2) Phase transition models: the Cahn-Hilliard model and the Modica-Mortola theorem 28.11.2024

<u>Classical Model</u>: $(n=3)$ Phase separation

1) Consider a container filled with 2 immiscible and incompressible fluids
example: oil and water; two different phases of the same fluid, like ice and water at $0°$.

2) In the classical theory of phase transitions it is assumed that, at equilibrium, the two liquids arrange themselves in order to minimize the area of the interface which separates the two phases.

<u>Remark</u>: We are neglecting any possible interaction of the fluids with the wall of the container and the effect of gravity.

· We would like to mathematically model the previous situation:

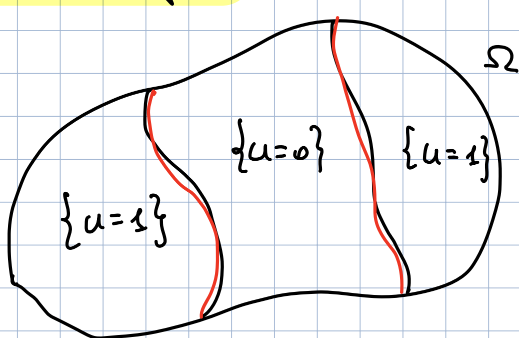
- Let $\Omega \subseteq \mathbb{R}^3$ be open, bounded and regular enough $\rightsquigarrow$ the container
- Let $u: \Omega \longrightarrow \{0,1\}$ $\rightsquigarrow$ every possible configuration of the system, where

  $\{u=0\}$ = set occupied by the first fluid

  $\{u=1\}$ = set occupied by the second fluid

- Denote S_u the singular set of u (set of discontinuity points of u), which is the interface between the two fluids.

$\Rightarrow$ By (2) the interface S_u is a minimal surface.



- Denote $vol(\Omega)$ the volume of the container. Then, the space of admissible configurations is

$$\left\{ u : \Omega \longrightarrow \{0,1\} \; : \; \int_\Omega u(x)\,dx = V \right\}$$

where V is the total volume of the second fluid s.t. $0 < V < vol(\Omega)$.

CLAIM: We postulate that the equilibrium configuration is obtained by minimizing the surface energy distributed on S_u and defined as

$$F(u) \doteq \sigma \mathcal{H}^2(S_u), \quad \text{with } u \text{ admissible configuration.}$$

Here σ is called the surface tension between the two fluids and $\mathcal{H}^2(S_u)$ is the 2D-Hausdorff measure of the interface S_u.

Van der Walls - Cahn - Hilliard Model: Phase transition

Assume that the transition is not given by a separating interface, but is rather a continuous phenomenon occurring in a thin layer (which is identified, on a macroscopic level, with the interface).

Remark: In this second case we allow for a fine mixture of the fluids.

Mathematically speaking:

- Let $u : \Omega \longrightarrow [0,1]$ denote the average volume density of the second fluid at any point $x \in \Omega$.

  Example: $u(x) = 0 \Rightarrow$ only the first fluid at x

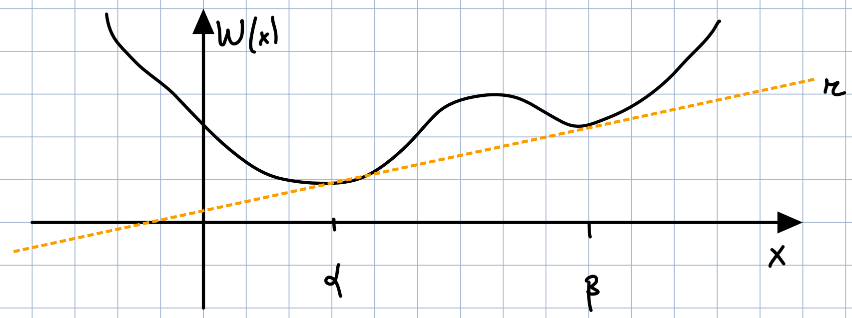
  $u(x) = \frac{1}{2} \Rightarrow$ both liquids with the same rate

  $u(x) = 1 \Rightarrow$ only the second fluid

- The space of admissible configurations then becomes

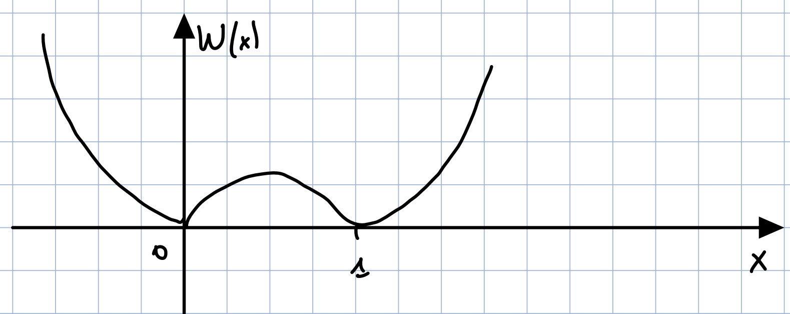
$$\left\{ u : \Omega \longrightarrow [0,1] \; : \; \int_\Omega u(x)\,dx = V \right\}.$$

· This theory also considers the so-called double-well potential $W : \mathbb{R} \longrightarrow [0,+\infty]$ which is a continuous and non-convex function with two local minimizers



Remark: Up to considering $W(x)-(ax+b)$ and up to translations and scalings, we can assume that the local minimizers satisfy:

- $\alpha = 0$, $\beta = 1$
- $W(\alpha) = W(\beta) = 0$



This new theory aims to minimize the (potential) energy

$$E(u) \doteq \int_{\Omega} W(u(x))\,dx \quad , \; u \text{ admissible configuration.}$$

Note that E attends its minima in configurations of the form

$$u(x) = \chi_A(x) = \begin{cases} 1, & \text{if } x \in A \\ 0, & \text{if } x \in \Omega \setminus A \end{cases}$$

where A satisfies the volume constraint $|A| = V$ (A should be a measurable set).

Remark: How can we minimize E? Remind that, in particular, W is non-convex.

Idea: (De Giorgi, Modica, Mortola) Fix $\varepsilon \in \mathbb{R}^+$ small and consider the sequence

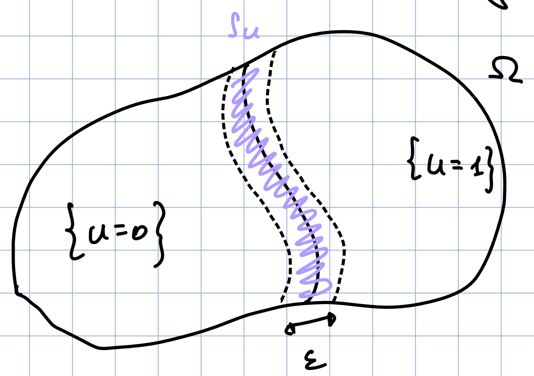
$$E_\varepsilon(u) \doteq \int_{\Omega} W(u(x))\,dx + \varepsilon^2 \int_{\Omega} |\nabla u(x)|^2\,dx \quad , \; u \in W^{1,2}(\Omega)$$

and use Γ-convergence. potential energy Kinetic energy

Remark: E_ε is well defined whenever $u \in W^{1,2}(\Omega)$.

Note that the term $\int_\Omega |\nabla u|^2 dx$ regularizes the potential energy $E(u)$, in the sense that, by continuity, any admissible configuration "u" is not allowed to jump between the values $u=0$ and $u=1$. For this reason, we talk about "phase transition", instead of phase separation.

$\varepsilon \in \mathbb{R}^+$ represents instead the thickness of the interface, in the following sense



Remark: Considering functionals F (classical model) and E (Cahn-Hilliard), is there a connection between σ and $W(u)$?

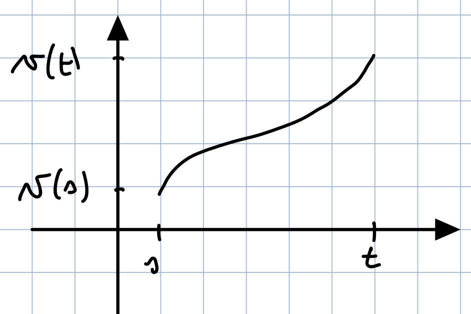
- Let $n=1$, $\Omega=(a,b)$ with $a<b$, $\varepsilon \in \mathbb{R}^+$, $v \in W^{1,2}(a,b)$ and let $s<t$ satisfy $(s,t) \subseteq (a,b)$. Then

$\alpha^2+\beta^2 \geq 2\alpha\beta \quad \forall \alpha, \beta \in \mathbb{R}$

$$\frac{1}{\varepsilon} E_\varepsilon(v)\Big|_{(s,t)} = \int_s^t \left[\frac{1}{\varepsilon} W(v(x)) + \varepsilon |v'(x)|^2\right] dx \geq 2\int_s^t \sqrt{W(v(x))} \cdot |v'(x)|\, dx$$

We will study this functionals soon

$$\geq 2\left|\int_s^t \sqrt{W(v(x))} \cdot \underbrace{(v'(x)\, dx)}_{= d(v(x))}\right|$$



c.v. $v(x)=\tau$

$$= 2\left|\int_{v(s)}^{v(t)} \sqrt{W(\tau)}\, d\tau\right|$$

- The quantity $2\left|\int_{v(s)}^{v(t)} \sqrt{W(\tau)}\, d\tau\right|$ is a lower bound of the energetic costs of a transition between $v(s)$ and $v(t)$. For $v(s)=0$ and $v(t)=1$ (or viceversa), we the get (in dimension 1)

$$2\int_0^1 \sqrt{W(\tau)}\, d\tau \doteq \sigma.$$

Before approaching the idea of De Giorgi, Modica and Mortola by means of Γ-convergence, let us underline the following property of Γ-convergence.

<u>Remark</u>: Assume that F_ε, F are functionals satisfying $F_\varepsilon \xrightarrow{\Gamma} F$ and assume that v_ε minimizes F_ε $\forall \varepsilon \in \mathbb{R}^+$. Then, v_ε minimizes also $\lambda_\varepsilon F_\varepsilon$ $\forall \lambda_\varepsilon > 0$.

· Consider now the sequence of functionals $\{G_\varepsilon\}_\varepsilon \doteq \{\lambda_\varepsilon F_\varepsilon\}_\varepsilon$ and assume that $\{v_\varepsilon\}_\varepsilon$ converges to v (and that equi-coercivity or equivalent compactness conditions are satisfied). Then, the following conditions hold true:

1) v_ε minimizes both F_ε and G_ε $\forall \varepsilon, \lambda_\varepsilon > 0$
2) $G_\varepsilon \overset{\Gamma}{\not\longrightarrow} F$
3) Different choice of λ_ε give different Γ-limits
4) v is a minimizer of F (by the fundamental th. of Γ-convergence)
5) Information about v are obtained also by studying the Γ-limits of the rescaled functionals $\{G_\varepsilon\}_\varepsilon$.

<u>Example</u>: If F is constant, any point v is a minimizer of F and so (4) gives no information about the nature of v (seen as the limit of $\{v_\varepsilon\}_\varepsilon$), while the Γ-limit of $\{G_\varepsilon\}_\varepsilon$ can provide more information (for suitable $\lambda_\varepsilon > 0$).

· Consider now our case, where we have

V.d. Waals-Cahn-Hilliard • $E_\varepsilon(u) \doteq \int_\Omega W(u(x))\,dx + \varepsilon^2 \int_\Omega |\nabla u(x)|^2 dx \,, \quad u \in W^{1,2}(\Omega)$

CLASSICAL MODEL • $F(u) \doteq \sigma \mathcal{H}^2(S_u) \,, \quad u \in BV(\Omega)$

<u>EX</u>: Show that w.r.t. the strong topology of $L^1(\Omega)$ as $\varepsilon \to 0$:

a) $E_\varepsilon \xrightarrow{\Gamma} E$, where $E(u) = \int_\Omega W(u(x))\,dx$

b) If $\lambda_\varepsilon \nearrow +\infty$ and $\varepsilon\lambda_\varepsilon \searrow 0$, then $\lambda_\varepsilon E_\varepsilon \xrightarrow{\Gamma} E$, where $E(u) = \begin{cases} 0, & \text{if } u \in \{0,1\} \\ +\infty, & \text{otherwise} \end{cases}$

c) If $\varepsilon\lambda_\varepsilon \nearrow +\infty$, then $\lambda_\varepsilon E_\varepsilon \xrightarrow{\Gamma} E$, where $E(u) = +\infty$ $\forall u$ admissible.

The question answered by (De Giorgi) - Modica - Mortola is the next one:

<u>Q</u>: Is there a certain scale $\lambda_\varepsilon > 0$ s.t. $\lambda_\varepsilon E_\varepsilon \xrightarrow{\Gamma} F$?

<u>Th</u>: Modica - Mortola (1977)

Let $\Omega \subseteq \mathbb{R}^m$ be open and bounded and denote the space of admissible configurations

$$X \doteq \left\{ u \in L^1(\Omega; [0,1]) \text{ s.t. } \int_\Omega u(x)\,dx = V \right\}$$

for $0 < V < vol(\Omega)$. Moreover, set $\sigma \doteq 2\int_0^1 \sqrt{W(s)}\,ds$ and for every $\varepsilon \in \mathbb{R}^+$ let

$$F_\varepsilon \doteq \frac{1}{\varepsilon} E_\varepsilon : X \longrightarrow \mathbb{R} \cup \{+\infty\}$$

$$u \longmapsto F_\varepsilon(u) = \begin{cases} \frac{1}{\varepsilon}\int_\Omega W(u(x))\,dx + \varepsilon \int_\Omega |\nabla u(x)|^2\,dx, & \text{if } u \in W^{1,2}(\Omega) \\ +\infty & \text{, if } u \in X \setminus W^{1,2}(\Omega) \end{cases}$$

and let $F: X \longrightarrow \mathbb{R} \cup \{+\infty\}$

$$u \longmapsto F(u) = \begin{cases} \sigma\, \mathcal{H}^{m-1}(S_u), & \text{if } u \in BV(\Omega; \{0,1\}) \\ +\infty & \text{, if } u \in X \setminus BV(\Omega; \{0,1\}) \end{cases}$$

Then, $\{F_\varepsilon\}_\varepsilon$ Γ-converges to F in the strong topology of $L^1(\Omega)$.

Moreover, $\{F_\varepsilon\}_\varepsilon$ are equicoercive and so the fundamental theorem of Γ-convergence can be applied.

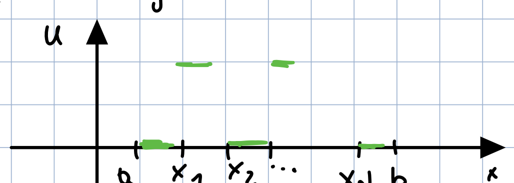
<u>Proof</u>: (We show the result in the 1-dimensional case)

- If $m = 1$, then $\Omega = (a,b)$, $vol(\Omega) = b - a$ $(b > a)$ and $V \in (0, b-a)$,

$$X \doteq \left\{ u \in L^1((a,b); [0,1]) \text{ s.t. } \int_a^b u(x)\,dx = V \right\},$$

$W: \mathbb{R} \longrightarrow \mathbb{R}^+_0$ is a double-well potential s.t. $\{s \in \mathbb{R} : W(s) = 0\} = \{0,1\}$,

$\sigma = 2\int_0^1 \sqrt{W(s)}\,ds$, $S_u = \{x_1, \dots, x_N\}$ Jump points and $\mathcal{H}^0(S_u)$ represents the number of Jumps.



Note that (in dimension $m=1$) $u \in BV((a,b); \{0,1\}) \Leftrightarrow u : (a,b) \longrightarrow \{0,1\}$ and $|S_u| = N < +\infty$.

As we already said, σ represents a lower bound of the energetic cost of the transition and so $\sigma \cdot \mathcal{H}^0(S_u)$ is the number of jumps times the cost.

STEP 1: (Γ-liminf-inequality) - Let $u_j, u \in X$ satisfy $u_j \longrightarrow u$ in $L^1(a,b)$-strong ($\Rightarrow u \in BV(a,b)$) and let $\varepsilon_j \searrow 0$ as $j \nearrow +\infty$. We show that

$$(*) \qquad F(u) \leq \liminf_{j \nearrow +\infty} F_{\varepsilon_j}(u_j).$$

First note that if $\liminf_{j \nearrow +\infty} F_{\varepsilon_j}(u_j) = +\infty$ the claim is trivial.

Assume then that $\liminf_{j \nearrow +\infty} F_{\varepsilon_j}(u_j) < +\infty$, that is, there exists a not relabeled subsequence s.t. $\lim_{j \nearrow +\infty} F_{\varepsilon_j}(u_j) < +\infty$.

Thus, there exists $C_1 \in \mathbb{R}$ such that $F_{\varepsilon_j}(u_j) \leq C_1$ and so, by the definition of F_{ε_j}:

1) (up to a further subseq.) $u_j \longrightarrow u$ a.e. in (a,b) (bounded seq. in L^1)

2) $u_j \in W^{1,2}(a,b)$ $\quad$ ($u_j \in L^\infty(a,b) \Rightarrow u_j \in L^2(a,b)$ + $\|\nabla u_j\|^2_{L^2} \leq F_{\varepsilon_j}(u_j) \leq C_1$)

3) $\displaystyle \frac{1}{\varepsilon_j}\int_a^b W(u_j(x))\,dx \leq C_1 \Rightarrow \int_a^b W(u_j(x))\,dx \leq C_1 \varepsilon_j \longrightarrow 0$ as $j \nearrow +\infty$

$\Rightarrow W(u_j) \longrightarrow 0$ in $L^1(a,b)$ $\Rightarrow W(u_j) \longrightarrow 0$ a.e. on (a,b)
(up to further subseq.)

· Since W is continuous, then (1) implies that

$$W(u_j) \longrightarrow W(u) \text{ a.e. in } (a,b)$$

and so, by (3), $W(u(x)) = 0$ a.e. $x \in (a,b)$. Therefore,

$$u(x) \in \{0,1\} \text{ a.e. } x \in (a,b)$$

being W a double-well potential.

<u>Remark</u>: Since $u_j \longrightarrow u$ in $L^1(a,b)$-strong (by hypothesis), there exists $\{u_{j_k}\}_k \subseteq \{u_j\}_j$ s.t.

$$u_{j_k} \longrightarrow u \text{ a.e. in } (a,b).$$

However, $\liminf_{k \nearrow +\infty} F_{\varepsilon_j}(u_{j_k})$ can be also $+\infty$.

We conclude by showing the validity of (*).

· Note that $\int_a^b u_j(x)\,dx = V \quad \forall j \in \mathbb{N}$ implies that $\int_a^b u(x)\,dx = V \quad (\Rightarrow u \in X)$.

Moreover, note that $S_u \neq \emptyset$. Otherwise, we have only two possibilities:

$$1)\quad u = 0 \Rightarrow \int_a^b u\,dx = 0 < V$$

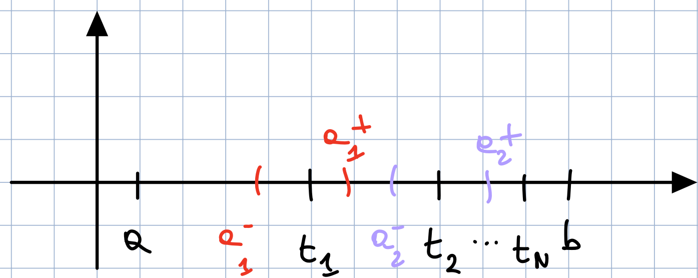
$$2)\quad u = 1 \Rightarrow \int_a^b u\,dx = b - a > V.$$

· Let $|S_u| = N$ and $t_1, \dots, t_N \in S_u$. For any $i \in \{1, \dots, N\}$ there exist $a_i^+, a_i^- \in (a,b)$ s.t.

i) $a_i^- < t_i < a_i^+ < a_{i+1}^-$

ii) $\lim\limits_{j \nearrow +\infty} u_j(a_i^\pm) = u(a_i^\pm)$ (being $u_j \longrightarrow u$ a.e. in (a,b))

iii) $u(a_i^-) \neq u(a_i^+)$



iv$_a$) $\begin{cases} u_j(a_i^-) \longrightarrow 0 \\ u_j(a_i^+) \longrightarrow 1 \end{cases}$ as $j \nearrow +\infty$ or

iv$_b$) $\begin{cases} u_j(a_i^-) \longrightarrow 1 \\ u_j(a_i^+) \longrightarrow 0 \end{cases}$ as $j \nearrow +\infty$

and so in any interval (a_i^-, a_i^+), u_j has a transition around "0" and "1".

Therefore, $$F_{\varepsilon_j}(u_j) \geq \sum_{i=1}^N \int_{a_i^-}^{a_i^+} \left[\frac{1}{\varepsilon_j} W(u_j(x)) + \varepsilon_j |u_j'(x)|^2 \right] dx$$

$$\geq \sum_{i=1}^N 2 \left| \int_{u_j(a_i^-)}^{u_j(a_i^+)} \sqrt{W(\tau)}\,d\tau \right| \longrightarrow \sum_{i=1}^N 2 \left| \int_0^1 \sqrt{W(z)}\,dz \right| = N\sigma$$

$$\Rightarrow \liminf_{j \nearrow +\infty} F_{\varepsilon_j}(u_j) \geq N\sigma = N\,\mathcal{H}^0(S_u).$$

If we repeat the same argument considering any possible jump, we finally get $(*)$.