Stripe Patterns and the Eikonal Equation

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1. Introduction

In this note we describe the behaviour of a stripe-forming system that arises in the modelling of block copolymers. Part of the analysis concerns a new formulation of the eikonal equation in terms of *projections*. For precise statements of the results, complete proofs, and references, we refer to [4] and [3].

1.1. **Diblock Copolymers.** In [4] we study 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 $\mathcal{G}_\varepsilon$ that admits locally minimizing stripe patterns of width $O(\varepsilon)$, and the aim is to study the properties of the system as $\varepsilon \to 0$. Below we will show that any sequence u_ε of patterns for which $\mathcal{G}_\varepsilon(u_\varepsilon)$ is bounded becomes stripe-like; in addition, the stripes become increasingly straight and uniform in width.

The energy functional is

$$\mathscr{F}_\varepsilon(u) = \begin{cases} \varepsilon \displaystyle\int_\Omega |\nabla u| + \frac{1}{\varepsilon} d(u, 1-u), & \text{if } u \in K, \\ \infty & \text{otherwise.} \end{cases} \tag{1}$$

Here Ω is an open, connected, and bounded subset of $\mathbb{R}^2$ with C^2 boundary, d is the Monge-Kantorovich distance, and

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

We introduce a rescaled functional $\mathcal{G}_\varepsilon$ defined by

$$\mathcal{G}_\varepsilon(u) := \frac{1}{\varepsilon^2}\Big(\mathscr{F}_\varepsilon(u) - |\Omega|\Big).$$

The interpretation of the function u and the functional $\mathscr{F}_\varepsilon$ are 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.

The functional $\mathscr{F}_\varepsilon$ contains two 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 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 ε in the scaling of (1).

1.2. **A non-oriented version of Eikonal equation.** At finite $\varepsilon > 0$, structures with small $\mathcal{G}_\varepsilon$ resemble parallel stripes of thickness roughly 2ε. As $\varepsilon \to 0$, these stripes become dense, and the limiting structure can be interpreted as a field of infinitesimal stripes—a field of orientations.

A natural mathematical object for the representation of such orientation fields, or line fields, is a *projection*. We define a projection to be a matrix P that can be written in terms of a unit vector m as $P = m \otimes m$. Such a projection matrix has a range and a kernel that are both one-dimensional, and if necessary one can identify a projection P with its range, i.e. with the one-dimensional subspace of $\mathbb{R}^2$ onto which it projects. Note that the independence of the sign of m—the unsigned nature of a projection—can be directly recognized in the formula $P = m \otimes m$.

We define $\operatorname{div} P$ as the vector-valued function whose i-th component is given by $(\operatorname{div} P)_i := \sum_{j=1}^{2} \partial_{x_j} P_{ij}$. We consider the following problem. Let Ω be an open subset of $\mathbb{R}^2$. Find $P \in L^\infty(\Omega; \mathbb{R}^{2\times 2})$ such that

$$P^2 = P \qquad \text{a.e. in } \Omega, \tag{2a}$$

$$\operatorname{rank}(P) = 1 \qquad \text{a.e. in } \Omega, \tag{2b}$$

$$P \text{ is symmetric} \qquad \text{a.e. in } \Omega, \tag{2c}$$

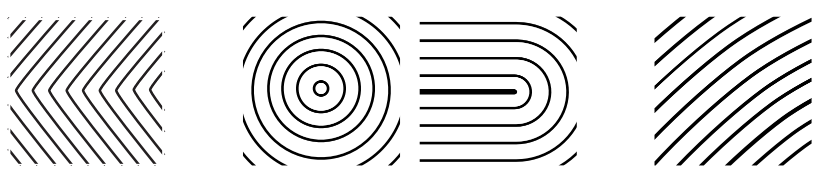
$$\operatorname{div} P \in L^2(\mathbb{R}^2; \mathbb{R}^2) \qquad \text{(extended to 0 outside } \Omega), \tag{2d}$$

$$P \operatorname{div} P = 0 \qquad \text{a.e. in } \Omega. \tag{2e}$$

The first three equations encode the property that $P(x)$ is a projection, in the sense above, at almost every x. The sense of property (2d) is that the divergence of P (extended to 0 outside Ω), in the sense of distributions in $\mathbb{R}^2$, is an $L^2(\mathbb{R}^2)$ function, which, in particular, implies

$$Pn = 0 \quad \text{in the sense of traces on } \partial\Omega.$$

The exponent 2 in (2d) is critical in the following sense. Obvious possibilities for singularities in a line field are jump discontinuities ('grain boundaries') and target patterns (see Figure 1).



(a) grain boundary

(b) target and U-turn patterns

(c) smooth directional variation

Figure 1: Canonical types of stripe variation in two dimensions. Types (a) and (b) are excluded by (2d).

At a grain boundary the jump in P causes $\operatorname{div} P$ to have a line singularity, comparable to the one-dimensional Hausdorff measure; condition (2d) clearly excludes that possibility. For a target pattern the curvature κ of the stripes scales as $1/r$, where r is the distance to the center; then $\int \kappa^p$ is locally finite for $p < 2$, and diverges logarithmically for $p = 2$. The cases $p < 2$ and $p \geq 2$ therefore distinguish between whether target patterns are admissible ($p < 2$) or not.

Given the regularity provided by (2d), the final condition (2e) represents the condition of parallelism, as a calculation for a smooth unit-length vector field $m(x)$ shows:

(3)

$$0 = P \operatorname{div} P = m(m \cdot (m \operatorname{div} m + \nabla m \cdot m)) = m \operatorname{div} m + m(m \cdot \nabla m \cdot m) = m \operatorname{div} m,$$

where the final equality follows from differentiating the identity $|m|^2 = 1$. For this smooth case the orientation field P can also be interpreted as a solution of the eikonal equation $|\nabla u| = 1$, as follows. The solution vector field m is divergence-free by (3), implying that its rotation over 90 degrees is a gradient ∇u; from $|m| = 1$ it follows that $|\nabla u| = 1$. This little calculation also shows that the interpretation of m in $P = m \otimes m$ is that of the stripe direction; P projects along the normal onto the tangent to a stripe.

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

Theorem 1. *The rescaled functional $\mathcal{G}_\varepsilon$ Gamma-converges to the functional*

$$\mathcal{G}_0(P) := \begin{cases} \dfrac{1}{8} \displaystyle\int_\Omega |\operatorname{div} P(x)|^2 dx & \text{if } P \in \mathcal{K}_0(\Omega) \\ +\infty & \text{otherwise} \end{cases}$$

Here the admissible set $\mathcal{K}_0(\Omega)$ is the set of solutions of (2). The topology of the Gamma-convergence in this case is the strong topology of measure-function pairs in the sense of Hutchinson [1]. The main tool in the proof of Theorem 1 is an explicit lower bound on the energy $\mathcal{G}_\varepsilon$ originally derived in [2]. This inequality gives a tight connection between low energy on one hand and specific properties of the geometry of the stripes on the other.

We refer to [3, 4] for the details and an extended discussion.

References

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