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MODELS OF PATTERN FORMATION

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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*) $\Omega_- := \left\{x \in \Omega : u(x) < \frac{\alpha+\beta}{2}\right\}$, $\Omega_+ := \left\{x \in \Omega : u(x) > \frac{\alpha+\beta}{2}\right\}$. 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) $\qquad \phi : \mathbf{R} \to \mathbf{R} \cup \{+\infty\}$ be lower semicontinuous and proper,

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

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

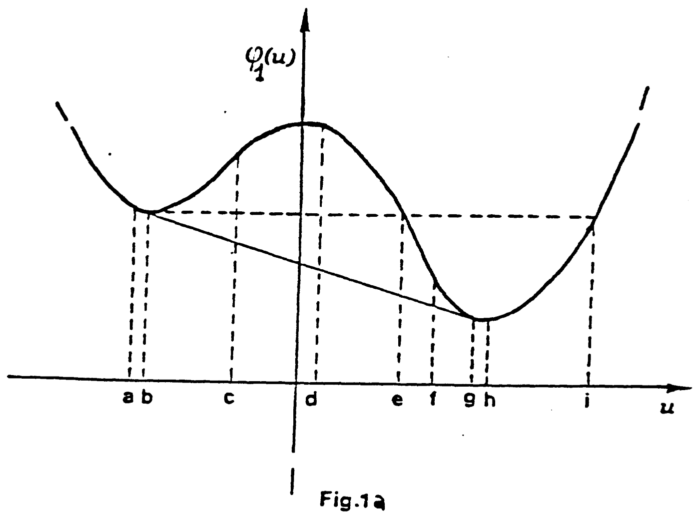

Fig.1a

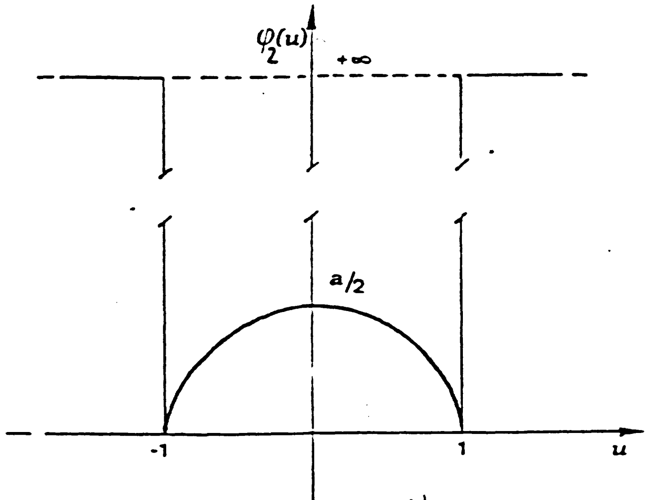

Fig. 1b

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

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

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

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

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

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

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

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

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 $\phi = \phi^{(2)}, \Phi_\theta$ 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*

$$(1.6) \qquad u = -1 \quad \text{where } \theta < 0, \qquad u = 1 \quad where \quad \theta > 0,\ a.e. in\, \Omega.$$

2. Relative minima

For suitable values of $\theta \in \mathbf{R}$, the non-convex real function $\phi_\theta : v \to \phi(v) - \theta v$ 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

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

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

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 $\theta \in L^\infty(\Omega), \phi_\theta$ 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 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

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

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

3. Surface tension

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

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

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

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

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 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 $\mu(A) << 1$, because

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

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

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

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*

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

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

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

$$\text{(4.3)} \qquad (\Phi + V)^{**}(u) = \Phi^{**}(u) + V(u).$$

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

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

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

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

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

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

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* :

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

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 Flerning-Rishel *coarea formula* [2,3]

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

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

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 $\wedge : L^1(\Omega) \to [0, +\infty]$ such that

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

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

If moreover

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

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

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

then, for suitable Φ and $\theta, \Psi_\theta^\wedge$ 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) $$\wedge_r(u) := \iint_{\Omega^2} |u(x) - u(y)| \cdot |x - y|^{-(N+r)} dx dy \qquad (0 < r < 1),$$

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

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

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

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

(5.9) $$Dom(\tilde{\wedge}_r) \underset{\neq}{\subset} Dom(\wedge_r) \qquad if \quad 0 < r < 1.$$

6. Fractal boundaries

By De Giorgi's theory [3], for any set $A \subset \Omega$ if $\chi_A \in Dom(V)(= BV(\Omega))$, then the *reduced boundary* $\partial^* A$ of A has finite $(N-1)$-dimensional Hausdorff measure. For any $r \in]0,1[\,, BV(\Omega) \subsetneqq Dom(\wedge_r)$ and $BV(\Omega) \subsetneqq Dom(\tilde{\wedge}_r)$; so the conditions $\chi_A \in Dom(\wedge_r)$ and $\chi_A \in Dom(\tilde{\wedge}_r)$ yield less regularity for the (essential) boundary of A, which can be regarded as a *fractal set* . Actually, both classes of functionals $\{\wedge_r\}_{0<r<1}$ and $\{\tilde{\wedge}_r\}_{0<r<1}$ 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

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

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

$$Dim_{\{\wedge_r\}}(\partial_e A) := N - sup\{r \in]0,1[\, : \wedge_r(\chi_A) < +\infty\}.$$

Under the condition that Ω be bounded, the *dimension of* $\partial_e A$ *relative to the functionals* $\{\tilde{\wedge}_r\}_{0<r<1}$ 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 $\wedge_r$ and $\tilde{\wedge}_r$ can be used to model very irregular interfaces, as in *dendritic* formations and in snowflakes; so $\wedge_r(\chi_A)$ and $\tilde{\wedge}_r(\chi_A)$ can be regarded as *generalized surface tension* contributions to the *free energy* .

References

[1] **B. Chalmers**: *Principles of solidification.* Wiley, New York (1964).

[2] **W.H. Fleming, R. Rishel**: *An integral formula for total gradient variation.* Arch. Math., **11** (1960), 218-222.

[3] **E. Giusti**: *Minimal surfaces and functions of bounded variation.* Birkhäuser, Boston (1984).

[4] **A. Visintin**: *Non-convex functionals related to multiphase systems.* (Preprint, 1987).

[5] **A.Visintin**: *Generalized coarea formula and fractal sets.* (Preprint 1988).

[6] **A. Visintin**: *Pattern evolution* (Preprint 1988).

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