Coupled second order singular perturbations for phase transitions

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Introduction

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- Let W be a nonnegative bulk free energy with

$$\{W = 0\} = \{a, b\}.$$

Introduction

Gibb's criteria for equilibria leads to the study of the problem

$$(P) \quad \text{minimize} \quad \int_\Omega W(u(x))\, dx \text{ under the constraint}$$

$$\int_\Omega u(x)\, dx = m$$

$$\text{where } m = (\theta a + (1 - \theta)b)\, \mathcal{L}^d(\Omega),\ 0 < \theta < 1.$$

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- In order to select physically preferred solutions, following the ideas of the gradient theory of phase transitions (Van der Waals, 1893), the following model was introduced by Cahn and Hilliard (1958) which assigns to each configuration u of the two-fluid system an energy of the form:

$$E_\varepsilon(u) = \int_\Omega W(u(x)) + \varepsilon^2 |\nabla u(x)|^2 \ dx,$$

where $\varepsilon > 0$ is a small parameter.

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- Gurtin (1983) conjectured that solutions of

$$(P_\varepsilon) \text{ minimize } E_\varepsilon(u) \text{ under the constraint } \int_\Omega u(x) \, dx = m$$

converge to minimizers of (P) having minimal interfacial energy.

Introduction

- Gurtin's conjecture was proved (using De Giorgi's notion of Γ-convergence and following the ideas of Modica and Mortola)) by Carr, Gurtin and Slemrod (1984) in the scalar case $d = 1$ and independently by Modica and Sternberg $(1987 - 1988)$ in the higher dimensional case $d \geq 2$.

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- The vectorial case $(u : \Omega \subset \mathbb{R}^d \to \mathbb{R}^N,\ d, N \geq 2)$ was considered by Fonseca and Tartar (1989), Sternberg (1991) and Barroso and Fonseca (1994).

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- coupled problem (Bouchitte', Owen and Sternberg, Fonseca and Popovici).

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- We refer also to Chermisi, Dal Maso, Fonseca, Leoni, for a model on pattern formation based on Ginzburg-Landau energy

$$\int_\Omega W(u) - q\epsilon^2 |\nabla u|^2 + \epsilon^4 |\nabla^2 u|^2 \, dx, \quad q > 0$$

Statement of the problem

In this work (two-wells, coupled, vectorial, dependence on second gradient) we consider the sequence of energy functionals

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where $u \in W^{2,2}(\Omega; \mathbb{R}^N)$ is a vector-valued function which describes the state of the mixture of N fluids $(N \in \mathbb{N},\ N \geq 2)$, Ω is an open bounded subset of $\mathbb{R}^d$ $(d \in \mathbb{N}, d \geq 2)$ with Lipschitz boundary which represents the container and $\varepsilon > 0$ is a small parameter.

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Therefore, the bulk energy density $f(x, u, \xi, \Lambda)$ is defined on $\Omega \times \mathbb{R}_+^N \times \mathbb{R}^{N \times d} \times \mathcal{T}^{N \times N \times d}$, where we denote by Sym^N the space of symmetric $N \times N$ matrices and by $\mathcal{T}^{N \times N \times d}$ the space of tensors $\Lambda = (\Lambda^1, \ldots, \Lambda^d)$, $\Lambda^i \in \mathrm{Sym}^N$, $i = 1, \ldots, d$.

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[(H1)] $f : \Omega \times \mathbb{R}_+^N \times \mathbb{R}^{N \times d} \times \mathcal{T}^{N \times N \times d} \to [0, +\infty)$ is continuous;

[(H2)] $f(x, u, \mathrm{O}, \mathrm{O}) = 0$ if and only if $u \in \{\alpha, \beta\} \subset \mathbb{R}_+^N$, $\alpha \neq \beta$;

Statement of the problem

[(H3)] there exists a continuous function
$g : \overline{\Omega} \times \mathbb{R}^N_+ \to [0, +\infty)$ such that

$$\frac{1}{C_0}\Big(g(x,u)+|\xi|^2+|\Lambda|^2\Big) \leq f\big(x,u,\xi,\Lambda\big) \leq C_0\Big(g(x,u)+|\xi|^2+|\Lambda|^2\Big)$$

for all $(x, u, \xi, \Lambda) \in \Omega \times \mathbb{R}^N_+ \times \mathbb{R}^{N \times d} \times \mathcal{T}^{N \times N \times d}$, where g satisfies

$$\frac{1}{C_0}|u|^q - C_0 \leq g(x,u) \leq C_0(1 + |u|^q)$$

for some $q \geq 2$, some $C_0 > 0$,
and for all $(x, u) \in \overline{\Omega} \times \mathbb{R}^N_+$;

Statement of the problem

[(H4)] for every $x_0 \in \Omega$ and every $\tau > 0$ there exists $\delta > 0$ such that $|x - x_0| < \delta$ implies

$$|f(x, u, \xi, \Lambda) - f(x_0, u, \xi, \Lambda)| \leq \tau f(x, u, \xi, \Lambda)$$

for all $(u, \xi, \Lambda) \in \mathbb{R}_+^N \times \mathbb{R}^{N \times d} \times \mathcal{T}^{N \times N \times d}$;

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for all $(u, \xi, \Lambda) \in \mathbb{R}_+^N \times \mathbb{R}^{N \times d} \times \mathcal{T}^{N \times N \times d}$;

[(H5)] for every $M > 0$ there exists $C_M > 0$ such that for every $u_1, u_2 \in \mathbb{R}_+^N$ with $|u_1|, |u_2| \leq M$, and every $(x, \xi, \Lambda) \in \Omega \times \mathbb{R}^{N \times d} \times \mathcal{T}^{N \times N \times d}$,

$$\left| f(x, u_1, \xi, \Lambda) - f(x, u_2, \xi, \Lambda) \right| \leq C_M |u_1 - u_2|(1 + |\xi|^2 + |\Lambda|^2);$$

Statement of the problem

[(H6)] there exist $\delta_0 > 0$ and $C > 0$ such that

$$f(x, u, O, O) \leq C|u - \alpha|^2$$

whenever $|u - \alpha| < \delta_0$ and $x \in \Omega$, and

$$f(x, u, O, O) \leq C|u - \beta|^2$$

whenever $|u - \beta| \leq \delta_0$ and $x \in \Omega$.

Statement of the problem

We also assume that the total amount of bulk material is preserved, i.e.,

$$\int_\Omega u(x)\, dx = V, \qquad (0.1)$$

for some $V = (V^1, \ldots, V^N) \in \mathbb{R}_+^N$ satisfying

$$|\Omega|\, \alpha^i \le V^i \le |\Omega|\, \beta^i, \qquad \text{for every } i = 1, \ldots, N, \qquad (0.2)$$

where α^i and β^i are the i-th components of α and β, respectively, and $|\Omega|$ denotes the Lebesgue measure of Ω. We write

$$\mathcal{V} := \{u : (0.1), (0.2) \text{ hold }\}.$$

Statement of the problem

The aim of this paper is to study the asymptotic behavior as, $\varepsilon \to 0^+$, of the sequence of functionals

$$E_\varepsilon(u;\Omega) \quad := \quad \frac{1}{\varepsilon} \int_\Omega f(x, u(x), \varepsilon \nabla u(x), \varepsilon^2 \nabla^2 u(x))\, dx,$$

$$\text{for } u \in W^{2,2}(\Omega; \mathbb{R}^N_+),$$

(0.3)

subject to the constraints (0.1) and (0.2).

BV functions

We briefly recall some basic facts about functions of bounded variation.

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A function $u \in L^1(\Omega; \mathbb{R}^N)$ is a *function of bounded variation*, briefly $u \in BV(\Omega; \mathbb{R}^N)$, if its distributional derivative Du is a bounded $N \times d$-valued Radon measure. This means that for all $\psi \in C_c^1(\Omega)$ the integration-by-parts formula

$$\int_\Omega \frac{\partial \psi}{\partial x_j} u^i \, dx = \int_\Omega \psi Du_j^i, \qquad i = 1, \ldots, N, \ j = 1, \ldots, d,$$

holds.

BV functions

Clearly, we have that $u \in W^{1,1}(\Omega; \mathbb{R}^N)$ when $Du \in L^1(\Omega; \mathbb{R}^N)$ and the measures Du_j^i are absolutely continuous with respect to the Lebesgue measure.

BV functions

Clearly, we have that $u \in W^{1,1}(\Omega; \mathbb{R}^N)$ when $Du \in L^1(\Omega; \mathbb{R}^N)$ and the measures Du_j^i are absolutely continuous with respect to the Lebesgue measure. Let Ω_u be the set of points where the approximate limit of u exists, i.e., $x \in \Omega$ such that there exist $z \in \mathbb{R}^N$ with

$$\lim_{\varepsilon \to 0} \fint_{Q(x,\varepsilon)} |u(y) - z| \, dy = 0.$$

If $x \in \Omega_u$ and $z = u(x)$ we say that u is *approximately continuous* at x (or that x is a Lebesgue point of u). The function u is approximately continuous $\mathcal{L}^d$-a.e. $x \in \Omega_u$ and

$$\mathcal{L}^d(\Omega \setminus \Omega_u) = 0. \tag{0.5}$$

BV functions

We have the following Lebesgue-Radon-Nikodým decomposition

$$Du = \nabla u \mathcal{L}^d \llcorner \Omega + D^s u$$

where $\nabla u \in L^1(\Omega; \mathbb{R}^{N \times d})$ is the density of the absolutely continuous part of Du and $D^s u$ is the singular part of Du with respect to $\mathcal{L}^d$.

BV functions

Let S_u be the *jump set* of this function, i.e., the set of points $x \in \Omega \setminus \Omega_u$ for which there exists a, $b \in \mathbb{R}^N$ and a unit vector $\nu \in S^{d-1}$, normal to S_u at x, such that $a \neq b$ and

$$\lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon^d} \int_{\{y \in Q_\nu(x,\varepsilon)\,:\,(y-x)\cdot\nu > 0\}} |u(y) - a|\, dy = 0 \qquad (0.6)$$

and

$$\lim_{\varepsilon \to 0^+} \frac{1}{\varepsilon^d} \int_{\{y \in Q_\nu(x,\varepsilon)\,:\,(y-x)\cdot\nu < 0\}} |u(y) - b|\, dy = 0. \qquad (0.7)$$

The triple (a, b, ν) uniquely determined by (0.6) and (0.7) up to permutation of (a, b), and a change of sign of ν and is denoted by $(u^+(x), u^-(x), \nu_u(x))$.

BV functions

We report the following Structure Theorem for BV-functions.

We need first some terminology: A $\mathcal{H}^{d-1}$-measurable set $E \subset \mathbb{R}^d$ is said to be a countably $\mathcal{H}^{d-1}$-rectifiable set if it can be covered $\mathcal{H}^{d-1}$ almost everywhere by a countable family of $(d-1)$-dimensional surfaces of class C^1.

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Theorem 0.2 (Structure Theorem for BV-functions). *If $\Omega \subset \mathbb{R}^d$ is open and $u \in BV(\Omega; \mathbb{R}^N)$, then S_u is a countably $\mathcal{H}^{d-1}$-rectifiable set oriented by ν_u, and $D^s u$ can be decomposed as $D^c u + D^j u$, where $|D^c u|(E) = 0$ for every Borel set E with $\mathcal{H}^{d-1}(E) < \infty$, and*

$$ D^j u = (u^+ - u^-) \otimes \nu_u \mathcal{H}^{d-1} \llcorner S_u. $$

Limiting energy

To describe the limiting energy and state the main theorem, we need to introduce some notation.

Given $\nu \in \mathbb{S}^{d-1} := \{x \in \mathbb{R}^d : \|x\| = 1\}$ let $\{\nu_1, \ldots, \nu_{d-1}, \nu\}$ be an orthonormal basis of $\mathbb{R}^d$,

Let S_ν be the strip:

$$S_\nu := \left\{ x \in \mathbb{R}^d : |y \cdot \nu| < \frac{1}{2} \right\}$$

and let Q_ν denote an open unit cube centered at the origin with two of its faces normal to ν.

Limiting energy

We define the class of admissible density functions by

$$
\mathcal{A}(\nu) := \left\{ w \in W^{2,2}_{\text{loc}}(S_\nu; \mathbb{R}^N_+) : w(y) = \alpha \text{ if } y \cdot \nu = -\frac{1}{2}, \right.
$$

$$
w(y) = \beta \text{ if } y \cdot \nu = \frac{1}{2},
$$

$$
w(y) = w(y + k\nu_i),
$$

$$
\left. \text{for all } y \in S_\nu, \quad i = 1, \ldots, d-1, \text{ and } k \in \mathbb{Z} \right\}.
$$

(0.8)

Limiting energy

We also introduce the surface energy density

$\sigma : \Omega \times \mathbb{S}^{d-1} \to [0, +\infty)$ defined by

$$\sigma(x, \nu) := \inf \left\{ \quad \int_{Q_\nu} \frac{1}{t} f\big(x, w(y), t\nabla w(y), t^2 \nabla^2 w(y)\big)\, dy \right.$$

$$\left. t > 0,\ w \in \mathcal{A}(\nu) \right\}. \tag{0.9}$$

Limiting energy

The limiting energy $F : L^1(\Omega; \mathbb{R}_+^N) \to [0, +\infty]$ is given by

$$F(u; \Omega) := \begin{cases} \displaystyle\int_{S_u} \sigma\big(x, \nu_u(x)\big) \, d\mathcal{H}^{d-1}(x) & \text{if } u \in BV\big(\Omega; \{\alpha, \beta\}\big) \cap \mathcal{V}, \\ +\infty & \text{otherwise,} \end{cases} \tag{0.10}$$

where S_u is the set of approximate jump points of u and ν_u is the generalized unit inner normal to S_u

Main result

Theorem 0.3. *Let Ω be a bounded open subset of $\mathbb{R}^d$ with Lipschitz boundary. Assume further that (H1)–(H6) hold. Then, for every $\varepsilon_n \to 0^+$ as $n \to +\infty$, the sequence of functionals $F_{\varepsilon_n} : L^1(\Omega; \mathbb{R}_+^N) \to [0, +\infty]$ defined by*

$$F_{\varepsilon_n}(u; \Omega) := \begin{cases} E_{\varepsilon_n}(u; \Omega) & \text{if } u \in W^{2,2}(\Omega; \mathbb{R}_+^N) \cap \mathcal{V}, \\ +\infty & \text{otherwise} \end{cases} \qquad (0.11)$$

Γ-converges, with respect to the $L^1(\Omega; \mathbb{R}_+^N)$-convergence, to the limiting functional $F : L^1(\Omega; \mathbb{R}_+^N) \to [0, +\infty]$ defined in (0.10).

Remark

Hypotheses $(H5)$ and $(H6)$ are needed in order to comply with the volume constraint.

Γ-convergence

Taking into account the definition of Γ-convergence, in order to prove Theorem 0.3 it suffices to show:

(Lower bound) For every $u \in L^1(\Omega; \mathbb{R}^N_+)$, for every sequence $\epsilon_n \to 0^+$ and for every sequence $u_n \to u$ in $L^1(\Omega; \mathbb{R}^N_+)$,

$$F(u) \leq \liminf_{n \to \infty} F_{\epsilon_n}(u_n),$$

Γ-convergence

(Upper bound) For every $\eta > 0$, every $u \in L^1(\Omega; \mathbb{R}_+^N)$, and every sequence $\epsilon_n \to 0^+$, there exists $\{u_n\} \subset L^1(\Omega; \mathbb{R}_+^N)$ such that $u_n \to u$ in $L^1(\Omega; \mathbb{R}_+^N)$ and

$$\limsup_{n \to \infty} F_{\epsilon_n}(u_n) \leq F(u) + \eta.$$

Sketch of proofs

The first step is to show that for every sequence
$u_n \in W^{2,2}(\Omega; \mathbb{R}_+^N) \cap \mathcal{V}$ such that $u_n \to u$ in $L^1(\Omega; \mathbb{R}_+^N)$ and for
every $\varepsilon_n \to 0^+$ we have that

$$\liminf_{n \to \infty} \int_\Omega \frac{1}{\varepsilon_n} f(x, u_n(x), \varepsilon_n \nabla u_n(x), \varepsilon_n^2 \nabla^2 u_n(x)) \, dx = +\infty,$$

unless $u \in BV(\Omega; \{\alpha, \beta\})$.

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$$\liminf_{n \to \infty} \int_\Omega \frac{1}{\varepsilon_n} f(x, u_n(x), \varepsilon_n \nabla u_n(x), \varepsilon_n^2 \nabla^2 u_n(x)) \, dx = +\infty,$$

unless $u \in BV(\Omega; \{\alpha, \beta\})$. The proof (by contradiction) relies on hypotheses (H_2) and (H_3) and follows the ideas in Fonseca-Tartar.

Sketch of proofs

Just an outline of the proof in the case we suppose
$u = \beta \chi_E + \alpha(1 - \chi_E)$ but $u \notin BV(\Omega; \mathbb{R}^N_+)$ (i.e. $\mathrm{Per}_\Omega E = +\infty$).
Suppose that there exist $\varepsilon_n \to 0^+$ and $u_n \to u$ in $L^1(\Omega; \mathbb{R}^N_+)$
such that

$$
\sup_n \int_\Omega \frac{1}{\varepsilon_n} f(x, u_n(x), \varepsilon_n \nabla u_n(x), \varepsilon_n^2 \nabla^2 u_n(x)) \, dx \leq C.
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Defining $\bar{g}(u) := \min_{x \in \bar{\Omega}} g(x, u)$ where g is the function in
(H_3) and

$$\Phi(v) \quad := \quad \inf \left\{ \int_{-1}^{1} \sqrt{\min\{\bar{g}(\psi(s)), M\}} |\psi'(s)| \, ds, \right.$$

$$\left. \psi \text{ continuous and piecewise } C^1 \ \ \psi(-1) = \alpha, \psi(1) = v \right\},$$

Sketch of proofs

we have that Φ is Lipschitz continuous and $\Phi \circ u = \chi_E \Phi(\beta)$ satisfies $|D(\Phi \circ u)|(\Omega) < +\infty$. Hence $\mathrm{Per}_\Omega(E) < \infty$, a contradiction.

Sketch of proofs

Given the target function:

$$u_0(x) := \begin{cases} \beta & \text{if } x \cdot \nu > 0, \\ \\ \alpha & \text{if } x \cdot \nu < 0, \end{cases}$$

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Using a slicing argument (similarly to Chermisi-Dal Maso-Fonseca - Leoni) we derive a technical lemma that allows us to replace a sequence $\{v_k\}$ converging to u_0 in $L^1(\Omega; \mathbb{R}^N_+)$ by a sequence $\{w_k\} \subset \mathcal{A}(\nu)$ still converging to u_0 in $L^1(\Omega; \mathbb{R}^N_+)$, without increasing the total energy.

Sketch of proofs

This sequence is obtained by an appropriate convex combination between v_k and the convolution of u_0 (on the cube Q_ν) and then extended by periodicity to the strip S_ν.

This technical result is used in both the lower and upper bound inequalities.

Sketch of proofs: lower bound

Since

$$f_n := \int_\Omega \frac{1}{\varepsilon_n} f(x, u_n(x), \varepsilon_n \nabla u_n(x), \varepsilon_n^2 \nabla^2 u_n(x)) \, dx$$

forms a sequence of nonnegative functions bounded in L^1 norm, (up to a subsequence) converges weakly* in the sense of measures to some nonnegative bounded Radon measure ζ.

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We just need to show that

$$\zeta^a(x) \geq \sigma(x, \nu_u(x)), \text{ for } \mathcal{H}^{d-1} \text{ a.e. } x \in \Omega \cap S_u,$$

where ζ^a denotes the absolutely continuous part of ζ w.r.to the measure $\mathcal{H}^{d-1} \lfloor \partial E$.

Sketch of proofs: lower bound

The result follows from Lebesgue Besicovitch derivation theorem since, choosing $r_k \to 0^+$ s.t. $\zeta(\partial(x + r_k Q_\nu)) = 0$, we have that

$$
\zeta^a(x) = \lim_{r \to 0^+} \frac{\zeta(Q_\nu(x; r))}{r^{d-1}}
$$

$$
= \lim_{k \to \infty} \frac{1}{r_k^{d-1}} \lim_{n \to \infty} E_{\varepsilon_n}(u_n; Q_\nu(x; r_k)).
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$$

Change variables (to the unit cube), diagonalization provedure and then apply the technical lemma in order to get a sequence in $\mathcal{A}(\nu)$.

Sketch of proofs: upper bound

- Recall: (Upper bound) For every $\eta > 0$, every $u \in L^1(\Omega; \mathbb{R}^N_+)$, and every sequence $\epsilon_n \to 0^+$, there exists $\{u_n\} \subset L^1(\Omega; \mathbb{R}^N_+)$ such that $u_n \to u$ in $L^1(\Omega; \mathbb{R}^N_+)$ and

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For all $(x_0, \nu) \in \Omega \times \mathbb{S}^{d-1}$ and $\tau > 0$ there exists $\delta > 0$ such $|x - x_0| < \delta$ implies that

$$|\sigma(x, \nu) - \sigma(x_0, \nu)| \leq \tau C \left(1 + |\alpha|^q + |\beta|^q + |\alpha - \beta|^2\right).$$

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- first for a cube assuming no explicit dependence on x,

- then for a cube allowing for dependence on x,

Sketch of proofs: upper bound

- first for a cube assuming no explicit dependence on x,

- then for a cube allowing for dependence on x,

- next for a planar interface (using Whitney's Covering Theorem),

Sketch of proofs: upper bound

- first for a cube assuming no explicit dependence on x,

- then for a cube allowing for dependence on x,

- next for a planar interface (using Whitney's Covering Theorem),

- then to a polygonal interface and finally for arbitrary sets of finite perimeter (by standard approximation results of sets of finite perimeter by polyhedral sets).

Upper bound

In each step we construct a sequence $v_{n,\eta}$ satisfying the upper bound inequality and then change it in order to comply with the volume constraint through:

$$u_{n,\eta} := v_{n,\eta} + b_{n,\eta}, \quad b_{n,\eta} := \frac{1}{|\Omega|} \int_\Omega u_0 - v_{n,\eta} \, dx,$$

and rely on (H_5) and (H_6) so that the upper bound inequality still holds.

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