Models of Phase Relaxation

Augusto Visintin - Trento (Italy)

Visintin@science.unitn.it

http://www-math.science.unitn.it/ visintin/

Contents

1. Phase Relaxation

Let us consider a solid-liquid system, and set

u: density of internal energy,

θ: temperature,

χ: phase function ($\chi := -1$ in the solid, $\chi := 1$ in the liquid).

Weak formulation of the multi-dimensional Stefan problem:

$$\frac{\partial u}{\partial t} - \kappa \varDelta \theta = f \qquad \text{in } \mathcal{D}'(Q), \tag{1.1}$$

$$u = C_V \theta + \frac{L}{2}\chi \qquad \text{in } Q := \varOmega \times]0,T[, \tag{1.2}$$

$$\chi \in \operatorname{sign}(\theta) \qquad \text{in } Q, \tag{1.3}$$

coupled with initial and boundary conditions (on u and θ, respect.).

(Henceforth constants will be normalized.)

Phase Relaxation. For fast processes *local thermodynamic equilibrium* cannot be assumed. (1.3) is then replaced by a *relaxation dynamics,* e.g.,

$$\varepsilon \frac{\partial \chi}{\partial t} + \mathrm{sign}^{-1}(\chi) \ni \theta \qquad \text{in } Q \ (\varepsilon > 0), \tag{1.4}$$

or the nonequivalent equation

$$\varepsilon \frac{\partial \chi}{\partial t} + \chi \in \mathrm{sign}(\theta) \qquad \text{in } Q. \tag{1.5}$$

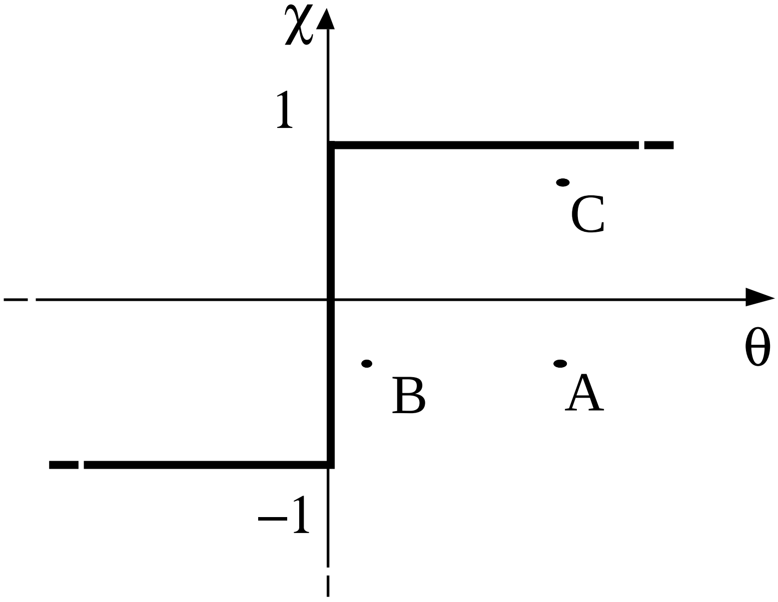
A.V.: *Stefan problem with phase relaxation.*
I.M.A. J. Appl. Math. **34** (1985), 225–245

The associated problems are well-posed in the framework of Sobolev spaces. As $\varepsilon \to 0$, their solutions converge to that of (1.1), (1.2), (1.3).

Modelling Objections. Either model is not completely satisfactory:

in (1.4) the rate of χ does not depend on χ,

in (1.5) this rate depends on θ only through its sign.



2. A More General Relaxation Dynamics

Let us fix a (Lipschitz-continuous) function $\varphi : \mathbf{R}^2 \to \mathbf{R}$ such that

$$\begin{aligned} &\varphi(\cdot,\chi) \ \text{ is nondecreasing} \quad \forall \chi \in \mathbf{R},\\ &\varphi(\theta,\cdot) \ \text{ is nonincreasing} \quad \forall \theta \in \mathbf{R}, \end{aligned} \tag{2.1}$$

$$\varphi(\theta,\chi) = 0 \ \text{ iff } \ \chi \in \operatorname{sign}(\theta) \quad \forall (\theta,\chi). \tag{2.2}$$

We then propose to deal with the more general relaxation dynamics

$$\varepsilon \frac{\partial \chi}{\partial t} = \varphi(\theta,\chi) \qquad \text{in } Q. \tag{2.3}$$

For instance,

$$\varepsilon \frac{\partial \chi}{\partial t} = g(\theta^+)\frac{1-\chi}{2} + g(-\theta^-)\frac{1+\chi}{2} \qquad \text{in } Q, \tag{2.4}$$

where $g(0) = 0$ and $g(\theta)\theta \geq 0$ for any θ.

Thus for $\theta > 0$, $\frac{\partial \chi}{\partial t}$ is proportional to the solid fraction, $\frac{1-\chi}{2}$. Indeed the melting driving force acts just on the solid *particles*.

Similarly, for $\theta < 0$, $\frac{\partial \chi}{\partial t}$ is proportional to the liquid fraction, $\frac{1+\chi}{2}$.

The initial- and boundary-value problem associated with

$$\frac{\partial}{\partial t}(\theta + \chi) - \kappa \Delta\theta = f \qquad \text{in } \mathcal{D}'(Q), \tag{2.5}$$

$$\varepsilon \frac{\partial \chi}{\partial t} = \varphi(\theta, \chi) \qquad \text{in } Q \tag{2.6}$$

is well-posed in natural spaces. We are interested in the limit as $\varepsilon \to 0$.

L^1**-Formulation of the Stefan Problem.** Let

$$\theta^0, \chi^0 \in L^1(\Omega), \qquad f \in L^1(Q). \tag{2.7}$$

Problem P. *To find* $\theta \in L^1\left(0, T; W_0^{1,1}(\Omega)\right)$ *and* $\chi \in L^1(Q)$ *such that*

$$\chi \in \operatorname{sign}(\theta) \qquad \textit{a.e. in } Q, \tag{2.8}$$

$$\frac{\partial}{\partial t}(\theta + \chi) - \Delta\theta = f \qquad \textit{in } \mathcal{D}'(\Omega)\textit{, a.e. in }]0, T[, \tag{2.9}$$

$$(\theta + \chi)|_{t=0} = \theta^0 + \chi^0 \qquad \textit{in } \mathcal{D}'(\Omega). \tag{2.10}$$

Thermodynamic Consistency.

Denoting the entropy density by s, and the absolute temperature by τ, we have

$$s = C_V \log \tau + \frac{L\chi}{2\tau_E} = C_V \log\left[\frac{1}{C_V}\left(u - \frac{L}{2}\chi\right)\right] + \frac{L\chi}{2\tau_E} =: \mathcal{S}(u,\chi),$$

whence

$$\frac{\partial \mathcal{S}}{\partial u}(u,\chi) = \frac{1}{\tau}\ , \qquad \frac{\partial \mathcal{S}}{\partial \chi}(u,\chi) = -\frac{L}{2\tau} + \frac{L}{2\tau_E} = \frac{L\theta}{2\tau\tau_E}\ .$$

Let us multiply the energy balance equation, $\frac{\partial u}{\partial t} + \nabla \cdot \vec{q} = f$, by $1/\tau$, and the relaxation dynamics, $\frac{\partial \chi}{\partial t} = \varphi(\theta,\chi)/\varepsilon$, by $L\theta/2\tau\tau_E$. We get

$$\begin{aligned}\frac{\partial s}{\partial t} &= \frac{\partial \mathcal{S}}{\partial u}\frac{\partial u}{\partial t} + \frac{\partial \mathcal{S}}{\partial \chi}\frac{\partial \chi}{\partial t}\\ &= -\nabla\cdot\frac{\vec{q}}{\tau} + \vec{q}\cdot\nabla\frac{1}{\tau} + \frac{f}{\tau} + \frac{\varphi(\theta,\chi)}{\varepsilon}\frac{L\theta}{2\tau\tau_E}\\ &=: -\nabla\cdot\frac{\vec{q}}{\tau} + \sigma + \frac{f}{\tau}\ .\end{aligned}$$

By the Fourier law $\vec{q}\cdot\nabla\frac{1}{\tau} \ge 0$; moreover, $\varphi(\theta,\chi)\theta \ge 0$ by the above assumptions on φ. Hence the entropy production rate, σ, is nonnegative:

$$\sigma := \vec{q}\cdot\nabla\frac{1}{\tau} + \frac{\varphi(\theta,\chi)}{\varepsilon}\frac{L\theta}{2\tau\tau_E} \ge 0.$$

Conclusion: the energy balance and the relaxation dynamics are consistent with the second principle of thermodynamics.

3. Convergence

Lemma. *For any* $(\theta_1, \chi_1), (\theta_2, \chi_2) \in \mathbf{R}^2$,

$$\big[\varphi(\theta_1, \chi_1) - \varphi(\theta_2, \chi_2)\big] \big[\mathrm{sign}_0(\theta_1 - \theta_2) - \mathrm{sign}_0(\chi_1 - \chi_2)\big] \geq 0.$$

Uniform estimates are then derived as follows:

(i) δ_t equation$_\varepsilon$ $|$ $\mathrm{sign}_\varepsilon(\delta_t \theta_\varepsilon)$

(ii) $\rho\delta_{x_i}$ equation$_\varepsilon$ $|$ $\mathrm{sign}_\varepsilon(\delta_{x_i} \theta_\varepsilon)$ $(i = 1, ..., N)$

Here δ_ξ represents the increment w.r.t. the variable ξ,
$\mathrm{sign}_\varepsilon$ is a single-valued regularization of the multi-valued function “sign”,
$\rho \in \mathcal{D}(\Omega)$ is a smooth cut-off: $\rho = 1$ far from $\partial\Omega$, $\rho = 0$ close to $\partial\Omega$.

Theorem 3.1 *(Convergence) Under natural assumptions, there exists a solution* (θ, χ) *of Problem 2.1 such that, as* $\varepsilon \to 0$ *along a suitable sequence,*

$$\theta_\varepsilon \to \theta, \quad \chi_\varepsilon \to \chi \qquad \textit{a.e. in } Q,$$

$$\frac{\partial \theta_\varepsilon}{\partial t} \to \frac{\partial \theta}{\partial t}, \ \frac{\partial \chi_\varepsilon}{\partial t} \to \frac{\partial \chi}{\partial t}, \ \Delta\theta_\varepsilon \to \Delta\theta \quad \textit{weakly star in } C_0^0(Q)'.$$

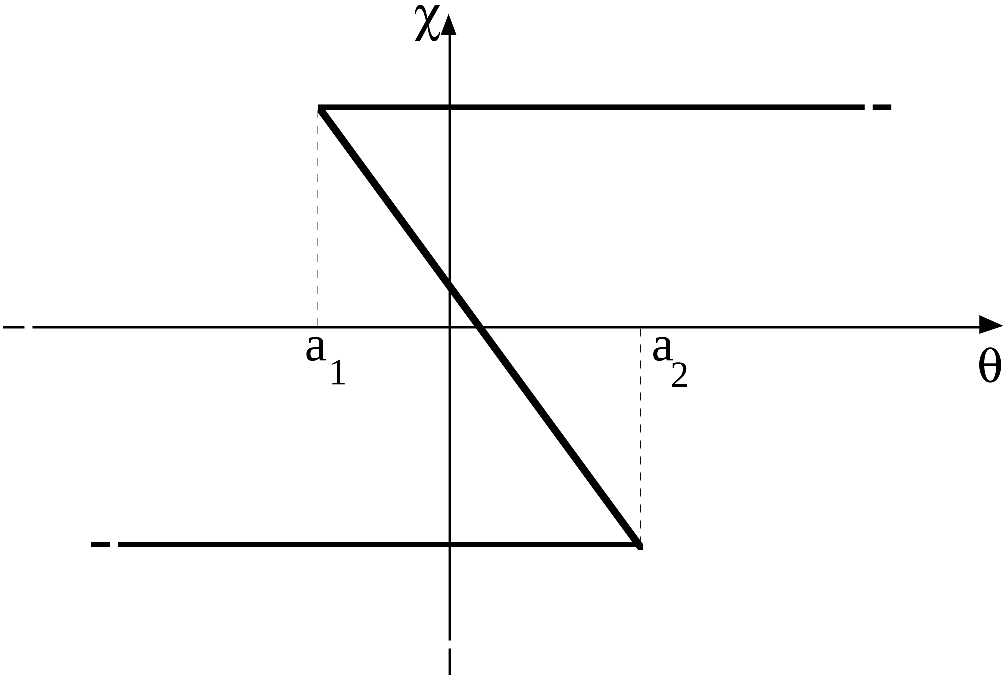
Moreover, (θ, χ) *is a solution of Problem P.*

If $N \leq 4$, then $\theta \in L^2(Q)$. Uniqueness follows from a classic result.

A.V.: *Models of phase-relaxation.*
Differential and Integral Equations **14** (2001), 1469-1486

4. Nonmonotone Constitutive Relation

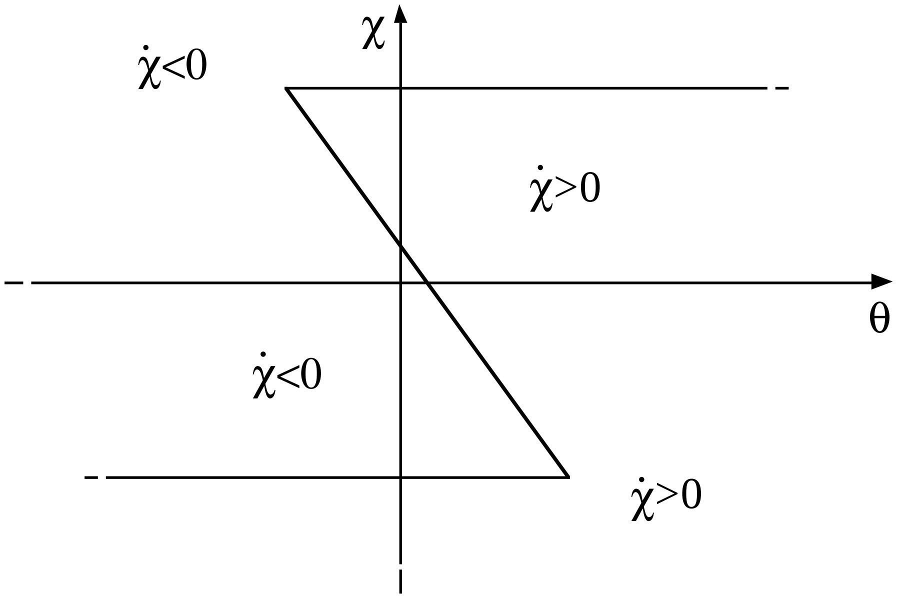
In presence of phase transitions, it is natural to consider a nonmonotone relation $\theta = \gamma(u\chi)$, e.g.,

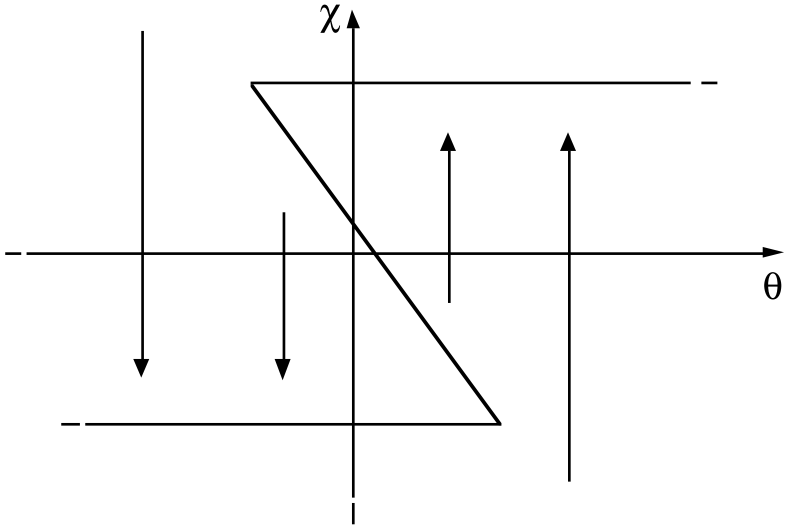


By coupling the equation $\frac{\partial}{\partial t}(\theta+\chi) - \Delta\theta = f$ with a nonmonotone relation $\theta = \gamma(\chi)$, a forward-backward parabolic equation is obtained.

First Relaxation Dynamics.

$$\varepsilon\frac{\partial\chi}{\partial t} + \gamma(\chi) = \theta \qquad \text{in } Q.$$

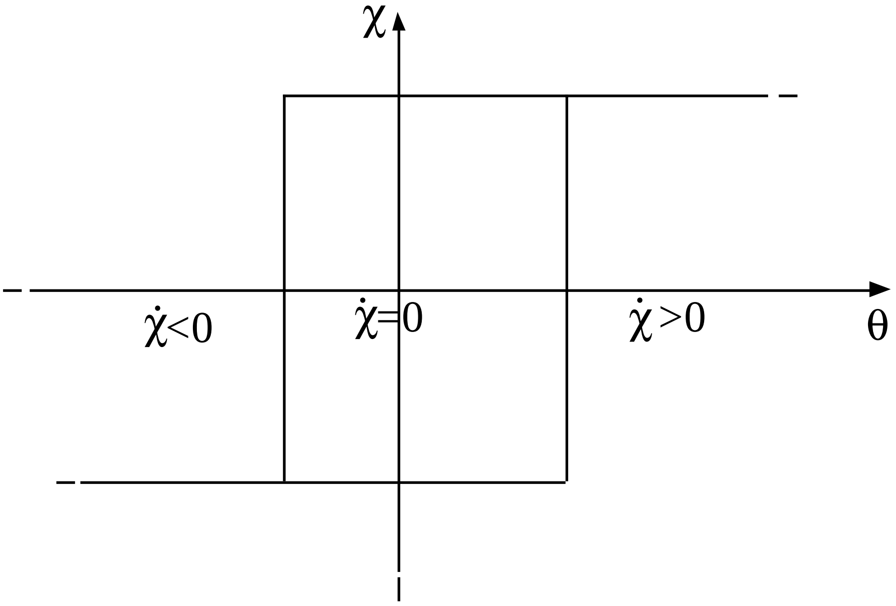




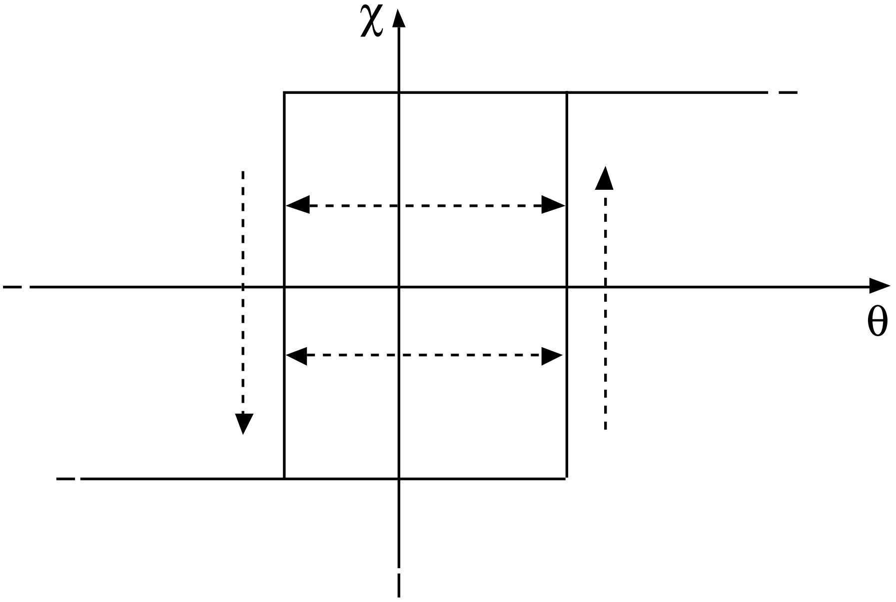
The ε-problems is easily studied, but difficulties arise as $\varepsilon \to 0$.

Modified Relaxation Dynamics.

$$\varepsilon \frac{\partial \chi}{\partial t} = \varphi(\theta, \chi) \qquad \text{in } Q.$$



Limit Dynamics: Hysteresis.



The ε-problem is easily studied, and the limit as $\varepsilon \to 0$ yields a hysteresis relation. A convergence result analogous to that above holds here.

This limit problem reads as follows, $\mathcal{F}$ being a *hysteresis operator:*

Problem P1. *To find $\theta \in H^1(Q)$ and $\chi \in L^1(Q)$ such that*

$$\chi \in \mathcal{F}(\theta) \qquad \textit{a.e. in } Q,$$

$$\frac{\partial}{\partial t}(\theta + \chi) - \varDelta\theta = f \qquad \textit{in } \mathcal{D}'(\varOmega), \textit{ a.e. in }]0, T[,$$

$$(\theta + \chi)|_{t=0} = \theta^0 + \chi^0 \qquad \textit{in } \varOmega.$$

This problem has a solution; cf.

A.V.: *Forward–backward parabolic equations and hysteresis.*
Calculus of Variations, 2002 (to appear)

Remark.

The boundary and initial-value problem for the following

quasilinear second-order hyperbolic equation with hysteresis

has a solution, as well:

$$\frac{\partial^2}{\partial t^2}\,[\theta + \mathcal{F}(\theta)] - \varDelta\theta = \tilde{f} \qquad \text{in } \mathcal{D}'(Q).$$

A.V.: *Quasi-linear hyperbolic equations with hysteresis.*
Ann. Inst. H. Poincaré. Analyse non lineaire 2002 (to appear)

5. A Vector Stefan-Type Problem in Ferromagnetism

The Ampère and Faraday laws

$$\begin{aligned} c\nabla \times \vec{H} &= 4\pi \vec{J} + \frac{\partial \vec{D}}{\partial t} \\ c\nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \end{aligned} \qquad (\nabla\times \ := \text{curl}) \tag{5.1}$$

coupled with the constitutive laws

$$\vec{D} = \epsilon \vec{E}, \qquad \vec{J} = \sigma(\vec{E} + \vec{g}) \tag{5.2}$$

yield

$$\epsilon \frac{\partial^2 \vec{B}}{\partial t^2} + 4\pi\sigma \frac{\partial \vec{B}}{\partial t} + c^2 \nabla \times \nabla \times \vec{H} = 4\pi c \sigma \nabla \times \vec{g}. \tag{5.3}$$

In metals $\epsilon \ll \sigma, c^2$. In the limit as $\epsilon \to 0$ we get the equation

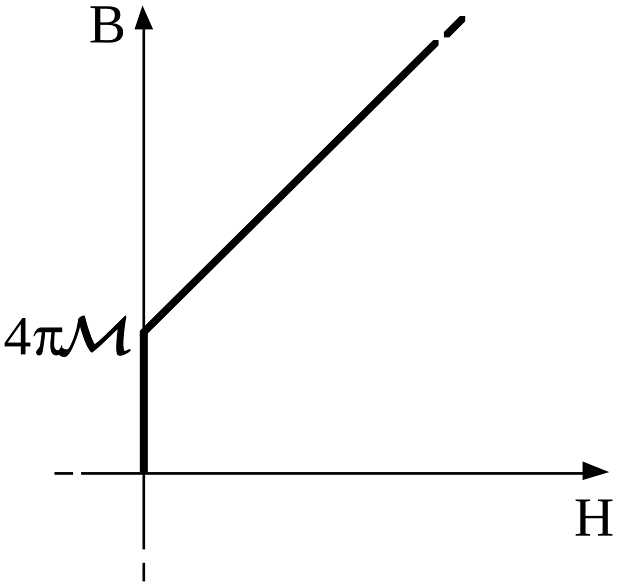
$$4\pi\sigma \frac{\partial \vec{B}}{\partial t} + c^2 \nabla \times \nabla \times \vec{H} = 4\pi c \sigma \nabla \times \vec{g}. \tag{5.4}$$

We assume that $\vec{B}$ and $\vec{H}$ are related by a maximal monotone graph:

$$\vec{B} \in \vec{H} + 4\pi\mathcal{M}\vec{\alpha}(\vec{H}) \qquad (\mathcal{M} := \text{constant } > 0). \tag{5.5}$$

E.g., $\vec{\alpha}$:= subdifferential of the modulus function:

$$\vec{\alpha}(\vec{v}) := \begin{cases} \dfrac{\vec{v}}{|\vec{v}|} & \text{if } \vec{v} \neq \vec{0}, \\ \{\vec{v} \in \mathbf{R}^3 : |\vec{v}| \leq 1\} & \text{if } \vec{v} = \vec{0}, \end{cases} \qquad \forall \vec{v} \in \mathbf{R}^3; \tag{5.6}$$



This may represent the behaviour of soft iron.

Well-posedness can be proved for the initial- and boundary-value problem corresponding to (5.4) and (5.5).

If the system has planar symmetry, (5.4) is reduced to a scalar equation.

A Free Boundary Problem. Formally the system (5.4), (5.5) is the weak formulation of a *two-phase problem:*

$$\begin{cases} \vec{B} = \vec{0} & \text{unmagnetized phase,} \\ |\vec{B}| \geq 4\pi\mathcal{M} & \text{magnetized phase.} \end{cases} \tag{5.7}$$

The system (5.4), (5.5) in the sense of distributions is formally equivalent to the same equations pointwise in $Q\setminus\mathcal{S}$, coupled with the interface conditions

$$4\pi\sigma v\,[[\vec{B}]] = c^2\vec{\nu} \times [[\nabla \times \vec{H}]] \qquad \text{a.e. on } \mathcal{S}, \tag{5.8}$$

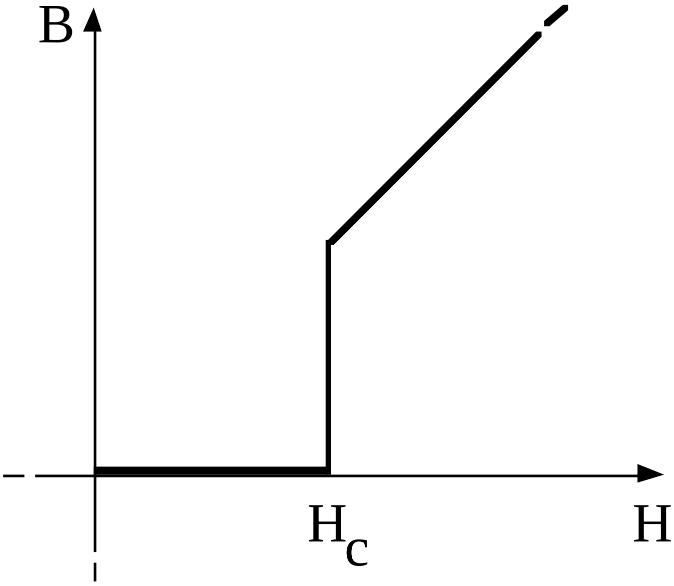
$$\vec{\nu} \times [[\vec{H}]] = \vec{0}, \quad \vec{\nu} \cdot [[\vec{B}]] = 0, \quad \vec{\nu} \cdot [[\nabla \times \vec{H}]] = 0 \qquad \text{a.e. on } \mathcal{S}; \tag{5.9}$$

here $\vec{\nu}$ is orthogonal to $\mathcal{S}_t$, v is the interface (normal) velocity, $[[\,\cdot\,]]$ is the jump across $\mathcal{S}$.

An Open Problem. In general the existence of an interface between the magnetically saturated and unsaturated phases is not obvious, even under regularity hypotheses. A priori a mixed phase (a sort of *magnetic mushy region)* characterized by $0 < |\vec{B}| < 4\pi\mathcal{M}$ might appear.

A.V.: *On some models of ferromagnetism.*
In: Free boundary problems, theory and applications, I
(N. Kenmochi, ed.), Gakkotosho (2000), 411-428

The previous discussion can be extended to a constitutive relation of the form below



which might be regarded as a naive model of *type-I superconductivity.*

H_c is the *critical field;* $|\vec{B}| = 0$, $0 < |\vec{B}| < H_c$, and $|\vec{B}| \geq H_c$, respect., correspond to the superconducting, intermediate, and normal states.

conference announcement

FREE BOUNDARY PROBLEMS

Trento (Italy), June 5–8, 2002

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