On Slow Motion for Phase Transitions

Calculus of Variations, PDE, and Geometric Measure Theory

Giovanni Leoni

Carnegie Mellon University

September 7, 2015

Papers:

- G. Dal Maso, I. Fonseca and G.L., 2015, Calc. Var. Partial Differential Equations,

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- R. Murray and M. Rinaldi, in preparation,
- I. Fonseca, G.L., G. Hayrapetyan, and M. Rinaldi, in preparation.

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- Motion of a curved antiphase boundary (APB)

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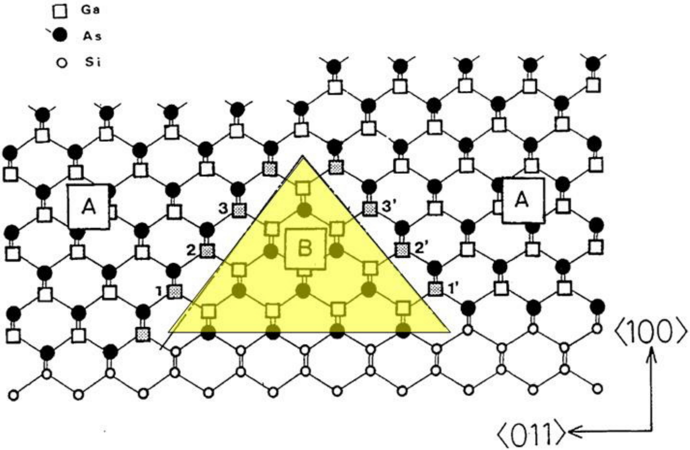
- APB: Planar defect in polycristalline materials



- Interfacial motion theory: Smoluchowski (1951), Turnbull (1951)

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- κ mean curvature of the interface.

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- $u : \Omega \times [0,\infty) \to \mathbb{R}$ order parameter,
- $\varepsilon > 0$,
- $f(s) = W'(s)$, W double-well potential.
  Prototype
  $$W(s) := \frac{1}{4}(s^2 - 1)^2.$$

Allen–Cahn Equation

$$\begin{cases} u_t = \varepsilon^2 \Delta u - u^3 + u & \text{in } \Omega \times (0,\infty), \\ \frac{\partial u}{\partial \nu} = 0 & \text{on } \partial\Omega \times (0,\infty), \\ u(x,0) = u_0(x) & \text{in } \Omega, \end{cases} \qquad \text{(ACE)}$$

$L^2(\Omega)$ gradient flow

$$F_\varepsilon(u) = \int_\Omega \left[\frac{1}{4}(u^2 - 1)^2 + \varepsilon^2 |\nabla u|^2 \right] dx.$$

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- $\varepsilon^2 |\nabla u|^2$ penalizes interfaces.

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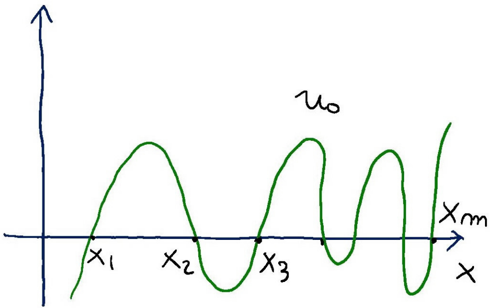
- Mugnai and Röger (2008): Gamma convergence by gradient flows Sandier and Serfaty (2004).

Dynamics

$$\begin{cases} u_t = \varepsilon^2 u_{xx} - u^3 + u & (x,t) \in (a,b) \times (0,\infty), \\ u_x(a,t) = u_x(b,t) = 0 & t \in (0,\infty), \\ u(x,0) = u_0(x) & x \in (a,b), \end{cases}$$

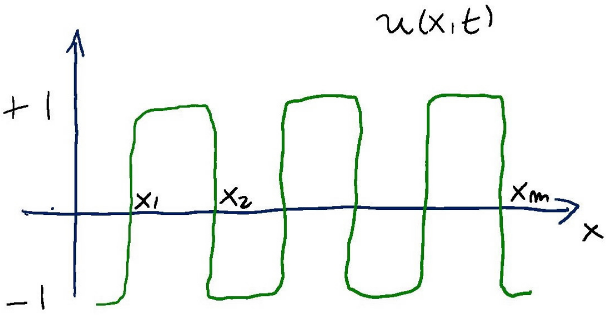
- u_0 smooth with m simple zeros



Phase I: Formation of Interfaces

$$u_t = \varepsilon^2 u_{xx} - u^3 + u$$

- $\varepsilon \ll 1$ for small times $t \ll 1$, $\varepsilon^2 u_{xx}$ negligible



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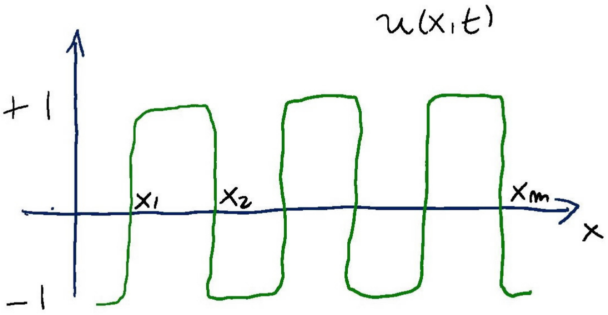
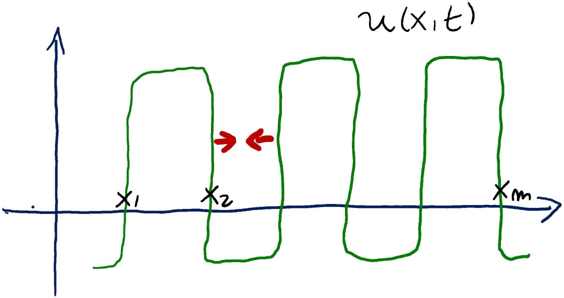
- $u_t \simeq -u^3 + u$



Phase II: Slow Motion

$$u_t = \varepsilon^2 u_{xx} - u^3 + u$$

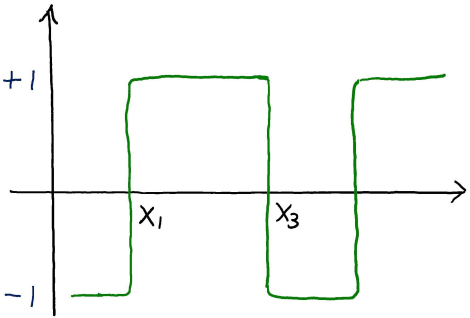
- $\varepsilon^2 u_{xx}$ no longer negligible



Phase III: Disappearance of Interfaces

$$u_t = \varepsilon^2 u_{xx} - u^3 + u$$

- when interfaces are close enough to a or b or to each other, they disappear quickly



Slow Motion: The Dynamical Approach

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- Carr and Pego (1989), speed of order $ce^{-c/\varepsilon}$:

$$\frac{dx_n(t)}{dt} = \frac{64}{\varepsilon}\left[e^{-\sqrt{2}(x_n(t)-x_{n-1}(t))/\varepsilon} - e^{-\sqrt{2}(x_{n+1}(t)-x_n(t))/\varepsilon}\right]$$

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- Chen (1992), $N \geq 1$.

Slow Motion: The Energy Approach

$$G_\varepsilon(u) = \int_a^b \left[\frac{1}{4\varepsilon}(u^2 - 1)^2 + \varepsilon |u'|^2 \right] dx.$$

- If $u_\varepsilon \in H^1(a,b)$ and $u_\varepsilon \longrightarrow u_0$ in $L^1(a,b)$, $u_0 \in BV((a,b);\{-1,1\})$,

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- Modica and Mortola (1979) $W(s) = \sin^2(\pi s)$,

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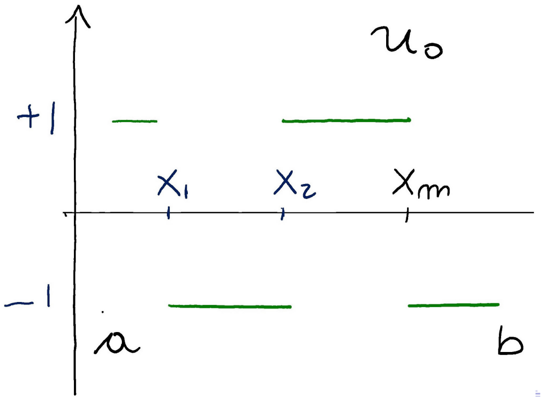

Slow Motion: The Energy Approach

Improved Energy Estimate, I

$$G_\varepsilon(u) = \int_a^b \left[\frac{1}{4\varepsilon}(u^2 - 1)^2 + \varepsilon |u'|^2 \right] dx.$$

Theorem (Bronsard and Kohn (1990))

For every $k \in \mathbb{N}$ there exist $\delta_k > 0$, $C_k > 0$ such that if $u \in H^1(a, b)$ and $\|u - u_0\|_{L^1} \leq \delta_k$,

$$G_\varepsilon(u) \geq c_0 m - C_k \varepsilon^k.$$

Slow Motion: The Energy Approach

Algebraic Slow Motion

$$\begin{cases} u_t = \varepsilon^2 u_{xx} - u^3 + u & (x,t) \in (a,b) \times (0,\infty), \\ u_x(a,t) = u_x(b,t) = 0 & t \in (0,\infty), \\ u(x,0) = u_{0,\varepsilon}(x) & x \in (a,b). \end{cases} \tag{AC}$$

Theorem (Bronsard and Kohn (1990))

For every $k \in \mathbb{N}$, if $u_{0,\varepsilon} \in H^1(a,b)$, $u_{0,\varepsilon} \to u_0$ in $L^1(a,b)$ and

$$G_\varepsilon(u_{0,\varepsilon}) \leq c_0 m + \varepsilon^k,$$

then solutions u_ε of (AC) satisfy for every $n > 0$,

$$\lim_{\varepsilon \to 0^+} \sup_{0 \leq t \leq n\varepsilon^{-k}} \int_a^b |u_\varepsilon(x,t) - u_0(x)| \, dx = 0.$$

Slow Motion: The Energy Approach

Improved Energy Estimate, II

$$G_\varepsilon(u) = \int_a^b \left[\frac{1}{4\varepsilon}(u^2 - 1)^2 + \varepsilon|u'|^2\right] dx.$$

Theorem (Grant (1995))

For every $L > 0$ there exist $\delta > 0$, $C > 0$ such that if $u \in H^1(a, b)$ and $\|u - u_0\|_{L^1} \leq \delta$,

$$G_\varepsilon(u) \geq c_0 m - Ce^{-L/\varepsilon}.$$

Slow Motion: The Energy Approach

Exponential Slow Motion

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Theorem (Grant (1995))

For every $L > 0$, if $u_{0,\varepsilon} \in H^1(a,b)$, $u_{0,\varepsilon} \to u_0$ in $L^1(a,b)$ and

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then solutions u_ε of (AC) satisfy

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Slow Motion: The Energy Approach

Sharp Energy Estimate, III

$$G_\varepsilon(u) = \int_{\mathbb{T}} \left[\frac{1}{4\varepsilon}(u^2 - 1)^2 + \varepsilon |u'|^2 \right] dx.$$

Theorem (Bellettini, Nayam, Novaga (2013))

For every $\{u_\varepsilon\} \subset H^1(\mathbb{T})$ with $u_\varepsilon \to u_0$ in $L^1(\mathbb{T})$, there exist $d_{n,\varepsilon} \to x_{n+1} - x_n$, $n = 1, \ldots, m$, such that

$$G_\varepsilon(u_\varepsilon) \geq c_0 m - 16\sqrt{2} \sum_{n=1}^{m} e^{-\sqrt{2} d_{n,\varepsilon}/\varepsilon} + o\left(e^{-3\sqrt{2} d_{n,\varepsilon}/(2\varepsilon)}\right),$$

- $\mathbb{T}$ *one-dimensional torus.*

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- $\mathbb{T}$ *one-dimensional torus.*
- *This inequality is sharp.*

Slow Motion: The Energy Approach

The gradient flow of

$$G_0(x_1,\ldots,x_m) := c_0 m - 16\sqrt{2}\sum_{n=1}^{m} e^{-\sqrt{2}(x_{n+1}-x_n)/\varepsilon}$$

is given by

$$\begin{aligned}\frac{dx_n(t)}{dt} &= \frac{\partial G_0}{\partial x_n}(x_1,\ldots,x_m)\\ &= \frac{64}{\varepsilon}\left[e^{-\sqrt{2}(x_n(t)-x_{n-1}(t))/\varepsilon} - e^{-\sqrt{2}(x_{n+1}(t)-x_n(t))/\varepsilon}\right].\end{aligned}$$

- recover the results of Carr and Pego (1989).

Slow Motion: The N-Dimensional Case

$$\begin{cases} u_t = \varepsilon^2 \Delta u - u^3 + u & \text{in } \Omega \times (0,\infty), \\ \frac{\partial u}{\partial \nu} = 0 & \text{on } \partial\Omega \times (0,\infty), \\ u(x,0) = u_0(x) & \text{in } \Omega, \end{cases}$$

Dynamical Approach:

- Kowalczyk (1997), dynamics of a straight interface on a special domain,

Energy Approach:

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Energy Approach:

- Bronsard and Kohn (1991), radial case.

Slow Motion: The Energy Approach

Van Der Waals– Cahn–Hilliard Theory for Phase Transitions

- Free energy

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- Van Der Waals (1893), Cahn and Hilliard (1958), Gurtin (1987)

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Slow Motion: The Energy Approach

Van Der Waals– Cahn–Hilliard Theory for Phase Transitions

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- Carr, Gurtin, and Slemrod (1984) for $N = 1$, Modica and Mortola (1979), Modica (1987), Sternberg (1988) for $N \geq 1$.

Slow Motion: The Energy Approach

Global minimizers u_0 of

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are of the form

$$u_0 = -1\chi_{\Omega \setminus E_0} + 1\chi_{E_0},$$

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- Gonzalez, Massari and Tamanini (1983), Grüter (1987)

Slow Motion: The Energy Approach

Sharp Energy Estimate

$$G_\varepsilon(u) = \int_\Omega \left[\frac{1}{4\varepsilon}(u^2-1)^2 + \varepsilon|\nabla u|^2 \right] dx.$$

Theorem (G.L. and Murray)

Let $\Omega \subset \mathbb{R}^N$ be open, bounded, of class $C^{2,\alpha}$, $\alpha > 0$. Then for $\mathcal{L}^1$ a.e. mass $\mathfrak{m}$ and for every $\{u_\varepsilon\} \subset H^1(\Omega)$ with $\int_\Omega u_\varepsilon\, dx = \mathfrak{m}$ and $u_\varepsilon \to u_0$ in $L^1(\Omega)$,

$$G_\varepsilon(u_\varepsilon) \geq c_0 \operatorname{Per}_\Omega(E_0) - \frac{(N-1)^2}{9}\kappa^2\varepsilon + o(\varepsilon).$$

- *This inequality is sharp.*

Slow Motion: The Energy Approach

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- Sternberg and Zumbrun (1998, 1999)

Slow Motion: Non Local Allen–Cahn Equation

Murray and Rinaldi

$$\begin{cases} u_t = \varepsilon^2 \Delta u - u^3 + u + \lambda & \text{in } \Omega \times (0, \infty), \\ \frac{\partial u}{\partial \nu} = 0 & \text{on } \partial\Omega \times (0, \infty), \\ u(x, 0) = u_{0,\varepsilon}(x) & \text{in } \Omega, \end{cases}$$

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- proposed by Rubinstein and Sternberg (1992).

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$$G_\varepsilon(u_{0,\varepsilon}) \le c_0 \operatorname{Per}_\Omega(E_0) + \varepsilon,$$

then for every $M > 0$ solutions u_ε of (NAC) satisfy

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- E_0 isolated local minimizer In preparation.

Slow Motion: Swift–Hohenberg Equation

Fonseca, G.L., Harapetyan and Rinaldi

$$u_t + \varepsilon^2 \gamma \Delta^2 u - \Delta u + \frac{1}{\varepsilon^2}\left(u - u^3\right) = 0.$$

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    - Cicalese, Spadaro and Zeppieri (2011), Chermisi, Dal Maso, Fonseca, and G.L. (2011), Fonseca, Hayrapetyan, G. L. and Zwicknagl (2014).

Gamma-Asymptotic Developments

Definition

X metric space, $F_\varepsilon^{(0)} : X \to (-\infty, \infty]$ has a Γ-asymptotic development of order k,

$$F_\varepsilon^{(0)} \stackrel{\Gamma}{=} F^{(0)} + \varepsilon F^{(1)} + \cdots + \varepsilon^k F^{(k)} + o\left(\varepsilon^k\right),$$

if

- $F_\varepsilon^{(0)} \xrightarrow{\Gamma} F^{(0)}$

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Gamma-Asymptotic Developments: First Example

Anzellotti and Baldo (1993)

$$F_\varepsilon^{(0)}(u) := \int_\Omega \left(W(u) + \varepsilon^2 |\nabla u|^2 \right) \, dx$$

if $u \in H^1(\Omega)$, $u = g$ on $\partial\Omega$, $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1(\Omega)$.

- $\Omega \subset \mathbb{R}^N$ open, bounded, connected, C^2 boundary,

Theorem (Anzellotti & Baldo)

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$$F^{(1)}(u) := 2c_0 \, \mathrm{Per}_\Omega\left(u^{-1}([c, d])\right) + 2 \int_{\partial\Omega} |\Phi(u) - \Phi(g)| \, d\mathcal{H}^{N-1}$$

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- $\Phi(t) := \int_b^t \sqrt{W(s)}\, ds$, $c_0 := \Phi(c) = \int_b^c \sqrt{W(s)}\, ds$

Modica (1987)

- $N = 1$, $\Omega = (0, 1)$, $g(0) := u_0 \in (a, b)$, $g(1) := u_1 \in (c, d)$,

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- $u^{-1}([c,d]) = (x_0, 1)$, *for some* $0 < x_0 < 1$,

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$$F_\varepsilon^{(0)}(u) := \int_0^1 \left(W(u) + \varepsilon^2 |u''|^2 \right) \, dx$$

if $u \in H^1(\Omega)$, $u = g$ on $\partial\Omega$, $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1(\Omega)$.

Theorem (Anzellotti & Baldo)

$F_\varepsilon^{(0)} \overset{\Gamma}{=} F^{(0)} + \varepsilon F^{(1)} + \varepsilon^2 F^{(2)} + o\left(\varepsilon^2\right)$, *where*
$F^{(2)}(u) := \int_0^1 |u''|^2 \, dx$ *if*

- $u \in [a,b] \cup [c,d]$ *a.e. in* $(0,1)$,
- $u^{-1}([c,d]) = (x_0, 1)$, *for some* $0 < x_0 < 1$,
- $u \in H^1((x_0,1)) \cap H^1((0,x_0))$,

- $N=1$, $\Omega=(0,1)$, $g(0):=u_0\in(a,b)$, $g(1):=u_1\in(c,d)$,

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- $u\in[a,b]\cup[c,d]$ *a.e. in* $(0,1)$,
- $u^{-1}([c,d])=(x_0,1)$, *for some* $0<x_0<1$,
- $u\in H^1((x_0,1))\cap H^1((0,x_0))$,
- $u(0)=u_0,\quad u_-(x_0)=b,\quad u_+(x_0)=c,\quad u(1)=u_1$

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- $u \in H^1((x_0,1)) \cap H^1((0,x_0))$,
- $u(0) = u_0$, $u_-(x_0) = b$, $u_+(x_0) = c$, $u(1) = u_1$
- *and* $F^{(2)}(u) := \infty$ *otherwise in* $L^1(\Omega)$.

Gamma-Asymptotic Developments: Second Example

Anzellotti, Baldo, and Orlandi (1996)

$$F_{\varepsilon}^{(0)}(u) := \int_{\Omega} \left(u^2 + \varepsilon^2 |\nabla u|^2\right) \, dx$$

if $u \in H^1(\Omega)$ and $u = g$ on $\partial\Omega$, and $F_{\varepsilon}^{(0)}(u) := \infty$ otherwise in $L^1(\mathbb{R}^N)$.

- $\Omega \subset \mathbb{R}^N$ open, bounded, connected, C^3 boundary,

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if $u \in H^1(\Omega)$ and $u = g$ on $\partial\Omega$, and $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1(\mathbb{R}^N)$.

- $\Omega \subset \mathbb{R}^N$ open, bounded, connected, C^3 boundary,
- $g \in C^2(\partial\Omega)$, $g > 0$

$$F_\varepsilon^{(0)}(u) := \int_\Omega \left(u^2 + \varepsilon^2 |\nabla u|^2\right) \, dx$$

if $u \in H^1(\Omega)$ and $u = g$ on $\partial\Omega$, and $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1(\Omega)$.

Theorem (Anzellotti, Baldo, & Orlandi)

$$F_\varepsilon^{(0)} \stackrel{\Gamma}{=} F^{(0)} + \varepsilon F^{(1)} + \varepsilon^2 F^{(2)} + o\left(\varepsilon^2\right),$$

where

- $F^{(0)}(u) := \int_\Omega u^2 \, dx$ *if* $u \in L^2(\Omega)$ *and* $F^{(0)}(u) := \infty$ *otherwise in* $L^1(\Omega)$,

$$F_\varepsilon^{(0)}(u) := \int_\Omega \left(u^2 + \varepsilon^2 |\nabla u|^2\right) \, dx$$

if $u \in H^1(\Omega)$ and $u = g$ on $\partial\Omega$, and $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1(\Omega)$.

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where

- $F^{(1)}(u) := \int_{\partial\Omega} g^2 \, d\mathcal{H}^{N-1}$ *if* $u = 0$ *a.e. in* Ω *and* $F^{(1)}(u) := \infty$ *otherwise in* $L^1(\Omega)$,

$$F_\varepsilon^{(0)}(u) := \int_\Omega \left(u^2 + \varepsilon^2 |\nabla u|^2\right)\, dx$$

if $u \in H^1(\Omega)$ and $u = g$ on $\partial\Omega$, and $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1(\Omega)$.

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$$F_\varepsilon^{(0)} \stackrel{\Gamma}{=} F^{(0)} + \varepsilon F^{(1)} + \varepsilon^2 F^{(2)} + o\left(\varepsilon^2\right),$$

where

- $F^{(2)}(u) := -\frac{1}{2}\int_{\partial\Omega} g^2 K_1 \, d\mathcal{H}^{N-1}$ *if* $u = 0$ *a.e. in* Ω *and* $F^{(2)}(u) := \infty$ *otherwise in* $L^1(\Omega)$,

$$F_\varepsilon^{(0)}(u) := \int_\Omega \left(u^2 + \varepsilon^2 |\nabla u|^2\right)\, dx$$

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- $F^{(2)}(u) := -\frac{1}{2}\int_{\partial\Omega} g^2 K_1 \, d\mathcal{H}^{N-1}$ *if* $u = 0$ *a.e. in* Ω *and* $F^{(2)}(u) := \infty$ *otherwise in* $L^1(\Omega)$,
- *for* $x \in \partial\Omega$, $K_1(x)$ *is the symmetric curvature of order* 1 *at* x.

Gamma-Asymptotic Developments: Cahn-Hilliard

$$F_\varepsilon^{(0)}(u) := \int_\Omega \left((u^2 - 1)^2 + \varepsilon^2 |\nabla u|^2 \right) \, dx$$

if $u \in H^1(\Omega)$, $\int_\Omega u \, dx = m$ and $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1(\Omega)$.

$$F_\varepsilon^{(0)} \stackrel{\Gamma}{=} F^{(0)} + \varepsilon F^{(1)} + \varepsilon^2 F^{(2)} + o\left(\varepsilon^2\right).$$

Anzellotti, Baldo, and Orlandi (1996)

Problem

Is $F^{(2)}$ a functional depending on the curvature of the jump surface?

$$F_\varepsilon^{(0)}(u) := \int_{\mathbb{R}^2} \left((u^2 - 1)^2 + \varepsilon^2 |\nabla u|^2 \right) \, dx$$

if $u \in H^1_{\text{loc}}(\mathbb{R}^2)$, $\int_{\mathbb{R}^2} (u(x) + 1) \, dx = 2$ and $F_\varepsilon^{(0)}(u) := \infty$ otherwise in $L^1_{\text{loc}}(\mathbb{R}^2)$.

Theorem (Dal Maso, Fonseca, Focardi, & G.L.)

$$F_\varepsilon^{(0)} \overset{\Gamma}{=} F^{(0)} + \varepsilon F^{(1)} + \varepsilon^2 F^{(2)} + o\left(\varepsilon^2\right),$$

where

$$F^{(2)} = 0.$$