Models of pattern formation

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MODELS OF PATTERN FORMATION

by

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Abstract.

Patterned structures are represented by means of a potential equal to the sum of a non-convex functional with the perimeter functional. This is also a model of stable and metastable states in two-phase systems with surface tension. A generalization based on an extension of Fleming-Rishel's coarea formula allows to deal with very irregular configurations, with boundary of fractional dimension.

1. Two phase systems

This note announces some of the results of [4,5]. The corresponding evolution model is developed in [6]. Here we shall deal just with two-phase systems; however the extension to more phases is obvious.

Let \( \Omega \) be a "smooth" bounded domain of \( \mathbb{R}^N (N \geq 1) \) and \( u \in L^1(\Omega) \). We shall denote by \( \mu \) the \( N \)-dimensional Lebesgue measure. If there exists an interval \([\alpha, \beta] \subset \mathbb{R}\) such that \( \mu(\{x \in \Omega : \alpha < u(x) < \beta\}) = 0 \), then it is natural to decompose \( \Omega \) in the sets (phases) \( \Omega_- := \{x \in \Omega : u(x) < \frac{\alpha + \beta}{2}\}, \Omega_+ := \{x \in \Omega : u(x) > \frac{\alpha + \beta}{2}\} \). Thus the system can be regarded as patterned. These phases can be very irregular; however they are stable for small \( L^\infty \)-perturbations of \( u \).

Now we shall see how two-(or more) phase systems can be represented by means of non-convex potentials. Let

\[
\phi : \mathbb{R} \rightarrow \mathbb{R} \cup \{+\infty\} \text{ be lower semicontinuous and proper,}
\]

\[
\lim_{|v| \rightarrow +\infty} \frac{\phi(v)}{|v|} = +\infty.
\]

The case of interest is that of non-convex \( \phi \), as in fig. 1.

![Fig.1a](image-url)
Fig. 1. Examples of non convex potentials. (1a) \( u = b, u = d \) and \( u = h \) are minimum, relative maximum and absolute minimum points of \( \phi^{(1)} \), respectively; \( u = c \) and \( u = f \) are flexi. The drawn segment is tangent to the graph of \( \phi^{(1)} \) at \( u = a, g \).

(1b) \( a \in \mathbb{R} \) and

\[
\phi^{(2)}(v) := \frac{1}{2}(1 - v^2) \quad \text{if} \quad |v| \leq 1; \quad \phi^{(2)}(v) = +\infty \quad \text{if} \quad |v| > 1.
\]

Then we fix any \( \theta \in L^\infty(\Omega) \) and set

\[
(1.3) \quad \Phi_\theta(v) := \int_\Omega [\phi(v(x)) - \theta(x)v(x)] \, dx \leq +\infty \quad \forall v \in L^1(\Omega).
\]

Note that there exists at least one \( u \in L^1(\Omega) \) such that \( \Phi_\theta(u) = \inf \Phi_\theta \). Moreover, setting \( \phi_\xi(v) := \phi(v) - \xi v \quad \forall \xi, v \in \mathbb{R} \), we have

\[
(1.4) \quad \begin{cases} 
\Phi_\theta(u) = \inf \Phi_\theta \iff \phi_\theta(x)(u(x)) = \inf \phi_\theta(x) \quad \text{a.e. in } \Omega \\
\iff \partial \phi_\theta(u(x)) \ni \theta(x) \quad \text{a.e. in } \Omega \iff \partial \phi_\theta(u(x)) \neq \emptyset \quad \text{a.e. in } \Omega.
\end{cases}
\]

Thus for \( \phi = \phi^{(i)}(i = 1, 2) \), we have

\[
(1.5) \quad \Phi_\theta = \inf \Phi_\theta \Rightarrow \begin{cases} 
\phi^{(1)} \quad \text{a.e. in } \Omega \text{ if } \phi = \phi^{(1)}; \\
\phi^{(2)} \quad \text{a.e. in } \Omega \text{ if } \phi = \phi^{(2)}
\end{cases}
\]

Thus any absolute minimum point of \( \phi^{(i)} \) corresponds to a patterned structure: \( \Omega = \{x : u(x) \leq a\} \cup \{x : u(x) \geq g\} \) for \( \phi = \phi^{(1)} \); \( \Omega = \{x : u(x) = -1\} \cup \{x : u(x) = 1\} \) for \( \phi = \phi^{(2)} \).

Physical interpretation for \( \phi = \phi^{(2)} \). We consider a solid-liquid system (water and ice, e.g.). Let \( \theta \) be (proportional to) the relative temperature; set \( u = -1 \) in ice and \( u = 1 \) in water. Then for \( \phi = \phi^{(2)}, \Phi_\theta \) represents the free energy, and the minimum condition “\( \partial \phi^{(2)}(u(x)) \ni \theta(x) \quad \text{a.e. in } \Omega \)” corresponds to the usual phase rule

\[
(1.6) \quad u = -1 \quad \text{where } \theta < 0, \quad u = 1 \quad \text{where } \theta > 0, \text{ a.e. in } \Omega.
\]
2. Relative minima

For suitable values of $\theta \in \mathbb{R}$, the non-convex real function $\phi_\theta : v \to \phi(v) - \theta v$ may have a relative (non-absolute) minimum (in $\mathbb{R}$). Note that also for relative minima an excluded zone appears, which may or may not coincide with that of absolute minima. Let us set

\[
\text{Abs}(\phi) := \{v \in \mathbb{R} : v \text{ is an absolute minimum point of } \phi_\theta \text{ for some } \theta \in \mathbb{R}\},
\]

\[
\text{Rel}(\phi) := \{v \in \mathbb{R} : \text{v is a relative minimum point of } \phi_\theta \text{ for some } \theta \in \mathbb{R}\};
\]

thus for instance

\[(2.1) \quad \text{Rel}(\phi^{(1)}) = ]-\infty, c[ \cup ]f, +\infty[, \quad \text{Abs}(\phi^{(1)}) = ]-\infty, a[ \cup [g, +\infty[,
\]

\[(2.2) \quad \text{Rel}(\phi^{(2)}) = \text{Abs}(\phi^{(2)}) = \{ -1, 1 \}.
\]

Note that in several cases (but not always!)

\[
\text{Abs}(\phi) = \{ v \in \mathbb{R} : \phi''(v) = \phi(v) \}, \quad \text{Rel}(\phi) = \{ v \in \mathbb{R} : \phi''(v) > 0 \}).
\]

The situation is different for space dependent systems:

**Proposition.** For any $\theta \in L^\infty(\Omega), \phi_\theta$ has no relative (non-absolute) minimum point with respect to the topology of $L^1(\Omega)$.

This can be easily understood by means of the following example. Let us take $\phi = \phi^{(1)}$ and $\theta \equiv 0$ in $\Omega$. We shall show that the function $u \equiv b$ in $\Omega$ is not a relative minimum point of $\phi_\theta$ with respect to the topology of $L^1(\Omega)$. For any set $A \subset \Omega$ with $\mu(A) > 0$, set

\[
u_A := b \quad \text{in } \Omega \setminus A, \quad u := h \text{ in } A.
\]

Then $\Phi_\theta(u_A) < \Phi_\theta(u)$ and $\|u - u_A\|_{L^1(\Omega)} \to 0$ as $\mu(A) \to 0$.

**Physical interpretation.** The points of absolute minimum of the potential can be interpreted as states of stable equilibrium, and those of relative minimum as states of metastable equilibrium. The latter can persist just for a limited time; they eventually decay, because thermodynamic fluctuations let the system explore nearby states. By proposition 1, metastable states cannot be represented by means of the potential $\Phi_\theta$, for any $\theta \in L^\infty(\Omega)$.  

3. Surface tension

We introduce a space interaction term, containing space derivatives:

\[ V(v) = \int_{\Omega} |\nabla v| := \sup \left\{ \int_{\Omega} v \text{div} \eta \, dx : \eta \in C^1_c(\Omega)^N, |\eta| \leq 1 \text{ in } \Omega \right\} (\leq +\infty) \forall v \in L^1(\Omega). \]

and define the potential functional (\( \sigma \) being a positive constant)

\[ \Psi_\theta(v) := \int_{\Omega} [\phi(v(x)) - \theta(x)v(x)] \, dx + \frac{\sigma}{2} V(v) (\leq +\infty) \forall v \in L^1(\Omega). \]

**Proposition 2.** For suitable \( \theta \in L^{\infty}(\Omega) \), \( \Psi_\theta \) has a relative (non-absolute) minimum with respect to the topology of \( L^1(\Omega) \).

In order to illustrate this statement, let us still consider the case of \( \phi = \phi^{(1)} \), \( \theta \equiv 0 \) in \( \Omega \), \( u \) and \( u_A \) as in section 2. Then, denoting by \( \chi_A \) the characteristic function of \( A \),

\[ \Psi_\theta(u_A) - \Psi_\theta(u) = [\phi(h) - \phi(b)] \mu(A) + (h - b) \frac{\sigma}{2} V(\chi_A); \]

the latter is positive for \( \mu(A) \ll 1 \), because

\[ \lim_{\mu(A) \to 0} \frac{V(\chi_A)}{\mu(A)} = +\infty. \]

**Physical interpretation.** By proposition 2, \( \Psi_\theta \) allows to represent states of metastable equilibrium. According to the previous model of ice and water systems, \( \frac{\sigma}{2} V(u) \) is the surface tension contribution to the free energy.

**Remark.** If in (3.2) \( V(u) \) where replaced by \( \int_{\Omega} |\nabla u|^p \, dx \) for some \( p \in [1, +\infty[ \), then proposition 2 would still hold. However, setting \( \Phi_\theta^p(u) := \Phi_\theta(u) + \int_{\Omega} |\nabla u|^p \, dx \),

\[ \phi_\theta^p(v) < +\infty \Rightarrow v \in W^{1,p}(\Omega) \Rightarrow v \text{ cannot jump along any (smooth) interior surface } \Rightarrow v \text{ does not represent a patterned structure.} \]

On the contrary the condition \( \Phi_\theta(u) < +\infty \) is obviously consistent with the presence of such discontinuities.
4. Main result

Theorem 1 [4]. Assume that (1.1), (1.2) hold and that

\[(4.1) \quad \text{any connected component of } \{ y \in \mathbb{R} : \phi^{**}(y) < \phi(y) \} \text{ is bounded.} \]

Then for any \( u \in L^1(\Omega) \)

\[(4.2) \quad \partial(\Phi + V)(u) = \partial\Phi(u) + \partial V(u) \quad \text{in } L^\infty(\Omega), \]

\[(4.3) \quad (\Phi + V)^**(u) = \Phi^{**}(u) + V(u). \]

In particular, for any \( u \in L^1(\Omega) \)

\[(4.4) \quad \begin{cases} 
\partial(\Phi + V)(u) \neq 0 \text{ in } L^\infty(\Omega) \Rightarrow \partial\Phi(u) \neq 0 \text{ in } L^\infty(\Omega) \Rightarrow \\
\partial\phi(u(x)) \neq 0 \text{ a.e. in } \Omega \Leftrightarrow u(x) \in \text{Abs}(\phi) \text{ a.e. in } \Omega; 
\end{cases} \]

hence, for any \( \theta \in L^\infty(\Omega) \),

\[(4.5) \quad \begin{cases} 
\text{if } u \text{ is an absolute minimum point of } \Psi_{\theta}(\text{i.e., } \partial(\Phi + V)(u) \in \Theta), \\
\text{then } u(x) \in \text{Abs}(\phi) \text{ a.e. in } \Omega. 
\end{cases} \]

A similar result can be shown for relative minima [4]:

\[(4.6) \quad \begin{cases} 
\text{if } u \text{ is a relative minimum point of } \Psi_{\theta} \text{ (with respect to} \\
\text{the topology of } L^1(\Omega), \text{ then } u(x) \in \text{Rel}(\phi) \text{ a.e. in } \Omega. 
\end{cases} \]

Physical interpretation of (4.5) and (4.6): points of either absolute or relative minimum of \( \Psi_{\theta} \), which were interpreted as stable and metastable states, respectively, have a phase structure.

If \( \phi = \phi^{(2)} \) and \( u \) is an either absolute or relative minimum of \( \Psi_{\theta} \), then by either (4.5) or (4.6), \(|u(x)| = 1 \) a.e. in \( \Omega \); namely \( u \) corresponds to a two-phase structure. Moreover if \( \theta \in C^0(\Omega) \) and the interface \( S \) between these phases is "smooth", then by a standard surface variation argument one gets the classical Gibbs-Thomson law:

\[(4.7) \quad \theta = -\sigma \kappa \quad \text{on } S, \]

where \( \kappa \) denotes the mean curvature of \( S \), assumed positive for an ice ball.

Theorem 1 also plays a crucial role in a model of the evolution of non-Cartesian surfaces of codimension 1 [6].
5. Generalized coarea formula.

The functional $V$ fulfils the classical Fleming-Rishel coarea formula [2,3]

\[ V(u) = \int_{\mathbb{R}} V(H_s(u)) ds(\leq +\infty) \quad \forall u \in L^1(\Omega), \]

where for any $y, s \in \mathbb{R}$, $H_s(y) := 0$ if $y < s$, $H_s(y) := 1$ if $y \geq s$.

This formula plays a crucial role in the proof of Theorem 1. Actually, as shown in [4], that result holds also if $V$ is replaced by any functional $\Lambda : L^1(\Omega) \to [0, +\infty]$ such that

\[ \Lambda \text{ is convex and lower semi-continuous (i.e., } \Lambda = \Lambda^{**}, \]

\[ \Lambda \text{ fulfils the "generalized coarea formula" (5.1).} \]

If moreover

\[ \text{the inclusion } \text{Dom}(\Lambda) \subset L^1(\Omega) \text{ is compact,} \]

then, for any $\phi$ fulfilling (1.1), (1.2), and for any $\theta \in L^\infty(\Omega)$, the functional $\Psi_\theta : u \to \Phi(u) + \Lambda(u) - \int_{\Omega} \theta u \, dx$ has an absolute minimum. And finally, if also

\[ \lim_{\mu(A) \to 0} \frac{\Lambda(\chi_A)}{\mu(A)} = +\infty, \]

then, for suitable $\Phi$ and $\theta$, $\Psi_\theta$ has also a relative (non-absolute) minimum point in $L^1(\Omega)$.

All of these conditions are fulfilled not only by $V$, but also by

\[ \Lambda_r(u) := \iint_{\Omega^2} |u(x) - u(y)| \cdot |x - y|^{-(N+r)} \, dx \, dy \quad (0 < r < 1), \]

and, setting $B_h(x) := \{ y \in \mathbb{R}^N : |x - y| \leq h \}$, by

\[ \tilde{\Lambda}_r(u) := \int_{\mathbb{R}^+} h^{-(1+r)} \, dh \int_{\Omega} \left( \text{ess sup}_{B_h(x) \cap \Omega} u - \text{ess inf}_{B_h(x) \cap \Omega} u \right) \, dx \quad (0 < r < 1). \]

Note that $\text{Dom}(\Lambda_r) = W^{r,1}(\Omega)$, fractional Sobolev space; also $\text{Dom}(\tilde{\Lambda}_r)$ is a Banach space. Moreover

\[ \text{Dom}(\Lambda_{r_2}) \subset \neq \text{Dom}(\Lambda_{r_1}), \quad \text{Dom}(\tilde{\Lambda}_{r_2}) \subset \neq \text{Dom}(\tilde{\Lambda}_{r_1}) \quad \text{if } 0 < r_1 < r_2 < 1; \]

\[ \text{Dom}(\tilde{\Lambda}_r) \subset \neq \text{Dom}(\Lambda_r) \quad \text{if } 0 < r < 1. \]
6. Fractal boundaries

By De Giorgi's theory [3], for any set \( A \subseteq \Omega \) if \( \chi_A \in \text{Dom}(V)(= BV(\Omega)) \), then the reduced boundary \( \partial^* A \) of \( A \) has finite \((N-1)\)-dimensional Hausdorff measure. For any \( r \in ]0,1[ \), \( BV(\Omega) \subseteq \text{Dom}(\lambda_r) \) and \( BV(\Omega) \subseteq \text{Dom}(\tilde{\lambda}_r) \); so the conditions \( \chi_A \in \text{Dom}(\lambda_r) \) and \( \chi_A \in \text{Dom}(\tilde{\lambda}_r) \) yield less regularity for the (essential) boundary of \( A \), which can be regarded as a fractal set. Actually, both classes of functionals \( \{\lambda_r\}_{0<r<1} \) and \( \{\tilde{\lambda}_r\}_{0<r<1} \) induce in a natural way two definitions of fractional dimension for set boundaries. For any measurable set \( A \subseteq \Omega \), let us denote by \( \partial_e A \) its essential boundary in \( \Omega \), that is

\[
\partial_e A := \{ x \in \Omega : \mu(B_h(x) \cap \Omega) > 0, \mu(B_h(x) \cap (\mathbb{R}^N \setminus \Omega)) < 0 \ \forall h > 0 \}.
\]

Assuming \( \partial_e A \neq \emptyset \), we then define the dimension of \( \partial_e A \) relative to the functionals \( \{\lambda_r\}_{0<r<1} \):

\[
\text{Dim}_{\{\lambda_r\}}(\partial_e A) := N - \sup\{ r \in ]0,1[ : \lambda_r(\chi_A) < +\infty \}.
\]

Under the condition that \( \Omega \) be bounded, the dimension of \( \partial_e A \) relative to the functionals \( \{\tilde{\lambda}_r\}_{0<r<1} \) can be defined similarly. The latter dimension is strictly related to the Minkowski-Bouligand dimension [5].

Physical applications. For any \( r \in ]0,1[ \), the functionals \( \lambda_r \) and \( \tilde{\lambda}_r \) can be used to model very irregular interfaces, as in dendritic formations and in snowflakes; so \( \lambda_r(\chi_A) \) and \( \tilde{\lambda}_r(\chi_A) \) can be regarded as generalized surface tension contributions to the free energy.

References


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