

Pattern formation in multi-component inhibitory systems

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Abstract

Pattern formation can be understood as an outcome of competing short range and long range interactions. This principle is demonstrated with a minimal, geometric model that assigns the free energy to each partition of a domain into two disjoint sets. The two sets represent the two components of a binary system. The free energy consists of two terms: a short range term that is the perimeter between the two sets, and a long range term that is given by a nonlocal quantity. The nonlocal term behaves as an inhibitor that limits growth and spreading. Because of this property, the system is termed a binary inhibitory system. The free energy functional is naturally defined on the class of Caccioppoli sets with a fixed volume, where one can also define the notion of stationary points. When the problem is posed in one dimension, all stationary points can be found. In higher dimensions, many stationary points have been discovered.

A pattern observed in the physical world is a stationary point with additional properties. First, it must be stable in some sense; second it must be somewhat periodic. Typically a physical pattern is an assembly of many copies of a geometric object. An example is a stationary assembly of discs. The construction of this assembly involves several intricate ideas, which can be applied to other stationary assemblies.

Recent studies also deal with a ternary inhibitory system of three components. The free energy of this system is again a sum of a short interaction energy of perimeter and a long range nonlocal energy. Unique in the ternary system is the phenomenon of triple junction where the three components come to meet at the same place. In an appropriate parameter range, there is a stable stationary assembly of two dimensional double bubbles.

1 A binary inhibitory system

Patterns appear in physical and biological systems as outcomes of self-organization principles. One finds examples in morphological phases of block copolymers, animal coats, and skin pigmentation. Common in these pattern-forming systems is that a deviation from homogeneity has a strong positive feedback on its further increase. On its own, it would lead to an unlimited increase and spreading. Pattern formation requires in addition a longer ranging confinement of the locally self-enhancing process.

Therefore at the minimum pattern formation requires two mechanisms: growth and inhibition. One of the most elegant inhibitory systems is a sharp interface limit model derived from the Ohta-Kawasaki [21] density functional theory. It was first introduced to the mathematical community by Nishiura and Ohnishi [20]. The system is binary because it consists of two components. It is a geometric variational problem on a bounded, open, and sufficiently smooth set D of \mathbb{R}^n . This set is partitioned into two disjoint subsets Ω

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and $D \setminus \Omega$, each of which is occupied by one of the two components of the system. The free energy functional takes the form

$$\mathcal{J}_B(\Omega) = \frac{1}{n-1} \mathcal{P}_D(\Omega) + \frac{\gamma}{2} \int_D |(-\Delta)^{-1/2}(\chi_\Omega - \omega)|^2 dx. \quad (1.1)$$

for subsets Ω of D of prescribed measure. Namely Ω is in

$$\mathcal{A} = \{\Omega \subset D : \Omega \text{ is Lebesgue measurable and } |\Omega| = \omega|D|\} \quad (1.2)$$

where $\omega \in (0, 1)$ is a parameter of the system. Here $|\Omega|$ and $|D|$ stand for the Lebesgue measures of Ω and D respectively. The constant $\frac{1}{n-1}$ in (1.1) and the half in $\frac{\gamma}{2}$ are not essential. We put them in (1.1) to have a better looking Euler-Lagrange equation later.

Growth is generated by the first term in (1.1). Here $\mathcal{P}_D(\Omega)$ is the perimeter of Ω in D . If Ω has C^1 boundary, then $\mathcal{P}_D(\Omega)$ is simply the area of the part of the boundary of Ω that is inside D , i.e. the area of $\partial\Omega \cap D$. For a general Lebesgue measurable set Ω , the perimeter is defined by

$$\mathcal{P}_D(\Omega) = \sup \left\{ \int_\Omega \operatorname{div} g(x) dx : g \in C_0^1(D, \mathbb{R}^n), |g(x)| \leq 1 \forall x \in D \right\} \quad (1.3)$$

where $\operatorname{div} g$ is the divergence of the C^1 vector field g on D with compact support and $|g(x)|$ stands for the Euclidean norm of the vector $g(x) \in \mathbb{R}^n$. The reader who is familiar with BV functions will recognize that $\mathcal{P}_D(\Omega) < \infty$ means that χ_Ω , the characteristic function of Ω ($\chi_\Omega(x) = 1$ if $x \in \Omega$ and $\chi_\Omega(x) = 0$ if $x \in D \setminus \Omega$), is a BV function in D . If $\mathcal{P}_D(\Omega) < \infty$, Ω is called a Caccioppoli set. See for instance [7, 9] for more on BV functions and Caccioppoli sets. To make this term small, Ω likes to form a large region bounded by a surface of small area, and shares the boundary with D as much as possible.

The number γ in (1.1) is a positive constant, the second parameter after ω . The second term in (1.1) is responsible for inhibition. The operator $(-\Delta)^{-1/2}$ is defined by the Poisson's equation. Given $f \in L^2(D)$ such that $\int_D f(x) dx = 0$, let u be the solution of the following Poisson's equation with the Neumann boundary condition:

$$-\Delta u = f \text{ in } D, \quad \partial_n u = 0 \text{ on } \partial D, \quad \int_D u(x) dx = 0. \quad (1.4)$$

In (1.4) ∂_n stands for the outward normal derivative at ∂D . Because the integral of f is 0, the partial differential equation with the boundary condition is solvable. The solution is unique up to an additive constant. The condition $\int_D u(x) dx$ fixes this constant and gives us a unique solution. The map $f \rightarrow u$ from the space of $\{f \in L^2(D) : \int_D f(x) dx = 0\}$ to itself given above is the operator $(-\Delta)^{-1}$. Since this operator is bounded, self-adjoint, and positive definite, it has a positive square root, which is $(-\Delta)^{-1/2}$ in (1.1). Like $(-\Delta)^{-1}$, $(-\Delta)^{-1/2}$ is a nonlocal operator. For the second term in (1.1) to be small, the function χ_Ω must have frequent fluctuation.

Therefore the two terms in (1.1) have different preferences. On the other hand, the two terms are effective at different length scales. The perimeter term is more central at a small length scale so it forces the boundary of Ω to be everywhere close to a surface of constant mean curvature. The second term is more important at a longer distance so that it often makes Ω to have a near periodic shape.

One can also study \mathcal{J}_B with the periodic boundary condition. In other words take D to be \mathbb{R}^n/Λ , where Λ is a discrete subgroup of \mathbb{R}^n isomorphic to \mathbb{Z}^n . This simplifies the problem somewhat because \mathbb{R}^n/Λ has no boundary. On the other hand there is translation invariance on \mathbb{R}^n/Λ , and one often needs to find ways to remove any degeneracy related to this invariance.

There is a related variational problem that allows the two components to mix. Instead of using a subset Ω of D , one uses a function u defined on D that represents the concentration of one of the two components. If $u(x) = 1$, then the point $x \in D$ is occupied by the first component; if $u(x) = 0$, then the point x is occupied by the second component; if $0 < u(x) < 1$, then the point is taken by a mixture of the two components. The situation $u(x) \notin [0, 1]$ is not physical and can be mathematically ruled out when one studies stationary

points. The free energy of this more complex system is

$$\mathcal{I}_{B,\epsilon} = \int_D \left[\frac{\epsilon^2}{2} |\nabla u|^2 + \frac{u^2(1-u)^2}{4} + \frac{\epsilon\gamma}{2} |(-\Delta)^{-1/2}(u-\omega)|^2 \right] dx \quad (1.5)$$

where u is in the admissible set

$$\mathcal{A}_I = \{u \in H^1(D) : \frac{1}{|D|} \int_D u(x) dx = \omega\}. \quad (1.6)$$

The additional parameter ϵ is positive. It is large if the temperature is high and small if the temperature is low. A stationary point of $\mathcal{I}_{B,\epsilon}$ is a solution to the following integro-differential equation.

$$-\epsilon^2 \Delta u + u(u-1/2)(u-1) + \epsilon\gamma(-\Delta)^{-1}(u-\omega) = \lambda \text{ in } D, \quad \partial_n u = 0 \text{ on } \partial D, \quad \int_D u(x) dx = 0. \quad (1.7)$$

In this model there are no longer clearly defined interfaces separating the two components in a stationary point. Instead, when ϵ is small, one can often identify regions whose width is of the order ϵ where the function u changes quickly between values close to 0 and values close to 1. These regions are viewed as interfaces, or more precisely, diffusive interfaces. The problem $\mathcal{I}_{B,\epsilon}$ is called a diffusive interface model.

De Giorgi's Gamma-convergence theory connects $\mathcal{I}_{B,\epsilon}$ to \mathcal{J}_B . As $\epsilon \rightarrow 0$, $\epsilon^{-1}\mathcal{I}_{B,\epsilon}$ Gamma-converges to \mathcal{J}_B . The reader may find the details of this story in [25]. One consequence of this theory is that as $\epsilon \rightarrow 0$, a global minimizer of $\mathcal{I}_{B,\epsilon}$ converges to a global minimizer of \mathcal{J}_B . Conversely, if \mathcal{J}_B has an isolated local minimizer Ω , then for small ϵ , $\mathcal{I}_{B,\epsilon}$ has a local minimizer u_ϵ such that

$$\int_D |u_\epsilon - \chi_\Omega| dx \rightarrow 0 \text{ as } \epsilon \rightarrow 0. \quad (1.8)$$

2 Global minimizer and first variation

I start this section by showing that \mathcal{J}_B always has a global minimizer.

Theorem 2.1 *There exists $\Omega_\star \in \mathcal{A}$ such that*

$$\mathcal{J}_B(\Omega_\star) = \inf_{\Omega \in \mathcal{A}} \mathcal{J}_B(\Omega).$$

Proof. The functional \mathcal{J}_B is bounded from below by 0, so there exists a sequence of Ω_j in \mathcal{A} such that

$$\lim_{j \rightarrow \infty} \mathcal{J}_B(\Omega_j) = \inf_{\Omega \in \mathcal{A}} \mathcal{J}_B(\Omega). \quad (2.1)$$

Recall that the BV norm is defined as follows. For any function $f \in L^1(D)$, let

$$[f]_{\text{BV}} = \sup \left\{ \int_D f(x) \operatorname{div} g(x) dx : g \in C_0^1(D, \mathbb{R}^n), |g(x)| \leq 1 \forall x \in D \right\}. \quad (2.2)$$

Clearly $[f]_{\text{BV}} = \mathcal{P}_D(\Omega)$ if $f = \chi_\Omega$. If $[f]_{\text{BV}} < \infty$, we say that f is a BV function (a function of bounded variation) and define the BV norm of f to be

$$\|f\|_{\text{BV}} = [f]_{\text{BV}} + \|f\|_{L^1(D)}. \quad (2.3)$$

It follows from (2.1) that the χ_{Ω_j} 's have bounded BV norms.

By the compactness theorem of BV functions [7, Theorem 4, Page 176] there exists $u \in BV(D)$ such that $\chi_{\Omega_j} \rightarrow u$ in $L^1(D)$. One can also assume that $\chi_{\Omega_j}(x) \rightarrow u(x)$ at every $x \in D$. Then $u(x) = 0$ or 1 for

every x , and one can identify u with χ_{Ω_*} for some measurable set $\Omega_* \subset D$. The convergence $\chi_{\Omega_j} \rightarrow \chi_{\Omega_*}$ in $L^1(D)$ also implies that $|\Omega_*| = \omega|D|$, i.e. $\Omega_* \in \mathcal{A}$. Next apply the lower semi-continuity of BV functions [7, Theorem 1, Page 172] to conclude that $\chi_{\Omega_*} \in BV(D)$ and

$$\mathcal{P}_D(\Omega_*) \leq \liminf_{j \rightarrow \infty} \mathcal{P}_D(\Omega_j). \quad (2.4)$$

Since χ_{Ω_j} is uniformly bounded by 1, $\chi_{\Omega_j} \rightarrow \chi_{\Omega_*}$ in $L^1(D)$ implies that $\chi_{\Omega_j} \rightarrow \chi_{\Omega_*}$ in $L^2(D)$. Then $(-\Delta)^{-1/2}(\chi_{\Omega_j} - \omega) \rightarrow (-\Delta)^{-1/2}(\chi_{\Omega_*} - \omega)$ in $L^2(D)$ and

$$\lim_{j \rightarrow \infty} \int_D |(-\Delta)^{-1/2}(\chi_{\Omega_j} - \omega)|^2 dx = \int_D |(-\Delta)^{-1/2}(\chi_{\Omega_*} - \omega)|^2 dx. \quad (2.5)$$

Combining (2.4) and (2.5) we deduce that

$$\mathcal{J}_B(\Omega_*) \leq \liminf_{j \rightarrow \infty} \mathcal{J}_B(\Omega_j). \quad (2.6)$$

This shows that Ω_* is a minimizer of \mathcal{J}_B in \mathcal{A} . \square

It is difficult to determine the exact shape of the global minimizer Ω^* . We will see that in one dimension, i.e. $D = (0, 1)$, a global minimizer is a periodic union of intervals; see Theorem 3.2. In higher dimensions, this question is far from being settled, although recent years have seen a number of results on this problem [2, 41, 17, 4, 16, 10] for various ranges of ω and γ , and some special shapes of D .

The functional \mathcal{J}_B has a complicated landscape. The global minimizer is not the only object of interest. This article is more about stationary points than global minimizers. Let $\varepsilon_0 > 0$ and $\Phi : \mathbb{R}^n \times (-\varepsilon_0, \varepsilon_0) \rightarrow \mathbb{R}^n$ be a smooth function. Φ is termed a deformation of D if

1. $\Phi(x, 0) = x$ for every $x \in \mathbb{R}^n$,
2. $\Phi(\cdot, \varepsilon) : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is one-to-one and onto for every $\varepsilon \in (-\varepsilon_0, \varepsilon_0)$,
3. Φ leaves D invariant, i.e. for every ε , $\Phi(x, \varepsilon) \in D$ if and only if $x \in D$.

Let $\Omega \in \mathcal{A}$, such that $\mathcal{J}_B(\Omega) < \infty$, and let Φ be a deformation. We say that Φ preserves the volume of Ω if

$$|\Phi(\Omega, \varepsilon)| = |\Omega|, \quad \forall \varepsilon \in (-\varepsilon_0, \varepsilon_0). \quad (2.7)$$

The first variation of \mathcal{J}_B under a volume preserving deformation Φ is

$$\left. \frac{d\mathcal{J}_B(\Phi(\Omega, \varepsilon))}{d\varepsilon} \right|_{\varepsilon=0}. \quad (2.8)$$

Since Ω is a Caccioppoli set, i.e., $\mathcal{P}_D(\Omega) < \infty$, the Riesz representation theorem asserts that the distributional derivative $D\chi_\Omega$ can be regarded as a vector valued measure on D . The total variation of this measure is a real valued, finite measure, denoted by $|D\chi_\Omega|$.

There are various natural ways to define the boundary of a Caccioppoli set measure theoretically. For instance one can use the support of the measure $|D\chi_\Omega|$ as the boundary of Ω . This support, denoted by $\text{supp}(|D\chi_\Omega|)$, is defined by its complement, i.e., $\text{supp}(|D\chi_\Omega|)$ is the subset of D whose complement in D is

$$\{x \in D : \exists \rho > 0 \text{ such that } B_\rho(x) \subset D \text{ and } |D\chi_\Omega|(B_\rho(x)) = 0\}. \quad (2.9)$$

In (2.9), $B_\rho(x)$ is the open ball centered at x of radius ρ .

Another concept for a measure theoretic boundary of Ω is called the reduced boundary, denoted by $\partial^*\Omega$. A point $x \in D$ is in $\partial^*\Omega$ if

1. $|D\chi_\Omega|(B_\rho(x) \cap D) > 0$ for any $\rho > 0$,

2. the limit $\nu(x) = \lim_{\rho \rightarrow 0} \nu_\rho(x)$ exists where

$$\nu_\rho(x) = \frac{D\chi_\Omega(B_\rho(x) \cap D)}{|D\chi_\Omega|(B_\rho(x) \cap D)},$$

3. $|\nu(x)| = 1$.

The reduced boundary $\partial^*\Omega$ is always a subset of $\text{supp}(|D\chi_\Omega|)$, but the converse is not always true. A simple counter-example is a rectangle in a two dimensional D . The four corner points are in $\text{supp}(|D\chi_\Omega|)$ but not in $\partial^*\Omega$. Of course, if the set Ω has C^1 boundary, then $\partial^*\Omega$ and $\text{supp}(|D\chi_\Omega|)$ all agree with the topological boundary $\partial\Omega \cap D$. I refer to [7, 9] for more on reduced boundaries.

Although $\text{supp}(|D\chi_\Omega|) \setminus \partial^*\Omega$ may not be empty, this set is always small. Actually the measure $|D\chi_\Omega|$ is nothing but the $n-1$ dimensional Hausdorff measure restricted to $\partial^*\Omega$:

$$|D\chi_\Omega|(E) = H^{n-1}(E \cap \partial^*\Omega) \quad (2.10)$$

for any $E \subset D$. The unit vector $\nu(x)$ in the definition of the reduced boundary is the normal vector of $\partial^*\Omega$ at x , inward with respect to Ω . With this normal vector, one obtains a tangent space to $\partial^*\Omega$ at every $x \in \partial^*\Omega$.

We introduce the term inhibitor variable, denoted I_Ω , for each $\Omega \in \mathcal{A}$ to be the solution of

$$-\Delta I_\Omega = \chi_\Omega - \omega \text{ in } D, \quad \partial_n I_\Omega = 0 \text{ on } \partial D, \quad \int_D u(x) dx = 0.$$

In other words, $I_\Omega = (-\Delta)^{-1}(\chi_\Omega - \omega)$.

Let

$$X(x) = \left. \frac{\partial \Phi(x, \varepsilon)}{\partial \varepsilon} \right|_{\varepsilon=0}, \quad \forall x \in \mathbb{R}^n \quad (2.11)$$

be the infinitesimal vector field of a deformation Φ . Since Φ leaves D invariant,

$$X(x) \in T_{\partial D}(x), \quad \forall x \in \partial D, \quad (2.12)$$

where $T_{\partial D}(x)$ is the tangent space of ∂D at x . Calculations show that

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \mathcal{P}_D(\Phi(\Omega, \varepsilon)) = \int_{\partial^*\Omega} \text{div}_{\partial^*\Omega} X dH^{n-1}. \quad (2.13)$$

Here $\text{div}_{\partial^*\Omega}$ is the divergence on $\partial^*\Omega$, made possible by the properties of the reduced boundary. More precisely, with $X = (X_1, X_2, \dots, X_n)$,

$$\text{div}_{\partial^*\Omega} X = \nabla_j^{\partial^*\Omega} X_j, \quad (2.14)$$

where $\nabla_j^{\partial^*\Omega}$ is the j -th component of the gradient $\nabla^{\partial^*\Omega}$ on $\partial^*\Omega$, namely,

$$\nabla^{\partial^*\Omega} f = \sum_{k=1}^{n-1} D_{\tau_k} f \tau_k \quad \text{and} \quad \nabla_j^{\partial^*\Omega} f = \nabla^{\partial^*\Omega} f \cdot e_j. \quad (2.15)$$

Here D_{τ_k} is the usual directional derivative in \mathbb{R}^n along the direction τ_k , the τ_k 's ($k = 1, 2, \dots, n-1$) form an orthonormal basis of the tangent space of $\partial^*\Omega$, and the e_j 's ($j = 1, 2, \dots, n$) are the standard unit vectors in \mathbb{R}^n . Also

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \frac{1}{2} \int_D |(-\Delta)^{-1/2}(\chi_{\Phi(\Omega, \varepsilon)} - \omega_\varepsilon)|^2 dx = - \int_{\partial^*\Omega} I_\Omega \nu \cdot X dH^{n-1} \quad (2.16)$$

where $\omega_\varepsilon = \frac{|\Phi(\Omega, \varepsilon)|}{|D|}$. Moreover

$$\left. \frac{d|\Phi(\Omega, \varepsilon)|}{d\varepsilon} \right|_{\varepsilon=0} = - \int_{\partial^*\Omega} \nu \cdot X dH^{n-1}. \quad (2.17)$$

See, for example [40], for the derivations of these formulas. Hence for a volume preserving deformation Φ of Ω , the infinitesimal vector field X satisfies

$$\int_{\partial^*\Omega} \nu \cdot X \, dH^{n-1} = 0. \quad (2.18)$$

Motivated by (2.13)-(2.17), we say that a Caccioppoli set $\Omega \in \mathcal{A}$ is a stationary point of \mathcal{J}_B if

$$\int_{\partial^*\Omega} (\operatorname{div}_{\partial^*\Omega} X - I_\Omega \nu \cdot X) \, dH^{n-1} = 0 \quad (2.19)$$

for every $X \in C^\infty(\mathbb{R}^n, \mathbb{R}^n)$ that satisfies (2.12) and (2.18).

If Ω has C^2 boundary and does not share boundary with D , then (2.19) is equivalent to the Euler-Lagrange equation,

$$H + \gamma I_\Omega = \lambda, \text{ on } \partial\Omega \cap D. \quad (2.20)$$

In (2.20), H is the mean curvature of the surface $\partial\Omega \cap D$, and the constant λ is a Lagrange multiplier corresponding to the constraint $|\Omega| = \omega|D|$. If Ω shares boundary with D , then one adds another condition that

$$\partial\Omega \cap D \perp \partial D \quad (2.21)$$

where $\partial\Omega \cap D$ and ∂D meet.

A stationary point with C^2 boundary is called a regular stationary point. Whether \mathcal{J}_B has non-regular stationary points is a difficult open question. This article only deals with regular stationary points.

3 Stationary points

In one dimension, $D = (0, 1)$, all stationary points of \mathcal{J}_B are known. For each positive integer K let $z_1, z_2, \dots, z_K \in (0, 1)$ be given by

$$z_1 = \frac{1 - \omega}{K}, \quad z_3 = z_1 + \frac{2}{K}, \quad z_5 = z_3 + \frac{2}{K}, \dots$$

and

$$z_2 = \frac{1 + \omega}{K}, \quad z_4 = z_2 + \frac{2}{K}, \quad z_6 = z_4 + \frac{2}{K}, \dots \quad (3.1)$$

Also define $z'_1, z'_2, \dots, z'_K \in (0, 1)$ by

$$z'_1 = \frac{\omega}{K}, \quad z'_3 = z'_1 + \frac{2}{K}, \quad z'_5 = z'_3 + \frac{2}{K}, \dots$$

and

$$z'_2 = \frac{2 - \omega}{K}, \quad z'_4 = z'_2 + \frac{2}{K}, \quad z'_6 = z'_4 + \frac{2}{K}, \dots \quad (3.2)$$

For each K we have two sets

$$\Omega_K = (z_1, z_2) \cup (z_3, z_4) \cup (z_5, z_6) \cup \dots \quad \text{and} \quad \Omega'_K = (0, z'_1) \cup (z'_2, z'_3) \cup (z'_4, z'_5) \cup \dots \quad (3.3)$$

It was proved by Ren and Wei [25] that the stationary points of \mathcal{J}_B on $(0, 1)$ are precisely these Ω_K 's and Ω'_K 's.

Theorem 3.1 ([25]) *If $D = (0, 1)$, then $\Omega \in \mathcal{A}$ is a stationary point of \mathcal{J}_B if and only if Ω is one of the sets Ω_K and Ω'_K , $K = 1, 2, \dots$. Moreover every stationary point is a local minimizer.*

The global minimizers of \mathcal{J}_B on $(0, 1)$ are also known. The energy of Ω_K and Ω'_K are equal, which we denote by $J(K)$. Calculations show that

$$J(K) = K + \frac{\gamma\omega^2(1-\omega)^2}{6K^2}. \quad (3.4)$$

If we minimize J among positive integers K , there are two possibilities: (1) J is minimized by one integer K_* ; (2) J is minimized by two consecutive integers K_* and $K_* + 1$. The first case is generic.

Theorem 3.2 ([25]) *If J is minimized by one integer, K_* , then \mathcal{J}_B has two global minimizers: Ω_{K_*} and Ω'_{K_*} ; if J is minimized by two integers, K_* and $K_* + 1$, then \mathcal{J}_B has four global minimizers: Ω_{K_*} , Ω'_{K_*} , Ω_{K_*+1} , and Ω'_{K_*+1} .*

The proofs of these theorems depend on the special structure of Caccioppoli sets in one dimension. A Caccioppoli set $\Omega \subset (0, 1)$ is, up to a set of Lebesgue measure 0, just a finite union of intervals. It can be identified by the endpoints of the intervals. Say there are K endpoints denoted by $x_1, x_2, \dots, x_K \in (0, 1)$. They are the interfaces separating Ω from $(0, 1) \setminus \Omega$. Then the measure $|D\chi_\Omega|$ is just the sum of delta measures centered at x_k , $k = 1, 2, \dots, K$, namely

$$|D\chi_\Omega| = \sum_{k=1}^K \delta_{x_k}. \quad (3.5)$$

Within the class of Caccioppoli sets in \mathcal{A} with K endpoints the energy \mathcal{J}_B is a function of x_1, x_2, \dots, x_K . For a stationary point, the equation (2.20) becomes a system of equations for these x_k 's. One can solve these equations and find two solutions, which are exactly (3.1) and (3.2).

To discuss whether a stationary point is a local minimizer, one needs a topology on \mathcal{A} . The natural topology is given by the $L^1(D)$ norm; namely, for $\Omega, \Omega' \in \mathcal{A}$ the distance between the two sets is

$$d(\Omega, \Omega') = \int_D |\chi_\Omega - \chi_{\Omega'}| dx. \quad (3.6)$$

Under this topology, in one dimension, the subclass of Caccioppoli sets in \mathcal{A} has an unusual structure, so that all stationary points of \mathcal{J}_B are local minimizers. There are no other type stationary points.

The functional \mathcal{J}_B on a higher dimensional set $D \in \mathbb{R}^n$, $n \geq 2$, is a much more difficult problem. One can certainly extend the one dimensional stationary points Ω_K and Ω'_K trivially to a stationary point on a rectangle

$$D = (0, 1) \times (0, w) \quad (3.7)$$

where $w > 0$ is the width. They would be good candidates for the stripe pattern observed in the lamellar phase of diblock copolymers, provided one can show that they were stable in D . It turns out that with given ω, γ and K , the stability of Ω_K and Ω'_K depends on the width w of the rectangle w .

There are several works addressing this issue, where stability is discussed from different perspectives. First, Ren and Wei [27] considered the diffusive interface problem (1.5). It was shown in [25] by De Giorgi's Gamma-convergence theory, that near each Ω_K (or Ω'_K) of Theorem 3.1, there exists a local minimizers $U_{\epsilon, K}$, or $U'_{\epsilon, K}$, of $\mathcal{I}_{B, \epsilon}$. When such a local minimizer on $(0, 1)$ is trivially extended to a stationary point on $(0, 1) \times (0, w)$, one can study its stability from the eigenvalue problem

$$-\epsilon^2 \Delta \phi + \left(3U_{\epsilon, K}^2 - 3U_{\epsilon, K} - \frac{1}{2} \right) \phi + \epsilon \gamma (-\Delta)^{-1} \phi = \lambda \phi + Const., \quad (3.8)$$

$$\partial_n \phi = 0 \text{ on } \partial D, \quad \int_D \phi(x) dx = 0.$$

In [27] the authors found asymptotic formulas for all the eigenvalues in terms of the small parameter ϵ . It turns out that only when w is small, all the eigenvalues are positive. If w is large, one can find a negative eigenvalue, and consequently $U_{\epsilon, K}$ is unstable.

Knowing the dependence of the eigenvalues on γ , the authors were able to find bifurcation solutions as γ crosses some critical values [31]. These solutions have wiggled interfaces. They are the first real two dimensional solutions.

Next, Choksi and Sternberg [6] considered the second variation of \mathcal{J}_B . Let $\Omega \in \mathcal{A}$ be a Caccioppoli set, and a deformation Φ be a volume preserving deformation mentioned in the last section. The second variation of Ω along Φ is

$$\frac{d^2 \mathcal{J}_B(\Phi(\Omega, \varepsilon))}{d\varepsilon^2} \Big|_{\varepsilon=0}. \quad (3.9)$$

They proved that when w is small, the second variation of Ω_K (or Ω'_K) along any deformation Φ is non-negative, and when w is large, there is always some deformation Φ long which, the second variation is negative. Actually they considered the periodic boundary condition case, but their result is also valid if the domain is a rectangle in \mathbb{R}^n .

In [1], Acerbi *et al* showed that the positivity of the second variation at a regular stationary point indeed implies that the stationary point is a local minimizer with respect to the metric given in (3.6). Using this result, Morini and Sternberg showed in [16] that when the width w is small, Ω_K and Ω'_K are local minimizers on $(0, 1) \times (0, w)$. Moreover, when w is small, a global minimizer on $(0, 1) \times (0, w)$ must be the extension of a global minimizer on $(0, 1)$.

Another one dimensional result was obtained by Ren and Wei [26] that there are stationary points on a disc in \mathbb{R}^2 which are unions of concentric annuli. There are also solutions of wiggled interfaces bifurcating out of these radial solutions [30].

The first higher dimensional result on a general domain, not by the bifurcation theory, was proved by Oshita [22].

Theorem 3.3 ([22]) *Let D be a bounded and smooth domain in \mathbb{R}^2 . There exists $\omega_0 > 0$ depending on D only such that if $\omega < \omega_0$, there is $\gamma_0 > 0$ so that when $\gamma < \gamma_0$, \mathcal{J}_B admits a stationary point which is close to a disc of radius $\sqrt{\frac{\omega|D|}{\pi}}$ and is centered near a global minimum of the function $z \rightarrow R(z, z)$.*

The function R in this theorem is the regular part of Green's function of Δ with the Neumann boundary condition. Recall that the Green's function, denoted $G(x, y)$, is the solution of the following problem

$$-\Delta G(\cdot, y) = \delta(\cdot - y) - \frac{1}{|D|} \text{ in } D; \quad \partial_n G(\cdot, y) = 0 \text{ on } \partial D; \quad \int_D G(x, y) dx = 0 \quad (3.10)$$

for each $y \in D \subset \mathbb{R}^2$. One can write G as a sum of two terms:

$$G(x, y) = \frac{1}{2\pi} \log \frac{1}{|x - y|} + R(x, y). \quad (3.11)$$

The first term $\frac{1}{2\pi} \log \frac{1}{|x - y|}$ is the fundamental solution of the Laplace operator in two dimensions; the second term R is the regular part of the Green's function, a smooth function of $(x, y) \in D \times D$. It is known that

$$R(z, z) \rightarrow \infty, \text{ as } z \rightarrow \partial D, \quad (3.12)$$

so the function $z \rightarrow R(z, z)$ has a global minimum in D .

The idea of Oshita's work is to view the nonlocal part of \mathcal{J}_B as a small perturbation of the perimeter term in \mathcal{J}_B . Then a disc centered at any general point $\xi \in D$ is a stationary point of the perimeter functional according to the isoperimetric inequality. With the addition of a small nonlocal term, one can make a small perturbation to the disc and find a set that almost solves (2.20). By "almost solves" we mean that this set is stationary with respect to all but two deformations. These two deformations are related to the translations of the set. However if one adjusts the center of the disc ξ in D , it turns out that there is a special place ξ^* in D such that if the disc is centered at ξ^* , then the perturbed disc is a stationary point with respect to all deformations. Asymptotically ξ^* converges to a minimum of $z \rightarrow R(z, z)$ as $\gamma \rightarrow 0$.

The next breakthrough came in [33] by Ren and Wei. They observed that a disc is not only a stationary point of the perimeter functional, it is also stationary with respect to the singular part of the nonlocal energy. Recall that in (2.20), the function I_Ω can be written, with the help of Green's function, as

$$I_\Omega(x) = \int_\Omega G(x, y) dy. \quad (3.13)$$

But by (3.11) we have

$$I_\Omega(x) = \int_\Omega \frac{1}{2\pi} \log \frac{1}{|x-y|} dy + \int_\Omega R(x, y) dy. \quad (3.14)$$

If we take Ω to be a disc B_ρ of radius ρ , centered at any $\xi \in D$ and insert it into the equation (2.20), then the curvature H of the boundary of $B_\rho(\xi)$ is obviously $\frac{1}{\rho}$, a constant. Moreover, the first term of I_{B_ρ} ,

$$\int_{B_\rho(\xi)} \frac{1}{2\pi} \log \frac{1}{|x-y|} dy,$$

is also constant for all $x \in \partial B_\rho(\xi)$. Only the term

$$\int_{B_\rho(\xi)} R(x, y) dy$$

is not constant on $\partial B_\rho(\xi)$. Based on this observation, Ren and Wei showed that an approximate disc exists as a stationary point for a much larger range of the parameter ω and γ .

Theorem 3.4 ([33]) *Let $\rho > 0$ be such that $\pi\rho^2 = \omega|D|$. For any $\eta > 0$ there exists $\delta > 0$ such that if ρ and γ satisfy*

$$1). \gamma\rho^3 < 12 - \eta, \quad 2). \gamma\rho^4 < \delta, \quad 3). \rho < \sqrt{\frac{\omega_0|D|}{\pi}},$$

then \mathcal{J}_B admits a stationary point that is close to a disc of radius ρ , and is centered near a minimum of $z \rightarrow R(z, z)$. In some sense, this stationary point is stable.

Here ω_0 is the same as the one in Theorem 3.3. So to have a disc-like stationary point, γ does not have to be small. If ω is small enough, we can again have a disc-like stationary point even if γ is large.

The claim of stability lies in the proof of the theorem. First, take a disc of radius ρ and place it inside D with the center being ξ . At this point, ξ is arbitrary and is not where the center of the solution is. Next, we perturb the disc by a function $\phi(\theta)$, so that the boundary of the perturbed disc is parametrized by

$$\theta \in \mathbb{S}^1 \rightarrow \sqrt{\rho^2 + 2\phi(\theta)}e^{i\theta}. \quad (3.15)$$

In (3.15), \mathbb{S}^1 is the unit circle, or the interval $[0, 2\pi]$ with identified endpoints. We write $e^{i\theta}$ for $(\cos \theta, \sin \theta)$ for simplicity. The function $\theta \rightarrow \sqrt{\rho^2 + 2\phi(\theta)}$ is really the radius variable in the polar coordinates centered at ξ . We do not use the radius variable to describe perturbation, but use the variable $\theta \rightarrow \phi(\theta)$ because the constraint $|\Omega| = \omega|D|$ is a simple affine condition

$$\int_0^{2\pi} \phi(\theta) d\theta = 0 \quad (3.16)$$

in terms of ϕ . Another condition on ϕ is that

$$\int_0^{2\pi} \phi(\theta) \cos \theta d\theta = \int_0^{2\pi} \phi(\theta) \sin \theta d\theta = 0. \quad (3.17)$$

This ensures that the set perturbed by ϕ is “centered” at ξ . We denote this set by Ω_ϕ .

Since our set Ω_ϕ is centered at an arbitrary point ξ , it is not realistic to find a ϕ so that Ω_ϕ solves (2.20). Instead we look for a ϕ that solves the “projected” equation, namely $H(\partial\Omega_\phi) + \gamma I_{\Omega_\phi}$ is in the linear span of $\{1, \cos \theta, \sin \theta\}$. In other words we look for ϕ , and three numbers λ , A_1 , and A_2 such that

$$H(\partial\Omega_\phi) + \gamma I_{\Omega_\phi} = \lambda + A_1 \cos \theta + A_2 \sin \theta. \quad (3.18)$$

To solve this equation, we use the exact disc $B(\xi)$ centered at ξ as an approximate solution. It corresponds to $\phi = 0$. We analyze the linearized operator of the equation (2.20) at $\phi = 0$. This linear operator turns out to be invertible and positive definite. The equation (3.18) may be written in a fixed point form near the approximate solution and is solved by the contraction mapping principle.

Denote this solution of (3.18) by ϕ^* and the corresponding set by Ω_{ϕ^*} . Recall that our starting point is a fixed center ξ , so this ϕ^* also depends on ξ . We emphasize this dependence by writing $\phi^* = \phi^*(\cdot, \xi)$ and $\Omega_{\phi^*} = \Omega_{\phi^*(\cdot, \xi)}$. The final step is to show that there is a particular ξ^* in D such that when $\xi = \xi^*$, the corresponding $\phi^*(\cdot, \xi^*)$ and $\Omega_{\phi^*(\cdot, \xi^*)}$ solves (3.18) with $A_1 = A_2 = 0$.

To do this, one minimizes the energy of $\Omega_{\phi^*(\cdot, \xi)}$ with respect to ξ . It turns out that since $\Omega_{\phi^*(\cdot, \xi)}$ was found near the exact disc $B(\xi)$, the energy of $\Omega_{\phi^*(\cdot, \xi)}$ is close to the energy of $B(\xi)$. The energy of $B(\xi)$ can be computed explicitly:

$$\mathcal{J}_B(B(\xi)) = 2\pi\rho + \frac{\pi^2\gamma\rho^4}{2} \left[\frac{1}{2\pi} \log \frac{1}{\rho} + \frac{1}{8\pi} + R(\xi, \xi) + \frac{\rho^2}{4|D|} \right]. \quad (3.19)$$

Clearly $\mathcal{J}_B(B(\xi))$ is minimized, with respect to ξ , at a minimum of the function $\xi \rightarrow R(\xi, \xi)$. It also implies that $\mathcal{J}_B(\Omega_{\phi^*(\cdot, \xi)})$ is minimized, with respect to ξ , at a point ξ^* which is close the minimum of $\xi \rightarrow R(\xi, \xi)$. As a minimum, ξ^* satisfies

$$\left. \frac{\partial \mathcal{J}_B(\Omega_{\phi^*(\cdot, \xi)})}{\partial \xi_i} \right|_{\xi=\xi^*} = 0, \quad i = 1, 2. \quad (3.20)$$

A careful reading of (3.20) shows that it implies that $A_1 = A_2 = 0$ in (3.18) at $\xi = \xi^*$.

This shows the existence of a stationary point. The stability of this point is ascertained from two facts. First, we constructed a fixed point $\phi^*(\cdot, \xi)$ with the help of the linearized operator at the exact disc $B(\xi)$. One can show that this linear operator is similar to the one at $\Omega_{\phi^*(\cdot, \xi)}$. Hence the latter linear operator is also positive definite. This shows that among the perturbations satisfying (3.16) and (3.17), $\phi^*(\cdot, \xi)$ is locally energy minimizing. We emphasize that $\phi^*(\cdot, \xi)$ is only locally energy minimizing among these special perturbations. Second, we minimized the energy of $\phi^*(\cdot, \xi)$ with respect to ξ . As we vary ξ , $\phi^*(\cdot, \xi)$ can be viewed as a family of perturbations. These perturbations do not satisfy the condition (3.17), so they are beyond the perturbations in the first step. Since $\phi^*(\cdot, \xi^*)$ is obtained from a minimum ξ^* , our stationary point locally minimizes in both steps. We therefore conclude that in this sense, $\phi^*(\cdot, \xi^*)$ is stable.

The sense of stability discussed above should be compared to the more standard notions of stability. One can define a stationary point to be if it is a local energy minimizer with respect to the metric d given in (3.6). Or one can define a stationary point to be stable if \mathcal{J}_B has positive second variation, (3.9), at the stationary point along any deformation whose infinitesimal element is non-trivial. Although we expect that these three notions of stability are more or less equivalent, the only known fact now is that the positivity of the second variation implies the local minimality of the energy functional by Acerbi *et al* [1] mentioned earlier.

For pattern formation problems, one really likes to find stationary points that are nearly periodic sets of multiple components. A stationary point that models a pattern should be an assembly of many similar geometric shapes. We call such a stationary point a stationary assembly. The single disc solutions in Theorems 3.3 and 3.4 are not stationary assemblies.

Fortunately Ren and Wei discovered that the techniques they developed in [33] can be elaborated to construct stationary assemblies. They showed that for each positive integer K there is an assembly of K small discs as a stationary point of \mathcal{J}_B , when ω is small and γ is in a particular range. To state this result,

define a function F by

$$F(\xi_1, \xi_2, \dots, \xi_K) = F(\xi_1, \xi_2, \dots, \xi_K) = \sum_{k=1}^K R(\xi_k, \xi_k) + \sum_{k=1}^K \sum_{l=1, l \neq k}^K G(\xi_k, \xi_l), \quad (3.21)$$

where $\xi_k \in D$, and $\xi_j \neq \xi_k$ if $j \neq k$, with the help of Green's function and its regular part. This function tends to infinity if one ξ^k approaches the boundary of D or if two distinct ξ^k and ξ^l become too close, so F always has a global minimum.

Theorem 3.5 ([32]) *Let $K \geq 2$ be an integer and ρ be such that $K\pi\rho^2 = \omega|D|$.*

1. *For every $\eta > 0$ there exists $\delta > 0$, depending on η , K and D only, such that if*

$$\frac{1 + \eta}{\rho^3 \log \frac{1}{\rho}} < \gamma < \frac{12 - \eta}{\rho^3}, \quad (3.22)$$

and

$$\rho < \delta, \quad (3.23)$$

then there exists a stationary point, stable in some sense.

2. *This stationary point is a union of K sets, each of which is close to a disc of radius ρ .*

3. *Let the centers of these approximate discs be ξ_1^* , ξ_2^* , ..., ξ_K^* . Then $\xi^* = (\xi_1^*, \xi_2^*, \dots, \xi_K^*)$ is close to a global minimum of the function F .*

As in the previous case, one takes K discs and place them inside D with centers at $\xi_1, \xi_2, \dots, \xi_K$. However unlike the last case, the radius of these discs is not fixed at ρ . Instead we introduce w_1, w_2, \dots, w_K , so that the area of the k -th disc is w_k . The w_k 's satisfy

$$\sum_{k=1}^K w_k = K\pi\rho^2. \quad (3.24)$$

Perturbed each $B_{r_k}(\xi_k)$, the disc centered at ξ of radius $r_k = \sqrt{\frac{w_k}{\pi}}$, by a function ϕ_k to Ω_{ϕ_k} . Each ϕ_k satisfies (3.16) and (3.17). One then finds $\phi^* = (\phi_1^*, \phi_2^*, \dots, \phi_K^*)$ such that the set $\Omega^* = \cup_{k=1}^K \Omega_{\phi_k^*}$ solves

$$H(\partial\Omega_{\phi_k}) + \gamma I_{\Omega_{\phi_k}} = \lambda_k + A_{1,k} \cos \theta + A_{2,k} \sin \theta \quad (3.25)$$

on each $\partial\Omega_{\phi_k}$.

As before ϕ^* is not a solution of (2.20) yet. There are the terms $A_{1,k} \cos \theta$ and $A_{2,k} \sin \theta$ in (3.25). Moreover the constants λ_k there depend on k , while the constant λ in (2.20) does not. We use the ξ_k 's and the w_k 's to fix these problems. Note that $\phi^* = \phi^*(\cdot, \xi, w)$ depends on $\xi = (\xi_1, \dots, \xi_K)$ and $w = (w_1, \dots, w_K)$. One minimizes $\mathcal{J}_B(\phi^*(\cdot, \xi, w))$ with respect to (ξ, w) . This energy is close to the energy of the approximate solution $\cup_{k=1}^K B_{r_k}(\xi_k)$, which is

$$\begin{aligned} \mathcal{J}_B(\cup_{k=1}^K B_{r_k}(\xi_k)) &= \sum_{k=1}^K 2\pi r_k + \frac{\gamma\pi^2}{2} \left[\sum_{k=1}^K \left(\frac{r_k^4}{2\pi} \log \frac{1}{r_k} + \frac{r_k^4}{8\pi} + r_k^4 R(\xi_k, \xi_k) \right) \right. \\ &\quad \left. + \sum_{k=1}^K \sum_{l \neq k} r_k^2 r_l^2 G(\xi_k, \xi_l) + \sum_{k=1}^K \sum_{l=1}^K \left(\frac{r_k^2 r_l^4}{8|D|} + \frac{r_k^4 r_l^2}{8|D|} \right) \right]. \end{aligned} \quad (3.26)$$

When ρ is small as in assumption (3.23) of Theorem 3.5 and the r_k 's are in a neighborhood of ρ , the leading order quantity of (3.26) is

$$\sum_{k=1}^K 2\pi r_k + \frac{\gamma\pi^2}{2} \sum_{k=1}^K \frac{r_k^4}{2\pi} \log \frac{1}{r_k}. \quad (3.27)$$

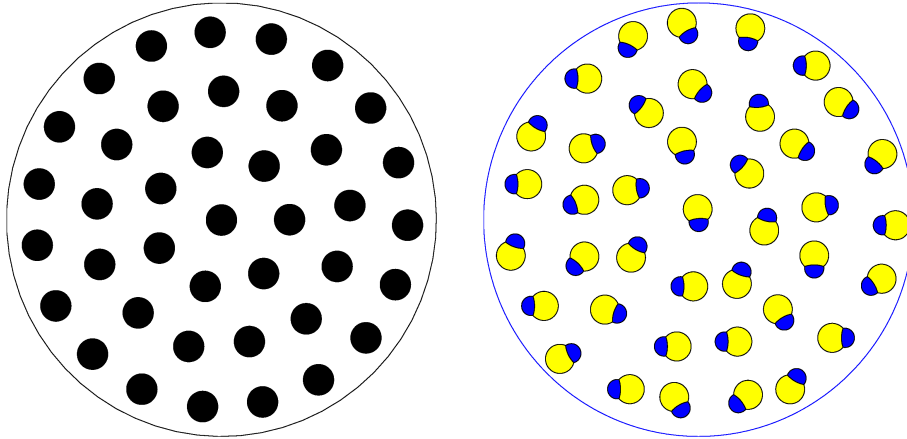


Figure 1: Left: a stationary assembly of \mathcal{J}_B with 40 discs. Right: a stationary assembly of \mathcal{J}_T with 40 double bubbles.

The lower bound $\frac{1+\eta}{\rho^3 \log \frac{1}{\rho}} < \gamma$ ensures that (3.27) is locally minimized at $r_1 = \dots = r_K = \rho$. One can take all the r_k 's to be ρ in (3.26) and minimize with respect to the ξ_k 's. This means minimizing F of (3.21).

In conclusion, $\mathcal{J}_B(\Omega_{\phi^*(\cdot, \xi, w)})$ is minimized with respect to (ξ, w) at (ξ^*, w^*) where $w^* = (w_1^*, \dots, w_K^*)$ and each w_k^* is close to $\pi\rho^2$, and ξ^* is close to a minimum of F . At (ξ^*, w^*) we have the equations

$$\frac{\partial \mathcal{J}_B(\phi^*(\cdot, \xi, w))}{\partial \xi_{k,j}} \Big|_{(\xi, w) = (\xi^*, w^*)} = 0, \quad \frac{\partial \mathcal{J}_B(\phi^*(\cdot, \xi, w))}{\partial w_k} \Big|_{(\xi, w) = (\xi^*, w^*)} = \lambda, \quad k = 1, \dots, K, \quad j = 1, 2. \quad (3.28)$$

The constant λ corresponds to the constraint (3.24) on the w_k 's. Using these equations we deduce that in (3.25), when $(\xi, w) = (\xi^*, w^*)$, the λ_k 's are actually independent of k , and the $A_{1,k}$'s and the $A_{2,k}$'s all vanish. This proves the theorem.

If D is the unit disc, the Green's function is known explicitly:

$$G(x, y) = \frac{1}{2\pi} \log \frac{1}{|x - y|} + \frac{1}{2\pi} \left[\frac{|x|^2}{2} + \frac{|y|^2}{2} + \log \frac{1}{|x\bar{y} - 1|} \right] - \frac{3}{8\pi} \quad (3.29)$$

where \bar{y} denotes the complex conjugate of $y \in D \subset \mathbb{R}^2 \cong \mathbb{C}$ and $x\bar{y}$ is the complex product of x and \bar{y} . Consequently F is also known explicitly. The left plot of Figure 1 shows a stationary point of \mathcal{J}_B that is an assembly of 40 discs. The locations of these discs are determined by numerically minimizing F .

This result has an analogy in three dimensions.

Theorem 3.6 ([34]) *Let $D \subset \mathbb{R}^3$ be a bounded and smooth domain, K be an integer, and ρ be such that $\frac{K4\pi\rho^3}{3} = \omega|D|$.*

1. *For every $\eta > 0$ there exists $\delta > 0$, depending on η , K and D only, such that if*

$$\frac{1.5 + \eta}{\rho^3} < \gamma < \frac{15 - \eta}{\rho^3}, \quad (3.30)$$

and

$$\rho < \delta, \quad (3.31)$$

then there exists a stationary point, stable in some sense.

2. The stationary point is a union of K sets, each of which is close to a ball of radius ρ .
3. The centers of the balls are determined by the analogous F in three dimensions in the same way.

One subtle difference between the two dimensional case and the three dimensional case is that in the three dimensions, the lower bound and the upper bound of γ in (3.30) are of the same order, while the corresponding bounds in two dimensions are of different orders. This difference can be ultimately attributed to the difference in the fundamental solutions of Δ in two and three dimensions: one is $\frac{1}{2\pi} \log \frac{1}{|x|}$ and the other is $\frac{1}{4\pi|x|}$.

4 The profile problem and ansatz solutions

As we mentioned earlier, Ren and Wei recognized in [33] that a disc is stationary with respect to the perimeter term and the singular part of the Green's function. The same idea was also used in [34] for a ball in the three dimensional analogy. In this section we elaborate on this idea and consider a profile problem that consists of the perimeter term and the singular part of the Green's function.

This profile problem is posed on the entire space \mathbb{R}^n . Let $m > 0$. For each Lebesgue measurable set Ω with the fixed Lebesgue measure m ,

$$|\Omega| = m, \quad (4.1)$$

define the energy

$$\mathcal{K}_B(\Omega) = \frac{1}{n-1} \mathcal{P}(\Omega) + \frac{\gamma}{2} \int_{\Omega} \mathcal{N}(\Omega)(x) dx. \quad (4.2)$$

In (4.2), $\mathcal{P}(\Omega)$ is the perimeter of Ω in \mathbb{R}^n , given by (1.3) with D being \mathbb{R}^n ; $\mathcal{N}(\Omega)$ is the Newtonian potential of Ω given by

$$\mathcal{N}(x) = \int_{\Omega} \Gamma(x-y) dy, \quad \forall x \in \mathbb{R}^n. \quad (4.3)$$

Here Γ is the fundamental solution of Δ in \mathbb{R}^n , i.e.,

$$\Gamma(x) = \begin{cases} \frac{1}{2\pi} \log \frac{1}{|x|} & \text{if } n = 2, \\ \frac{1}{n(n-1)\alpha(n)|x|^{n-2}} & \text{if } n \geq 3, \end{cases} \quad (4.4)$$

where $\alpha(n)$ is the volume of the unit ball in \mathbb{R}^n .

A regular stationary point Ω of \mathcal{K}_B satisfies

$$H(\partial\Omega) + \gamma \mathcal{N}(\Omega) = \lambda \quad (4.5)$$

on its boundary $\partial\Omega$. Often times we use a solution of (4.5) as a building block to construct a stationary assembly to (2.20), as in Theorems 3.4, 3.5, and 3.6. We call such a solution of the profile equation (4.5) an ansatz solution. We know that the unit disc in \mathbb{R}^2 and the unit ball in \mathbb{R}^3 are ansatz solutions.

In order to make a stable stationary assembly of (2.20) from an ansatz, the ansatz itself must be stable. For equation (4.5) the relevant concept here is the linearly stability. It turns out that the unit disc is linearly stable if

$$0 < \gamma < 12, \quad (4.6)$$

The number 12 is a bifurcation point. For γ near 12, (4.5) has an oval shaped bifurcation solution. This oval solution may also be used as an ansatz for an oval shaped solution of \mathcal{J}_B ; see Ren and Wei [35] for detail. In three dimensions the unit ball is linearly stable if

$$0 < \gamma < 15. \quad (4.7)$$

Interestingly, there are other ansatz solutions of (4.5). Kang and Ren proved that in two dimensions there is a ring like solution.

Theorem 4.1 ([12]) *There exists $\gamma_0 > 0$ such that if $\gamma > \gamma_0$, equation (4.5) admits a ring shaped solution $\Omega = \{x \in \mathbb{R}^2 : R_1 < |x| < R_2\}$ and $|\Omega| = \pi$. There is another value γ_1 (greater than γ_0) such that the ring is linearly stable if $\gamma > \gamma_1$ and linearly unstable if $\gamma \in (\gamma_0, \gamma_1)$.*

This ring ansatz was used by Kang and Ren in [13] to build a stationary assembly of rings, and also a stationary assembly of both rings and discs. The first assembly is stable, but the second is not.

In three dimensions, the obvious analogy of a ring is a shell, that is the set bounded by two concentric spheres. However it was proved in [24] by Ren that any shell solution of (4.5) must be linearly unstable. It is not known at the moment whether (4.5) has any linearly stable solution in \mathbb{R}^3 , which is not a ball.

There is one solution found by Ren and Wei which may play a role in three dimensions.

Theorem 4.2 ([36]) *When γ is sufficiently large, equation (4.5) has an approximately torus shaped, tube like solution in \mathbb{R}^3 of volume 1.*

Let $f = f(\gamma)$ be a function given by its inverse

$$\gamma = \frac{2}{f^3 \log \frac{1}{2\pi^2 f^3}},$$

Note $\lim_{\gamma \rightarrow \infty} f(\gamma) = 0$. If p_γ and q_γ are the two radii of the torus solution ($p_\gamma > q_\gamma$), then $2\pi^2 p_\gamma q_\gamma^2 = 1$ and

$$\lim_{\gamma \rightarrow \infty} \frac{q_\gamma}{f(\gamma)} = 1 \quad \text{and} \quad \lim_{\gamma \rightarrow \infty} 2\pi^2 f^2(\gamma) p_\gamma = 1$$

A cross section of this ansatz is approximately a round disc of radius q_γ . It is not known whether this solution is linearly stable.

5 A ternary inhibitory system

The functional \mathcal{J}_B of (1.1) can easily be generalizied to study inhibitory systems with more than two componetns. We consider a three component system in this section. This ternary system was originally derived by Ren and Wei in [28] from Nakazawa and Ohta's density functional formulation for triblock copolymers [19]. Again let D be a bounded and open set of \mathbb{R}^n . Suppose that ω_1 and ω_2 are two positive numbers such that $\omega_1 + \omega_2 < 1$. For two measurable subsets Ω_1 and Ω_2 of D satisfying $|\Omega_1| = \omega_1|D|$, $|\Omega_2| = \omega_2|D|$, and $|\Omega_1 \cap \Omega_2| = 0$, set $\Omega_3 = D \setminus (\Omega_1 \cup \Omega_2)$. The free energy of the system is

$$\mathcal{J}_T(\Omega_1, \Omega_2) = \frac{1}{2} \sum_{i=1}^3 \mathcal{P}_D(\Omega_i) + \sum_{i,j=1}^2 \int_D \frac{\gamma_{ij}}{2} \left((-\Delta)^{-1/2} (\chi_{\Omega_i} - \omega_i) \right) \left((-\Delta)^{-1/2} (\chi_{\Omega_j} - \omega_j) \right) dx. \quad (5.1)$$

Although experimentally an almost unlimited number of architectures can be synthetically accessed in ternary systems like triblock copolymers [3, Figure 5 and the magazine's cover], the mathematical study of \mathcal{J}_T is still in an early stage due to its complexity. Found by Ren and Wei in [29] is a one dimensional local minimizer of \mathcal{J}_T , consisting of alternating A , B , and C micro-domains. The functional \mathcal{J}_T is posed on the unit interval with the periodic boundary condition there. The matrix $\gamma = [\gamma_{ij}]$ is assumed to be positive definite in [29].

Another one dimensional stationary point, again a local minimizer of \mathcal{J}_T , was found by Choksi and Ren in [5]. This time one eigenvalue of γ is positive but the other one is 0 whose eigenvector is (ω_1, ω_2) . It models a diblock copolymer/homopolymer blend. Such a blend is a mixture of an AB diblock copolymer with a homopolymer of monomer species C , where the species C is thermodynamically incompatible with both the A and B monomer species. In this blend there is a *macroscopic phase separation* into homopolymer-rich and copolymer-rich domains followed by *micro-phase separation* within the copolymer-rich domains into A -rich and B -rich subdomains. The stationary point has the $ABAB\dots ABACC\dots C$ pattern.

A new challenge in a higher dimensional ternary system is the phenomenon of triple junction, where the three components come to meet. In two dimensions a triple junction occurs on points and in three dimensions a triple junction occurs on curves.

Two dimensional results came only recently in [37, 38, 39] by Ren and Wei. The stationary points they found are related to the fascinating structure of the double bubble; see Figure 2. This structure arises as the optimal configuration of the two component isoperimetric problem. The usual isoperimetric problem is a one component problem which asserts that the round sphere is the least-perimeter way to enclose a given volume. For the two component isoperimetric problem, one finds two disjoint sets E_1 and E_2 in \mathbb{R}^n of the prescribed Lebesgue measures such that the size of $\partial E_1 \cup \partial E_2$ is minimum. The double bubble is the unique solution to this isoperimetric problem by the works of Foisy *et al* [8], Hutchings *et al* [11], and Reichardt [23]. In two dimensions the planar double bubble is enclosed by three circular arcs that meet at two triple junction points, or triple points. The angles between the arcs at a triple point are all 120 degrees.

To state Ren and Wei's two dimensional results, introduce a fixed number $m \in (0, 1)$ and a small ϵ so that $\omega_1|D| = \epsilon^2 m$ and $\omega_2|D| = \epsilon^2(1 - m)$. The area constraints $|\Omega_1| = \omega_1|D|$ and $|\Omega_2| = \omega_2|D|$ takes the form

$$|\Omega_1| = \epsilon^2 m \quad \text{and} \quad |\Omega_2| = \epsilon^2(1 - m). \quad (5.2)$$

Instead of ω_1 and ω_2 , ϵ becomes one parameter of our problem. The fixed number m measures the relative area of $|\Omega_1|$ vs $|\Omega_2|$ since $\frac{|\Omega_1|}{|\Omega_2|} = \frac{m}{1-m}$.

The other parameter is the matrix γ . It must be positive definite and satisfy a uniform positivity condition. Namely, there exists $\iota > 0$ so that $\iota \bar{\lambda}(\gamma) \leq \bar{\lambda}(\gamma)$ where $\bar{\lambda}(\gamma)$ and $\bar{\bar{\lambda}}(\gamma)$ are the two eigenvalues of γ such that $0 < \bar{\lambda}(\gamma) \leq \bar{\bar{\lambda}}(\gamma)$. The matrix γ must also have a lower bound and an upper bound.

Theorem 5.1 ([39]) *Let D be a bounded and connected open set of \mathbb{R}^2 with smooth boundary, $m \in (0, 1)$, $n \in \mathbb{N}$, and $\iota \in (0, 1]$. There exist positive numbers δ , $\bar{\sigma}$, and σ depending on D , m , n , and ι only, such that if the following three conditions hold*

1. $0 < \epsilon < \delta$,
2. $\frac{\bar{\sigma}}{\epsilon^3 \log \frac{1}{\epsilon}} \leq \bar{\lambda}(\gamma) \leq \bar{\bar{\lambda}}(\gamma) < \frac{\sigma}{\epsilon^3}$,
3. $\iota \bar{\bar{\lambda}}(\gamma) \leq \bar{\lambda}(\gamma)$,

then there is a stationary assembly of n perturbed double bubbles, satisfying the constraints (5.2). Each perturbed double bubble is bounded by three smooth curves that meet at two triple junction points.

This solution is stable in some sense. If $n = 1$, the lower bound $\frac{\bar{\sigma}}{\epsilon^3 \log \frac{1}{\epsilon}} \leq \bar{\lambda}(\gamma)$ is not needed.

All the perturbed double bubbles in the stationary assembly have almost the same size and shape. The locations of the double bubbles are determined by the same function F of (3.21). This theorem was first proved for the $n = 1$ and symmetric ($m = \frac{1}{2}$) case in [37], then for the $n = 1$ and asymmetric ($m \in (0, 1)$) case in [38], and finally for the general case ($n \geq 2$ and $m \in (0, 1)$) in [39].

The right plot of Figure 1 illustrates this theorem with an assembly of 40 double bubbles in D which is the unit disc. As in Theorem 3.5 the locations of the double bubbles in the assembly are obtained by minimizing F . Theorem 5.1 does not tell what the directions of the double bubbles are, so the directions of the double bubbles in the figure are not the true directions in the stationary assembly.

In two dimensions, a regular stationary point (Ω_1, Ω_2) of \mathcal{J}_T is a solution to the following equations:

$$\kappa_1 + \gamma_{11}I_{\Omega_1} + \gamma_{12}I_{\Omega_2} = \lambda_1 \quad \text{on } \partial\Omega_1 \setminus \partial\Omega_2 \quad (5.3)$$

$$\kappa_2 + \gamma_{12}I_{\Omega_1} + \gamma_{22}I_{\Omega_2} = \lambda_2 \quad \text{on } \partial\Omega_2 \setminus \partial\Omega_1 \quad (5.4)$$

$$\kappa_0 + (\gamma_{11} - \gamma_{12})I_{\Omega_1} + (\gamma_{12} - \gamma_{22})I_{\Omega_2} = \lambda_1 - \lambda_2 \quad \text{on } \partial\Omega_1 \cap \partial\Omega_2 \quad (5.5)$$

$$\nu_1 + \nu_2 + \nu_0 = \vec{0} \quad \text{at } \partial\Omega_1 \cap \partial\Omega_2 \cap \partial\Omega_3. \quad (5.6)$$

Here we assume that Ω_1 and Ω_2 do not touch the boundary of D . Otherwise we need to add another condition that the boundary of Ω_1 (or Ω_2) meets the boundary of D perpendicularly.

In (5.3)-(5.5) κ_1 , κ_2 , and κ_0 are the curvatures of the curves $\partial\Omega_1 \setminus \partial\Omega_2$, $\partial\Omega_2 \setminus \partial\Omega_1$, and $\partial\Omega_1 \cap \partial\Omega_2$, respectively. These are signed curvatures defined with respect to a choice of normal vectors. For instance a circle has positive curvature if the normal vector is inward pointing. On $\partial\Omega_1 \setminus \partial\Omega_2$ the normal vector points inward into Ω_1 . On $\partial\Omega_2 \setminus \partial\Omega_1$, the normal vector points inward into Ω_2 . On $\partial\Omega_1 \cap \partial\Omega_2$, the normal vector points from Ω_2 towards Ω_1 , i.e. inward with respect to Ω_1 and outward with respect to Ω_2 .

As in the binary case I_{Ω_1} and I_{Ω_2} are inhibitors of Ω_1 and Ω_2 , respectively. The constants λ_1 and λ_2 are Lagrange multipliers corresponding to the constraints (5.2).

In the last equation, (5.6), ν_1 , ν_2 , and ν_0 are the inward pointing, unit tangent vectors of the curves $\partial\Omega_1 \setminus \partial\Omega_2$, $\partial\Omega_2 \setminus \partial\Omega_1$, and $\partial\Omega_1 \cap \partial\Omega_2$ at triple points. The requirement that the three unit vectors sum to zero is equivalent to the condition that the three curves meet at 120 degree angles.

The proof of Theorem 5.1 consists of several steps. In the first step, one constructs an assembly of exact double bubbles and compute its energy. Take K exact double bubbles B^k whose two bubbles are B_1^k and B_2^k for $k = 1, 2, \dots, K$. The area of B_i^k is w_i^k . Take K distinct points ξ^k in D and K angles $\theta^k \in \mathbb{S}^1$, where \mathbb{S}^1 is the unit circle. Scale down each B^k by a factor ϵ , rotate by the angle θ^k and place it in D centered at ξ^k . More precisely, let $T^k = T_{\epsilon, \xi^k, \theta^k}$ be the affine transformation

$$T^k(\hat{x}) = T_{\epsilon, \xi^k, \theta^k}(\hat{x}) = \epsilon e^{i\theta^k} \hat{x} + \xi^k, \quad (5.7)$$

and then map B^k into D by T^k . The image is a small double bubble denoted $T^k(B^k)$, and the collection $(T^1(B^1), T^2(B^2), \dots, T^K(B^K))$ is an assembly of exact double bubbles denoted by $T(B)$. This $T(B)$ depends on $\xi = (\xi^1, \dots, \xi^K)$, $\theta = (\theta^1, \dots, \theta^K)$, and $w = \{w_i^k\}$. One finds the energy of $T(B)$ as follows.

$$\begin{aligned} \mathcal{J}_T(T(B)) &= \epsilon \sum_{k=1}^K \sum_{i=0}^2 2a_i^k r_i^k + \left(\log \frac{1}{\epsilon}\right) \epsilon^4 \sum_{k=1}^K \sum_{i,j=1}^2 \frac{\gamma_{ij} w_i^k w_j^k}{4\pi} + \epsilon^4 \sum_{k=1}^K \sum_{i,j=1}^2 \frac{\gamma_{ij}}{2} \int_{B_i^k} \int_{B_j^k} \frac{1}{2\pi} \log \frac{1}{|\hat{x} - \hat{y}|} d\hat{x} d\hat{y} \\ &+ \epsilon^4 \sum_{k=1}^K \sum_{i,j=1}^2 \frac{\gamma_{ij}}{2} w_i^k w_j^k R(\xi^k, \xi^k) + \epsilon^4 \sum_{k \neq l} \sum_{i,j=1}^2 \frac{\gamma_{ij}}{2} w_i^k w_j^l G(\xi^k, \xi^l) + O(|\gamma|\epsilon^5). \end{aligned} \quad (5.8)$$

In the second step, perturb each B^k in a special way to define a restricted class of perturbed double bubble assemblies. There are actually two parts in the perturbation. First move the two triple points of B^k vertically in opposite directions by the same amount. Connect the new triple points by three circular arcs. The two sets bounded by the new arcs still have the areas w_1^k and w_2^k respectively and the radii ρ_i^k of the new arcs satisfy the condition $(\rho_1^k)^{-1} - (\rho_2^k)^{-1} = (\rho_0^k)^{-1}$. However the 120 degree angle condition at triple points no longer holds for the new arcs. In the second part of the restricted perturbation, the arcs are changed to more general curves, while the areas of the two enclosed sets remain to be w_i^k and the triple points are unchanged. This perturbed double bubble is denoted P^k . It is scaled down by ϵ and mapped into D by the same T^k . The collection $T(P) = (T^1(P^1), T^2(P^2), \dots, T^K(P^K))$ is an assembly of perturbed double bubbles. All assemblies obtained this way form a restricted class of perturbed double bubble assemblies. This class is specified by ξ , θ , and w .

It turns out that each assembly in a restricted class is identified by an element of a Hilbert space. The element consists of $3K$ functions ϕ_i^k and K numbers η^k for $k = 1, 2, \dots, K$ and $i = 1, 2, 0$. Collectively they are denoted by (ϕ, η) where $\phi = (\phi^1, \phi^2, \dots, \phi^K)$, $\phi^k = (\phi_1^k, \phi_2^k, \phi_0^k)$, and $\eta = (\eta^1, \eta^2, \dots, \eta^K)$. Within the restricted class \mathcal{J}_T becomes a functional on the Hilbert space.

In each restricted class there is an element (ϕ^*, η^*) that locally minimizes \mathcal{J}_T within the restricted class. This third step is most technical, involving an error estimate of the exact double bubble assembly $T(B)$, proving the positivity of the second variation of \mathcal{J}_T at $T(B)$, and a fixed point argument. It is shown that (ϕ^*, η^*) satisfies a weakened version of (5.3)-(5.5) where the constants λ_1 and λ_2 may vary from one perturbed double bubble to another perturbed double bubble in the assembly.

To fix this problem and also to have the 120 degree angle condition (5.6) satisfied, revisit the restricted class of perturbed double bubble assemblies. Since this class is specified by (ξ, θ, w) , the energy minimizing

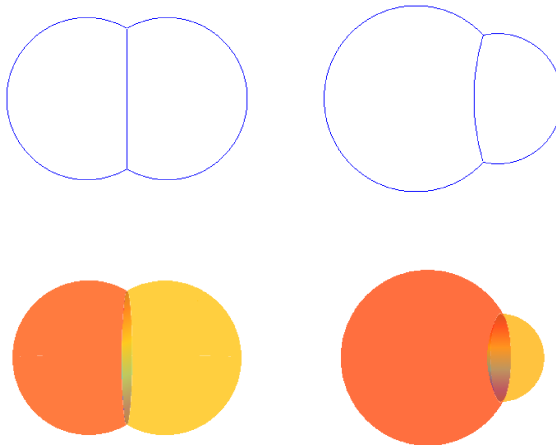


Figure 2: First row: two dimensional symmetric and asymmetric double bubbles. Second row: three dimensional symmetric and asymmetric double bubbles.

element (ϕ^*, η^*) in this class should be denoted by $(\phi^*(\cdot, \xi, \theta, w), \eta^*(\xi, \theta, w))$. In the fourth step one finds that the energy $\mathcal{J}(\phi^*(\cdot, \xi, \theta, w), \eta^*(\xi, \theta, w))$ of this element is close to that of $\mathcal{J}_T(T(B))$ given in (5.8). Treating this quantity as a function of ξ , θ , and w , one minimizes it with respect to (ξ, θ, w) and finds a minimum (ξ^*, θ^*, w^*) . If one uses the restricted class of assemblies specified by this particular (ξ^*, θ^*, w^*) , then the locally energy minimizing element $(\phi^*(\cdot, \xi^*, \theta^*, w^*), \eta^*(\xi^*, \theta^*, w^*))$ solves (5.3)-(5.5) exactly and also satisfies the 120 degree angle condition (5.6) at triple points. This completes the sketch of the proof.

6 Conclusions

I have mainly discussed stationary assemblies of the functionals \mathcal{J}_B and \mathcal{J}_T in this article. But implications go beyond these two functionals.

In the study of biological processes of organism development, the Gierer-Meinhardt system [14, 15, 18] is an often used model for morphogenesis patterns on animal coats and skin pigmentation. This is an activator-inhibitor type system of two partial differential equations on a bounded domain D :

$$u_t = \epsilon^2 \Delta u - u + \frac{u^p}{(1 + \kappa u^p)v^q}; \quad \tau v_t = d \Delta v - v + \frac{u^r}{v^s}, \quad (6.1)$$

with the zero Neumann boundary condition for both variables u and v . One can show formally that if d is of the order $\frac{1}{\epsilon}$, the u component of a stationary solution has a limit as $\epsilon \rightarrow 0$. This limit is a positive constant on a subset Ω of D and is 0 on $D \setminus \Omega$. The Lebesgue measure $|\Omega|$ is determined by the parameters in (6.1), and most interestingly Ω satisfies the same equation (2.20); see [36] for detail.

Despite the lack of a free energy functional, the Gierer-Meinhardt system contains mechanisms that produce growth and inhibition. The Euler-Lagrange equation (2.20) of \mathcal{J}_B can be regarded as a singular limit of (6.1), a simplification that retains the key properties of (6.1).

This article should have convinced the reader that the functionals \mathcal{J}_B and \mathcal{J}_T , although minimalist, are powerful enough to model pattern formation. I hope that more sophisticated patterns of interest will emerge from deep analysis of these inhibitory systems.

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