Stripe patterns and a projection-valued formulation of the eikonal equation

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We describe recent work on striped patterns in a system of block copolymers. A by-product of the characterization of such patterns is a new formulation of the eikonal equation. In this formulation, the unknown is a field of projection matrices of the form $P = e \otimes e$, where $e$ is a unit vector field. We describe how this formulation is better adapted to the description of striped patterns than the classical eikonal equation, and illustrate this with examples.

Keywords: modulated patterns; roll patterns; diblock copolymers; director formulation

1. Introduction

(a) Stripe patterns

Stripe patterns appear in a wide variety of natural systems. The simplest examples are those in which the stripes are predetermined—typically, as the result of how the material has been created. Examples of this are layered composites and geological strata (see [1–3] in this issue, as well as earlier studies [4–9]). Deformation of such predetermined stripes while preserving their width leads to various types of striped patterns.

In other systems, the stripes are not predetermined, but arise as the result of the dynamics of the system. This class includes the example of this paper—block copolymer melts—but also other amphiphilic systems [10,11], activator–inhibitor dynamics [12], liquid crystals [13], electric discharges [14] and thin magnetic films [15]. Various mathematical systems are used to study such stripe-forming properties, such as the Swift–Hohenberg equation [16–18] and the Ohta–Kawasaki, or non-local Cahn–Hilliard equation [19–23]. Such systems are characterized by an order parameter that typically takes values within a finite range. Taking this range to be $[0, 1]$, and identifying values in $[0, 1/2)$ with ‘black’ and $(1/2, 1]$ with ‘white’ gives rise to black-and-white patterns that—for

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Figure 1. The eikonal equation in the formulation (1.1) on a domain in the form of a stadium. The initial position of the wavefront is on the boundary; as time progresses, the wave front propagates inward. The solution $u$ of (1.1) is given by $u(x) = \text{dist}(x, \partial \Omega)$. A level curve at level $t$ is a snapshot of the wavefront at time $t$. Collecting snapshots at different times creates a striped pattern.

some values of the parameters—may look like stripes. (This property tends to be strongly parameter dependent; for other values of the parameters, either no patterns appear or, for instance, a spotted pattern appears [24–27].)

Often, one is interested in a more high level, or large-scale, description of the striped patterns, in which stripes are not described individually. In this setup, stripes are assumed to be locally parallel to each other and uniform in width, but their orientation and width can vary at a larger spatial scale. The properties of such patterns are then described in terms of local stripe orientation and relative spacing. One example of such a description is the Cross–Newell or ‘phase-diffusion’ equation [16–18,28], which characterizes the relative phase of a striped pattern. In this context, the ‘phase’ at $x$ counts the number of oscillations between $x$ and some reference position, and the relative phase is the difference between the phase and what the phase would be for a ‘perfect’ stripe pattern.

Going even further up the scale, one might make an assumption that the stripe width is fixed across the whole domain, leading to a representation in terms of solutions of the eikonal equation. This equation has its origin in models of wave propagation, and because this origin is relevant for the discussion below, we briefly describe it here. The eikonal equation describes the position of a wavefront at different times $t$. For a homogeneous and isotropic medium, in which the wave velocity is constant, the equation can be written in the form

$$|\nabla u| = 1. \tag{1.1}$$

The wavefront at time $t$ is given by the level set $\{x : u(x) = t\}$, and the function $u$ has the interpretation of the time needed for a wave to arrive at the point $x$. Figure 1 shows the solution of the eikonal equation on a well-known test case, that of the stadium domain. The wavefront is assumed to start at $t = 0$ at the outer boundary of the domain, and propagates inwards. The level curves indicate the solution at subsequent times.

(b) The eikonal equation as a kinematical description

We now turn back to the case of striped patterns and the aim of this paper. The first step in any modelling process is the choice of the degrees of freedom, the kinematics, of the system. In a system with stripes of a fixed width, the stripes
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Figure 2. Two wave-propagation histories in similar setups. Both start from the fat line and propagate in the direction of the arrow. (a) A singularity (corner) developing when the curvature becomes too high. In (b) the wave starts from the final front of (a), propagates in the opposite direction and instantly smoothes out the corner. If time were reversible, then the two diagrams would be identical. Their differences illustrate the irreversible effects in wavefront dynamics, in other words, the arrow of time.

are parallel, implying that (at least intuitively) knowing one stripe is enough to fix the neighbouring stripes, and therefore by repetition all stripes. Because of the similarities in this description with wave propagation, the eikonal equation has been used extensively to describe the kinematics of striped patterns [17,18,29]. In such a setup, the stripes are assumed to be level curves of a function that solves equation (1.1) in an appropriate sense. In many cases, it turns out that the kinematics are even sufficient to fully determine the solution; for instance, once the boundary of the stadium in figure 1 is chosen to be a stripe (wavefront), then all the other stripes (wavefronts) are fixed.

However, there are some peculiarities with the application of the eikonal equation, originally derived for wave propagation, to the context of striped patterns. These are mostly clearly illustrated by the behaviour at singularities, which we discuss in §2. The main message of this paper is that while the idea of using the eikonal equation for the kinematics of striped patterns is sound, there is good reason to use not the usual formulation (1.1) but an alternative formulation that we introduce in §3.

2. Singularities

Singularities can be mathematical, physical or both. A mathematical singularity is, for instance, a discontinuity of one of the objects in the mathematical formulation. A physical singularity corresponds to an extreme event, often an event that causes the modelling to break down.

The eikonal-equation solution of figure 1 is a good example. The ridge of the ‘roof’ function $u$ is both a mathematical and a physical singularity. It is a mathematical singularity because the function $u$ has a discontinuous derivative along the ridge. The physical singularity is the annihilation event: the wavefronts arriving from the two sides meet and cancel each other. These two singularities are related: the mathematics and physics match.

Singularities in the eikonal equation are related to the arrow of time. Wavefronts move forward, not backward, and they behave differently in ‘forward’ time than in ‘backward’ time. Figure 2 illustrates this: the wavefronts in the right-hand diagram start at the final front of the left-hand diagram, and propagate in the opposite direction. The result is a different form of the wavefronts.
When representing striped patterns by level curves of solutions \( u \) of the eikonal equation (1.1) (figure 3a), mathematical singularities arise that have no physical counterpart, such as the ridge line in (a). When replacing the vector-valued description of (1.1) by a projection-valued description (figure 3b), the ridge discontinuity disappears. Both descriptions also have a curvature discontinuity at the two end points, which is mirrored by a physical discontinuity.

Both diagrams in figure 2 correspond to solutions of equation (1.1). This shows that there is a lack of uniqueness because both solutions have the same boundary at the top; therefore, an additional condition is necessary to decide upon a unique evolution starting from the top wavefront. A common condition is that of a viscosity solution \([30]\), which can be interpreted as using the arrow of time as a selection criterion.

We now turn back again to the use of the eikonal equation in various descriptions of striped patterns. For instance, the Cross–Newell equation leads in the limit of scale separation (small deviation from straight, parallel stripes) to the eikonal equation (1.1) \([16,17]\). In a completely different context and derivation, a modified eikonal equation also arises as a scale-separation limit in a system of block copolymers (§3). As fronts at different times are parallel, the equation is indeed a natural candidate for the description of systems with stripe-like behaviour.

However, some of the mathematical singularities in the eikonal equation do not correspond to physical singularities. The same example of the stadium domain illustrates this. When viewing the level curves of \( u \) as a striped pattern (as in figure 3a), the ridge line is a stripe like any other. Therefore, the mathematical singularity has no physical counterpart.

This issue was discussed by Ercolani et al. \([18]\), and a suggestion was made to switch to director fields; however, the implementation chosen in Ercolani et al. \([18]\) was based on Riemannian surfaces, which appear slightly artificial to us, and indeed lead to mathematical complications. In contrast, in recent work, we encountered a formulation of the eikonal equation in director form (projection form, to be precise), which arose completely naturally from the analysis of the microscopic system. We now describe this system and the formulation in some detail.

3. Diblock copolymers

In Peletier & Veneroni \([31]\), we studied the formation of stripe-like patterns in a specific two-dimensional system that arises in the modelling of AB diblock copolymers. This system is defined by an energy \( G_\varepsilon \) that admits locally minimizing stripe patterns of width \( O(\varepsilon) \), and the aim was to study the properties of the system as \( \varepsilon \to 0 \). Although we do not impose any restrictions on the geometry of
Figure 4. A section of a domain $\Omega$ with (a) a general admissible pattern and (b) a stripe-like pattern. We prove that in the limit $\varepsilon \to 0$, all patterns with bounded energy $G_\varepsilon$ resemble (b). Areas: grey ($u = 1$) and white ($u = 0$).

the structures (figure 4a), it turns out that any sequence $u_\varepsilon$ of patterns for which $G_\varepsilon(u_\varepsilon)$ is bounded becomes stripe-like; in addition, the stripes become increasingly straight and uniform in width.

The energy functional is

$$G_\varepsilon(u) = \begin{cases} \frac{1}{\varepsilon} \int_\Omega |\nabla u| + \frac{1}{\varepsilon^3} d(u, 1 - u) - \frac{1}{\varepsilon^2} |\Omega|, & \text{if } u \in K, \\ \infty, & \text{otherwise.} \end{cases}$$

(3.1)

Here, $\Omega$ is an open, connected and bounded subset of $\mathbb{R}^2$ with $C^2$ boundary with area $|\Omega|$, $d$ is the Monge–Kantorovich distance (see Villani [32]) and

$$K := \left\{ u \in BV(\Omega; \{0, 1\}) : \frac{1}{|\Omega|} \int_\Omega u(x) \, dx = \frac{1}{2} \text{ and } u = 0 \text{ on } \partial \Omega \right\}.$$

The interpretation of the function $u$ and the functional $G_\varepsilon$ is as follows.

The function $u$ is a characteristic function, whose support corresponds to the region of space occupied by the A part of the diblock copolymer; the complement (the support of $1 - u$) corresponds to the B part. The boundary condition $u = 0$ in $K$ reflects a repelling force between the boundary of the experimental vessel and the A phase. Figure 4 shows two examples of admissible patterns.

The functional $G_\varepsilon$ contains two non-constant terms. The first term penalizes the interface between the A and the B parts, and arises from the repelling force between the two parts; this term favours large-scale separation. In the second term, the Monge–Kantorovich distance $d$ appears; this term is a measure of the spatial separation of the two sets $\{u = 0\}$ and $\{u = 1\}$, and favours rapid oscillation. The combination of the two leads to a preferred length scale, which is of order $\varepsilon$ in the scaling of (3.1).

4. A non-oriented version of the eikonal equation

In the analysis of this system in the limit $\varepsilon \to 0$, we encountered a new formulation of the eikonal equation that eliminates the unphysical mathematical singularity described earlier (figure 3). The central object in this formulation is a projection:
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A matrix \( P \) that can be written in terms of a unit vector \( m \) as \( P = m \otimes m \), or in coordinates \( P_{ij} = m_i m_j \) (Figure 5). Such a projection matrix has a range and a kernel that are both one dimensional; the range is parallel to \( m \), and the kernel orthogonal. Note that the independence of the sign of \( m \)—the unsigned nature of a projection—can be directly recognized in the formula \( P = m \otimes m \).

If \( m \) is a unit vector, then \( P = m \otimes m \) projects onto the one-dimensional subspace spanned by \( m \). If \( m(x) \) is parallel to the layering at \( x \), then the one-dimensional range of \( P(x) \) is also parallel to the layering. It is in this sense that we interpret \( P \) as characterizing the direction of the layering. In this description, one can already detect that \( P \) is a better descriptor of layering than \( m \) because a given layer direction can be characterized by two different vectors \( m \), but only by one projection.

In terms of this projection, the eikonal equation takes the form of a number of conditions. The first is that at every point \( x \), \( P(x) \) is a projection in the sense above, which can be written as

\[
P^2 = P, \quad P \text{ is symmetric, and } \text{rank}(P) = 1 \quad \text{a.e. in } \Omega.
\]

We write it in this way to avoid the implicit use of a vector field \( m \). The second condition is that the projection-valued function \( P \) has a divergence at every point,

\[
\text{div } P \in L^1(\Omega).
\]

Here, the divergence of the matrix \( P \) with elements \( P_{ij} \) is the vector \( \sum_j \partial_j P_{ij} \). With a little linear algebra, it can be shown that this implies that all partial derivatives \( \partial_i P_{ij} \) exist in \( L^1(\Omega) \) [33] (published in abridged form in Peletier & Veneroni [34]).

This divergence has two contributions, as can be seen by assuming that \( P \) is given by \( P = m \otimes m \) in terms of a smooth unit-length vector field \( m \), and expanding \( \text{div } P \),

\[
(\text{div } P)_i = \sum_j \partial_j (m_i m_j) = \sum_j [m_j \partial_i m_j + m_i \partial_j m_j],
\]

or in vector notation,

\[
\text{div } P = \nabla m \cdot m + m \text{ div } m.
\]
Because \( m \) has unit length, the matrix \( \nabla m \) can be written as a scalar curvature \( \kappa \) times the rank-one matrix \( m^\perp \otimes m \), where \( m^\perp \) is the rotation of \( m \) over \( \pi/2 \). Therefore,

\[
\text{div } P = \kappa m^\perp + m \text{div } m.
\]

The vector \( \text{div } P \), therefore, consists of two parts: a part orthogonal to \( m \), which measures the curvature of the layers, and a part parallel to \( m \) that captures the divergence of the layers, i.e. the degree to which the layers are parallel or not. Therefore, parallel layers can be imposed by requiring that the second component of \( \text{div } P \) vanishes, or equivalently that

\[
P \text{div } P = 0.
\]

Indeed, this equation arises naturally in the limit analysis of the functional \( \mathcal{G}_\varepsilon \). Note that if this equation holds, then \( |\text{div } P| = |\kappa| \), the (absolute value of) scalar curvature of the layers.

Collecting the various requirements, we define the projection-valued eikonal equation to be the following problem:

find \( P \in L^\infty(\Omega; \mathbb{R}^{2 \times 2}) \) such that

\[
P^2 = P \quad \text{a.e. in } \Omega, \tag{4.1a}
\]

\[
\text{rank}(P) = 1 \quad \text{a.e. in } \Omega, \tag{4.1b}
\]

\[
P \text{ is symmetric a.e. in } \Omega, \tag{4.1c}
\]

\[
\text{div } P \in L^1(\Omega; \mathbb{R}^2) \tag{4.1d}
\]

and

\[
P \text{div } P = 0 \quad \text{a.e. in } \Omega. \tag{4.1e}
\]

The precise relation between the solutions of the non-oriented eikonal equation and the block copolymer energy functionals is the following.

**Theorem 4.1.** The re-scaled functional \( \mathcal{G}_\varepsilon \) gamma converges to the functional

\[
\mathcal{G}_0(P) := \begin{cases} 
\frac{1}{8} \int_\Omega |\text{div } P(x)|^2 \, dx, & \text{if } P \in \mathcal{K}_0(\Omega), \\
+\infty, & \text{otherwise.}
\end{cases}
\]

Here, the admissible set \( \mathcal{K}_0(\Omega) \) is the set of solutions of (4.1). The topology of the gamma convergence in this case is the strong topology of measure-function pairs in the sense of Hutchinson [35]. The main tool in the proof of theorem 4.1 is an explicit lower bound on the energy \( \mathcal{G}_\varepsilon \), originally derived in Peletier & Röger [36]. This inequality gives a tight connection between low energy, on the one hand, and specific properties of the geometry of the stripes, on the other hand.

While there is much to be said about the interpretation of this theorem in the context of block copolymers (see Peletier & Veneroni [31, §1.7]), in this paper, we concentrate instead on the role of the projection-valued eikonal equation. In §5, we discuss the influence of the regularity of \( P \).

5. Regularity and singularities

There is a subtle relation between the regularity of the projection field \( P \) and the type of singularities that it may represent. Natural possibilities for singularities
in a line field are jump discontinuities (‘grain boundaries’) and target and U-turn patterns (figure 6). At a grain boundary, the jump in $P$ causes $\text{div} P$ to have a line singularity, comparable with the one-dimensional Hausdorff measure; condition (4.1d) excludes that possibility. For a target pattern, the curvature $\kappa$ of the stripes scales as $1/r$, where $r$ is the distance to the centre; then $\int \kappa^p$ is locally finite for $p < 2$, and diverges logarithmically for $p = 2$. Therefore, target patterns are admissible if and only if $\text{div} P$ may be in $L^1 \setminus L^2$. For instance, if $\mathcal{G}_0(P) < \infty$, then $\text{div} P \in L^2$, and only smooth variations are allowed (figure 6c).

The requirement that $\text{div} P \in L^1$ arises from the need to evaluate the product $P \text{div} P$ in a pointwise manner, but a consequence is that no grain boundaries are allowed. Because grain boundaries are certainly observed (for instance, in experimental block copolymer systems [37,38] and in the Swift–Hohenberg equation [18,39]), this calls for an appropriate generalization. This is a topic of current research.

6. Other applications of the projection-valued eikonal equation

We mentioned in §1 that striped patterns arise in a wide variety of systems. We expect that the projection-valued eikonal equation (4.1) will find applications in such systems, and theorem 4.1 illustrates its possible role. In line with the discussion in §1b, in the functional $\mathcal{G}_0$, equation (4.1) plays the role of characterization of kinematics: it describes the set of admissible deformations of the structure. The functional $\mathcal{G}_0$ incorporates this description by being equal to $+\infty$ for any projection field that does not satisfy equation (4.1). Within the constraints of admissibility, i.e. within the class of solutions of (4.1), the energy of the limiting system is given by the expression $(1/8) \int |\text{div} P|^2$. This integral can be interpreted as a constitutive law because it attributes energy to a given deformation (and because stress is the derivative of energy, it also characterizes the stress–strain relationship). Incidentally, because $|\text{div} P|$ is the magnitude of the local curvature of stripes, this constitutive law amounts to the same bending energy as is present in the classical model of the Euler elastica.

In the same way as for block copolymers, we expect the projection-valued eikonal equation to function as a kinematical description of the system, by characterizing all patterns of constant stripe width, in a way that avoids the problems of the vector-valued eikonal equation. Within the freedom allowed by this kinematical description, other properties, such as energies, forces and boundary conditions, will then determine the exact behaviour of the system.
7. Conclusion

In this paper, we have described a recently developed formulation of the eikonal equation, in terms of projections rather than vectors. This formulation is better suited to the description of striped patterns because it avoids singularities in the vector-valued eikonal equation that are meaningless in the context of spatial patterns. We expect that it will find many applications in the characterization of the kinematics of striped-pattern systems.

References