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)
Consider the evolution equation:

\[ u_t = \Delta[\phi(u)], \quad (1) \]

where \( \phi \) is a regular nonmonotonic function.

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

- forward diffusion where \( \phi' > 0 \) (\( \leftrightarrow \) stable phases);
- backward diffusion where \( \phi' < 0 \) (\( \leftrightarrow \) 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:

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

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

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

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 $\alpha_1, \alpha_2 > 0 \Rightarrow \text{double well potential}$ (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*

$$\phi(u, T) := \frac{\partial F}{\partial u}(u, T) = K.$$  (2)
For the Landau theory

$$F_K(u, T) = F_0(T) - Ku + \alpha_1(T - T_c)u^2 + \alpha_2u^4,$$

and equation (2) reads

$$\phi(u, T) \equiv 2\alpha_1(T - T_c)u + 4\alpha_2u^3 = K. \quad (3)$$

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!):

$$F(u, T) = F_0(T) - Ku + \alpha_1(T - T_c)u^2 - \alpha_2u^4 + \alpha_3u^6.$$
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

$$I[u] := \int_{\Omega} \left\{ F(u(x), T) - K(x)u(x) \right\} \, dx.$$  \hspace{1cm} (4)

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

$$\phi(u(x), T) = K(x) \quad (x \in \Omega \subseteq \mathbb{R}^n).$$  \hspace{1cm} (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** $u_t = -\text{div} \, j$. By the **Fourier law** there holds $j = -\nabla K$, (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:

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

- 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

\[
\Rightarrow \quad u_t + \text{div}[f(u)] = \epsilon \Delta u
\]

\Rightarrow \quad \text{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

\[
\phi(u(x), T) - \kappa \Delta u(x) = K(x) ,
\] (7)

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

\[
 u_t = \Delta \left[ \phi(u) - \kappa \Delta u \right] .
\] (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

\[ u_t = \Delta \left[ \phi(u) - \kappa \Delta u + \epsilon u_t \right]. \]  

(9)

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

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

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

\[ u_t = \Delta \left[ \phi(u) + \epsilon u_t \right], \]  

(10)

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

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

\[ u_t = \left\{ I - \epsilon \Delta \right\}^{-1} \Delta \phi(u), \]

*bounded operator*

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

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Motivations

Population dynamics

Let \( u^k_j = u(j\lambda, k\tau) \) be the population density at the location \( j\lambda \) at time \( k\tau \) in a linear array of locations \((j = 1, \ldots, 1/\lambda \in \mathbb{N}, \tau > 0)\). Let \( P(u^k_j) \) 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.
Heat transfer in a stratified turbulent shear flow in one space dimension ([BBDPU])

The temperature \( w \geq 0 \) satisfies the equation

\[
wt = [kw_x]_x,
\]

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

\[
\phi(p) = \frac{p}{1 + p^2}, \quad \phi(p) = p e^{-p}.
\]

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**

\[ \chi(p) = \log(1 + p^2) . \]
Some references

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 \( \psi : \mathbb{R} \rightarrow \mathbb{R} \) is odd, \( \psi'(s) > 0 \) and
   \[ \psi(s) \rightarrow \pm \gamma \in \mathbb{R} \quad \text{as} \quad s \rightarrow \pm \infty. \]

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

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

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

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

where \( \psi(u) := -\phi(u) + \int_0^u k_0(p) \, dp. \)

A typical choice is

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

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** $\implies$ **Entropy solutions** ([Plotnikov], [Evans-Portilheiro]);

- **Vanishing viscosity limit** of the regularized problem ([Plotnikov]);

- **Young measure-valued solutions** ([Plotnikov], [Smarrazzo]).
of cubic type: Main features of the problem

Consider the problem

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

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

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

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 $L^2((0, T); H^1_0(\Omega))$, **uniform with respect to $\epsilon$,** whence
  
  - weak* compactness in $L^\infty(Q_T)$ of the families $\{u_\epsilon\}$ and $\{v_\epsilon\}$,
  - weak compactness in $L^2((0, T); H^1_0(\Omega))$ 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 $\bar{\Omega}$

  \[
  \int \int_{Q_T} (u\zeta_t - \nabla v \cdot \nabla \zeta) \, dx \, dt + \int_\Omega u_0 \zeta(x, 0) \, dx = 0.
  \]

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

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

  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,

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

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 (\(\leftrightarrow\) usual solution if \(\phi\) is monotonic).