= \{ze^{2\pi i\mathbf{k}\cdot\mathbf{x}}Q^- : z \in \mathbf{C}\} \end{aligned}$$

where

$$Q^+ = \begin{bmatrix} a & 0 & ic \\ 0 & b & 0 \\ ic & 0 & -a-b \end{bmatrix} \quad \text{and} \quad Q^- = \begin{bmatrix} 0 & g & 0 \\ g & 0 & hi \\ 0 & hi & 0 \end{bmatrix} \quad (2.9)$$

with the specific values $a, b, c, g, h \in \mathbf{R}$ being chosen by \mathbf{L} (cf. [10, §5.7]).

Moreover, since \mathbf{L} commutes with τ we can further split

$$V_{\mathbf{k}}^+ = V_{\mathbf{k}}^{++} \oplus V_{\mathbf{k}}^{+-} \quad \text{and} \quad V_{\mathbf{k}}^- = V_{\mathbf{k}}^{-+} \oplus V_{\mathbf{k}}^{--}$$

into subspaces on which τ acts trivially and by minus the identity, and each of these subspaces is \mathbf{L} -invariant. Since

$$\tau Q \tau = \begin{bmatrix} a & g & -ic \\ g & b & -ih \\ -ic & -ih & -a-b \end{bmatrix}$$

we see that $V_{\mathbf{k}}^{\pm\pm} = \{ze^{2\pi i\mathbf{k}\cdot\mathbf{x}}Q^{\pm\pm} : z \in \mathbf{C}\}$, where the matrices $Q^{\pm\pm}$ are as given in (2.1).

Finally, note that $\ker \mathbf{L}$ is invariant under the action of ξ . It follows that on the square lattice

$$\ker \mathbf{L} = V_{\mathbf{k}}^{\pm\pm} \oplus \xi(V_{\mathbf{k}}^{\pm\pm})$$

whereas on the hexagonal lattice

$$\ker \mathbf{L} = V_{\mathbf{k}}^{\pm\pm} \oplus \xi^2(V_{\mathbf{k}}^{\pm\pm}) \oplus \xi^4(V_{\mathbf{k}}^{\pm\pm})$$

thus verifying (2.2),(2.3) and completing the proof of Theorem (2.1). \square

Axial Subgroups

The scalar and pseudoscalar actions of $\mathbf{E}(2)$ on the eigenfunctions on the square and hexagonal lattices are computed in [2]. The results are given in Table 2 in terms of the coefficients z_j in (2.2) and (2.3).

\mathbf{D}_4	Action	\mathbf{D}_6	Action
$\mathbf{1}$	(z_1, z_2)	$\mathbf{1}$	(z_1, z_2, z_3)
ξ	(\bar{z}_2, z_1)	ξ	$(\bar{z}_2, \bar{z}_3, \bar{z}_1)$
ξ^2	(\bar{z}_1, \bar{z}_2)	ξ^2	(z_3, z_1, z_2)
ξ^3	(z_2, \bar{z}_1)	ξ^3	$(\bar{z}_1, \bar{z}_2, \bar{z}_3)$
κ	$\epsilon(z_1, \bar{z}_2)$	ξ^4	(z_2, z_3, z_1)
$\kappa\xi$	$\epsilon(\bar{z}_2, \bar{z}_1)$	ξ^5	$(\bar{z}_3, \bar{z}_1, \bar{z}_2)$
$\kappa\xi^2$	$\epsilon(\bar{z}_1, z_2)$	κ	$\epsilon(z_1, z_3, z_2)$
$\kappa\xi^3$	$\epsilon(z_2, z_1)$	$\kappa\xi$	$\epsilon(\bar{z}_2, \bar{z}_1, \bar{z}_3)$
		$\kappa\xi^2$	$\epsilon(z_3, z_2, z_1)$
		$\kappa\xi^3$	$\epsilon(\bar{z}_1, \bar{z}_3, \bar{z}_2)$
		$\kappa\xi^4$	$\epsilon(z_2, z_1, z_3)$
		$\kappa\xi^5$	$\epsilon(\bar{z}_3, \bar{z}_2, \bar{z}_1)$
$[\theta_1, \theta_2]$	$(e^{-2\pi i\theta_1} z_1, e^{-2\pi i\theta_2} z_2)$	$[\theta_1, \theta_2]$	$(e^{-2\pi i\theta_1} z_1, e^{-2\pi i\theta_2} z_2, e^{2\pi i(\theta_1+\theta_2)} z_3)$

Table 2: (Left) $\mathbf{D}_4 \dot{+} \mathbf{T}^2$ action on square lattice; (right) $\mathbf{D}_6 \dot{+} \mathbf{T}^2$ action on hexagonal lattice. Here $[\theta_1, \theta_2] = \theta_1 \ell_1 + \theta_2 \ell_2$ as in Table 1. For scalar representation $\epsilon = +1$; for pseudoscalar representation $\epsilon = -1$.

The axial subgroups for each of the four irreducible representations of $\Gamma_{\mathcal{L}}$ are given in Table 3, together with generators $(z_1, z_2) \in \mathbf{C}^2$ or $(z_1, z_2, z_3) \in \mathbf{C}^3$ (fixed vectors) of the corresponding 1-dimensional fixed-point subspaces (axial eigenspaces) in $\ker \mathbf{L}$, and descriptions of the associated patterns (planforms).

The results in Table 3 summarize known results for scalar actions with and without the midplane reflection [5, 12] and the less well known results for pseudoscalar actions [1, 2]. See also [10]. More precisely, on the hexagonal lattice, the scalar⁺ action is identical to the action studied in Bénard convection [4, 5] and the scalar⁻ action is identical to the one studied in Bénard convection with the midplane reflection [12]. The pseudoscalar⁺ action is identical to that studied in [1, 2], whereas the pseudoscalar⁻ action is again the same as the one in Bénard convection with the midplane reflection — but with different isotropy subgroups, as Figures 5 and 6 show.

Lattice	Planform	Axial Isotropy Subgroup	Fixed Vector
Scalar Representation ($\epsilon = +1$); $\tau = +1$			
Square	squares	$\mathbf{D}_4(\kappa, \xi) \oplus \mathbf{Z}_2(\tau)$	(1, 1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^2, \tau) \oplus \mathbf{O}(2)[\theta_2, \kappa]$	(1, 0)
Hexagonal	hexagons ⁺	$\mathbf{D}_6(\kappa, \xi) \oplus \mathbf{Z}_2(\tau)$	(1, 1, 1)
	hexagons ⁻	$\mathbf{D}_6(\kappa, \xi) \oplus \mathbf{Z}_2(\tau)$	(-1, -1, -1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^3, \tau) \oplus \mathbf{O}(2)[\theta_2, \kappa]$	(1, 0, 0)
Pseudoscalar Representation ($\epsilon = -1$); $\tau = +1$			
Square	squares	$\mathbf{D}_4(\kappa[\frac{1}{2}, \frac{1}{2}], \xi) \oplus \mathbf{Z}_2(\tau)$	(1, 1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^2[\frac{1}{2}, 0], \tau) \oplus \mathbf{O}(2)[\theta_2, \kappa[\frac{1}{2}, 0]]$	(1, 0)
Hexagonal	hexagons	$\mathbf{Z}_6(\xi) \oplus \mathbf{Z}_2(\tau)$	(1, 1, 1)
	triangles	$\mathbf{D}_3(\kappa\xi, \xi^2) \oplus \mathbf{Z}_2(\tau)$	(i, i, i)
	rectangles	$\mathbf{Z}_2^3(\kappa, \xi^3, \tau)$	(0, 1, -1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^3[\frac{1}{2}, 0], \tau) \oplus \mathbf{O}(2)[\theta_2, \kappa[\frac{1}{2}, 0]]$	(1, 0, 0)
Scalar Representation ($\epsilon = +1$); $\tau = -1$			
Square	squares	$\mathbf{D}_4(\kappa, \xi) \oplus \mathbf{Z}_2(\tau[\frac{1}{2}, \frac{1}{2}])$	(1, 1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^2, \tau[\frac{1}{2}, 0]) \oplus \mathbf{O}(2)[\theta_2, \kappa]$	(1, 0)
Hexagonal	hexagons	$\mathbf{D}_6(\kappa, \xi)$	(1, 1, 1)
	triangles	$\mathbf{D}_6(\kappa, \tau\xi)$	(i, i, i)
	rectangles	$\mathbf{Z}_2^3(\tau\kappa, \xi^3, \tau[0, \frac{1}{2}])$	(0, 1, -1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^3, \tau[\frac{1}{2}, 0]) \oplus \mathbf{O}(2)[\theta_2, \kappa]$	(1, 0, 0)
Pseudoscalar Representation ($\epsilon = -1$); $\tau = -1$			
Square	squares	$\mathbf{D}_4(\tau\kappa, \xi) \oplus \mathbf{Z}_2(\tau[\frac{1}{2}, \frac{1}{2}])$	(1, 1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^2[\frac{1}{2}, 0], \tau[\frac{1}{2}, 0]) \oplus \mathbf{O}(2)[\theta_2, \kappa[\frac{1}{2}, 0]]$	(1, 0)
Hexagonal	hexagons	$\mathbf{D}_6(\tau\kappa, \xi)$	(1, 1, 1)
	triangles	$\mathbf{D}_6(\tau\kappa, \tau\xi)$	(i, i, i)
	rectangles	$\mathbf{Z}_2^3(\kappa, \xi^3, \tau[0, \frac{1}{2}])$	(0, 1, -1)
	rolls	$\mathbf{Z}_2^2(\kappa\xi^3[\frac{1}{2}, 0], \tau[\frac{1}{2}, 0]) \oplus \mathbf{O}(2)[\theta_2, \kappa[\frac{1}{2}, 0]]$	(1, 0, 0)

Table 3: Summary of axial subgroups. On the hexagonal lattice in the scalar case with $\tau = +1$ the points (1, 1, 1) and (-1, -1, -1) have the same isotropy subgroup ($\mathbf{D}_6(\kappa, \xi) \oplus \mathbf{Z}_2(\tau)$) — but are not conjugate by any element of $\Gamma_{\mathcal{L}}$. Therefore, the associated eigenfunctions generate different planforms.

The Planforms

We now consider 2-dimensional patterns by disregarding the z -coordinate in \mathbf{x} (but not in Q) and restricting attention to equilibrium states that are periodic with respect to a square or hexagonal lattice in the xy -plane.

To visualize the patterns of bifurcating solutions we assume a layer of liquid crystal material in the xy -plane that to first order has the form

$$Q(\mathbf{x}) = Q_0 + \varepsilon E(\mathbf{x})$$

where E is an axial eigenfunction, ε is small, and Q_0 is either isotropic ($\eta = -1$) or homeotropic ($\eta = +1$). At each point (x, y) we choose the eigendirection corresponding to the largest eigenvalue of the symmetric 3×3 matrix $Q(\mathbf{x})$ at $\mathbf{x} = (x, y)$ and we plot only the x, y components of that line field. In this picture, a line element that degenerates to a point corresponds to a vertical eigendirection, so the initial solution looks like an array of points.

Suppose that Q_0 is homeotropic. Then in our simulations no pattern will appear in bifurcations for which $Q(\mathbf{x})$ is fixed by the action of τ . For, if $E(\mathbf{x}) \in V_{\mathbf{k}}^{++}$ or $V_{\mathbf{k}}^{-+}$ then

$$Q(\mathbf{x}) = \begin{bmatrix} A & 0 \\ 0 & b \end{bmatrix}$$

where A is a 2×2 block and b is a scalar. Since b is close to 2 (the largest eigenvalue of Q_0) it is also the largest eigenvalue for $Q(\mathbf{x})$ for ε small. Hence, the leading eigendirection (corresponding to the largest eigenvalue) is always vertical and no patterns appear that are determined by changes in eigendirection. However, since variation in the vertical eigenvalue of $Q(\mathbf{x})$ represents variation in the propensity of molecules to align vertically it is plausible that indistinct patterns could nevertheless be observed in practice.

In Figures 3 and 4 we plot solutions corresponding to scalar and pseudoscalar square lattice patterns. In Figures 5–10 we plot those for a hexagonal lattice. Observe the dislocations that occur where the leading eigendirection changes discontinuously. The two competing directions are necessarily orthogonal in \mathbf{R}^3 .

3 Free Energy Models

These results imply that for a planar liquid crystal there are four types of steady-state bifurcations, scalar, pseudoscalar and $\tau = \pm 1$ of each type, that

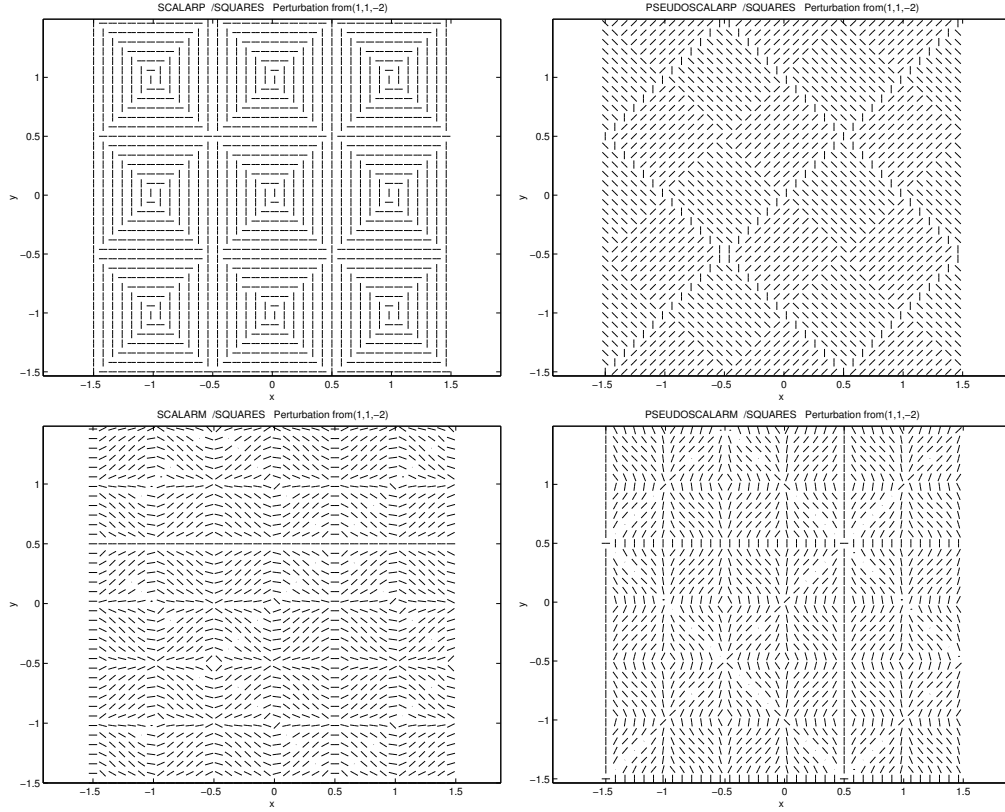


Figure 3: Square lattice bifurcations from isotropic ($\eta < 0$) liquid crystal to square patterns: (upper left) scalar $\tau = +1$; (upper right) pseudoscalar $\tau = +1$; (lower left) scalar $\tau = -1$; (lower right) pseudoscalar $\tau = -1$. Corresponding rolls patterns can be found in Figures 1 and 7-10.

can occur from a spatially homogeneous equilibrium to spatially periodic equilibria. Whichever bifurcation occurs, then generically all of the planforms that we listed in the relevant section of Table 3 will be solutions. We have not discussed the difficult issue of stability of these solutions since these are model dependent results, whereas the classification of equilibria that we have given is independent of the model.

What remains is to complete a linear calculation to determine when a steady-state bifurcation occurs and whether it is scalar or pseudoscalar. The outline of such a calculation goes as follows. We first compute a *dispersion curve* for both scalar and pseudoscalar eigenfunctions. That is, for each wave

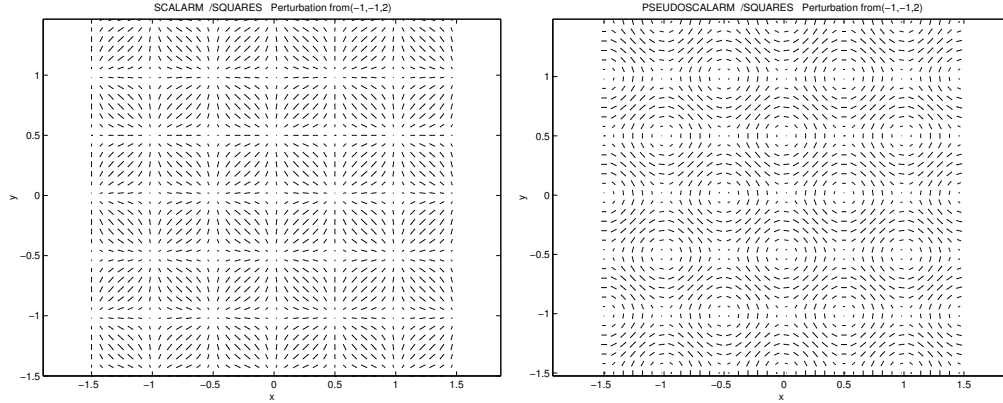


Figure 4: Square lattice bifurcations from homeotropic ($\eta > 0$) to squares with $\tau = -1$: (left) scalar; (right) pseudoscalar. Corresponding rolls patterns can be found in Figures 5-6.

length $k = |\mathbf{k}|$ we determine the first value λ_k of the bifurcation parameter λ where \mathbf{L} has a nonzero kernel. The curve (k, λ_k) is called the dispersion curve. We then find the minimum value $\lambda_* = \lambda_{k_*}$ on the dispersion curve; the corresponding wave length k_* is the *critical* wave length. We expect the first instability of the spatially homogeneous equilibrium to occur at the value λ_* of the bifurcation parameter. A bifurcating branch can consist of stable solutions only if the branch emanates from the first bifurcation (at λ_*).

As an illustration we now carry out these calculations for a Landau – de Gennes type model with appropriate planar symmetry. Related calculations were carried out for bifurcation from the 3-dimensional isotropic phase in [13]. In this model we show that there are bifurcations corresponding to each of the four irreducible representations of $\Gamma_{\mathcal{L}}$, and which of them occurs first depends on the action of τ .

Dispersion Curves for a 2-Dimensional Landau – de Gennes Model

The free energy F is expressed as an integral per unit volume of a *free energy density* \mathcal{F} which has two principal components \mathcal{F}_0 and \mathcal{F}_d corresponding to *bulk terms* and *deformation terms* respectively: we write F accordingly as $F = F_0 + F_d$. For a system in 3 dimensions these typically (see *e.g.* [13])

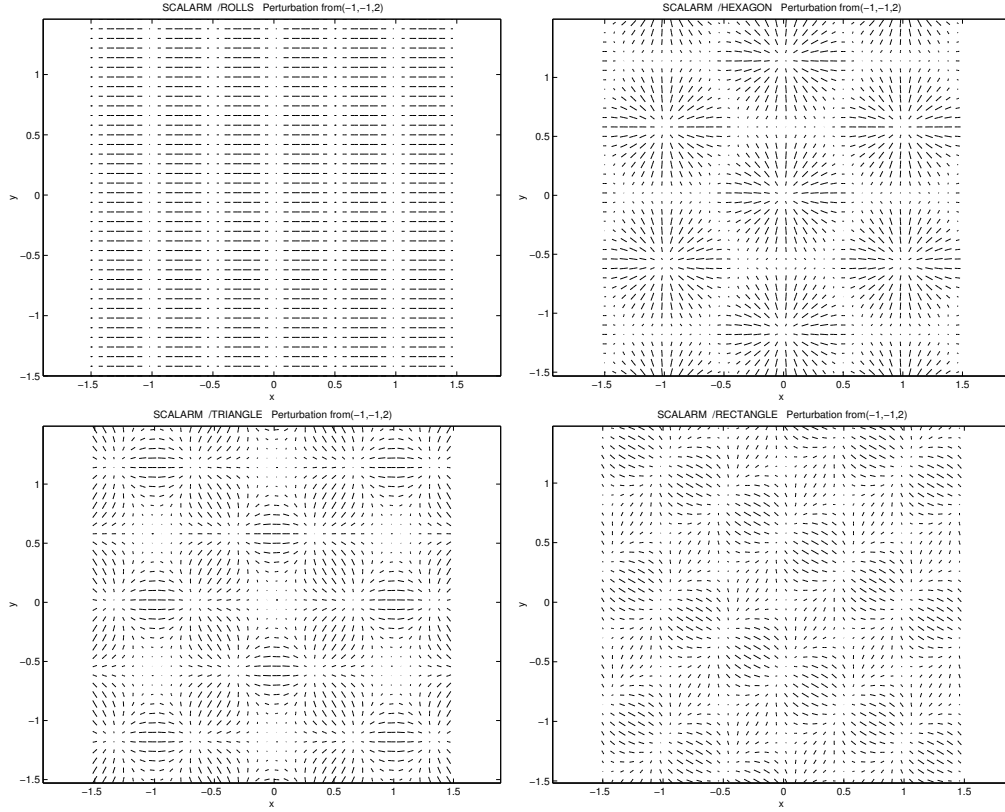


Figure 5: Hexagonal lattice bifurcations from homeotropic ($\eta > 0$) with scalar $\tau = -1$ representation: (upper left) rolls; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

take the form

$$\begin{aligned}\mathcal{F}_0(Q) &= \frac{1}{2}\lambda|Q|^2 - \frac{1}{3}B \operatorname{tr} Q^3 + \frac{1}{4}C|Q|^4 \\ \mathcal{F}_d(Q) &= c_1|\nabla Q|^2 + c_2|\nabla \cdot Q|^2 + c_3|Q \cdot \nabla \wedge Q|\end{aligned}$$

respectively, where $|R|^2$ denotes the sum of the squares of the coefficients of the tensor R . The expression for \mathcal{F}_0 represents the simplest $\mathbf{SO}(3)$ -invariant function on V exhibiting nontrivial interaction of local minima close to $Q = 0$, while \mathcal{F}_d consists of those $\mathbf{SO}(3)$ -invariant terms of at most order 2 in spatial first derivatives (the chiral term $|Q \cdot \nabla \wedge Q|$ is not reflection-invariant).

For a 2-dimensional problem this choice of free energy function is not fully appropriate: the relevant symmetry group is now $\Gamma = \mathbf{E}(2) \times \mathbf{Z}_2(\tau)$.

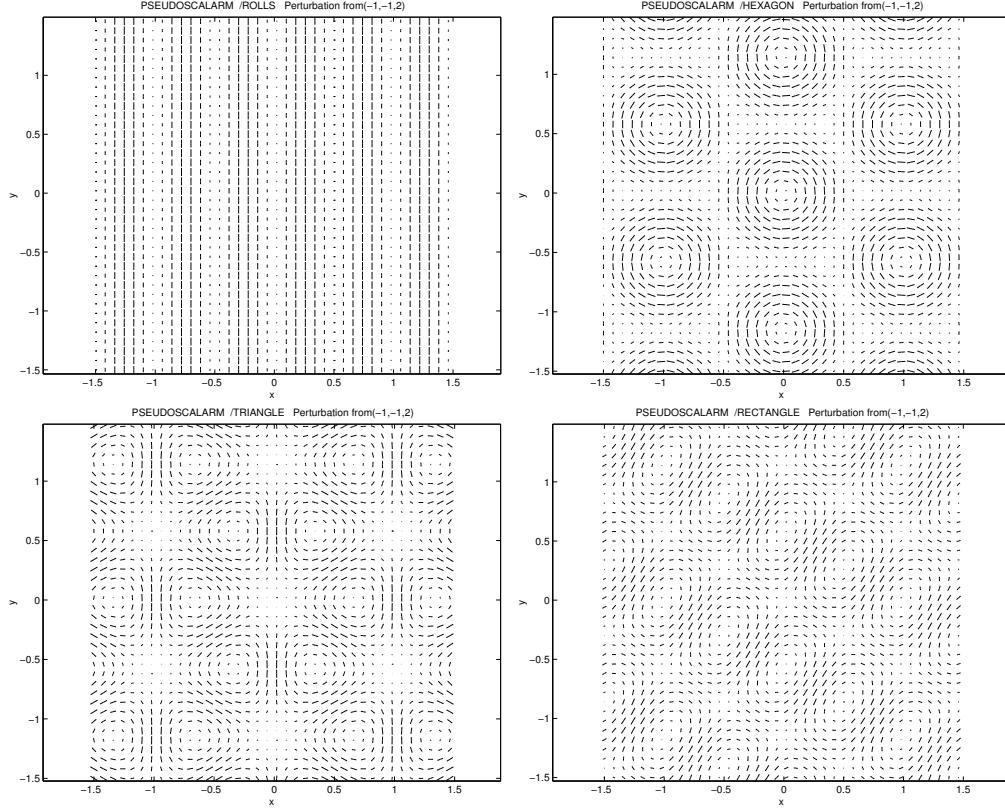


Figure 6: Hexagonal lattice bifurcations from homeotropic ($\eta > 0$) with pseudoscalar $\tau = -1$ representation: (upper left) rolls; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

Consequently a wider range of terms can appear in \mathcal{F}_0 , while the $|Q \cdot \nabla \wedge Q|$ term will no longer appear in \mathcal{F}_d .

We are interested in planforms that bifurcate from either the bulk homeotropic state or isotropic state, represented by Q_0 with $\eta > 0$ or $\eta < 0$ respectively. An example of a bulk term with $\mathbf{E}(2) \times \mathbf{Z}_2(\tau)$ invariance is $(Q_0 \cdot Q)^2$, and a candidate for a deformation term to replace the chiral term is $|\Delta Q|^2$ representing longer range interactions of molecules. Accordingly we consider a free energy density $\mathcal{F} = \mathcal{F}_0 + \mathcal{F}_d$ where now

$$\begin{aligned}\mathcal{F}_0(Q) &= \frac{1}{2}\lambda|Q|^2 - \frac{1}{3}B \operatorname{tr} Q^3 + \frac{1}{4}C|Q|^4 + \frac{1}{12}D(Q_0 \cdot Q)^2 \\ \mathcal{F}_d(Q) &= c_1|\nabla Q|^2 + c_2|\nabla \cdot Q|^2 + c_4|\Delta Q|^2.\end{aligned}$$

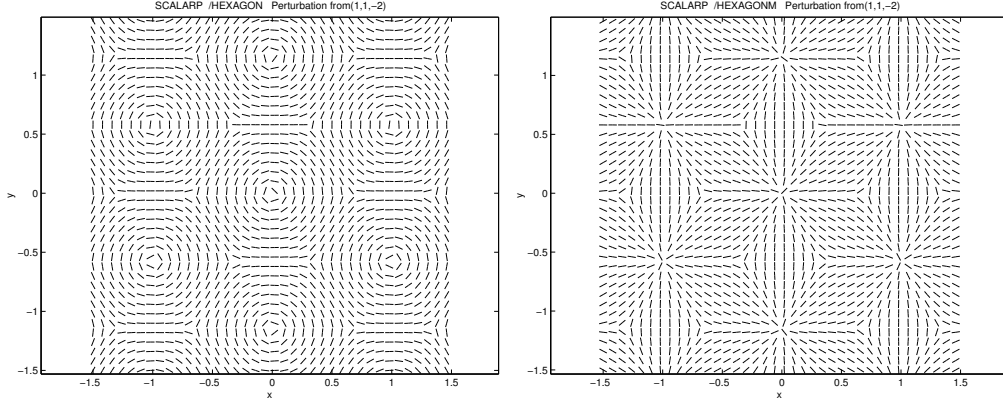


Figure 7: Hexagonal lattice bifurcations from isotropic ($\eta < 0$) with scalar $\tau = +1$ representation: rolls in Figure 1; (left) hexagons⁺; (right) hexagons⁻.

Equilibrium states are critical points of F , and for \mathcal{F}_0 we have

$$d\mathcal{F}_0(Q)R = \lambda Q \cdot R - BQ^2 \cdot R + C|Q|^2 Q \cdot R + \frac{1}{6}D(Q_0 \cdot Q)(Q_0 \cdot R)$$

for arbitrary 3×3 real symmetric matrices Q, R ; thus restricted to Q with trace zero we have $d\mathcal{F}_0(Q) = 0$ when

$$\lambda Q - B(Q^2 - \frac{1}{3}|Q|^2 I) + C|Q|^2 Q + \frac{1}{6}D(Q_0 \cdot Q)Q_0 = 0$$

and we easily verify the following

$$d\mathcal{F}_0(Q_0) = 0 \iff \lambda - B\eta + (6C + D)\eta^2 = 0. \quad (3.1)$$

Observe that $dF(Q)R = 0$ automatically for any spatially-periodic state R with zero mean, as the integral of an expression linear in R or its derivatives remains bounded as the volume tends to infinity. Therefore (3.1) is the condition for Q_0 to be an equilibrium state in our free energy model.

To study stability of the state Q_0 we evaluate the second derivative of the free energy at Q_0 . For $R \in V$ we find

$$d^2 F_0(Q_0)R^2 = \lambda|R|^2 - 2BQ_0 \cdot R^2 + C(2(Q_0 \cdot R)^2 + |Q_0|^2|R|^2) + \frac{1}{6}D(Q_0 \cdot R)^2$$

and (integrating over unit area)

$$d^2 F_d(Q_0)R^2 = c_1 \int |\nabla R|^2 + c_2 \int |\nabla \cdot R|^2 + c_4 \int |\Delta R|^2$$

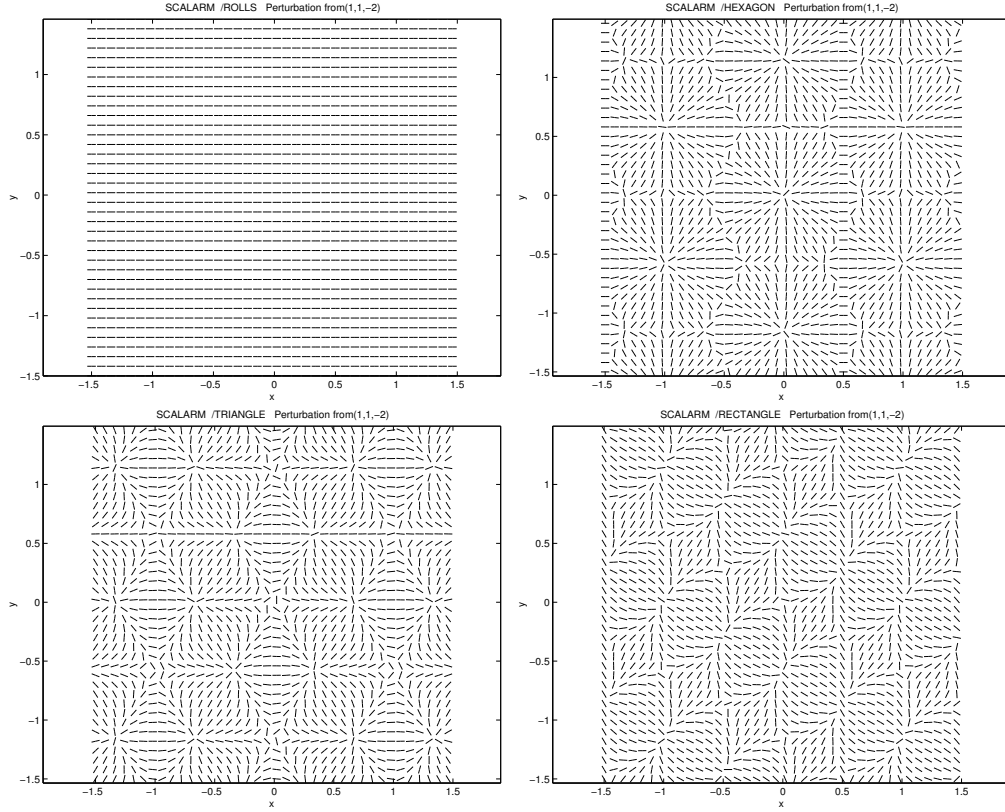


Figure 8: Hexagonal lattice bifurcations from isotropic ($\eta < 0$) with scalar $\tau = -1$ representation: (upper left) rolls; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

since Q_0 is spatially constant and terms linear in R integrate to zero.

We have already seen from Theorem 2.1 that the $\mathbf{E}(2) \times \mathbf{Z}_2(\tau)$ invariance of the free energy implies that generically the eigenfunctions of $d^2F(Q_0)$ on the space of \mathcal{L} -periodic matrix functions are linear combinations of functions belonging to one of the four subspaces $V_{\mathbf{k}}^{\pm\pm}$ and their rotations under $\frac{\pi}{2}$ (square lattice) or $\pm\frac{2\pi}{3}$ (hexagonal lattice). We next seek dispersion relations for each of the spaces $V_{\mathbf{k}}^{\pm\pm}$ in turn. When $R = e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q + c.c.$ it is easy to check that

$$\frac{1}{4\pi^2} \int |\nabla R|^2 = 2k^2|Q|^2, \quad \frac{1}{4\pi^2} \int |\nabla \cdot R|^2 = 2|Q\mathbf{k}|^2, \quad \frac{1}{16\pi^4} \int |\Delta R|^2 = 2k^4|Q|^2$$

where $k = |\mathbf{k}|$. Without loss of generality we can take $\mathbf{k} = (k, 0, 0)$ and

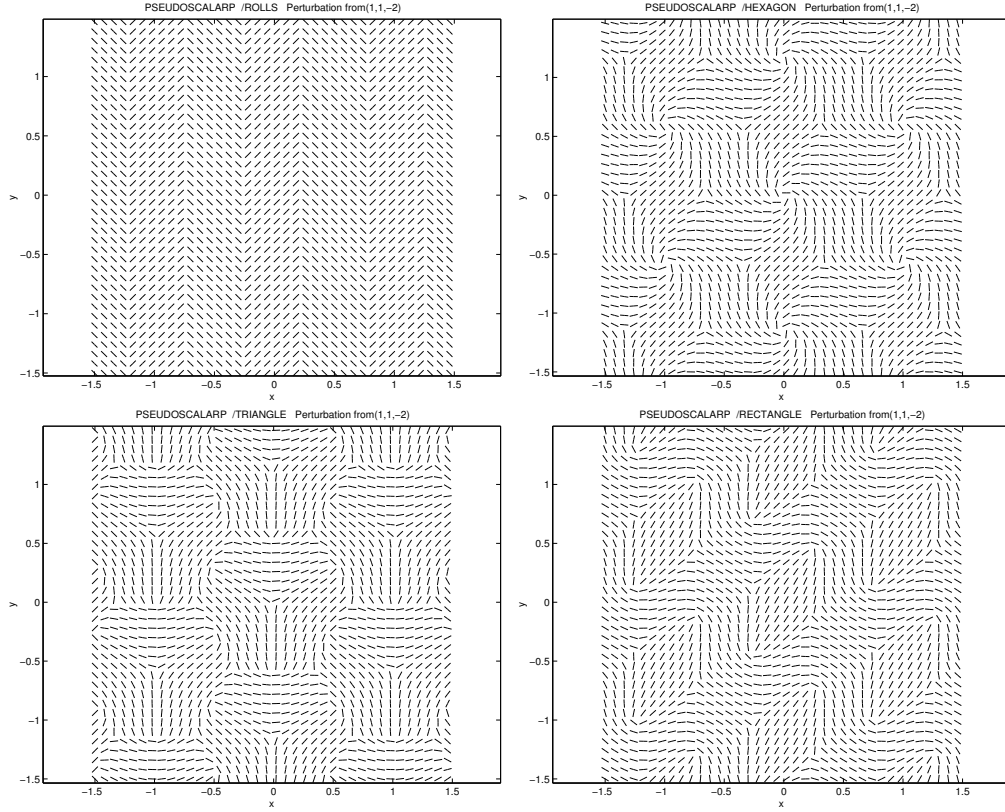


Figure 9: Hexagonal lattice bifurcations from isotropic ($\eta < 0$) with pseudoscalar $\tau = +1$ representation: (upper left) rolls; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

then after rescaling k by a factor of 2π the evaluations of $d^2F_0(Q_0)R^2$ and $d^2F_d(Q_0)R^2$ are given in Table 4.

If we normalize by choosing D so that (3.1) is satisfied by $\eta = 1$ (corresponding to homeotropy) then we find the conditions for a zero eigenvalue in each of the last three (1-dimensional) eigenspaces are respectively

$$\begin{aligned}
 \lambda - B + 6C + (c_1 + \frac{1}{2}c_2)k^2 + c_4k^4 &= 0 \\
 \lambda + 2B + 6C + (c_1 + \frac{1}{2}c_2)k^2 + c_4k^4 &= 0 \\
 \lambda - B + 6C + c_1k^2 + c_4k^4 &= 0
 \end{aligned} \tag{3.2}$$

with the analogous expressions for $\eta = -1$ (bifurcation from 2-dimensional isotropy) obtained by merely reversing the sign of B in these equations.

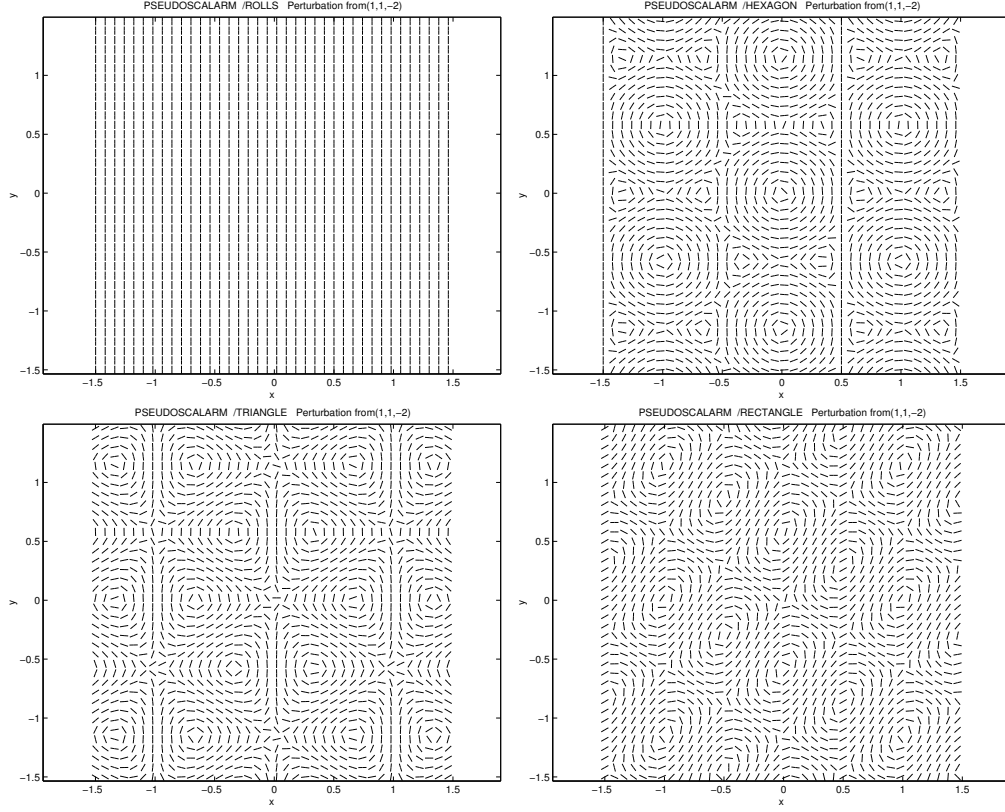


Figure 10: Hexagonal lattice bifurcations from isotropic ($\eta < 0$) with pseudoscalar $\tau = 1$ representation: (upper left) rolls; (upper right) hexagons; (lower left) triangles; (lower right) rectangles.

Stationary values of λ as a function of k occur where

$$k^2 = -(c_1 + \frac{1}{2}c_2)/2c_4$$

for $V_{\mathbf{k}}^{+-}$ and $V_{\mathbf{k}}^{-+}$, or

$$k^2 = -c_1/2c_4$$

for $V_{\mathbf{k}}^{--}$, giving values

$$\lambda = \begin{cases} B - 6C + (c_1 + \frac{1}{2}c_2)^2/4c_4 & \text{for } V_{\mathbf{k}}^{+-} \\ -2B - 6C + (c_1 + \frac{1}{2}c_2)^2/4c_4 & \text{for } V_{\mathbf{k}}^{-+} \\ B - 6C + c_1^2/4c_4 & \text{for } V_{\mathbf{k}}^{--} \end{cases} \quad (3.3)$$

R	$d^2 F_0(Q_0)R^2$	$d^2 F_d(Q_0)R^2$
$V_{\mathbf{k}}^{++}$	$\lambda(a^2 + b^2 - 2ab)$ $-B(a^2 + b^2 + 10ab)\eta$ $+6C(7(a^2 + b^2) + 10ab)\eta^2$	$2k^2(c_2 a^2 +$ $(a^2 + b^2 + (a + b)^2)(c_1 + c_4 k^2))$
$V_{\mathbf{k}}^{+-}$	$4(\lambda - B\eta + 6C\eta^2)$ $= -4D\eta^2$ by (3.1)	$(4c_1 + 2c_2)k^2 + 4c_4 k^4$
$V_{\mathbf{k}}^{-+}$	$4(\lambda + 2B\eta + 6C\eta^2)$	$(4c_1 + 2c_2)k^2 + 4c_4 k^4$
$V_{\mathbf{k}}^{--}$	$4(\lambda - B\eta + 6C\eta^2)$ $= -4D\eta^2$	$4c_1 k^2 + 4c_4 k^4$

Table 4: Computation of $d^2 F(Q_0)R^2$.

Finally, if $R \in V_{\mathbf{k}}^{++}$ then the matrix for $d^2 F_0(Q_0)R^2$ as a quadratic form in a, b is

$$\begin{bmatrix} \lambda - B + 42C & -\lambda - 5B + 30C \\ -\lambda - 5B + 30C & \lambda - B + 42C \end{bmatrix}$$

and for $d^2 F_d(Q_0)R^2$ is

$$\begin{bmatrix} 4c_1 k^2 + 2c_2 k^2 + 4c_4 k^4 & 2c_1 k^2 + 2c_4 k^4 \\ 2c_1 k^2 + 2c_4 k^4 & 4c_1 k^2 + 4c_4 k^4 \end{bmatrix}$$

and so $d^2 F(Q_0)|V_{\mathbf{k}}^{++}$ has a nontrivial kernel when the determinant of the sum of these two matrices vanishes.

With $c_2 = 0$ (that is, in physical terms, with no energy cost to the molecules for ‘splay’) the algebra simplifies to yield the dispersion relation

$$\lambda = -2B - 6C + \frac{c_1^2}{4c_4}. \quad (3.4)$$

From (3.2) and (3.4) we therefore see that with $c_2 = 0$ the values of λ for $V_{\mathbf{k}}^{\pm\pm}$ depend only on the second \pm , that is on whether bifurcating solutions have vertical reflection symmetry ($\tau = +1$) or not ($\tau = -1$) and are the same for the scalar and the pseudoscalar representations. Moreover, as λ decreases, the first bifurcation from the homeotropic state ($\eta > 0$) has $\tau = -1$ while the first bifurcation from the isotropic state ($\eta < 0$) has $\tau = +1$. These statements remain true for sufficiently small $|c_2|$.

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