Bridge to Research Seminar:

Applications of Singular Perturbations in Calculus of Variations

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Outline of Talks

- Examples of interfaces and defects in physical system and concept of singular perturbation
- A simple one-dimensional example illustrating **selection principle, microstructure, and multiple length scales**
- Connection with minimal surfaces
- Connection to point vortices

Research Interests: Applied Mathematics, Partial Differential Equations, Calculus of Variations, Probability Theory, Geometric Evolutions, Modeling in Materials Science, Stochastic Optimizations

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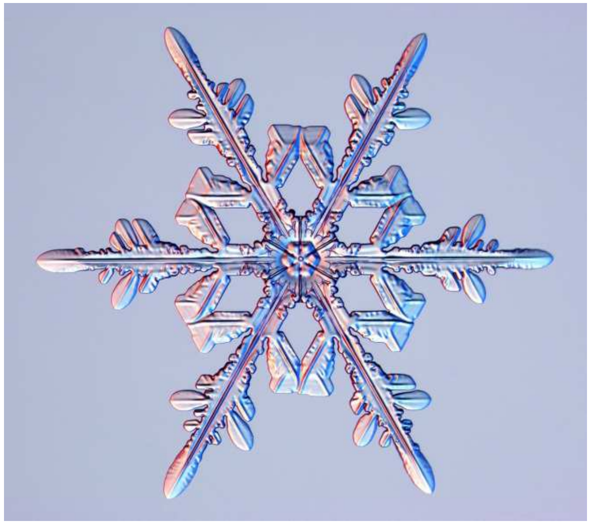
Examples of Interfaces and Defects

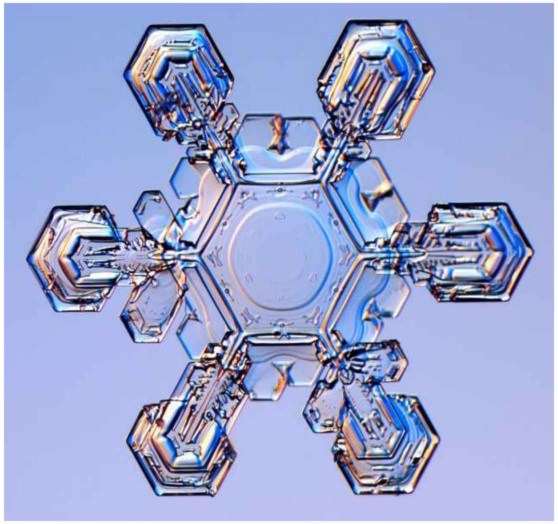
Interface: surface separating two regions

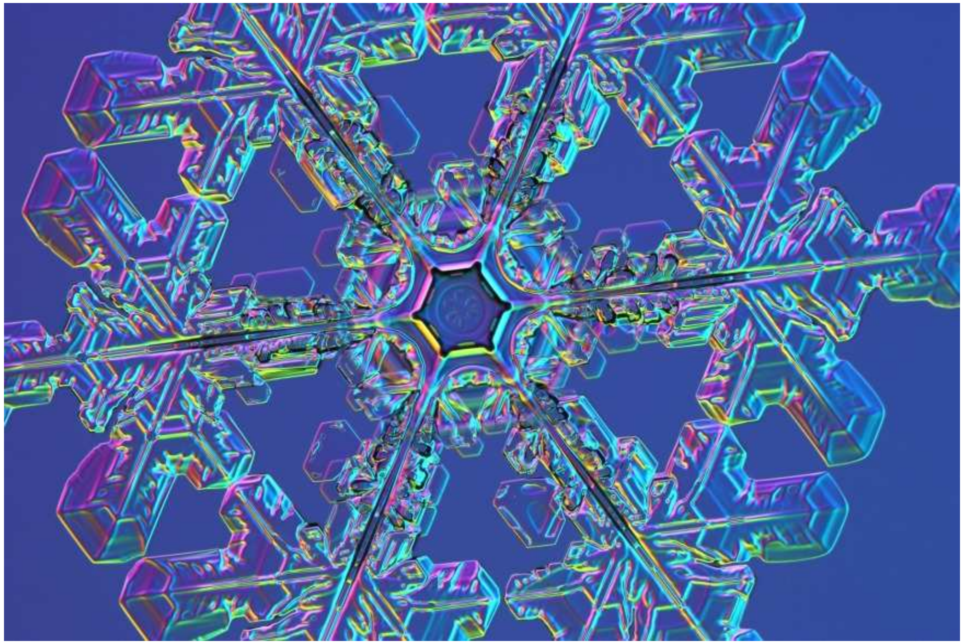
Defect: localized deviations in structure from the background environment

- phase boundaries between ice and water in crystal growth
- interfaces between two immiscible fluids
- grain boundaries
- triple junctions
- soap films and soap bubbles
- dislocation lines in materials
- vortices in superconductivity

Example of Interfaces: Crystal Growth







Example of Interfaces: Bubble Growth

Motion of Defects

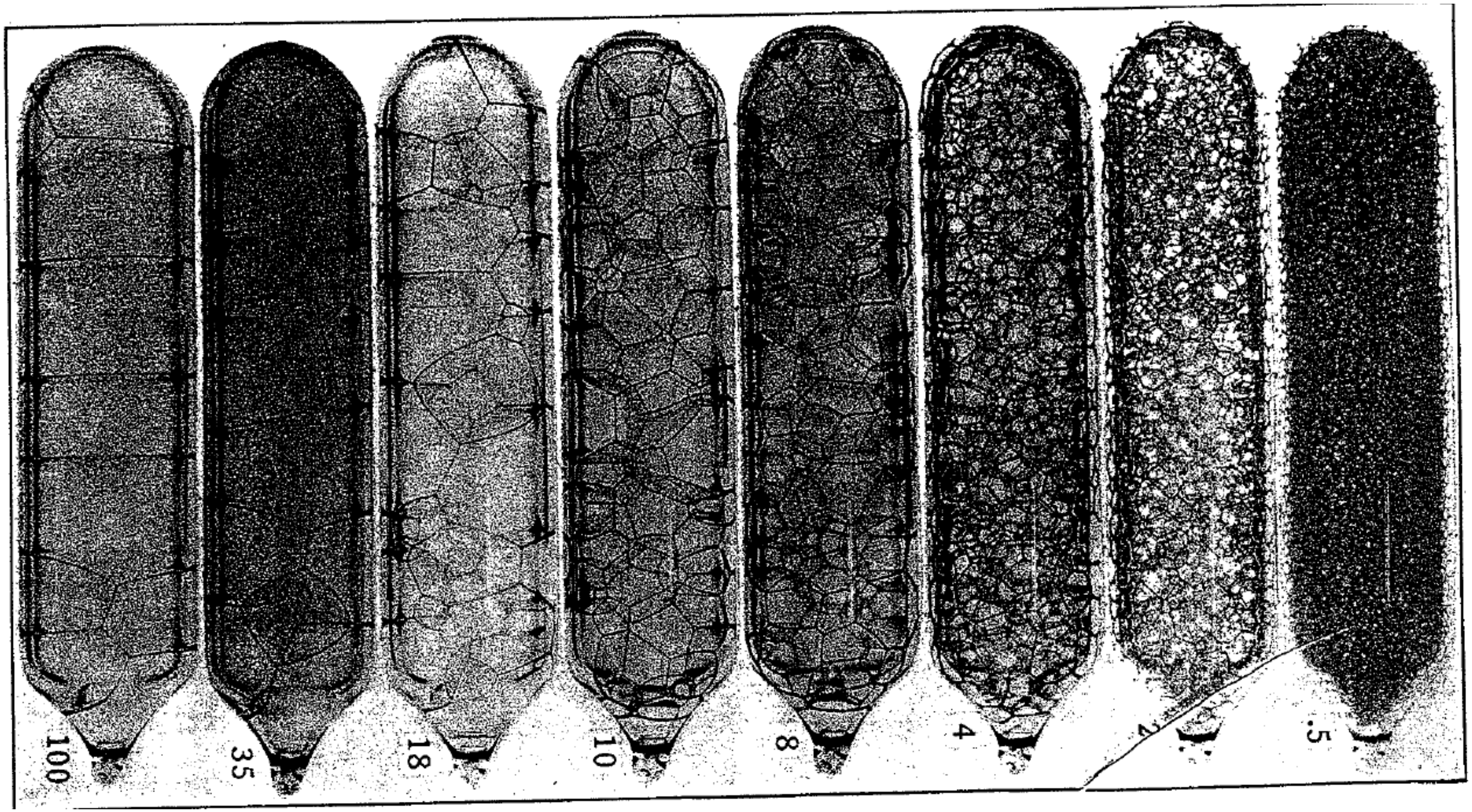


Fig. 11—Growth of Bubbles by Diffusion in Glass Tube Under Reduced Pressure. (Numbers indicate time in minutes after cessation of agitation.)

Example of Interfaces: Bubble Growth–2

Motion of Defects

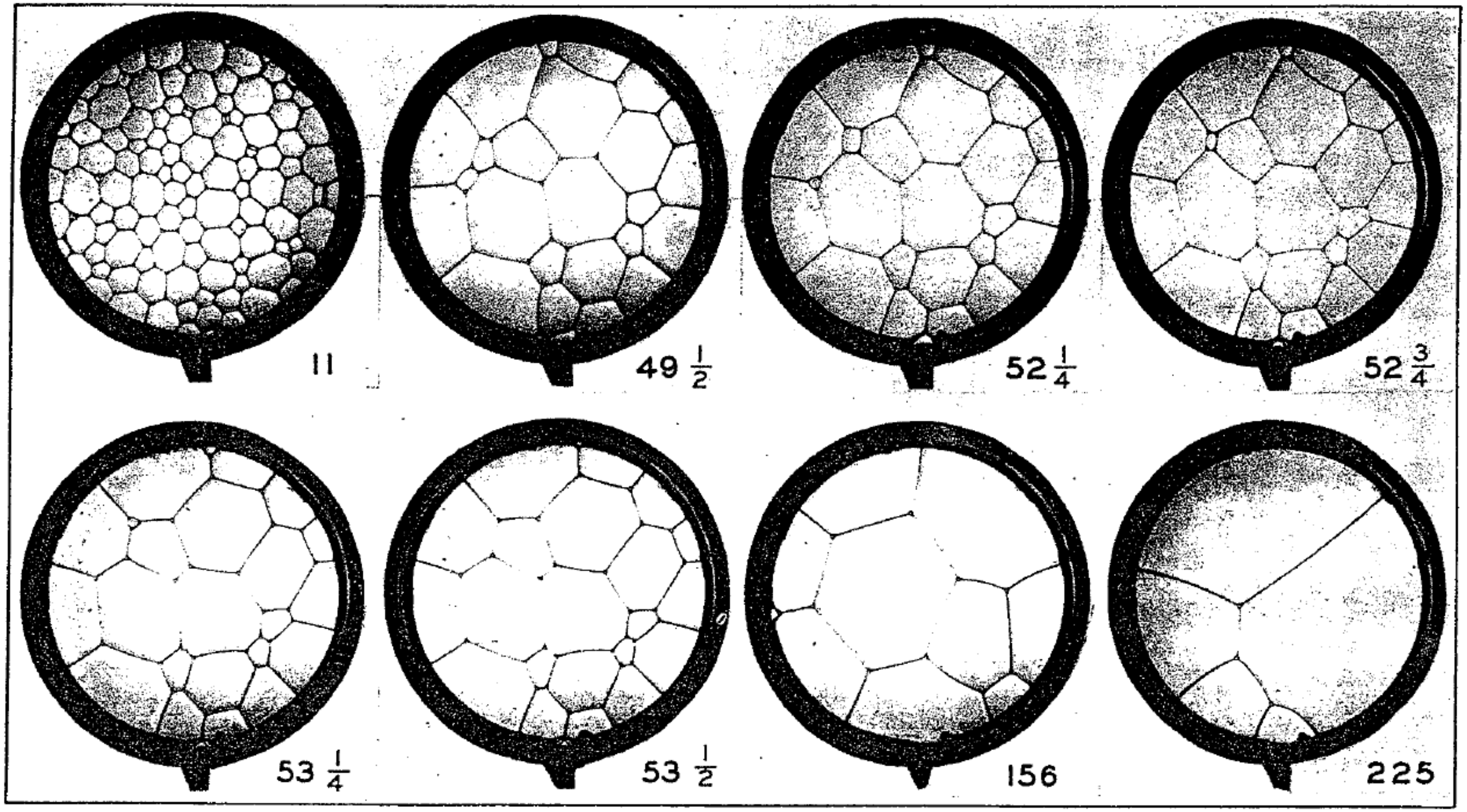


Fig. 12—Growth and Disappearance of Bubbles in a Flat Cell

Examples of Interfaces: Grain Growth

Motion of Defects

Fig. 3—The Grain Boundaries Between a Large Recrystallized Grain and the Small Strained Grains, Which Are Being Absorbed, Move in a Direction Toward Their Centers of Curvature, as in Grain Growth. Al-Zn alloy, strained and annealed at 450 °C. × 50. *(Lacombe and Berghezan.)*

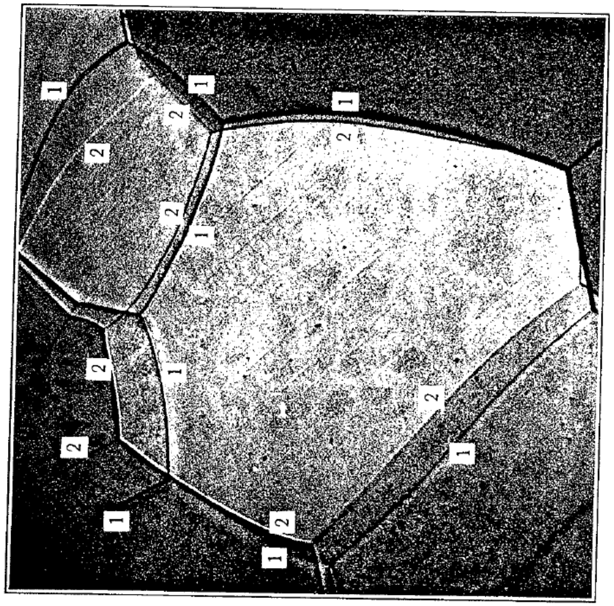
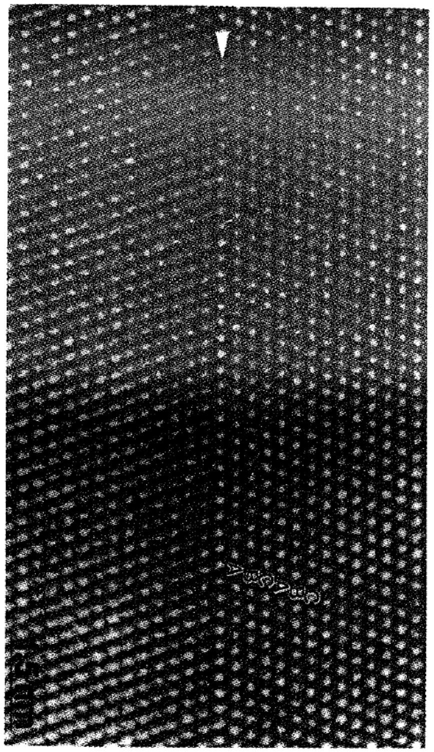
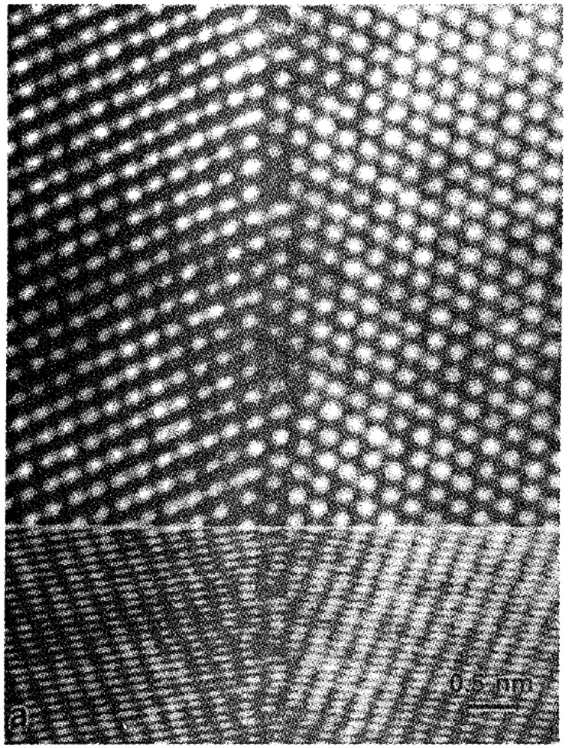


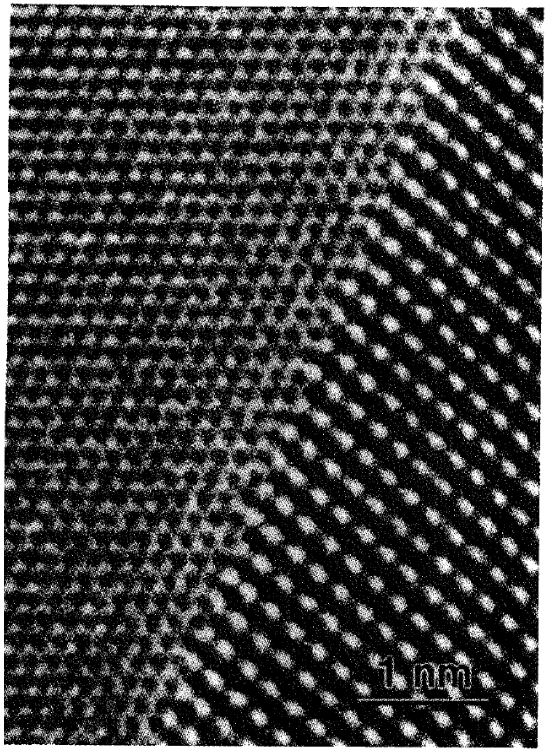
Fig. 2—In Grain Growth, Grain Boundaries Migrate Toward Their Centers of Curvature. Boundaries in high purity aluminum, after annealing 2 minutes at 600 °C (1), and after an additional anneal of 30 seconds at 600 °C (2). Anodic film and sensitive tint illumination. × 75. (Reference 20.)

Examples of Interfaces: Grain Growth–2

Structure of Defects







Examples of Interfaces: Grain Growth–3

Seeing the Structure and Motion of Defects with your Naked Eyes:

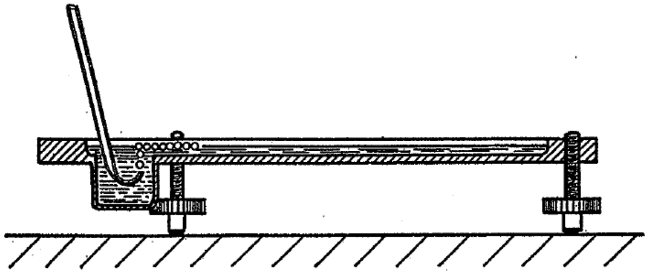
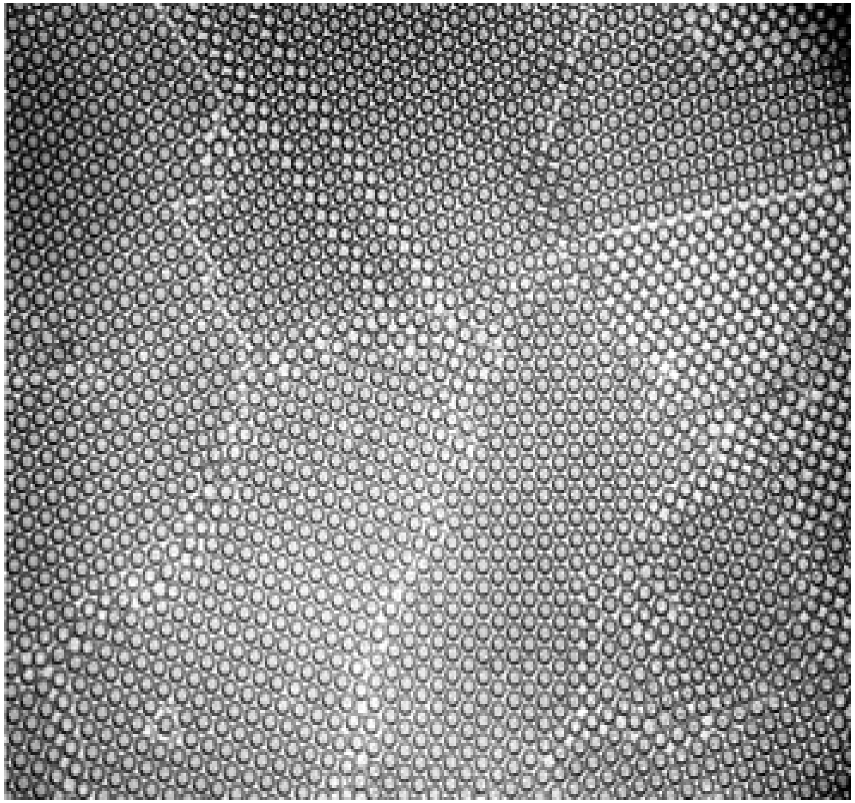


Figure 1. Apparatus for producing rafts of bubbles.



Example of Interfaces – Images

Image De-Noising

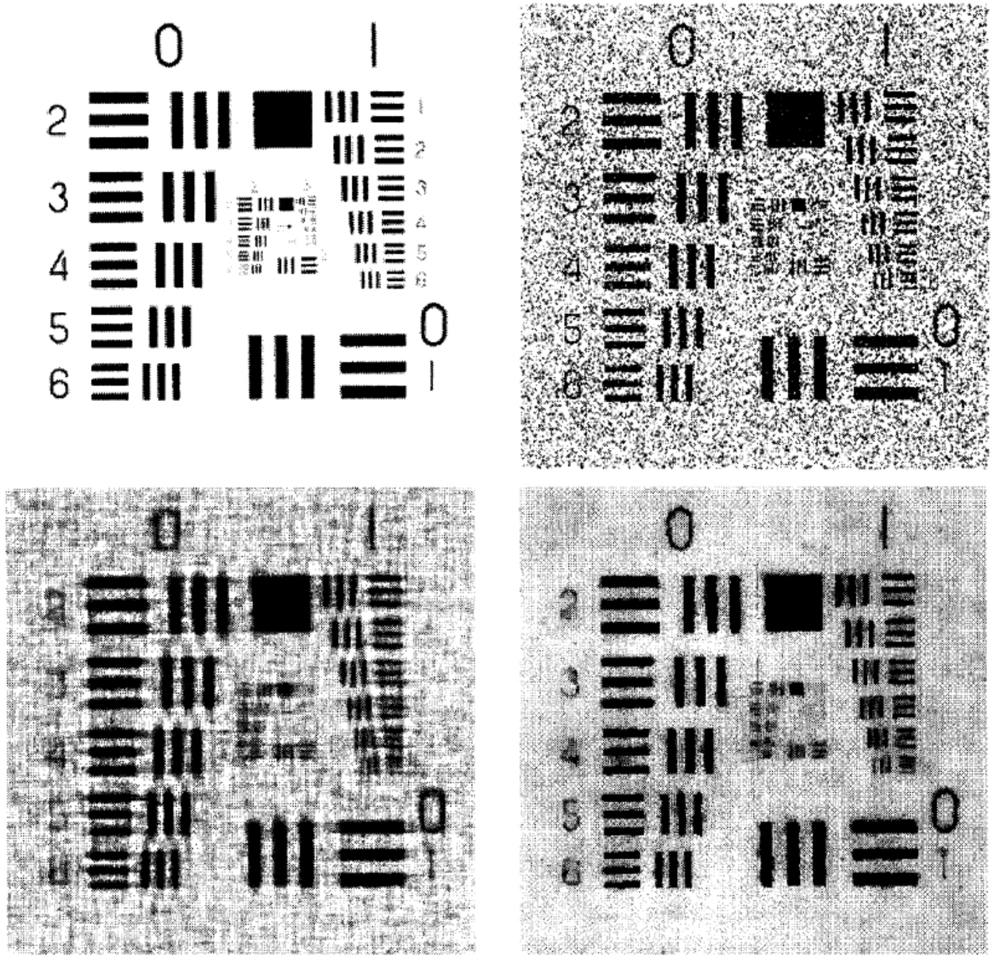


Fig. 3. (a) "Resolution Chart". (b) Noisy "Resolution Chart", SNR = 1.0. (c) Wiener filter reconstruction from (b). (d) TV reconstruction from (b).

Singular Perturbations

Higher Order Perturbations

How are the solutions of

$$F(u) = 0$$

in particular, the **structures and locations of their singularities**, if any, related to those of

$$F(u) + \epsilon G(u, \nabla u, \nabla^2 u) = 0$$

for $\epsilon \ll 1$?

The ϵ can be some physical parameter or even numerical discretization length scales. The key is to understand the **limiting behavior as** $\epsilon \longrightarrow 0$.

Some Well Known Examples of Singular Perturbatio

Method of Vanishing Viscosity and Selection Principle

- **Entropy Solution for Conservation Law**

$$U_t + F(U)_x = \epsilon^2 U_{xx}$$

converges, as $\epsilon \longrightarrow 0$ to **the entropy solution** of

$$U_t + F(U)_x = 0$$

- **Viscosity Solution for Hamilton-Jacobi Equation**

$$u_t + H(\nabla u) = \epsilon^2 \triangle u$$

converges, as $\epsilon \longrightarrow 0$ to **the viscosity solution** of

$$u_t + H(\nabla u) = 0$$

A Common Example in Calculus of Variations

$$\mathcal{F}(u) = \int \epsilon^2 \left|\nabla u\right|^2 + W(u)$$

or

$$\mathcal{F}(u) = \int \epsilon^2 \left|\nabla^2 u\right|^2 + W(\nabla u)$$

where

- W is some function which is **positive** and **vanishes on some finite set or manifold**;
- u can be a **scalar or vector-valued function**.

The main goal is to **minimize** $\mathcal{F}$ subject to some boundary conditions for u.

An Example from Calculus of Variations

Consider the following minimization problem:

$$\min \left\{ \int_0^1 (1 - u_x^2)^2 \, dx, \quad u(0) = 0, \;\; u(1) = 0 \right\}$$

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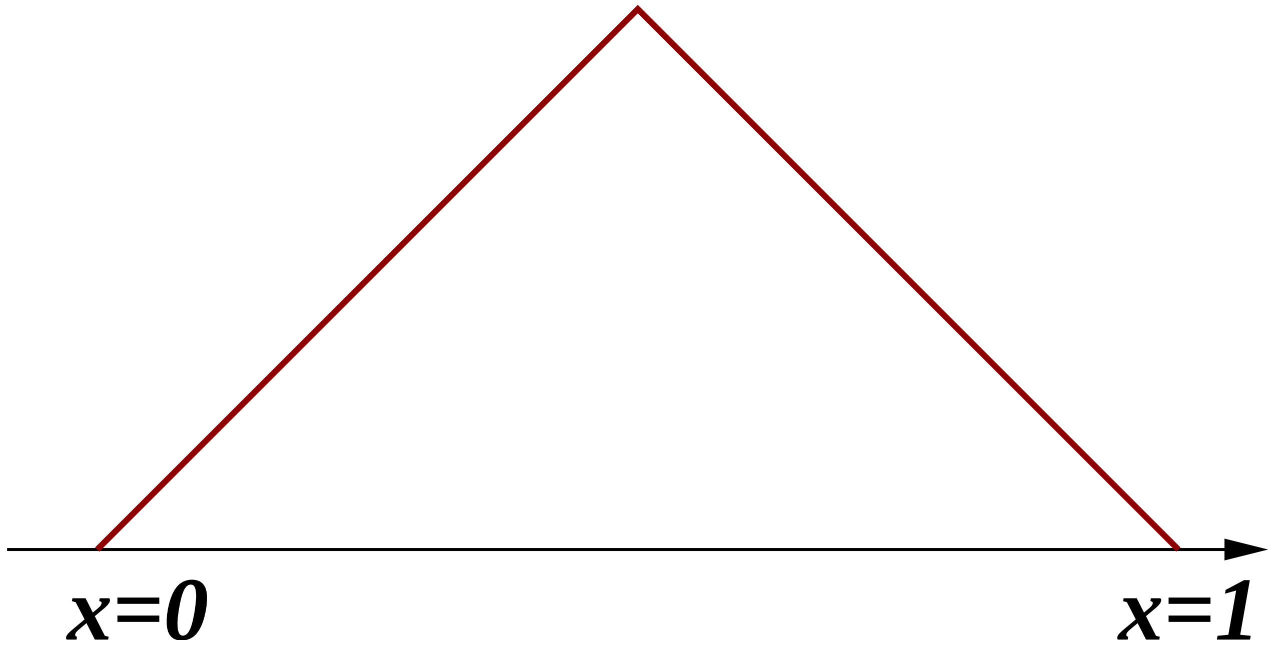

The functional attains the **minimum value zero**.

An Example from Calculus of Variations

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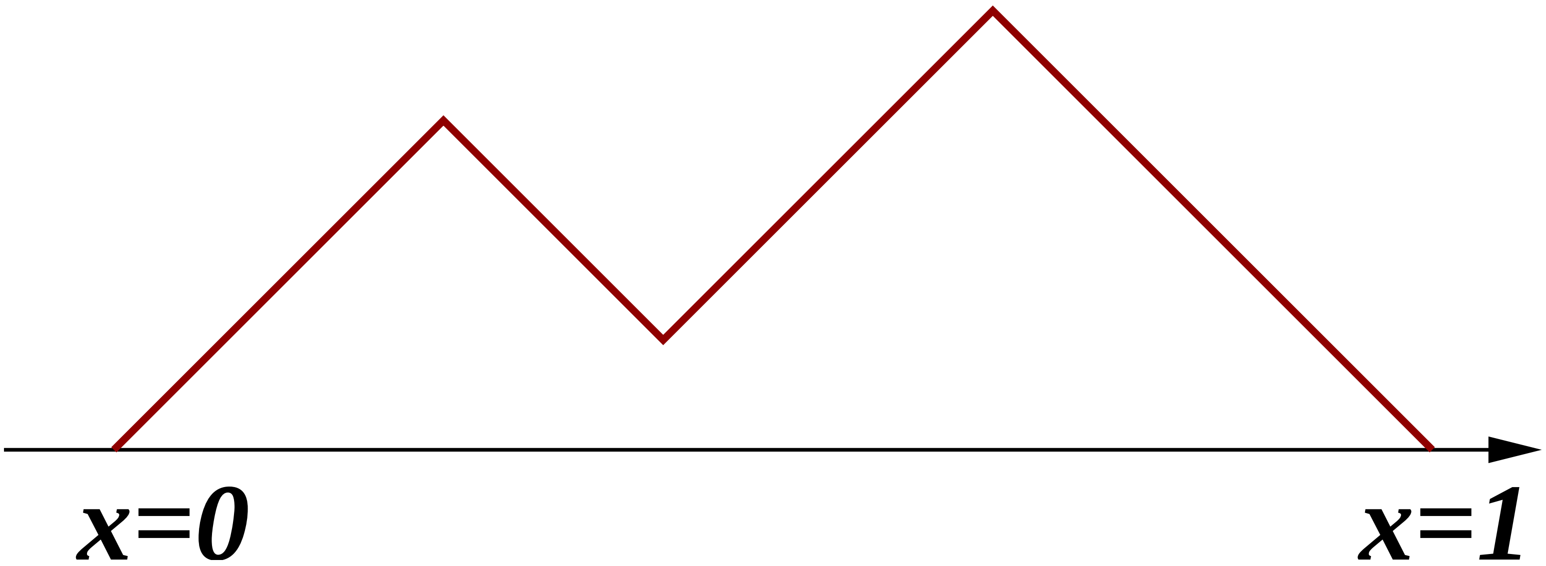

Another example of global minimizer.

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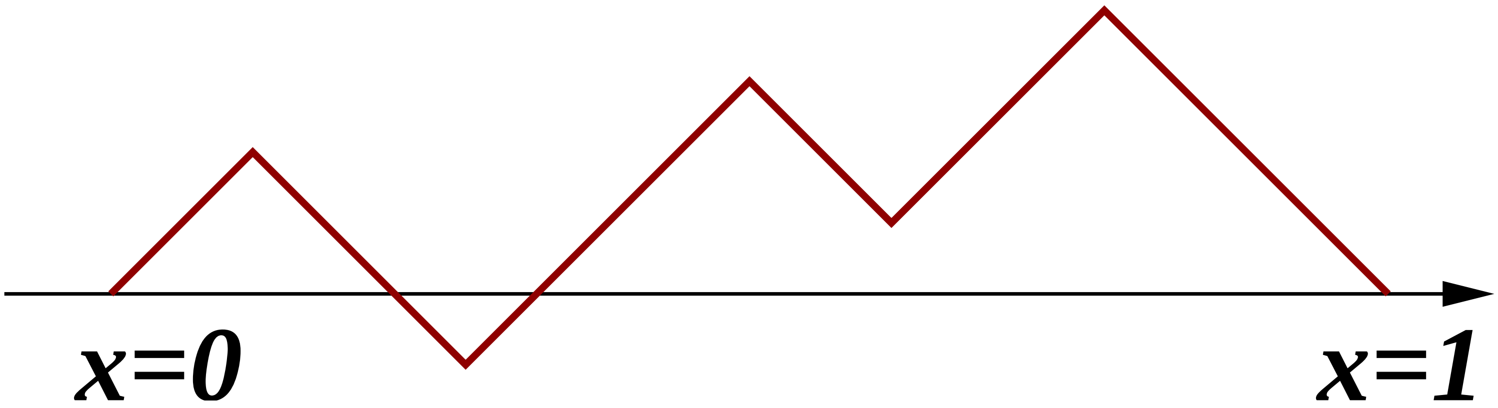

Yet another example of a minimizer.

Hence there are *lots of examples of global minimizers, i.e. the solutions are highly non-unique!*

An Example from Calculus of Variations

Consider the following **singularly perturbed** version:

$$\min\left\{\int_0^1 \epsilon^2 u_{xx}^2 + (1-u_x^2)^2\,dx, \quad u(0)=0,\ \ u(1)=0\right\}$$

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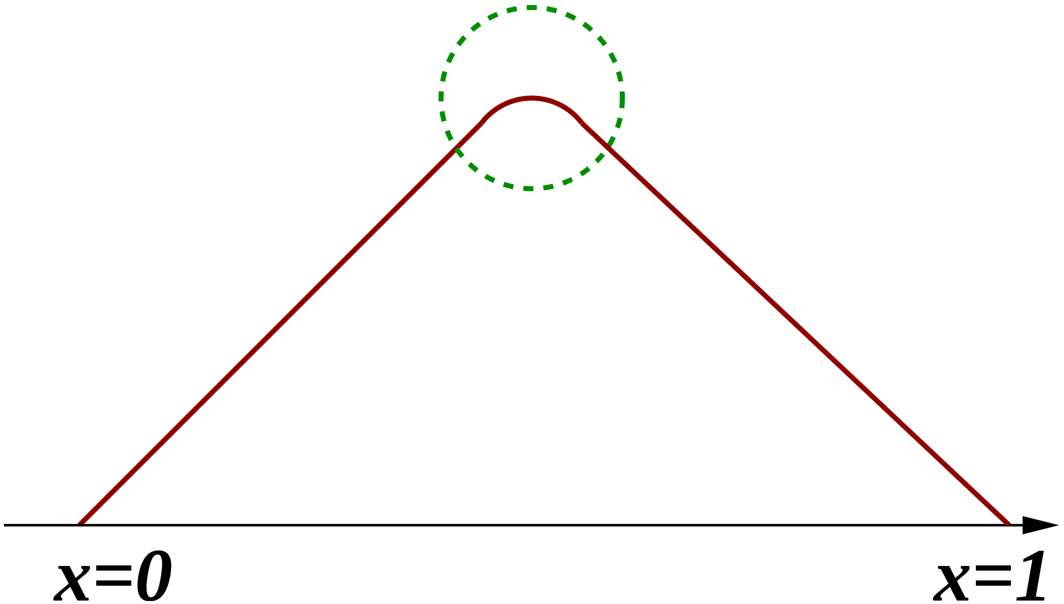

The minimizer have **smoothed out** corners.

An Example from Calculus of Variations

Consider the following **singularly perturbed** version:

$$\min\left\{\int_0^1 \epsilon^2 u_{xx}^2 + (1-u_x^2)^2\,dx, \quad u(0)=0,\ \ u(1)=0\right\}$$

1. each corner gives rise to a **delta function in the second derivative** which leads to **infinite** functional value;
2. the singular functional thus smoothes out the corner;
3. the amount of smoothing depends on the parameter ϵ;
4. still, each smoothed corner contributes to some energy;
5. hence **global minimizer** likes to have **as few corners** as possible.
6. thus the one with only **one corner** is the **global minimizer**.

Variant of the Previous Example

Consider the minimization problem:

$$\min\left\{\int_0^1 (1-u_x^2)^2 + u^2\,dx, \quad u(0)=0,\ \ u(1)=0\right\}$$

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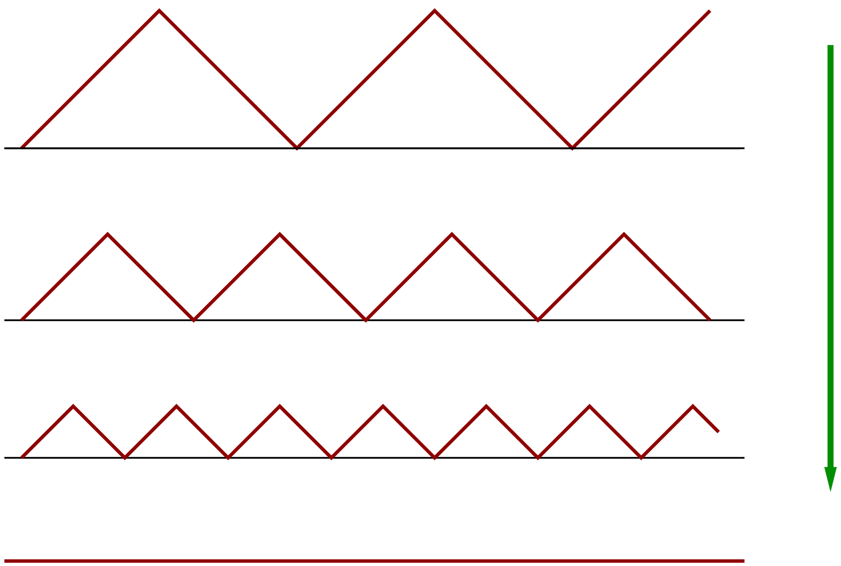

increasing number of oscillations: the sequence of functions converge to the ZERO function which is NOT the minimizer.

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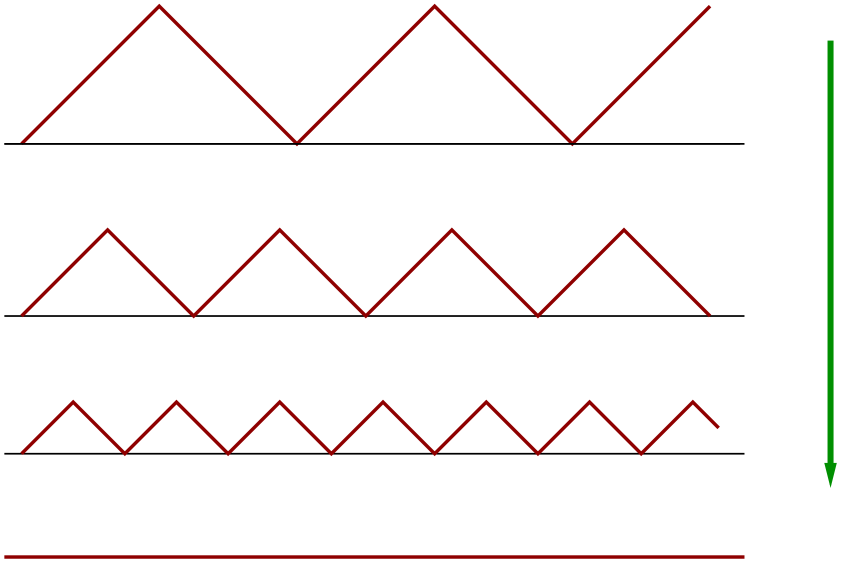

increasing number of oscillations: the sequence of functions converge to the ZERO function which is NOT the minimizer.

There is a **minimizing sequence but no minimizer**! This is an example of a functional which is **not lower-semi-continuous**.

Variant of the Previous Example

Consider the following **singularly perturbed** version:

$$\min \left\{ \int_0^1 \epsilon^2 u_{xx}^2 + (1 - u_x^2)^2 + u^2 \, dx, \quad u(0) = 0, \; u(1) = 0 \right\}$$

Variant of the Previous Example

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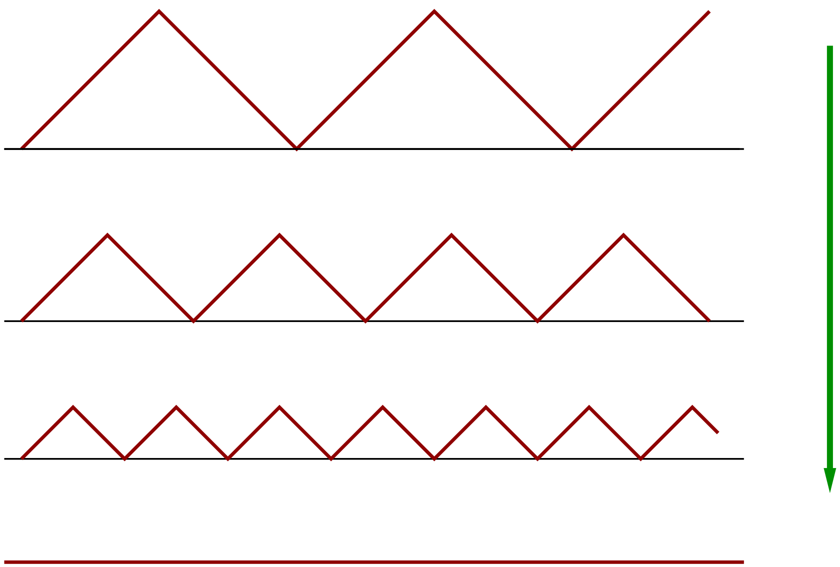


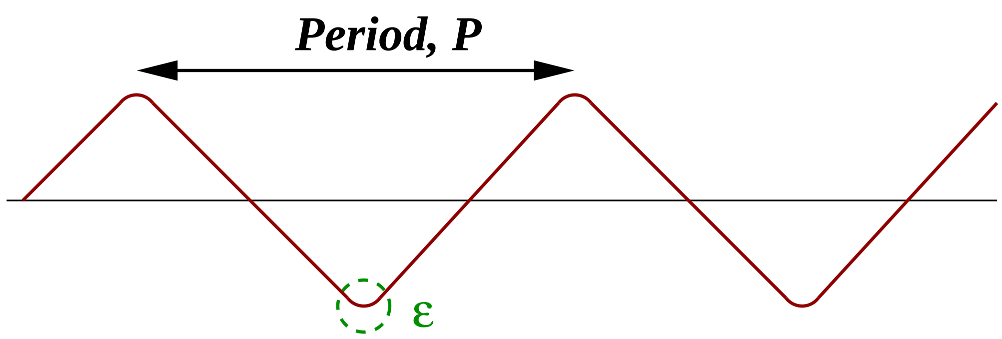
small number of smoothed corners
but large contribution from u

large number of smoothed corners
but small contribution from u

There is a **balance** or **competition** between the terms $\int \epsilon^2 u_{xx}^2$ and $\int u^2$.

Structure of Global Minimizer

S. Müller: the global minimizer exists and is **unique** and **periodic** with period $P = O(\epsilon^{\frac{1}{3}})$.



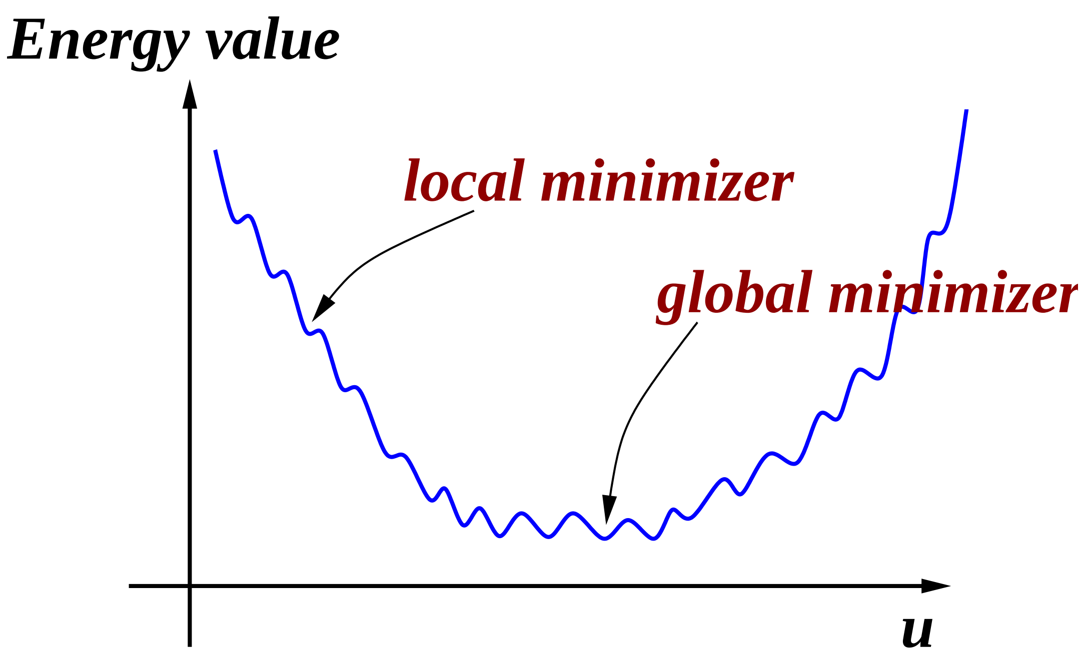
Note the existence of **multiple (three) length scales**:

- scale of the smoothed corners, **defects** ϵ;
- scale of the **pattern** $P = O(\epsilon^{\frac{1}{3}})$;
- scale of the **domain** $O(1)$.

$$\epsilon \ll \epsilon^{\frac{1}{3}} \ll O(1)$$

Structure of Local Minimizer

Y.: At **low energy level**, all the **local minimizers** are **periodic**. As the **period decreases**, periodic critical points become **unstable**. The length scale at which this happens is also characterized.



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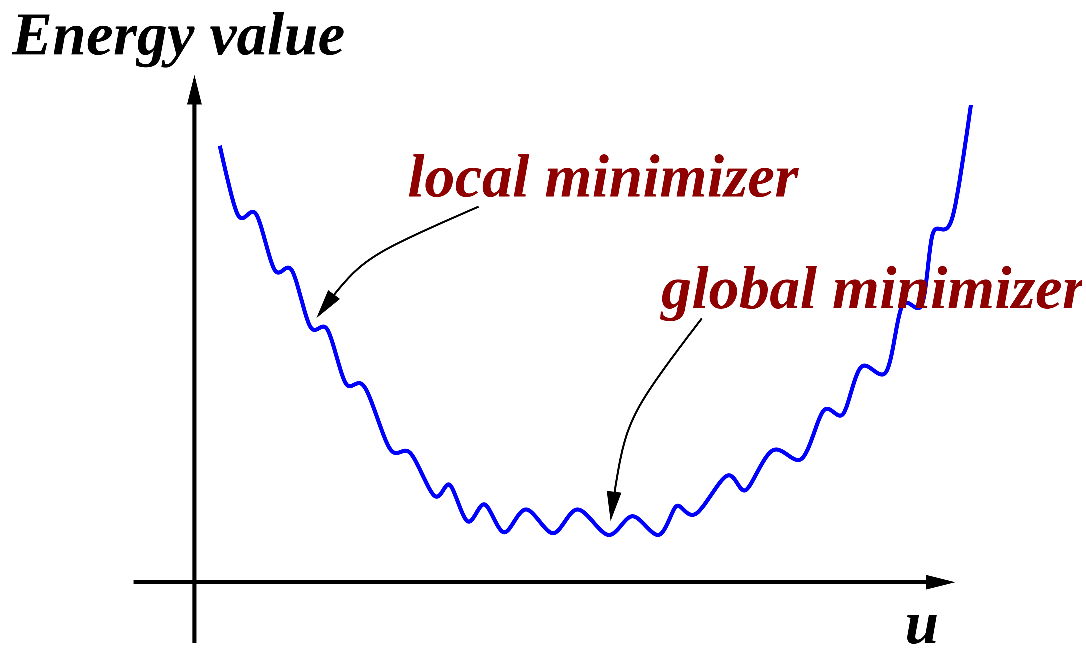
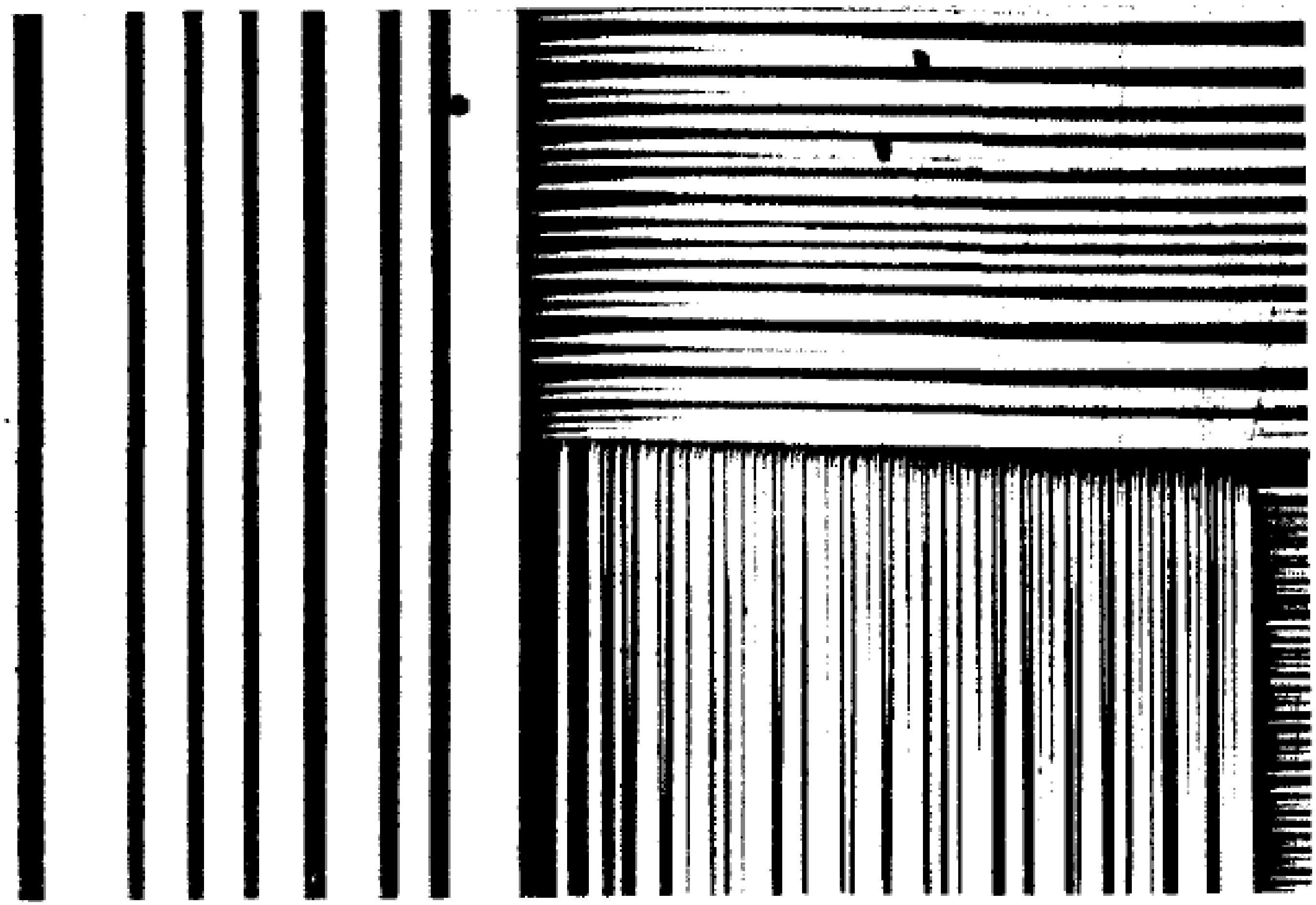


The **dynamics** on the energy landscape is in fact controlled by **local minimizers**, **saddle points**, or more generally **metastable states**!

An Actual Example of Microstructure

Martensitic Transformation



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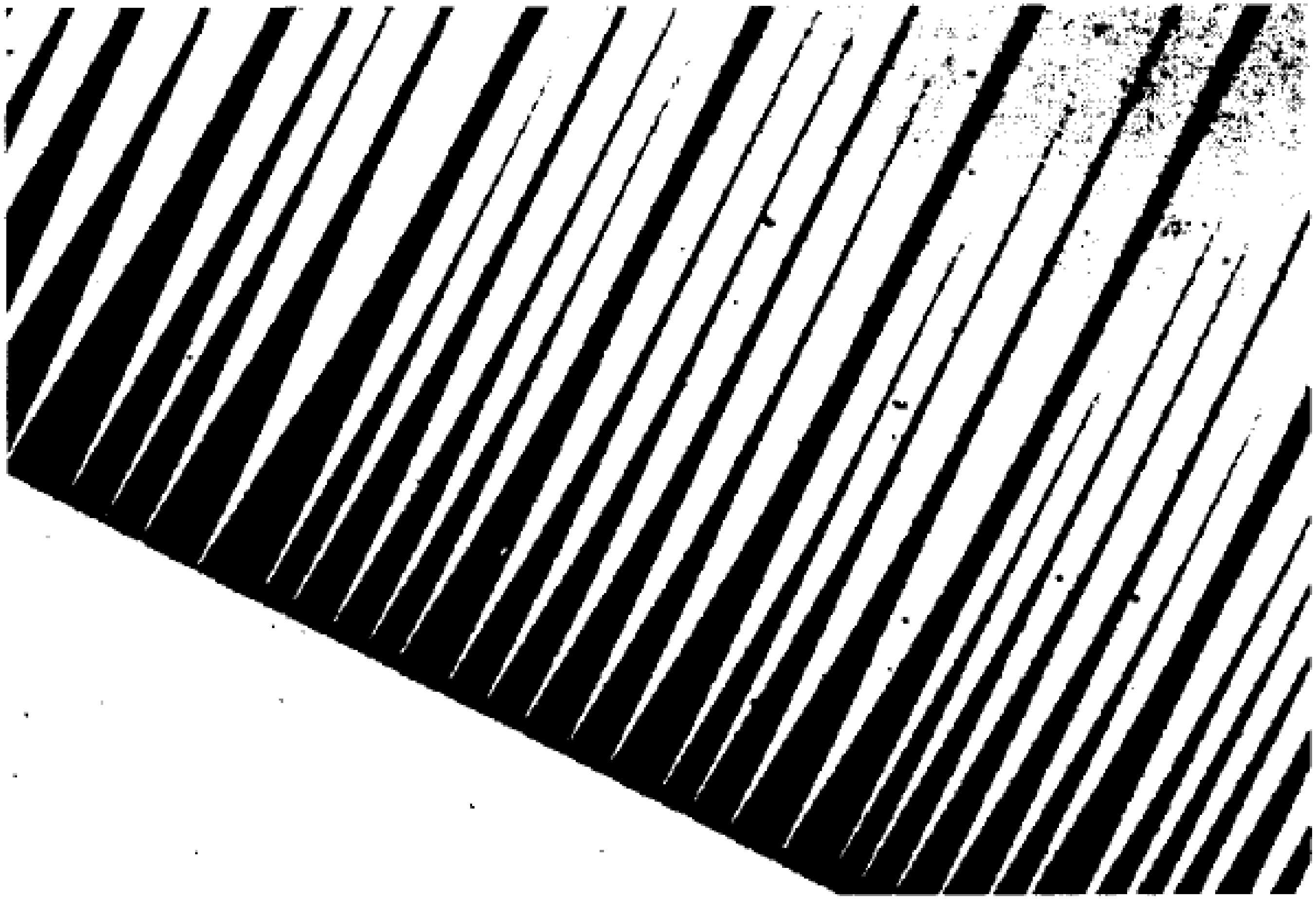

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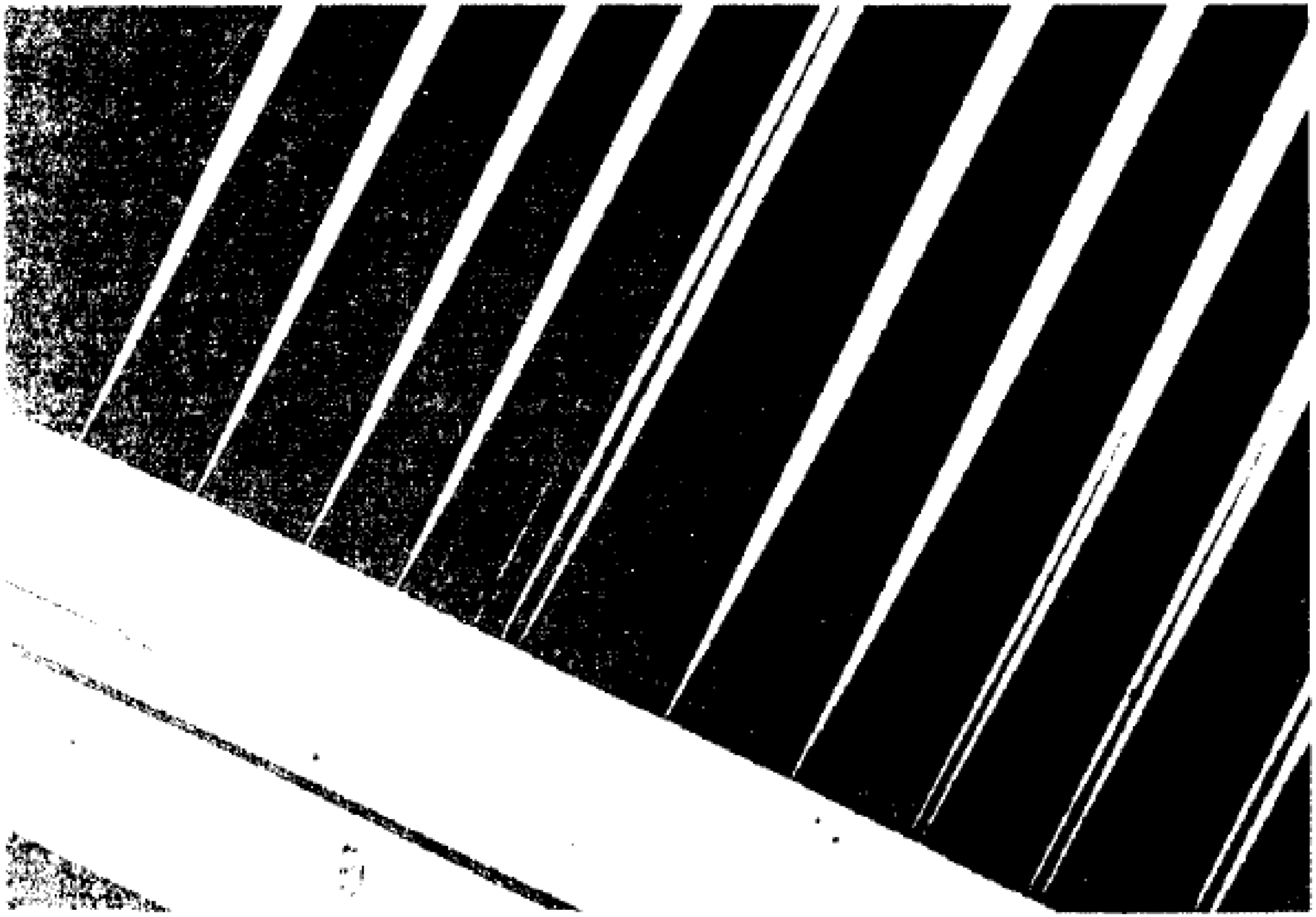
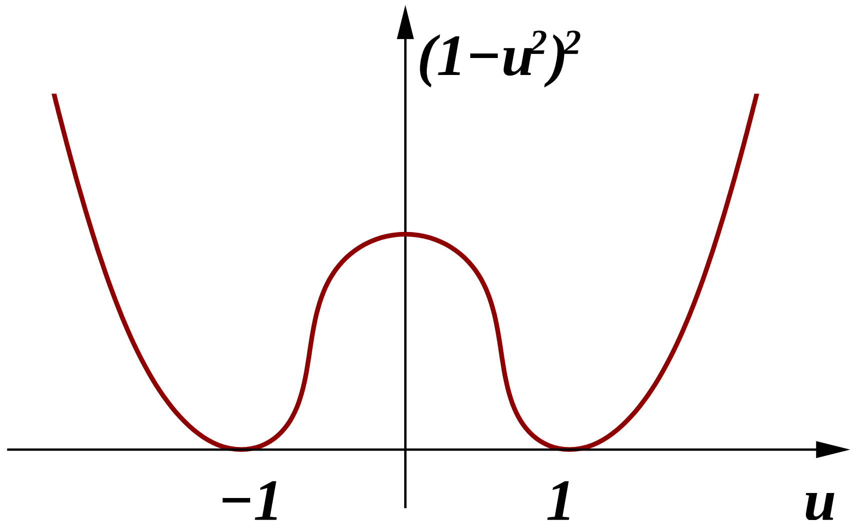


An Example from Higher Dimension

Consider the following minimization problem:

$$\min \left\{ \mathcal{F}(u) = \int_\Omega (1-u^2)^2\,dx, \quad \int_\Omega u = m \right\}$$



(In the above, u is a **scalar-valued** function. It is an example of a more general **Ginzburg-Landau** functional in which u can be **vector-valued**.)

An Example from Higher Dimension

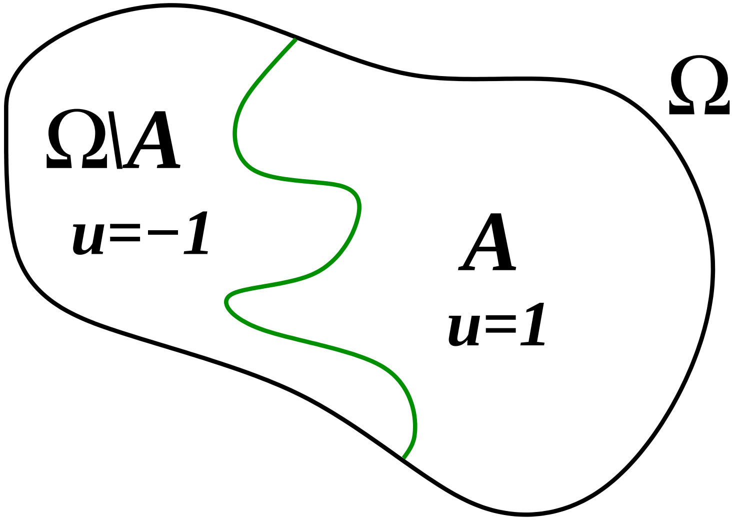
Consider the following minimization problem:

$$\min \left\{ \mathcal{F}(u) = \int_\Omega (1-u^2)^2 \, dx, \quad \int_\Omega u = m \right\}$$

The minimzer is represented **any subset** $A \subset \Omega$ such that

$$\text{Area}(A) = \frac{m + \text{Area}(\Omega)}{2} : \quad u = 1 \text{ on } A \text{ and } u = -1 \text{ on } \Omega \backslash A.$$

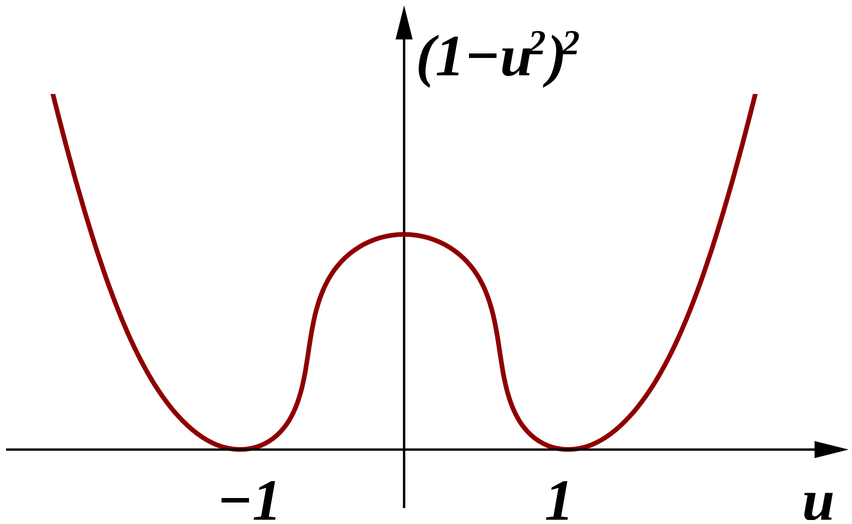
and hence there are **infinitely many solutions**. The **boundary** of A acts as an **interface** separating the regions $\{u = 1\}$ and $\{u = -1\}$.

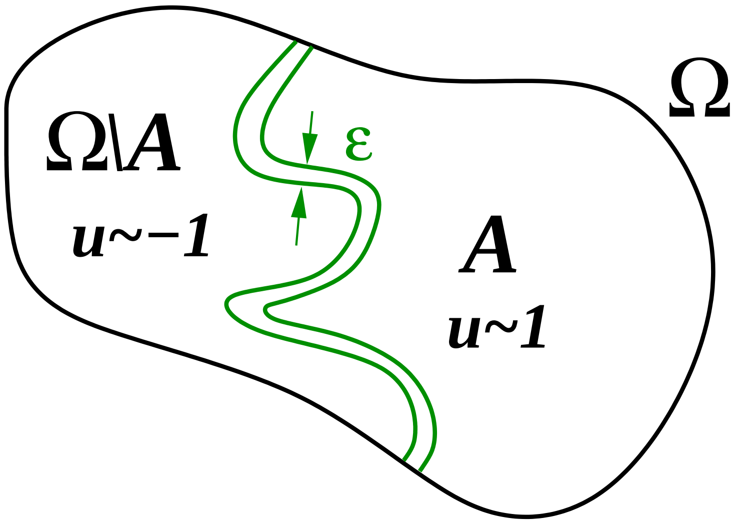


An Example from Higher Dimension

Consider the following **singular perturbation of $\mathcal{F}$ (often called the Allen-Cahn Functional)**:

$$\mathcal{F}_\epsilon(u) = \int_\Omega \epsilon^2 \, |\nabla u|^2 + (1-u^2)^2, \qquad \int_\Omega u = m$$





The term $\int_\Omega |\nabla u|^2$ **penalizes rapid changes** of u.

An Example from Higher Dimension

The minimizer can be represented by a subset $A \subset \Omega$ such that

$$\text{Area}(A) = \frac{m + \text{Area}(\Omega)}{2}$$

but with **minimum boundary length (or area)**

so as to minimize the contribution from $\int |\nabla u|^2$**.**

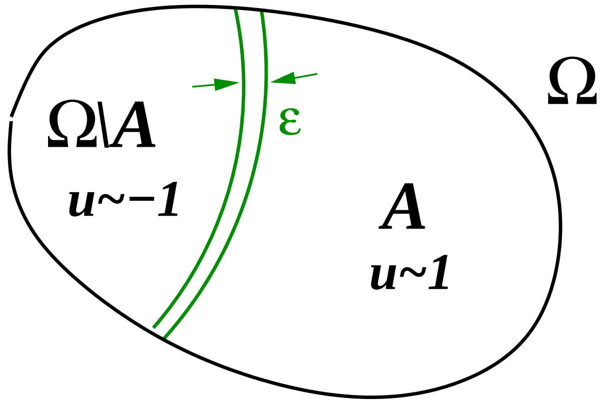
An Example from Higher Dimension

The minimizer can be represented by a subset $A \subset \Omega$ such that

$$\text{Area}(A) = \frac{m + \text{Area}(\Omega)}{2}$$

but with **minimum boundary length (or area)**

In dimension two: the boundary will be a **circular arc: curve with constant curvature** which minimizes length with prescribed volume;



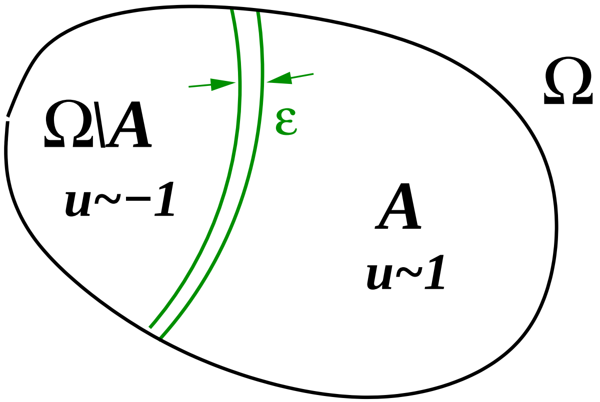
An Example from Higher Dimension

The minimizer can be represented by a subset $A \subset \Omega$ such that

$$\text{Area}(A) = \frac{m + \text{Area}(\Omega)}{2}$$

but with **minimum boundary length (or area)**

In dimension three: the boundary will be a **surface with constant mean curvature** which minimizes area with prescribed volume.



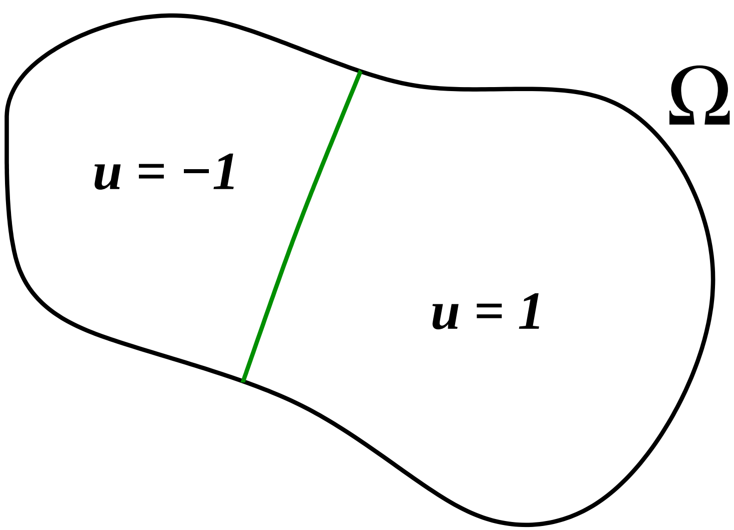
Limit of the Allen-Cahn Functional

Modica-Mortola; Sternberg. $\frac{1}{\epsilon}\mathcal{F}_\epsilon \longrightarrow (\text{“}\Gamma\text{”})\ \mathcal{F}_*$ where

$$\mathcal{F}_* : L^1(\Omega) \longrightarrow \bar{R}_+, \quad \mathcal{F}_*(u) = \int_\Omega |\nabla u|$$

for $u : \Omega \longrightarrow \{-1, 1\}$ and $\int_\Omega u = m$. ($\mathcal{F}_*(u) = \infty$ otherwise.)

Note: $\mathcal{F}_*(u) = \mathcal{H}^{n-1}(\partial\{u = 1\}) =$ **length** or **area** of $\partial\{u = 1\}$.

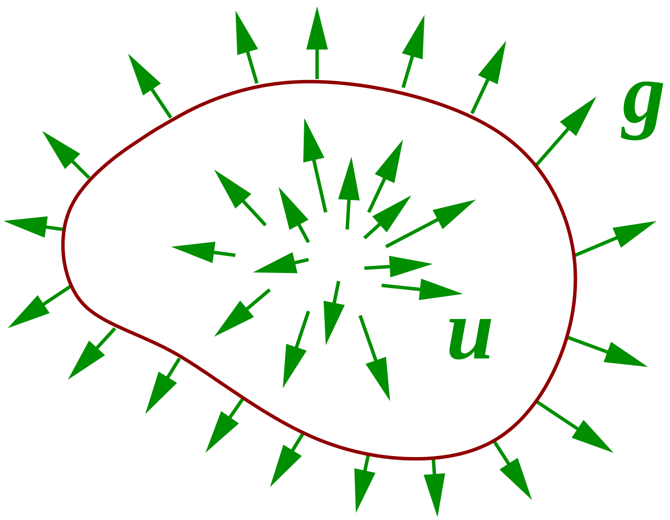


Modeling of Point Defects – Vortices

Given $g : \partial\Omega \longrightarrow S^1$, $|g| = 1$, $\deg(g, \partial\Omega) = 1$, $\Omega \subset \mathbb{R}^2$. Consider the minimization problem:

$$\min \int_\Omega \frac{1}{2}|\nabla u|^2, \quad u : \Omega \longrightarrow S^1, \quad u_{\partial\Omega} = g$$

A **singularity – point defect** must occur somewhere inside Ω:



Energy of a Point Defect

Point Defect (Vortex) has infinite energy:

Near the singularity,

$$u \sim e^{i\theta} \quad \text{so that} \quad |\nabla u|^2 = |\nabla \theta|^2 \sim \frac{1}{r^2}$$

$$\text{hence} \quad \int_0^1 \int_0^{2\pi} \frac{1}{r^2} r\,dr\,d\theta = 2\pi \int_0^1 \frac{1}{r}\,dr = \infty$$

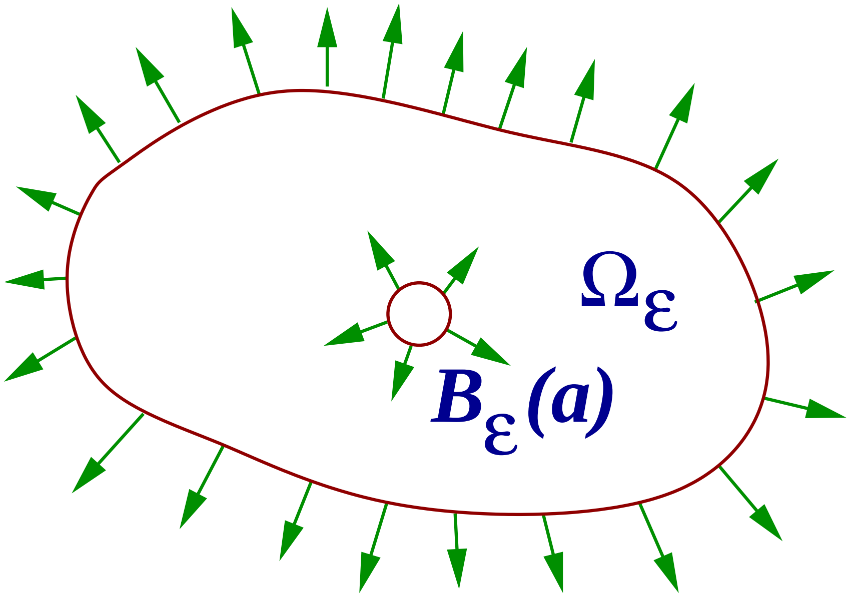
To remedy this, need to **exclude the point singularity**.

Modeling of Point Defects

Given $g : \partial\Omega \longrightarrow S^1$, $|g| = 1$, $\deg(g, \partial\Omega) = 1$, consider the minimization problem:

$$\min \int_{\Omega_\epsilon} \frac{1}{2}|\nabla u|^2, \quad u : \Omega_\epsilon \longrightarrow S^1, \quad u_{\partial\Omega} = g, \quad \deg(u, \partial B_\epsilon(a)) = 1$$

where $\Omega_\epsilon = \Omega \backslash B_\epsilon(a)$.



Modeling of Point Defects – Canonical Harmonic Ma

Now the energy of u in Ω_ϵ is finite:

$$\int_\epsilon^1 \int_0^{2\pi} \frac{1}{r^2} r dr d\theta = 2\pi \int_\epsilon^1 \frac{1}{r} dr = \pi \ln \frac{1}{\epsilon}$$

The **limit of the minimizer**, u^ϵ, as $\epsilon \longrightarrow 0$ is called the **canonical harmonic map** (as u will be a **harmonic function**) on $\Omega \backslash \{a\}$.

(Note that the energy of u will still go to ∞ as $\epsilon \longrightarrow 0$.)

Modeling of Point Defects – Renormalized Energy

Depending on the number of defects and the degree of u around each defect, the energy of u^ϵ can be shown to be:

$$\int_{\Omega_\epsilon} \frac{1}{2}|\nabla u|^2 = \pi \left(\sum_{i=1}^{N} d_i^2 \right) \ln \frac{1}{\epsilon} + O(1)$$

In order to further investigate the **location of the defects**, consider the next term in the expansion:

$$\int_{\Omega_\epsilon} \frac{1}{2}|\nabla u|^2 = \pi \left(\sum_{i=1}^{N} d_i^2 \right) \ln \frac{1}{\epsilon} + W(a_1, a_2, \ldots, a_N) + o(1)$$

The function W can be shown to exist and is called the **renormalized energy which is a function of the defect locations, a_i's**.

Modeling of Point Defects – Ginzburg-Landau Energ

Another Example of Singular Perturbation

Let $u : \Omega \longrightarrow \mathbb{C}(\equiv \mathbb{R}^2)$.

$$\mathcal{F}_\epsilon(u) = \int_\Omega \frac{1}{2}|\nabla u|^2 + \frac{1}{\epsilon^2}(1-|u|^2)^2, \quad u_{\partial\Omega} = g$$

Upon minimization of u, subject to appropriate Dirichlet boundary condition, it can be shown that the energy of a minimizer u_ϵ satisfies:

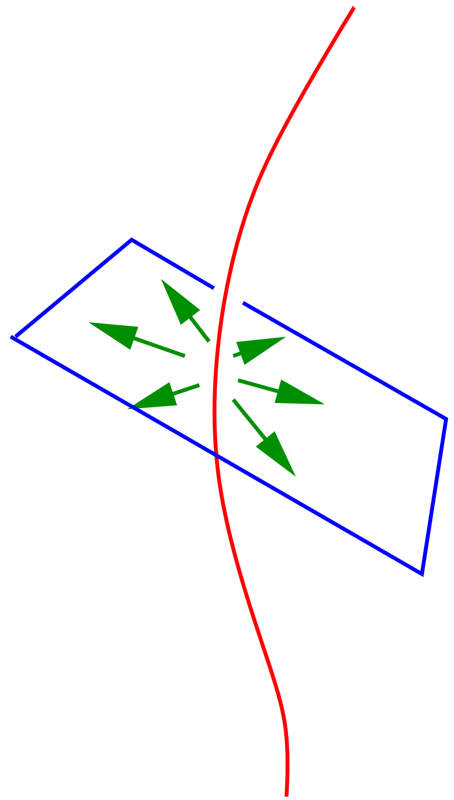
$$\mathcal{F}_\epsilon(u_\epsilon) \approx N\pi \ln\frac{1}{\epsilon} + W(a_1^*, a_2^*, \ldots, a_N^*) + N\gamma$$

where $N = \deg(g, \partial\Omega)$ and γ is some universal constant. The location of the vortices a_i^*'s minimizes the renormalized energy W.

Modeling of Curves (Filaments) in R^3

Let $u : \Omega \subset \mathbb{R}^3 \longrightarrow \mathbb{C}(\equiv \mathbb{R}^2)$.

$$\mathcal{E}(u) = \int_\Omega \frac{1}{2}\,|\nabla u|^2 + \frac{1}{\epsilon^2}(1 - |u|^2)^2$$



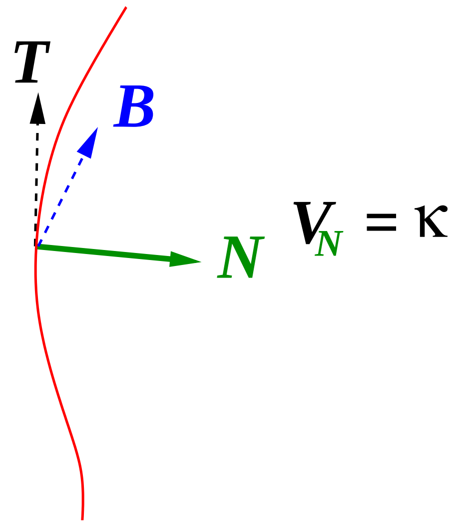
Dynamics of Curves (Filaments) in R^3

Heat Flow (Negative Gradient Flow):

$$u_t = \triangle u + \frac{1}{\epsilon^2} u(1 - |u|^2)$$

converges to **Motion by Mean Curvatrue**:

$$V_N = \kappa$$ (N is the normal direction).



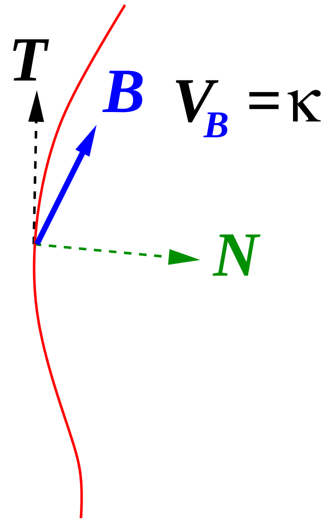
Dynamics of Curves (Filaments) in R^3

Schrödinger Flow:

$$\frac{1}{i}u_t = \triangle u + \frac{1}{\epsilon^2}u(1 - |u|^2)$$

converges to **bi-normal Mean Curvature Motion**:

$V_B = \kappa$ ($B = T \times N$ is the bi-normal direction).



Thank you for your attention.