

# The Cahn-Hilliard equation

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The Cahn–Hilliard equation : recent advances and applications

## The Cahn-Hilliard equation :

Cahn-Hilliard system :

$$\begin{aligned}\frac{\partial u}{\partial t} &= \kappa \Delta w, \quad \kappa > 0 \\ w &= -\alpha \Delta u + f(u), \quad \alpha > 0\end{aligned}$$

Equivalently :

$$\frac{\partial u}{\partial t} + \alpha \kappa \Delta^2 u - \kappa \Delta f(u) = 0$$

Describes the phase separation process in a binary alloy : spinodal decomposition, coarsening

$u$  : order parameter (in general : rescaled density of atoms taking values between  $-1$  and  $1$ )

$w$  : chemical potential

$\kappa$  : mobility

$\alpha$  : related to the surface tension at the interface



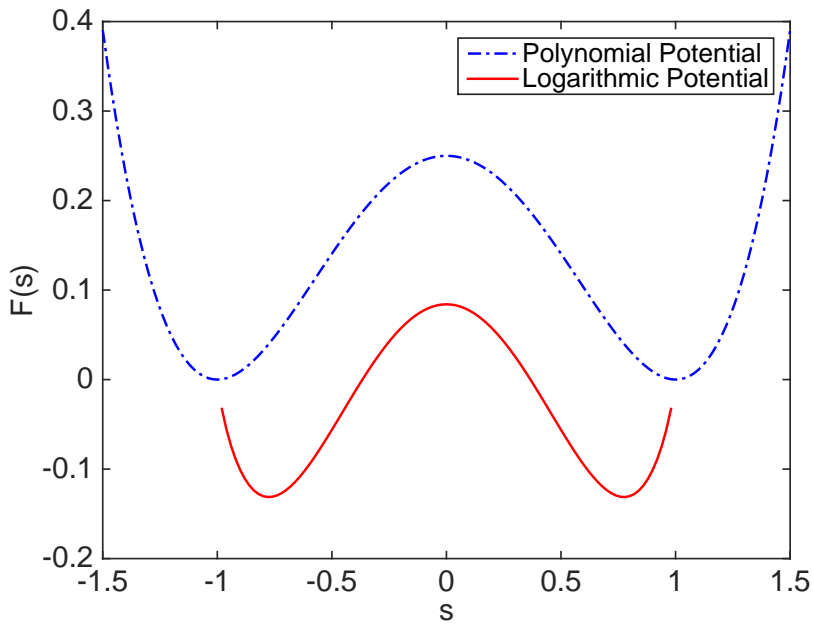
$f$  : derivative of a double-well potential  $F$

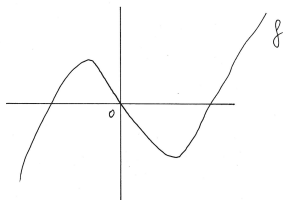
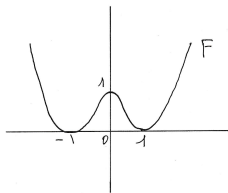
Typical choice :

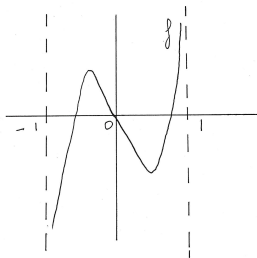
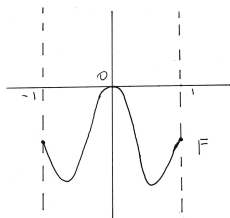
$$\begin{aligned} F(s) &= \frac{1}{4}(s^2 - 1)^2 \\ f(s) &= s^3 - s \end{aligned}$$

Thermodynamically relevant potential :

$$\begin{aligned} F(s) &= -\theta_0 s^2 + \theta_1 ((1+s) \ln(1+s) \\ &\quad + (1-s) \ln(1-s)) \\ f(s) &= -2\theta_0 s + \theta_1 \ln \frac{1+s}{1-s} \\ s &\in (-1, 1), \quad 0 < \theta_1 < \theta_0 \end{aligned}$$







**Remark :**  $\kappa$  should more generally depend on  $u$  and degenerate :

$$\frac{\partial u}{\partial t} = \operatorname{div}(\kappa(u) \nabla w)$$

$$\kappa(s) = 1 - s^2$$

Restricts the diffusion process to the interfacial region

Is observed when the movements of atoms are confined to this region

Derivation of the Cahn-Hilliard system :

Mass balance :  $\frac{\partial u}{\partial t} = -\operatorname{div} h$

$h$  : mass flux

Constitutive equation :  $h = -\kappa \nabla w$

Ginzburg-Landau free energy :  $\Psi_{\Omega}(u, \nabla u) = \int_{\Omega} (\frac{\alpha}{2} |\nabla u|^2 + F(u)) dx$

$\Omega$  : domain occupied by the material

Usual definition of  $w$  : derivative of  $\Psi_{\Omega}$  w.r.t.  $u$

→ No longer valid

New definition : variational derivative of  $\Psi_\Omega$  w.r.t.  $u$

$$\rightarrow w = -\alpha \Delta u + f(u)$$

Energy decay (compatible boundary conditions) :

$$\frac{d\Psi_\Omega}{dt} = -\kappa \|\nabla w\|_{L^2(\Omega)^n}^2 \leq 0$$

$$\frac{d\Psi_\Omega}{dt} = -\frac{1}{\kappa} \left\| \frac{\partial u}{\partial t} \right\|_{H^{-1}(\Omega)}^2 \leq 0$$

**Remark :** If A and B are the two components :  $u_A + u_B = 0$  (after rescaling)  
The Cahn-Hilliard equation is equivalent to a system of 2 Cahn-Hilliard equations

Free energy :

$$\Psi_{\Omega}(u_A, \nabla u_A, u_B, \nabla u_B) = \frac{1}{2} \int_{\Omega} \left( \frac{\alpha}{2} |\nabla u_A|^2 + \frac{\alpha}{2} |\nabla u_B|^2 + F(u_A) + F(u_B) \right) dx$$

Equations :

$$\frac{\partial u_A}{\partial t} = \kappa \Delta w_A, \quad w_A = \frac{1}{2} (-\alpha \Delta u_A + f(u_A)) \quad (= \partial_{u_A} \Psi_{\Omega})$$

$$\frac{\partial u_B}{\partial t} = \kappa \Delta w_B, \quad w_B = \frac{1}{2} (-\alpha \Delta u_B + f(u_B)) \quad (= \partial_{u_B} \Psi_{\Omega})$$

$$u_A + u_B = 0, \quad w_A + w_B = 0$$

$$w_A - w_B = -\alpha \Delta u_A + f(u_A)$$

Gradient term in the Ginzburg-Landau free energy : the interactions between the material's components are short-ranged

Obtained by approximation of a nonlocal term which also accounts for long-ranged interactions

Nonlocal Cahn-Hilliard equation : G. Giacomin-J.L. Lebowitz

Rigorous derivation based on stochastic arguments

Free energy :

$$\Psi_{\Omega}(u) = \int_{T^n} [f(u(x)) + u(x) \int_{T^n} \mathcal{K}(|x - y|)(1 - u(y))dy]dx$$

$T^n$  :  $n$ -dimensional torus,  $\mathcal{K}$  : smooth kernel

Mathematical analysis : C.G. Gal, H. Gajewski, M. Grasselli, ...

Usual boundary conditions :

$$\begin{aligned}\frac{\partial w}{\partial \nu} &= 0 \text{ on } \Gamma \\ \frac{\partial u}{\partial \nu} &= 0 \text{ on } \Gamma\end{aligned}$$

$\Omega \subset \mathbb{R}^N$ ,  $N \leq 3$  : bounded and regular domain

$\Gamma = \partial\Omega$

$\nu$  : unit outer normal vector

→ Mass conservation :  $\frac{d}{dt} \int_{\Omega} u \, dx = 0$

Equivalently :

$$\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0 \text{ on } \Gamma$$

## **Regular potentials :**

- Well-posedness, regularity : C.M. Elliott-S. Zheng, B. Nicolaenko-B. Scheurer, D. Li-C. Zhong, ...
- Existence of finite-dimensional attractors : B. Nicolaenko-B. Scheurer-R. Temam, D. Li-C. Zhong, ...
- Convergence of solutions to steady states : S. Zheng, P. Rybka-K.-H. Hoffmann

## Logarithmic (singular) potentials :

Main difficulty : prove that  $u$  remains in  $(-1, 1)$

**Remark :** Not true for regular potentials

We can prove that

$$|u(t, x)| < 1 \text{ a.e } (t, x)$$

In one and two space dimensions :

$$\|u(t)\|_{L^\infty(\Omega)} \leq 1 - \delta, \quad t > 0, \quad \delta \in (0, 1)$$

- Well-posedness, regularity : C.M. Elliott-S. Luckhaus, C.M. Elliott-H. Garcke, A. Debussche-L. Dettori, A. Miranville-S. Zelik
- Existence of finite-dimensional attractors : A. Debussche-L. Dettori, A. Miranville-S. Zelik
- Convergence of solutions to steady states : H. Abels-M. Wilke

## **Dynamic boundary conditions :**

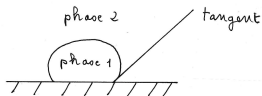
Influence of the walls for confined systems

Mainly studied for polymer mixtures

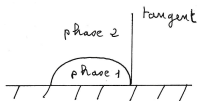
Technological applications

Problem : define the boundary conditions (we need 2 boundary conditions)

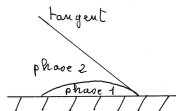
Variational boundary condition : static contact angle (not realistic)



$$\theta > \frac{\pi}{2}$$



$$\theta = \frac{\pi}{2}$$



$$\theta < \frac{\pi}{2}$$

First boundary condition : no mass flux at the boundary :

$$\frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma$$

→ Bulk mass conservation :  $\frac{d}{dt} \int_{\Omega} u dx = 0$

Second boundary condition : we consider, in addition to the Ginzburg-Landau free energy

$$\Psi_{\Omega}(u, \nabla u) = \int_{\Omega} \left( \frac{\alpha}{2} |\nabla u|^2 + F(u) \right) dx$$

the surface free energy

$$\Psi_{\Gamma}(u, \nabla_{\Gamma} u) = \int_{\Gamma} \left( \frac{\alpha_{\Gamma}}{2} |\nabla_{\Gamma} u|^2 + G(u) \right) dx$$

$$\alpha_{\Gamma} > 0$$

$\nabla_{\Gamma}$  : surface gradient

Original surface potential :  $G(s) = \frac{1}{2} a_{\Gamma} s^2 - b_{\Gamma} s$

$a_{\Gamma} > 0$  : accounts for a modification of the effective interaction between the components

$b_{\Gamma}$  : characterizes the preferential attraction of one of the components by the walls

Total energy :  $\Psi = \Psi_{\Omega} + \Psi_{\Gamma}$

The system tends to minimize the excess surface energy :

$$\frac{1}{d} \frac{\partial u}{\partial t} - \alpha_{\Gamma} \Delta_{\Gamma} u + g(u) + \alpha \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma$$

$d > 0$  : relaxation parameter

$\Delta_{\Gamma}$  : Laplace-Beltrami operator

$g = G'$

→ Dynamic boundary condition

Energy decay :

$$\frac{d\Psi}{dt} = -\frac{1}{\kappa} \left\| \frac{\partial u}{\partial t} \right\|_{H^{-1}(\Omega)}^2 - \frac{1}{d} \left\| \frac{\partial u}{\partial t} \right\|_{L^2(\Gamma)}^2 \leq 0$$

Second approach : G.R. Goldstein-A. Miranville-G. Schimperna

Total mass conservation :  $\frac{d}{dt}(\int_{\Omega} u dx + \int_{\Gamma} u d\sigma) = 0$

$\rightarrow \frac{\partial u}{\partial t} = \beta_{\Gamma} \Delta_{\Gamma} w - \kappa \frac{\partial w}{\partial \nu}$  on  $\Gamma$ ,  $\beta_{\Gamma} \geq 0$

Second boundary condition :  $w$  is a variational derivative of the total free energy  $\Psi$  w.r.t.  $u$

$\rightarrow w = -\alpha_{\Gamma} \Delta_{\Gamma} u + g(u) + \alpha \frac{\partial u}{\partial \nu}$  on  $\Gamma$

Cahn-Hilliard type equation on the boundary

Energy decay :

$$\frac{d\Psi_{\Omega}}{dt} = -\kappa \|\nabla \mu\|_{L^2(\Omega)^n}^2 \leq 0$$

Third approach : C. Liu-H. Wu

Based on energetic principles

Similar boundary conditions + no mass flux at the boundary

Conservation of mass in the bulk and on the boundary separately

Regular potentials : the system is well understood

Contributors : R. Chill, C.G. Gal, E. Fašangová, A. Miranville, J. Pruess, R. Racke, H. Wu, S. Zelik, S. Zheng, ...

Singular potentials : more complicated and less understood

Possible nonexistence of classical solutions

Other applications of the Cahn-Hilliard equation :

- Dealloying (corrosion processes)
- Population dynamics
- Bacterial films
- Thin films
- Image processing (denoising, inpainting)
- Astronomy (rings of Saturn)
- Clustering of mussels





**A variant of the Cahn-Hilliard equation :**

$$\frac{\partial u}{\partial t} + \alpha \kappa \Delta^2 u - \kappa \Delta f(u) + g(x, u) = 0$$

**First model :** The Cahn-Hilliard-Oono equation (Y. Oono-S. Puri, 1987)

$$g(x, s) = \beta s, \beta \geq 0$$

$\beta = 0$  : Cahn-Hilliard equation

$\beta > 0$  : models long-ranged (nonlocal) interactions

Introduced also to simplify numerical simulations

Associated free energy :

$$\Psi = \int_{\Omega} \left( \frac{\alpha}{2} |\nabla u|^2 + F(u) + \int_{\Omega} u(y) h(y, x) u(x) dx \right) dy$$

(Cahn-Hilliard equation :  $\Psi = \int_{\Omega} \left( \frac{\alpha}{2} |\nabla u|^2 + F(u) \right) dx$ )

$h$  : models the long-ranged interactions ; Oono's model (N=3) :

$$h(y, x) = \frac{\beta}{4\pi|y - x|}$$

The long-ranged interactions are repulsive when  $u(y)$  and  $u(x)$  have the same sign

→ Favors the formation of interfaces

Evolution equation :

$$\frac{\partial u}{\partial t} = \kappa \Delta \frac{\delta \Psi}{\delta u}$$

$\frac{\delta}{\delta u}$  : variational derivative

$-\frac{1}{4\pi|y-x|}$  : Green's function associated with the Laplace operator

Mathematical analysis : A. Miranville, JAAC ; A. Giorgini-M. Grasselli-A. Miranville, M3AS

## Remarks :

a) Variant of the model (R. Choksi-X. Ren, 2003) :

$$g(x, s) = \beta(s - \frac{1}{\text{Vol}(\Omega)} \int_{\Omega} u_0(x) dx)$$

$u_0$  : initial condition

Models microphase separation of diblock copolymers

Conservation of mass

Efficient numerical simulations (multigrid solvers) : A. Aristotelous-O.  
Karakashian-S. Wise

b) Coupling with the incompressible Navier-Stokes equations (Y. Huo-X. Jiang-H. Zhong-Y. Yang, 2003) :

Models a chemically reacting incompressible binary fluid in a bounded domain

Mathematical Analysis : S. Bosia-M. Grasselli-A. Miranville, M2AS

**Second model** : A Cahn-Hilliard/Allen Cahn equation (M. Hildebrandt-A. Mikhailov, 1996)

System of equations :

$$\begin{aligned}\frac{\partial u}{\partial t} &= \epsilon^2 D \Delta w - w \\ w &= -\Delta u + \frac{f(u)}{\epsilon^2}, \quad D, \epsilon > 0\end{aligned}$$

Equivalent formulation :

$$\frac{\partial u}{\partial t} + \epsilon^2 D \Delta^2 u - \Delta(Df(u) + u) + \frac{f(u)}{\epsilon^2} = 0$$

Models microscopic mechanisms such as surface diffusion and adsorption/desorption

Mathematical analysis : H. Israel

**Third model** : A Cahn-Hilliard model with a proliferation term (E. Khain-L. Sander, 2008)

$$g(x, s) = \beta s(s - 1), \beta > 0$$

Models wound healing and tumor growth (1D) or clustering of malignant brain tumor cells (2D)

Deals with cells which move, proliferate and interact via diffusion and cell-cell adhesion

$u$  : local density of cells

$F$  : local free energy,  $F(s) = \frac{1}{4}a(s - \frac{1}{2})^4 + \frac{1}{2}b(s - \frac{1}{2})^2$ ,  $a > 0$

$\beta$  : proliferation rate

Mathematical analysis : L. Cherfils-A. Miranville-S. Zelik, DCDS B

**Fourth model :** A Cahn-Hilliard model for binary image inpainting (A. Bertozzi-S. Esedoglu-A. Gillette, 2007)

$$g(x, s) = \lambda_0(s - h(x))\chi_{\Omega \setminus D}(x), \quad \lambda_0 > 0, \quad D \subset\subset \Omega$$

Equation :

$$\frac{\partial u}{\partial t} + \epsilon \Delta^2 u - \frac{1}{\epsilon} \Delta f(u) + g(x, u) = 0, \quad \epsilon > 0$$

$h(x)$  : given image ( $h \in L^2(\Omega)$ )

$D$  : inpainting domain (damaged region)

$$f(s) = 4s^3 - 6s^2 + 2s$$

$g(x, u)$  : added to keep  $u$  close to the image  $h(x)$  outside the inpainting region (fidelity term)

Mathematical Analysis : L. Cherfils-H. Fakhir-A. Miranville, IPI, SIIMS

Other variants of the Cahn-Hilliard equation :

### **Viscous Cahn-Hilliard equation**

$$-\beta \Delta \frac{\partial u}{\partial t} + \frac{\partial u}{\partial t} + \alpha \kappa \Delta^2 u - \kappa \Delta f(u) = 0, \beta > 0$$

Proposed by A. Novick-Cohen to account for viscosity effects in the phase separation of polymer/polymer systems

Further generalizations : Microforce balance (M. Gurtin)

Take into account anisotropy, deformations of the material (e.g., elastic or visco-elastic materials), heat transfers

## Hyperbolic Cahn-Hilliard equation

$$\beta \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} + \alpha \kappa \Delta^2 u - \kappa \Delta f(u) = 0, \quad \beta > 0$$

Proposed by P. Galenko et al. to model the early stages of spinodal decomposition in certain glasses

No mass conservation

Main difficulty : good notion of a solution in 2 and 3D

Bounded energy solutions : uniqueness in 2D

Logarithmic nonlinear terms : open problem ; already very difficult for the weakly damped wave equation :

$$\beta \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} - \Delta u + f(u) = 0, \quad \beta > 0$$

## Convective Cahn-Hilliard equation

$$\frac{\partial u}{\partial t} + \alpha \kappa \Delta^2 u + u \cdot \nabla u - \kappa \Delta f(u) = 0$$

Describes the dynamics of driven systems such as faceting of growing thermodynamically unstable crystal surfaces

Mass conservation

Cubic nonlinear term : A. Eden-V. Kalantarov

Logarithmic nonlinear terms : open problems (uniqueness, regularity)

## Higher-order Cahn-Hilliard models

Free energy :

$$\Psi_{\text{HOGL}} = \int_{\Omega} \left( \frac{1}{2} \sum_{i=1}^M \sum_{|k|=i} a_k |\mathcal{D}^k u|^2 + F(u) \right) dx, \quad M \in \mathbb{N}$$

$$|k| = k_1 + k_2 + k_3, \quad k = (k_1, k_2, k_3) \in (\mathbb{N} \cup \{0\})^3$$

$$\mathcal{D}^k = \frac{\partial^{|k|}}{\partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}}$$

Proposed by G. Caginalp-E. Esenturk to account for anisotropy effects

Corresponding equation :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^M (-1)^i \sum_{|k|=i} a_k \mathcal{D}^{2k} u - \Delta f(u) = 0$$

Examples :

Anisotropic Cahn-Hilliard equation :

$$\frac{\partial u}{\partial t} + \Delta \sum_{i=1}^3 a_i \frac{\partial^2 u}{\partial x_i^2} - \Delta f(u) = 0$$

Sixth-order anisotropic Cahn-Hilliard equation :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i,j=1}^3 a_{ij} \frac{\partial^4 u}{\partial x_i^2 \partial x_j^2} + \Delta \sum_{i=1}^3 b_i \frac{\partial^2 u}{\partial x_i^2} - \Delta f(u) = 0$$

Other sixth-order models :

- Strong anisotropy effects
- Atomistic models of crystal growth
- Description of growing crystalline surfaces with small slopes which undergo faceting
- Oil-water-surfactant mixtures
- Mixtures of polymer molecules

Regular nonlinear terms : well understood (L. Cherfils, M. Grasselli, A. Miranville, S. Peng, G. Schimperna, H. Wu, ...)

Logarithmic nonlinear terms : existence of classical solutions is open

Variational solutions : A. Miranville

## **Systems of Cahn-Hilliard equations**

Multi-component materials

## **Stochastic Cahn-Hilliard equation**

Also called Cahn-Hilliard-Cook equation

Takes into account thermal fluctuations

## **Coupling with the Allen-Cahn equation**

Allen-Cahn equation :

$$\frac{\partial u}{\partial t} - \Delta u + f(u) = 0$$

Models the ordering of atoms during the phase separation

## Coupling with the incompressible Navier-Stokes equations

Models mixtures of two incompressible immiscible fluids

$$\frac{\partial u}{\partial t} - \xi \operatorname{div} D(u) + (u \cdot \nabla)u + \nabla p = \varepsilon w \nabla \rho$$

$$\operatorname{div} u = 0$$

$$\frac{\partial \rho}{\partial t} + (u \cdot \nabla)\rho = \kappa \Delta w$$

$$w = -\varepsilon \Delta \rho + \frac{1}{\varepsilon} f(\rho)$$

$D(u) = \frac{1}{2}(\nabla u + {}^t\nabla u)$  : deformation tensor

$\varepsilon w \nabla \rho$  : Korteweg force

Boundary conditions : No slip boundary condition not realistic, dynamic boundary conditions

$$u \cdot \nu = 0, \quad \frac{\partial \mu}{\partial \nu} = 0 \text{ on } \Gamma$$

$$\xi(D(u) \cdot \nu)_\Gamma + \beta u_\Gamma = \mathcal{L}(\rho) \nabla_\Gamma \rho \text{ on } \Gamma$$

$$\frac{\partial \rho}{\partial t} + u_\Gamma \cdot \nabla_\Gamma \rho = -l_0 \mathcal{L}(\rho) \text{ on } \Gamma$$

$$\mathcal{L}(\rho) = -\gamma \Delta_\Gamma \rho + \varepsilon \frac{\partial \rho}{\partial \nu} + \zeta \rho + g(\rho)$$

$l_0, \beta, \zeta, \gamma > 0$  : phenomenological parameters

$\beta$  : slip coefficient

For  $v : \Gamma \rightarrow \mathbb{R}^n$  :  $v_\nu = v \cdot \nu$  (normal component),  $v_\Gamma = v - (v_\nu)\nu$  (tangential component)

Uniqueness : logarithmic nonlinear terms, dynamic boundary conditions  
(cubic and logarithmic nonlinear terms)

Variants : Cahn-Hilliard-Hele-Shaw, Cahn-Hilliard-Brinkman, Compressible  
Navier-Stokes equations