Bifurcation and Planar Pattern Formation for a Liquid Crystal

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Abstract. We consider the Landau – de Gennes model for the free energy of a liquid crystal, and discuss the geometry of its equilibrium set (critical points) for spatially uniform states in the absence of external fields. Using equivariant bifurcation theory we classify (on the basis of symmetry considerations independent of the model) square and hexagonally periodic patterns that can arise when a homeotropic nematic state becomes unstable, perhaps as a consequence of an applied magnetic or electric field.

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 field of symmetric 3×3 tensors $Q(\mathbf{x})$, $\mathbf{x} \in \mathbf{R}^3$ with trace $\mathrm{tr}(Q) = 0$ (the tensor order parameter) [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].

Symmetries in the order parameter. The complex linear space V of traceless symmetric 3×3 matrices Q is 5-dimensional over ${\bf C}$ with unitary basis

$$\frac{1}{2}\{M_0, M_{\pm 1}, M_{\pm 2}\}$$

where

$$M_0 = \sqrt{\frac{2}{3}} \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad M_{\pm 1} = \begin{pmatrix} 0 & 0 & \pm 1 \\ 0 & 0 & i \\ \pm 1 & i & 0 \end{pmatrix} \quad M_{\pm 2} = \begin{pmatrix} 1 & \pm i & 0 \\ \pm i & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

A state (phase) of the liquid crystal in \mathbb{R}^3 is given by the real part of a map $Q: \mathbb{R}^3 \to V$. At each point \mathbf{x} in space the rod-like molecule is assumed to align along the eigendirection corresponding to the largest eigenvalue of $Q(\mathbf{x})$.

The action of rigid motions in \mathbf{R}^3 on a state is defined as follows. Let $\gamma \in \mathbf{O}(3)$ and let $T_{\mathbf{v}}$ be translation by $\mathbf{y} \in \mathbf{R}^3$. Then

$$(T_{\mathbf{y}}Q)(\mathbf{x}) = Q(\mathbf{x} - \mathbf{y}) (\gamma \cdot Q)(\mathbf{x}) = \gamma Q(\gamma^{-1}\mathbf{x})\gamma^{-1}.$$
(1.1)

That is, translations just translate $Q(\mathbf{x})$ while rotations and reflections act simultaneously by rigid motion on the domain of $Q(\mathbf{x})$ and by conjugacy in the range.

THE FREE ENERGY FORMULATION. Equilibrium states of the liquid crystal (ignoring boundary effects which in physical situations do play a crucial role) are taken to be critical points of a smooth real-valued free energy functional

$$F(Q) = \frac{1}{\text{Vol}} \int \mathcal{F}(Q(\mathbf{x})) d\mathbf{x}$$

defined for real Q, where the free energy density \mathcal{F} is invariant under the Euclidean action (1.1). A standard free energy is given by the Landau-de Gennes model [9]

$$\mathcal{F}(Q) = \frac{1}{2}\tau \operatorname{tr}(Q^2) - \frac{1}{3}B\operatorname{tr}(Q^3) + \frac{1}{4}C(\operatorname{tr}(Q^2))^2 + C_1|\nabla Q|^2 + C_2|\nabla \cdot Q|^2 - 2DQ \cdot \nabla \wedge Q$$
(1.2)

where B, C, C_1, C_2, D are constants of the material and τ represents deviation from a critical temperature. The notation here is

$$|\nabla Q|^2 = \sum_{i,j} |\nabla Q_{ij}|^2,$$

$$|\nabla \cdot Q|^2 = \sum_j |\nabla \cdot Q_j|^2,$$

$$Q \cdot \nabla \wedge Q = \sum_j Q_j \cdot \nabla \wedge Q_j$$

where Q_j is the jth column of Q. This is a general O(3)-invariant function of degree at most four in Q [8] and at most two in the first-order spatial derivatives of Q.

In this paper we discuss aspects of bifurcations of spatially homogeneous states (Section 2) and spatially periodic nematic liquid crystal states (Section 3).

2. Spatially uniform equilibrium states

For a spatially uniform state the derivatives of Q are zero and we are reduced to considering critical points of $F:V\to\mathbf{R}$ restricted to real matrices. Symmetry implies that every equilibrium state corresponds to a group orbit of equilibria. Since every symmetric matrix can be diagonalized by an orthogonal matrix, it follows that every group orbit of equilibria contains a diagonal trace zero matrix. Thus, to study bifurcation of equilibria, we can restrict attention to the 2-dimensional

au range	equilibria	stability
$\tau > \tau_0$	Q = 0	stable
$\tau_0 > \tau > 0$	Q = 0	stable
	$Q=Q_i:=\eta_iQ(0,1)$	i = 1 stable
	$\eta_1 < \eta_2 < 0$	
	$Q = \widetilde{Q}_i := -\frac{1}{2}\eta_i Q(\pm\sqrt{3}, 1)$	i = 2 unstable
$0 > \tau$	Q = 0	unstable
	$Q = Q_1, \widetilde{Q}_1, \eta_1 < 0$	stable
	$Q = Q_2, \widetilde{Q}_2, \eta_2 > 0$	unstable

TABLE 1. Equilibria as a function of τ where $\tau_0 = \frac{B^2}{24C}$ and $Q(\rho, \eta)$ is defined in (2.1).

space of diagonal traceless matrices as in [8, XV, $\S6$]. We express such Q in the form

$$Q = Q(\rho, \eta) = -\eta \sqrt{\frac{3}{2}} M_0 + \rho \frac{\sqrt{3}}{2} (M_2 + M_{-2})$$
 (2.1)

since, in these coordinates,

$$tr(Q^2) = 6(\rho^2 + \eta^2) \tag{2.2}$$

$$\operatorname{tr}(Q^3) = 6\eta(3\rho^2 - \eta^2) = 6\operatorname{Im}(\rho + i\eta)^3.$$
 (2.3)

The function F restricted to the space $U \cong \mathbf{R}^2$ of matrices (2.1) is invariant with respect to the action of \mathbf{D}_3 in the (ρ, η) -plane generated by rotation by $2\pi/3$ and reflection in the η -axis. Thus

Proposition 2.1. Every nonzero critical orbit of F meets U in a \mathbf{D}_3 -symmetric configuration.

By first considering the restriction of F to the η -axis and then exploiting symmetry it is straightforward to deduce the description of equilibria for the system $\dot{Q} = -\operatorname{grad} F(Q)$ on U given in Table 1.

As τ decreases through $\tau_0=\frac{B^2}{24C}$ there are simultaneous saddle-node creations of pairs of equilibria at $(\rho,\eta)=(0,\eta_0)$ and $-\frac{1}{2}\eta_0(\pm\sqrt{3},1)$ where $\eta_0=-2\tau_0/B$; subsequently the innermost equilibria approach the origin and coalesce at a degenerate critical point there as τ decreases to 0, emerging on the other side as τ becomes negative. See Figures 1 and 2.

The physical interpretation is that for $\tau > \tau_0$ the only stable phase is isotropic (Q=0) while for $\tau < \tau_0$ there are further stable nematic phases with molecules aligned in a particular direction: any one alignment has the same free energy as any other. The isotropic phase loses stability when τ becomes negative. This familiar transition is described for example in [15].

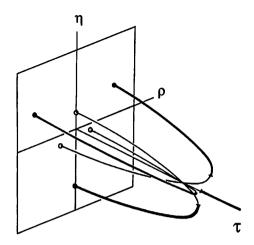


FIGURE 1. Bifurcation diagram for critical points of $\operatorname{grad} F$ on U.

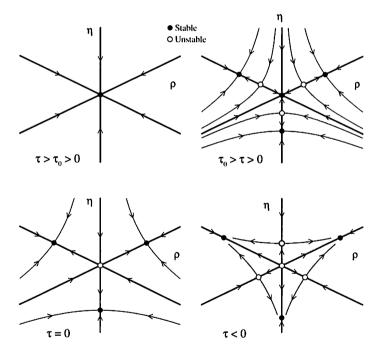


Figure 2. Schematic phase portraits for $\dot{Q} = -\operatorname{grad} F(Q)$.

REMARKS ON EQUILIBRIA IN A SHEAR FLOW. In the presence of a constant shear flow the system loses its O(3) symmetry and most of the equilibria disappear.

However, some do remain, along with a variety of interesting dynamical phenomena including Hopf bifurcations, Takens-Bogdanov bifurcation and period-doubling that come into play as τ decreases [14, 16]. A rigorous geometric analysis of some of these phenomena is given in [3], where it is shown that all equilibria are invariant under reflection in the plane of the shear flow, with the curious exception of a continuum (ellipse) of out-of-plane equilibria that arise with codimension 1. This non-generic behavior casts doubt on the robustness (structural stability) of the Landau-de Gennes model in the presence of a shear flow.

3. Spatially periodic equilibrium states

Suppose a spatially uniform equilibrium Q_0 loses stability to a spatially periodic state. In this section we use group representation theory (following [8, 7, 4]) to extract information about nonlinear behavior at bifurcation that is independent of the model.

Specifically, we consider local bifurcation from a planar layer of a homeotropic nematic liquid crystal Q_0 that is assumed to have constant alignment in the vertical direction to one that has spatially varying alignment in the planar directions. We assume that the new states are spatially periodic with respect to some planar lattice. The symmetry group for this discussion is the planar Euclidean group rather than the Euclidean group in three dimensions, as in the previous sections.

The fact that liquid crystals can display spatial periodicity with respect to a planar lattice is well known by experiment. For example, Figure 3 illustrates a so-called prewavy pattern [13, 10] while Figure 4 shows two types of chevron [10]. (We are grateful to the authors of the abstracts [11],[12] for these pictures.) Several striking photographs of periodic patterns can also be found in [6].

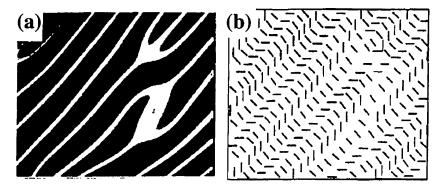


FIGURE 3. Prewavy pattern seen with crossed polarizers (a), and corresponding director field (b). The scale bar is $200\mu m$. (Courtesy J.-H.Huh.)

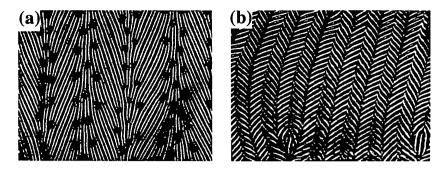


FIGURE 4. Two types of chevrons: (a) defect-mediated, (b) defect-free. The scale bar is $200\mu m$. (Courtesy J.-H.Huh.)

Linear Theory

Let L denote the linearization of the governing system of PDEs at Q_0 (for the free energy model we have $\mathsf{L} = D^2 F(Q_0)$). Bifurcation occurs at parameter values where L has a nonzero kernel. Planar translation symmetry implies that eigenfunctions of L have the plane wave form

$$e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q + c.c. \tag{3.1}$$

where $Q \in V$ is a constant matrix and $\mathbf{k} \in \mathbf{R}^2$ is a wave vector. Let

$$W_{\mathbf{k}} = \{e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q + c.c. : Q \in V\}$$
(3.2)

be the ten-dimensional L-invariant real linear subspace consisting of such functions. Rotations and reflections $\gamma \in \mathbf{O}(2)$ act on $W_{\mathbf{k}}$ by

$$\gamma(e^{2\pi i \mathbf{k} \cdot \mathbf{x}} Q) = e^{2\pi i (\gamma \mathbf{k}) \cdot \mathbf{x}} \gamma Q \gamma^{-1}. \tag{3.3}$$

Rotation symmetry implies that ker L is infinite-dimensional, since it contains all possible rotations of the eigenfunction (3.1). Restricting to planar lattices (which restricts the allowable rotations to a finite number) typically makes the kernel finite-dimensional.

When looking for nullvectors we can assume, after rotation, that $\mathbf{k} = k(1,0,0)$ and that nullvectors of L are in $W_{\mathbf{k}}$. Bosch Vivancos, Chossat, and Melbourne [1] observed that reflection symmetries can further decompose $W_{\mathbf{k}}$ into two L-invariant subspaces. To see why, consider the reflection

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

Note that the action (3.3) of κ on $W_{\mathbf{k}}$ (dropping the +c.c.) is

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

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

$$W_{\mathbf{k}} = W_{\mathbf{k}}^+ \oplus W_{\mathbf{k}}^- \tag{3.4}$$

where κ acts trivially on $W_{\mathbf{k}}^+$ and as minus the identity on $W_{\mathbf{k}}^-$. 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.

To determine the form of the scalar and pseudoscalar matrices (that is, those matrices Q^+, Q^- appearing in $W_{\mathbf{k}}^+$ and $W_{\mathbf{k}}^-$ respectively), we need to compute the effect of conjugacy by $\kappa \in \mathbf{O}(3)$ on V. The subspace of V where κ acts as the identity is

$$V^+ = \text{span}\{M_0, M_1 - M_{-1}, M_2 + M_{-2}\}$$

and the space where κ acts as minus the identity is

$$V^{-} = \text{span}\{M_1 + M_{-1}, M_2 - M_{-2}\}.$$

A further simplification can be made. Consider $R_{\pi} \in \mathbf{O}(3)$ given by $(x, y, z) \mapsto (-x, -y, z)$. Since (dropping the +c.c.)

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

the associated action of R_{π} on V is related to the conjugacy action by

$$R_{\pi}(Q) = \overline{R_{\pi} \cdot Q}.$$

Since L commutes with R_{π} and $R_{\pi}^2 = 1$, the subspaces of the kernel of L where $R_{\pi}(Q) = Q$ and $R_{\pi}(Q) = -Q$ are L-invariant. Therefore, we can assume that Q is in one of these two subspaces. Note that translation by $\ell = \frac{1}{4}\mathbf{k}/k^2$ implies that if $v(\mathbf{x},Q) = e^{2\pi i \mathbf{k} \cdot \mathbf{x}}Q$ is an eigenfunction then $iv(\mathbf{x},Q)$ is a (symmetry related) eigenfunction. It follows from (3) that if R_{π} acts as minus the identity on Q, then R_{π} acts as the identity on iQ. Thus we can assume without loss of generality that

$$R_{\pi}(Q) = \overline{Q},$$

that is, Q is R_{π} -invariant. Therefore we have proved

Lemma 3.1. Generically eigenfunctions in $V_{\mathbf{k}}$ have the form $e^{2\pi i \mathbf{k} \cdot x} Q + c.c.$ where Q is nonzero, R_{π} -invariant, and either even or odd.

Lemma 3.1 implies that typically eigenspaces are two-dimensional subspaces of $W_{\bf k}^+$ or $W_{\bf k}^-$ and have the form

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

where Q^+ and Q^- are R_{π} -invariant. We check easily that

$$R_{\pi} \cdot M_0 = \overline{M}_0$$
, $R_{\pi} \cdot M_{\pm 1} = M_{\mp 1}$, $R_{\pi} \cdot M_{\pm 2} = M_{\mp 2}$

and so by R_{π} -invariance we may assume that

$$Q^{+} = aM_{0} + b(M_{2} + M_{-2}) + ic(M_{1} - M_{-1}), \quad a, b, c \in \mathbf{R}$$

$$Q^{-} = g(M_{1} + M_{-1}) + ih(M_{2} - M_{-2}), \quad g, h \in \mathbf{R}$$
(3.5)

where $a, b, c, g, h \in \mathbf{R}$ are specific values chosen by L (cf. [7, §5.7]).

The Planforms

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

THE SQUARE LATTICE. The holohedry (the rotations and reflections that preserve the lattice) is \mathbf{D}_4 generated by κ and ξ , where ξ is counterclockwise rotation of the plane by $\frac{\pi}{2}$. We study the case where the critical dual wave vectors have shortest length and the kernel of L is four-dimensional:

$$V_{\mathbf{k}}^{+} \oplus \xi \left(V_{\mathbf{k}}^{+}\right)$$
 or $V_{\mathbf{k}}^{-} \oplus \xi \left(V_{\mathbf{k}}^{-}\right)$.

Therefore, we can write the general eigenfunction in the scalar case as

$$R^{+}(\mathbf{x}) = z_1 e^{2\pi i \mathbf{k}_1 \cdot \mathbf{x}} Q^{+} + z_2 e^{2\pi i \mathbf{k}_2 \cdot \mathbf{x}} \xi Q^{+} \xi^{-1} + c.c.$$
 (3.6)

and in the pseudoscalar case as

$$R^{-}(\mathbf{x}) = z_1 e^{2\pi i \mathbf{k}_1 \cdot \mathbf{x}} Q^{-} + z_2 e^{2\pi i \mathbf{k}_2 \cdot \mathbf{x}} \xi Q^{-} \xi^{-1} + c.c.$$
(3.7)

In each case there are two axial subgroups (isotropy subgroups with 1-dimensional fixed-point spaces, that we call axial directions), so the equivariant branching lemma [8, 4, 7] predicts that bifurcations from a spatially uniform nematic state will occur along these axial directions at least. Up to conjugacy by an element of $\mathbf{D}_4 \dot{+} \mathbf{T}^2$, the direction $(z_1, z_2) = (1, 0)$ corresponds to rolls and the direction $(z_1, z_2) = (1, 1)$ corresponds to squares.

To visualize the patterns of bifurcating solutions we assume a layer of liquid crystal material in the x, y-plane, possibly with an applied magnetic field in the z direction. We assume that the initial solution corresponds to a nematic phase with all molecules oriented in the z direction and that a symmetry-breaking bifurcation occurs as the strength of the magnetic field, temperature or other parameter is decreased. 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 at array of points. In Figures 5 and 6 we plot solutions corresponding to scalar and pseudoscalar rolls and squares. Note that pseudoscalar rolls form a chevron pattern that can be compared to Figure 4(b).

THE HEXAGONAL LATTICE. The holohedry is D_6 and is generated by κ and ξ , where ξ is counterclockwise rotation of the plane by $\frac{\pi}{3}$. The action of ξ on Q is

$$\xi(Q) = \xi Q \xi^{-1}.$$

On the hexagonal lattice, we also study the case where the dual wave vectors have shortest length and the kernel of L is six-dimensional. The dual wave vectors can be chosen to be

$$\mathbf{k}_1 = (1,0)$$
 $\mathbf{k}_2 = \frac{1}{2}(-1,\sqrt{3})$ $\mathbf{k}_3 = \frac{1}{2}(-1,-\sqrt{3}).$

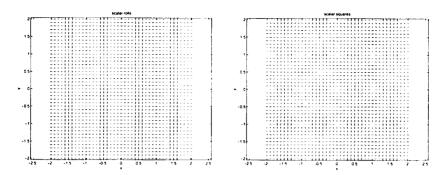


FIGURE 5. Square lattice with scalar representation: (left) rolls; (right) squares.

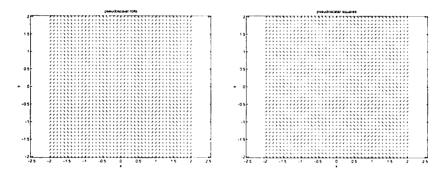


FIGURE 6. Square lattice with pseudoscalar representation: (left) antirolls; (right) anti-squares.

The eigenspaces are then

$$V_{\mathbf{k}}^{+} \oplus \xi^{2} \left(V_{\mathbf{k}}^{+} \right) \oplus \xi^{4} \left(V_{\mathbf{k}}^{+} \right) \quad \text{or} \quad V_{\mathbf{k}}^{-} \oplus \xi^{2} \left(V_{\mathbf{k}}^{-} \right) \oplus \xi^{4} \left(V_{\mathbf{k}}^{-} \right).$$

Therefore, we can write the general eigenfunction in the scalar case as

$$z_1e^{2\pi i\mathbf{k}_1\cdot\mathbf{x}}Q^+ + z_2e^{2\pi i\mathbf{k}_2\cdot\mathbf{x}}\xi^2Q^+\xi^4 + z_3e^{2\pi i\mathbf{k}_3\cdot\mathbf{x}}\xi^4Q^+\xi^2 + c.c.$$

and in the pseudoscalar case as

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

It is well-known from analyses of Bénard convection (see [8]) that on the scalar hexagonal lattice there are two branches of axial solutions – hexagons and rolls – and that the hexagons come in two types hexagons⁺ and hexagons⁻. For rolls we may take $(z_1, z_2, z_3) = (1, 0, 0)$ and for hexagons⁺ and hexagons⁻ we may take $(z_1, z_2, z_3) = \pm (1, 1, 1)$. Sample hexagon planforms are shown in Figure 7. Rolls are the same as those in Figure 5.

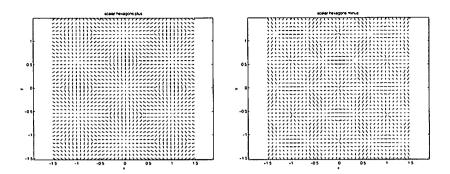


FIGURE 7. Hexagons on hexagonal lattice with scalar representation: (left) hexagons⁺; (right) hexagons⁻.

Bosch Vivancos et al. [1] and Bressloff et al. [2] show that in the pseudoscalar representation hexagons are given by $(z_1, z_2, z_3) = (1, 1, 1)$, triangles by $(z_1, z_2, z_3) = (i, i, i)$, and rectangles by $(z_1, z_2, z_3) = (1, -1, 0)$. Rolls are the same as in Figure 6. The remaining planforms are shown in Figure 8.

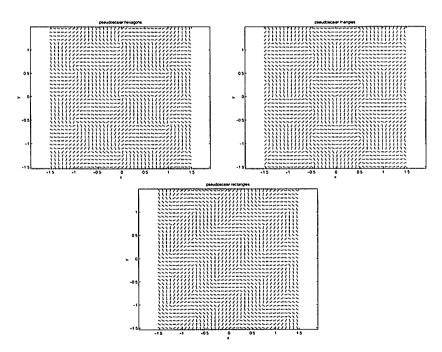


FIGURE 8. Hexagonal lattice with pseudoscalar representation: (upper left) hexagons; (upper right) triangles; (lower) rectangles.

Free energy interpretations

These results imply that there are two types of steady-state bifurcations, scalar and pseudoscalar, that can occur from a spatially homogeneous equilibrium to spatially periodic equilibria. If a scalar bifurcation occurs, then generically all of the scalar planforms that we listed (rolls, squares, hexagons⁺, hexagons⁻) will be solutions. Similarly, if a pseudoscalar bifurcation occurs, then generically all of the planforms that we listed (anti-rolls, anti-squares, hexagons, triangles, rectangles) will be solutions. We have not discussed the difficult issue of stability of these solutions.

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 need to compute a dispersion curve for both scalar and pseudoscalar eigenfunctions. That is, for each wave length $k = |\mathbf{k}|$ we must determine the first value of the bifurcation parameter λ where L has a nonzero kernel. Call that value λ_k . 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.

In principle, these calculations can be completed for the model equations (1.2) or a similar model, extending related calculations for bifurcation from the isotropic phase carried out by [9]. We defer the completion of this task to a future paper.

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