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# Two topics in the theory of reaction-diffusion equations

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# Forward-backward parabolic equations, 1

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# Plan of the lecture

- Statement of the problem
- Motivations:
  - phase transitions
  - population dynamics
  - oceanography
  - Perona-Malik equation
- Choice of the regularization
- Singular limit (general ideas)

# Introduction

Consider the evolution equation:

$$u_t = \Delta[\phi(u)]\,, \tag{1}$$

where $\phi$ is a regular **nonmonotonic** function.

Equation (1) is of **forward-backward** parabolic type:

- forward diffusion where $\phi' > 0$ ($\leftrightsquigarrow$ stable phases);
- backward diffusion where $\phi' < 0$ ($\leftrightsquigarrow$ unstable phases).

Therefore the corresponding Cauchy problem (like any other initial-boundary value problem) is **ill-posed**.

# Assumptions on $\phi$

The nonlinearities $\phi$ considered in the literature are of the following types:

- **cubic-like** functions:

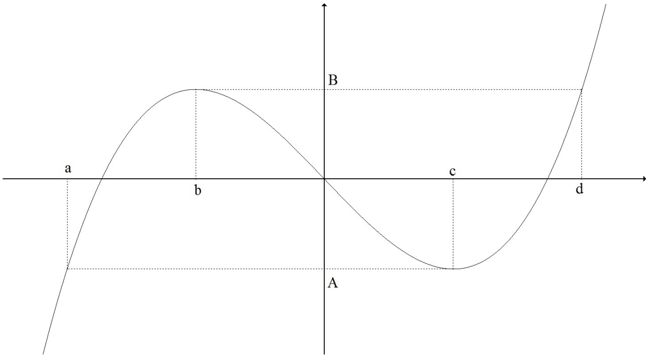
$$(H_1) \qquad \begin{cases} \phi(s) \to \pm\infty \ \text{ as } s \to \pm\infty, \\ \phi'(s) > 0 \ \text{ if } s < b \text{ and } s > c, \\ \phi'(s) < 0 \ \text{ if } b < s < c, \\ \phi''(b) \neq 0, \quad \phi''(c) \neq 0, \end{cases}$$

- **"Perona-Malik"** functions (degeneracy at infinity):

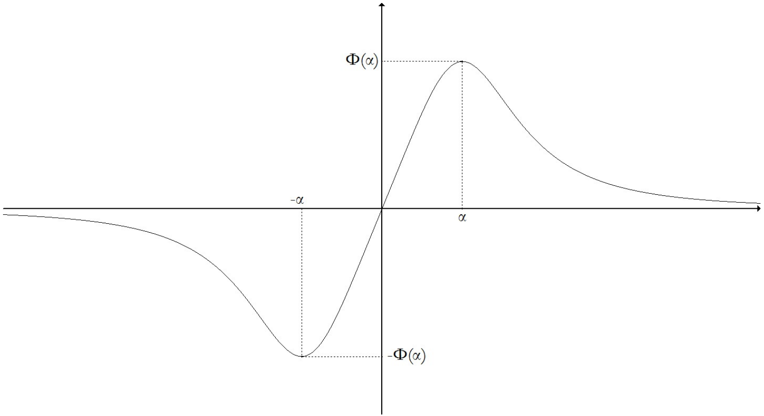
$$(H_2) \qquad \begin{cases} \phi \text{ is odd}, \ \phi(s) > 0 \ \text{ if } s > 0, \\ \phi'(s) > 0 \ \text{ if } 0 \leq s < \alpha, \ \phi'(s) < 0 \ \text{ if } s > \alpha, \\ \phi'(\alpha) = 0\,, \ \phi''(\alpha) \neq 0\,, \ \phi(s) \to 0 \text{ as } s \to +\infty, \\ \phi \in L^p(\mathbb{R}) \text{ for some } p \in [1, \infty). \end{cases}$$

**Different nonlinearities are related to different mathematical models.**

# In phase transitions: $\phi$ of cubic type



# In image processing, population dynamics, oceanography: $\phi$ of Perona-Malik type




**DIFFERENT BEHAVIOUR AT INFINITY!**

# Motivations

## Phase transitions

The so-called *phenomenological theories of PT* rely on:

(*i*) an *order parameter u* of the PT (*e.g.*, concentration, magnetization, polarization...);

(*ii*) an *equation of state*, which links the *free energy density F* with the order parameter $u$ and the temperature $T$.

The Landau theory postulates the free energy

$$F(u, T) := F_0(T) + \alpha_1 (T - T_c) u^2 + \alpha_2 u^4$$

for some $\alpha_1, \alpha_2 > 0 \Rightarrow$ *double well potential* (when $T < T_c$).

If an *external field K* is present, the free energy becomes $F_K(u, T) = F(u, T) - Ku$. Hence *the equilibria are the roots of*

$$\phi(u, T) := \frac{\partial F}{\partial u}(u, T) = K\,. \tag{2}$$

For the Landau theory

$$F_K(u,T) = F_0(T) - Ku + \alpha_1(T - T_c)u^2 + \alpha_2 u^4\,,$$

and equation (2) reads

$$\phi(u,T) \equiv 2\alpha_1(T - T_c)u + 4\alpha_2 u^3 = K\,. \qquad (3)$$

When $T < T_c$ the lhs of (3) is a cubic with roots

$$u_0 = 0\,, \quad u_\pm = \pm\sqrt{\frac{\alpha_1(T_c - T)}{2\alpha_2}}\,.$$

Three solutions of (3) exist if $|K| < K_c := \frac{2}{3\sqrt{3}}\frac{[\alpha_1(T_c - T)]^{3/2}}{\sqrt{\alpha_2}}$ . Therefore, when $T < T_c$ a *field-induced phase transition with hysteresis* is possible for $|K| < K_c$ .

REMARK: *Devonshire free energy density* (more complicated!):

$$F(u,T) = F_0(T) - Ku + \alpha_1(T - T_c)u^2 - \alpha_2 u^4 + \alpha_3 u^6\,.$$

*The Landau theory does not include space dependence, nor time evolution*.

To address space dependence, consider the *phase field* $u = u(x)$, the external field $K = K(x)$ and the *functional*

$$\mathcal{I}[u] := \int_{\Omega} \{F(u(x), T) - K(x)u(x)\}\, dx\,. \tag{4}$$

The isothermal equilibria are now described by the *Euler equation*, which is formally the same of equation (2):

$$\phi(u(x), T) = K(x) \qquad (x \in \Omega \subseteq \mathbb{R}^n)\,. \tag{5}$$

**Remark:** The nature of the external field depends on the specific PT. For instance, for *phase separation in mixtures* the order parameter is the *concentration* and the external field is the *difference of chemical potentials*.

**Remark:** Since the Landau free energy is the double-well potential, the functional in (4) is *nonconvex*.

**Question:** How to include dynamics in the above model?

To address time evolution, let the phase field $u = u(x,t)$ satisfy the *conservation law*

$$\frac{d}{dt}\int_{\Omega} u(x,t)\,dx = 0\,,$$

which gives the *continuity equation* $u_t = -div\,\mathbf{j}$. By the *Fourier law* there holds $\mathbf{j} = -\nabla K\,,$ (namely, *flux* $\propto$ *gradient of thermodynamic force*), thus

$$u_t = \Delta K\,.$$

The above equality becomes an evolution equation for $u$, if we have a *constitutive equation* to link $u$ with $K$. This is given by the so-called **Cahn dynamical principle**, which makes use of equality (2). Then we obtain:

$$u_t = \Delta[\phi(u,T)] \qquad (6)$$

- namely, equation (1) for any fixed $T < T_c$.

**"Near equilibrium" dynamical principle** ([Cahn]): The order parameter $u = u(x, t)$ is the only *”slow variable”*, every other quantity having already relaxed at the equilibrium $\Leftrightarrow$ *time-delay effects are disregarded.*

*This assumption is not satisfied in important physical cases* (polymer glass transition, solid metallic alloys, separation of phases in fluid mixtures). Mathematically, *it is not rigorous* since it makes use of a constitutive equation, which is only valid in equilibrium conditions, to derive an evolution equation.

Therefore, *it is not surprising that the resulting equation is "ill-posed"* (in the sense that the associated initial boundary value problems are ill-posed).

# Regularizations

**Philosophy (singular limit)**

*"True" equation:* $u_t = \Delta[\phi(u)] + \epsilon\,\mathcal{F}(u)\,,$
where $\mathcal{F}$ is some physically meaningful differential operator.

*"Reduced" equation:* $u_t = \Delta[\phi(u)]\,,$
plus **additional conditions**.

*Conjecture:* The reduced problem is ill-posed because some relevant physical term has been neglected.

**Question:** Is it possible to define "properly" solutions of the reduced problem by studying the *vanishing viscosity limit of the regularized problem*?

**Remark:** Analogy with the theory of first order hyperbolic conservation laws

$$\Rightarrow \quad u_t + div[f(u)] = \epsilon\,\Delta u$$

$\Rightarrow$ Rankine–Hugoniot condition, entropy inequalities…

# The "proper" regularization should be suggested by physics...

Taking *non-local spatial effects* into account suggests the *Landau-Ginzburg functional*

$$\mathcal{I}[u] := \int_\Omega \left\{ F(u(x),T) - K(x)u(x)(x + \frac{\kappa}{2}|\nabla u|^2(x) \right\} dx\,.$$

Arguing as above, instead of (5) we obtain

$$\phi(u(x),T) - \kappa\Delta u(x) = K(x)\,, \tag{7}$$

and instead of (6) the *"well-posed" Cahn-Hilliard equation*:

$$u_t = \Delta\Big[\phi(u) - \kappa\Delta u\Big]\,. \tag{8}$$

However, also the Cahn-Hilliard equation is derived by assuming the validity of (7) *even with time dependence* - namely, by using again the Cahn dynamical principle.

If *time delay effects* are taken into account, we obtain the more complete equation

$$u_t = \Delta\left[\phi(u) - \kappa\Delta u + \epsilon\, u_t\right]. \tag{9}$$

This suggests *two possible regularizations* of the equation $u_t = \Delta\phi(u)$:

($i$) if $\epsilon = 0 \quad \Rightarrow$ *Cahn–Hilliard;*

($ii$) if $\kappa = 0 \quad \Rightarrow$ *Sobolev equation:*

$$u_t = \Delta\left[\phi(u) + \epsilon\, u_t\right], \tag{10}$$

which is often called *viscous regularization* of (6).

**Remark:** The Sobolev equation can be rewritten as

$$u_t \;=\; \underbrace{\{I - \epsilon\,\Delta\}^{-1}\Delta}_{\textit{bounded operator}} \;\; \phi(u)\,,$$

thus it is clearly "well-posed". Moreover, its solution satisfies infinitely many *viscous entropy inequalities*.

# Motivations

## Population dynamics

Let $u_j^k = u(j\lambda, k\tau)$ be the population density at the location $j\lambda$ at time $k\tau$ in a linear array of locations ($j = 1, \dots, \frac{1}{\lambda} \in N, \tau > 0$). Let $P(u_j^k)$ be the *transition probability* of a jump of $\pm\lambda$, starting from the location $j\lambda$ at time $k\tau$. [Padrón]

In the *diffusion approximation* we obtain

$$u_t = [\phi(u)]_{xx} ,$$

with $\phi(u) := u\,P(u)$. Then:

($i$) *dispersing populations* $\Rightarrow$ $P$ increasing $\Rightarrow$ equation is "well-posed" (*e.g.*, $\phi(p) = p^{1+m}$);

($ii$) *aggregating populations* $\Rightarrow$ $P$ decreasing $\Rightarrow$ equation is *"ill-posed"* (*e.g.*, $\phi(p) = pe^{-p}$).

**Remark:** Different choices of $\phi$ arise when modelling phenomena like *swarming* or *fish schooling* .

# Motivations

## Oceanography

*Heat transfer in a stratified turbulent shear flow* in one space dimension ([BBDPU]): The temperature $w \geq 0$ satisfies the equation

$$w_t = [k w_x]_x \,,$$

where $k = \sigma(w_x)$ is the *temperature diffusivity*. Since $k$ decreases when $w_x$ is large, a typical choice of $\sigma$ is

$$\sigma(p) = \frac{1}{1+p^2} \,.$$

Then the above equation reads

$$w_t = [\phi(w_x)]_x \,, \quad \phi(p) := p\,\sigma(p) = \frac{p}{1+p^2} \tag{11}$$

Setting $u = w_x$ gives equation (1) (under assumption $(H_2)$) in one space dimension.

# Motivations

**Image processing**

Observe that equation (11) is the one-dimensional *Perona-Malik equation*. Here $w(\cdot, t)$ represents sequentially *restored versions* of the grey level distribution of some distorted picture.

As before, typical choices of $\phi$ are

$$\phi(p) = \frac{p}{1+p^2}\,, \quad \phi(p) = pe^{-p}\,.$$

The diffusion coefficient $\sigma(w_x)$ is designed to be

- *big* at points where $|w_x| \sim 0$;
- *small* near edge points, where $|w_x| >> 1$.

Hence *small disturbances are smoothed out*, while *sharp edges are preserved*.

# Motivations

**Concluding remark:** Equation (1) arises when studying time evolution of systems with **nonconvex energy density**.

In fact, in phase transitions the prototype was

$$\mathcal{I}[u] = \int_\Omega \chi(u)\, dx \,,$$

with the *Landau double well potential*

$$\chi(p) = (1 - p^2)^2 \,.$$

In image processing we have

$$\mathcal{I}[w] = \int_\Omega \chi(w_x)\, dx \,,$$

with the *Perona-Malik potential*

$$\chi(p) = \log(1 + p^2) \,.$$

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# Regularizations

To sum up, the following regularizations have been used:

1. *Pseudoparabolic* ([Novick-Cohen & Pego], [Plotnikov]):

$$u_t = \Delta[\phi(u)] + \epsilon \Delta u_t \,.$$

2. *Degenerate pseudo-parabolic* ([BBDPU]):

$$u_t = \Delta[\phi(u)] + \epsilon\, \Delta[\psi(u)]_t \,,$$

where $\psi : \mathbb{R} \to \mathbb{R}$ is odd, $\psi'(s) > 0$ and

$$\psi(s) \to \pm\gamma \in \mathbb{R} \quad \text{as} \quad s \to \pm\infty \,.$$

3. *Cahn-Hilliard* ([Plotnikov], [Bellettini]):

$$u_t = \Delta[\phi(u)] - \epsilon\, \Delta^2 u \,.$$

4. *Time/space discretization* ([Kinderlehrer], [Demoulini],...).

**Remark:** Regularizations [1, 3, 4] are usually associated with $\phi$ *"of cubic type"*, [2] with $\phi$ *"of Perona-Malik type"*.

# Motivating the choice [2] [Barenblatt]:

By taking into account *time delay effects*, the "true" equation is

$$u_t(x,t) = \Delta\left[u(x,t)\,k_0(u(x,t-\epsilon))\right] \quad \text{with } k_0(u) := \frac{\phi(u)}{u}\,,$$

where the small parameter $\epsilon$ represents a *relaxation time* [BBDPU]. A *formal development* with respect to $\epsilon$ gives

$$u_t = \Delta[\phi(u)] + \epsilon\Delta[\psi(u)]_t\,,$$

$$\text{where} \quad \psi(u) := -\phi(u) + \int_0^u k_0(p)\,dp\,.$$

A typical choice is

$$\phi(u) = \frac{u}{1+u^2} \quad \Rightarrow \quad \psi(u) = -\frac{u}{1+u^2} + \mathrm{arctg}\,u \to \pm\frac{\pi}{2} \quad \text{as } u \to \pm\infty\,.$$

The regularization is degenerate pseudoparabolic, since $\psi'(u) \to 0$ as $u \to \pm\infty$.

# Many open problems...

- Does the solution obtained as the *vanishing viscosity limit of the regularized problem* depend on the regularization itself?
- Lack of a general uniqueness result
- Development of singularities for the degenerate pseudoparabolic case (choice [2]), if $\phi$ is of Perona-Malik type $\Rightarrow$ *need to consider* *Radon measure-valued solutions*
- Qualitative properties (*e.g.*, asymptotic behaviour for large time)
- Numerics

# Keynotes for the cubic-like case

**Sobolev regularization**

- **Regularized problem** (*e.g.*, [Novick-Cohen & Pego] for the Neumann IBVP for equation (1));
- **Entropy inequalities** $\Longrightarrow$ **Entropy solutions** ([Plotnikov], [Evans-Portilheiro]);
- **Vanishing viscosity limit** of the regularized problem ([Plotnikov]);
- **Young measure-valued solutions** ([Plotnikov], [Smarrazzo]).

# $\phi$ of cubic type: Main features of the problem

Consider the problem

$$(C) \qquad \begin{cases} u_t = \Delta[\phi(u)] & \text{in } \Omega \times (0,T) =: Q \\ u = 0 & \text{in } \partial\Omega \times (0,T) \\ u = u_0 \in L^\infty(\Omega) & \text{in } \Omega \times \{0\}\,. \end{cases}$$

**Main idea** ([Plotnikov, 1994]): To define *weak entropy solutions* of problem $(C)$ by the Sobolev regularization

$$(C_\epsilon) \qquad \begin{cases} u_t = \Delta v & \text{in } Q \\ v = 0 & \text{in } \partial\Omega \times (0,T) \\ u = u_0 \in L^\infty(\Omega) & \text{in } \Omega \times \{0\}\,, \end{cases}$$

letting $\epsilon \to 0$ in the *chemical potential* $v := \phi(u) + \epsilon u_t$ .

**Remark:** For every $\epsilon > 0$ there exists a unique strong solution $(u_\epsilon, v_\epsilon)$ of the regularized problem $(C_\epsilon)$. [Novick-Cohen & Pego]

If $\phi$ satisfies assumption $(H_1)$ [cubic type]:

- *Estimates* of $u_\epsilon$, $v_\epsilon$ in $L^\infty(Q_T)$, and of $v_\epsilon$ in $L^2((0,T);H_0^1(\Omega))$, *uniform with respect to* $\epsilon$, whence
  - weak* compactness in $L^\infty(Q_T)$ of the families $\{u_\epsilon\}$ and $\{v_\epsilon\}$,
  - weak compactness in $L^2((0,T);H_0^1(\Omega))$ of the family $\{v_\epsilon\}$.
- *Existence* of a couple $u \in L^\infty(Q_T)$, $v \in L^2((0,T);H^1(\Omega)) \cap L^\infty(Q_T)$ such that for any $\zeta \in C^1(\bar{Q}_T)$, $\zeta(\cdot,T) = 0$ in $\bar{\Omega}$

$$\iint_{Q_T} (u\zeta_t - \nabla v \cdot \nabla \zeta)\, dxdt + \int_\Omega u_0 \zeta(x,0)\, dx = 0\,.$$

- *Characterization of the* limiting Young measures *associated with* $\{u_\epsilon\}$ *and* $\{v_\epsilon\}$, whence

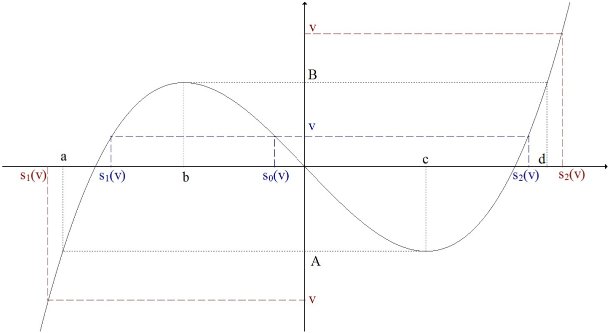
$$u = \sum_{i=0}^{2} \lambda_i s_i(v) \geq 0 \quad (\leftrightsquigarrow \quad u = \phi^{-1}(v) \text{ if } \phi \text{ is monotonic})\,.$$

Here $0 \leq \lambda_i = \lambda_i(x,t) \leq 1$, $\sum_{i=0}^{2} \lambda_i = 1$, and $s_i(v)$ are the three roots of the equation $\phi(u) = v$.

More explicitly,

$$u(x,t) = \begin{cases} s_1(v(x,t)) & \text{if } v(x,t) < A \\ \sum_{i=0}^{2} \lambda_i(x,t) s_i(v(x,t)) & \text{if } A \le v(x,t) \le B \\ s_2(v(x,t)) & \text{if } v(x,t) > B\,. \end{cases}$$

In particular, $\lambda_1 = 1$ if $v < A$ and $\lambda_2 = 1$ if $v > B$.




Therefore, the couple $(u, v)$ is a solution of problem $(P)$ *in the sense of Young measures* ($\leftrightsquigarrow$ usual solution if $\phi$ is monotonic).