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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 Ω be a "smooth" bounded domain of \mathbf{R}^N ($N \geq 1$) and $u \in L^1(\Omega)$. We shall denote by μ the N -dimensional Lebesgue measure. If there exists an interval $]\alpha, \beta[\subset \mathbf{R}$ such that $\mu(\{x \in \Omega : \alpha < u(x) < \beta\}) = 0$, then it is natural to decompose Ω 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^∞ -perturbations of u .

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

$$(1.1) \quad \phi : \mathbf{R} \rightarrow \mathbf{R} \cup \{+\infty\} \text{ be lower semicontinuous and proper,}$$

$$(1.2) \quad \lim_{|v| \rightarrow +\infty} \frac{\phi(v)}{|v|} = +\infty.$$

The case of interest is that of *non-convex* ϕ , as in fig. 1.

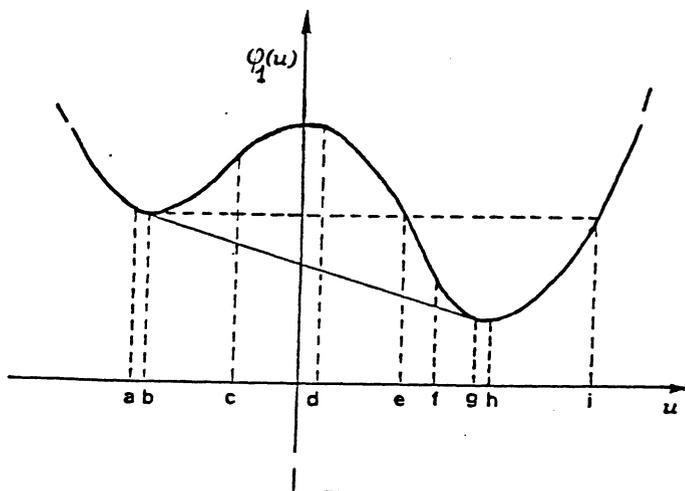


Fig.1a

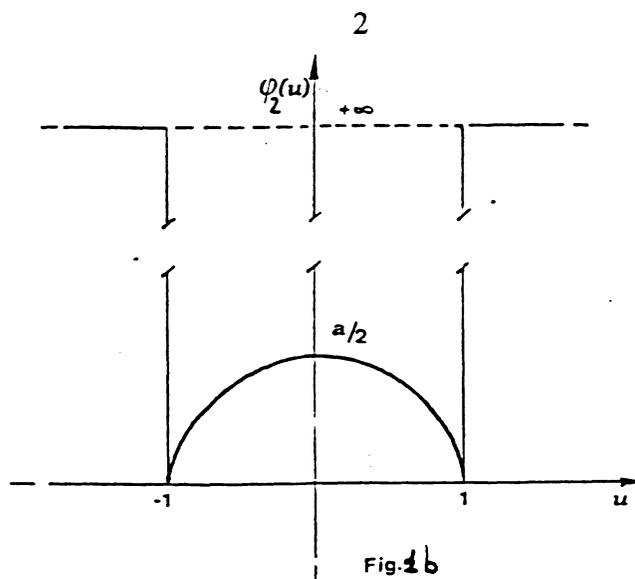


Fig. 1. Examples of non convex potentials. **(1a)** $u = b, u = d$ and $u = h$ are minimum, relative maximum and absolute minimum points of $\phi^{(1)}$, respectively; $u = c$ and $u = f$ are flexi. The drawn segment is tangent to the graph of $\phi^{(1)}$ at $u = a, g$.

(1b) $a \in \mathbf{R}$ and

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

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 $\phi_\xi(v) := \phi(v) - \xi v \quad \forall \xi, v \in \mathbf{R}$, we have

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

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

$$(1.5) \quad \Phi_\theta = \inf \Phi_\theta \implies \begin{cases} u(x) \notin]a, g[\quad \text{a.e. in } \Omega \text{ (if } \phi = \phi^{(1)}); \\ |u(x)| = 1 \quad \text{a.e. in } \Omega \text{ (if } \phi = \phi^{(2)}) \end{cases}$$

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 θ be (proportional to) the relative temperature; set $u = -1$ in ice and $u = 1$ in water. Then for $\phi = \phi^{(2)}$, Φ_θ represents the *free energy*, and the minimum condition " $\partial\phi^{(2)}(u(x)) \ni \theta(x)$ a.e. in Ω " 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 $\theta \in \mathbf{R}$, the non-convex real function $\phi_\theta : v \rightarrow \phi(v) - \theta v$ may have a relative (non-absolute) minimum (in \mathbf{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

$$\begin{aligned} \text{Abs}(\phi) &:= \{v \in \mathbf{R} : v \text{ is an } \textit{absolute} \text{ minimum point of } \phi_\theta \text{ for some } \theta \in \mathbf{R}\}, \\ \text{Rel}(\phi) &:= \{v \in \mathbf{R} : v \text{ is a } \textit{relative} \text{ minimum point of } \phi_\theta \text{ for some } \theta \in \mathbf{R}\}; \end{aligned}$$

thus for instance

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

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

Note that in several cases (but not always!)

$$\text{Abs}(\phi) = \{v \in \mathbf{R} : \phi^{**}(v) = \phi(v)\}, \quad \text{Rel}(\phi) = \{v \in \mathbf{R} : \phi''(v) > 0\}.$$

The situation is different for space dependent systems:

Proposition. For any $\theta \in L^\infty(\Omega)$, ϕ_θ 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 Ω . We shall show that the function $u \equiv b$ in Ω is *not* a relative minimum point of ϕ_θ with respect to the topology of $L^1(\Omega)$. For any set $A \subset \Omega$ with $\mu(A) > 0$, set

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

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

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 Φ_θ , for any $\theta \in L^\infty(\Omega)$.

3. Surface tension

We introduce a *space interaction term*, containing space derivatives:

$$(3.1) \quad V(v) = \int_{\Omega} |\nabla v| := \sup \left\{ \int_{\Omega} v \operatorname{div} \eta \, dx : \eta \in C_c^1(\Omega)^N, |\eta| \leq 1 \text{ in } \Omega \right\} (\leq +\infty) \forall v \in L^1(\Omega).$$

and define the potential functional (σ being a positive constant)

$$(3.2) \quad \Psi_{\theta}(v) := \int_{\Omega} [\phi(v(x)) - \theta(x)v(x)] \, dx + \frac{\sigma}{2} V(v) (\leq +\infty) \quad \forall v \in L^1(\Omega).$$

Proposition 2. For suitable $\theta \in L^{\infty}(\Omega)$, Ψ_{θ} 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 Ω , u and u_A as in section 2. Then, denoting by χ_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

$$(3.3) \quad \lim_{\mu(A) \rightarrow 0} \frac{V(\chi_A)}{\mu(A)} = +\infty.$$

Physical interpretation. By proposition 2, Ψ_{θ} 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) $V(u)$ were replaced by $\int_{\Omega} |\nabla u|^p dx$ for some $p \in [1, +\infty[$, then proposition 2 would still hold. However, setting $\Psi_{\theta}^p(u) := \Phi_{\theta}(u) + \int_{\Omega} |\nabla u|^p dx$,

$$(3.4) \quad \left\{ \begin{array}{l} \Psi_{\theta}^p(v) < +\infty \Rightarrow v \in W^{1,p}(\Omega) \Rightarrow v \text{ cannot jump along} \\ \text{any (smooth) interior surface} \Rightarrow v \text{ does not represent a} \\ \text{patterned structure} . \end{array} \right.$$

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

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

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 $u \in L^1(\Omega)$

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

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

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

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

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

Physical interpretation of (4.5) and (4.6): points of either absolute or relative minimum of Ψ_θ , 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 Ψ_θ , then by either (4.5) or (4.6), $|u(x)| = 1$ a.e. in Ω ; namely u corresponds to a two-phase structure. Moreover if $\theta \in C^0(\Omega)$ and the interface \mathcal{S} between these phases is “smooth”, then by a standard surface variation argument one gets the classical *Gibbs-Thomson law* :

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

where κ denotes the mean curvature of \mathcal{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]

$$(5.1) \quad V(u) = \int_{\mathbf{R}} V(H_s(u)) ds (\leq +\infty) \quad \forall u \in L^1(\Omega),$$

where for any $y, s \in \mathbf{R}$, $H_s(y) := 0$ 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 $\wedge : L^1(\Omega) \rightarrow [0, +\infty]$ such that

$$(5.2) \quad \wedge \text{ is convex and lower semi-continuous (i.e., } \wedge = \wedge^{**}),$$

$$(5.3) \quad \wedge \text{ fulfils the "generalized coarea formula" (5.1).}$$

If moreover

$$(5.4) \quad \text{the inclusion } \text{Dom}(\wedge) \subset L^1(\Omega) \text{ is compact,}$$

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

$$(5.5) \quad \lim_{\mu(A) \rightarrow 0} \frac{\wedge(\chi_A)}{\mu(A)} = +\infty,$$

then, for suitable Φ and θ , Ψ_θ^\wedge 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

$$(5.6) \quad \wedge_r(u) := \iint_{\Omega^2} |u(x) - u(y)| \cdot |x - y|^{-(N+r)} dx dy \quad (0 < r < 1),$$

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

$$(5.7) \quad \tilde{\wedge}_r(u) := \int_{\mathbf{R}^+} h^{-(1+r)} dh \int_{\Omega} \left(\text{ess sup}_{B_h(x) \cap \Omega} u - \text{ess inf}_{B_h(x) \cap \Omega} u \right) dx \quad (0 < r < 1).$$

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

$$(5.8) \quad \text{Dom}(\wedge_{r_2}) \subsetneq \text{Dom}(\wedge_{r_1}), \quad \text{Dom}(\tilde{\wedge}_{r_2}) \subsetneq \text{Dom}(\tilde{\wedge}_{r_1}) \quad \text{if } 0 < r_1 < r_2 < 1;$$

$$(5.9) \quad \text{Dom}(\tilde{\wedge}_r) \subsetneq \text{Dom}(\wedge_r) \quad \text{if } 0 < r < 1.$$

6. Fractal boundaries

By De Giorgi's theory [3], for any set $A \subset \Omega$ 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 $r \in]0, 1[$, $BV(\Omega) \subsetneq \text{Dom}(\Lambda_r)$ and $BV(\Omega) \subsetneq \text{Dom}(\tilde{\Lambda}_r)$; 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 $A \subset \Omega$, let us denote by $\partial_e A$ its *essential boundary in* Ω , that is

$$\partial_e A := \{x \in \Omega : \mu(B_h(x) \cap \Omega) \neq 0, \mu(B_h(x) \cap (\mathbf{R}^N \setminus \Omega)) \neq 0 \quad \forall h > 0\}.$$

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 Ω 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 Λ_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*.

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