INTERNATIONAL ATOMIC ENERGY AGENCY
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INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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SMR.398/11

TOPICAL MEETING ON VARIATIONAL PROBLEMS IN ANALYSIS

(28 August - 8 September 1989)

Crystal Microstructure, Young Measures, and Variational Problems of Elasticity Theory

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These are preliminary lecture notes, intended only for distribution to participants

Crystal microstructure, Young measures, and variational problems of Elasticity theory.

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A course of 3 lectures, ICTP Trieste, September 4-8, 1989

Lecture 1

Elastic materials

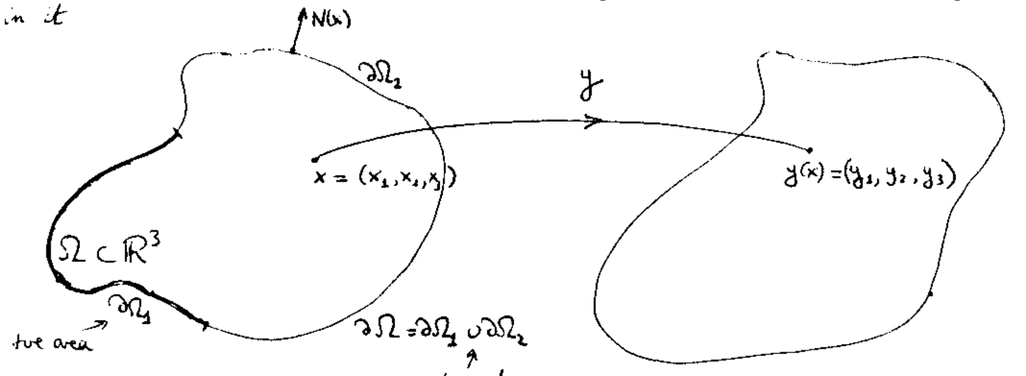
Examples: rubber, steel, glass, skin, rock, quartz, air, paper, wood ...

all these materials exhibit elastic properties in certain ranges of deformation; the typical characteristic of elastic behaviour is the ability of the material to recover a previous state.

There are various closely related mathematical theories of elasticity which aim to model this aspect of material behaviour: such theories may concern only equilibrium configurations (elastostatics) or aim to predict motions of elastic bodies (elastodynamics). Different theories of elastodynamics may give rise to the same theory of elastostatics if we look for time-independent solutions.

Kinematics

To describe different configurations of an elastic body we fix on one such configuration and label the particles by the positions they occupy in it



Reference configuration — Typical deformed configuration

We always suppose that Ω is a bounded domain with sufficiently smooth boundary $\partial\Omega$ (strongly Lipschitz will do).

So a typical deformed configuration is described by a mapping

$$y : \Omega \longrightarrow \mathbb{R}^3.$$

Configurations y should be invertible to avoid interpenetration of matter (this gives rise to serious mathematical difficulties).

The deformation gradient is

$$F = Dy(x) = \left(\frac{\partial y_i}{\partial x_\alpha}\right) = (y_{i,\alpha}).$$

In keeping with invertibility we require that

$$\det Dy(x) > 0,$$

i.e. $Dy(x) \in M^{3\times3}_+ = \{A \in M^{3\times3} : \det A > 0\}$

$M^{3\times3}$: 3×3 real matrices

nlinear (finite) elastostatics

$$\text{Elastic energy} = \int_\Omega W(x, Dy(x))\, dx$$

free-energy function of material
(sometimes called stored-energy or strain energy)

l energy $I(y)$ = elastic energy + other bits

$$= \int_\Omega \left[W(x, Dy(x)) + \psi(x, y(x)) \right] dx - \int_{\partial\Omega_2} t_R(x) \cdot y(x)\, dA$$

potential energy of external body forces
(e.g. $\psi = \rho_R(x)\, g\, x_3$ for gravity)

pot. energy due to applied surface force $t_R(x)$ on $y(\partial\Omega_2)$.

oblem: Find the configuration(s) y minimizing $I(y)$ subject to $y|_{\partial\Omega_1} = \bar{y}$).

Suppose y is a sufficiently smooth minimizer. Let $\varphi|_{\partial\Omega_1} = 0$.

Then
$$0 = \frac{d}{dt} I(y + t\varphi)\Big|_{t=0}$$
$$= \int_\Omega \left[\frac{\partial W}{\partial A_{i\alpha}}(x, Dy)\, \varphi_{i,\alpha} + \frac{\partial \psi}{\partial y_i}(x,y)\, \varphi_i \right] dx - \int_{\partial\Omega_2} t_R(x) \cdot \varphi(x)\, dA$$

True for all φ.

$$\boxed{\begin{aligned} \frac{\partial}{\partial x_\alpha} \frac{\partial W}{\partial A_{i\alpha}} &= \frac{\partial \psi}{\partial y_i} \quad \text{in } \Omega \qquad i = 1,2,3 \\ \frac{\partial W}{\partial A_{i\alpha}} N_\alpha &= t_{Ri} \quad \text{on } \partial\Omega_2 \end{aligned}}$$

quasilinear system

or
$$\begin{cases} \operatorname{Div} T_R = \operatorname{grad} \psi & \text{in } \Omega \\ T_R N = t_R & \text{on } \partial\Omega_2 \end{cases} \qquad (1)$$

where $T_R = \dfrac{\partial W}{\partial A}$ = 1st Piola-Kirchhoff stress tensor.

(Often we will consider the simplified special case when the material is homogeneous, i.e. $W = W(Dy)$, and the applied forces are absent, i.e. $t_R = 0$, $\psi = 0$. Then we have to minimize
$$I(y) = \int_\Omega W(Dy(x))\, dx$$
subject to $y|_{\partial\Omega_1} = \bar{y}$)

Questions: What is W? What properties of W distinguish different types of material? Is the minimum of I attained? If not, what happens? If the minimum is attained, how smooth are the minimizers? Do they satisfy (1)? If there are singularities what is their physical significance? How can we calculate minimizers numerically? etc. etc. ....

and Why minimize I?

This is a deep question; a rough answer is 'because of the 2nd Law of Thermodynamics'. At this level of modelling (i.e. continuum mechanics) an appropriate statement of the 2nd Law is the Clausius-Duhem $\leq$, which in certain cases implies that the equations of motion for momentum and energy possess a Lyapunov function V. For nonlinear thermoelasticity

$$V = \int_{\Omega} \rho_R \left[\tfrac{1}{2}|v|^2 + \varepsilon - \theta_0\,\eta\right] + \psi \; dx \;-\; \int_{\partial\Omega_2} t_R \cdot y \, dA,$$

where $v = \dot{y}(x,t)$ = velocity,
$\varepsilon = \varepsilon(x, \theta(x,t), Dy(x,t))$ = internal energy,
$\eta = \eta(x, \theta(x,t), Dy(x,t))$ = entropy,
θ_0 = constant boundary temperature,

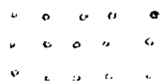
$$\frac{dV}{dt} \leq 0 .$$

As $t \to \infty$, we expect $\theta \to \theta_0$, $v \to 0$; in this limit V equals I, with $W = \rho_R\big(\varepsilon(x,\theta_0,Dy) - \theta_0\,\eta(x,\theta_0,Dy)\big)$.
This motivates the study of <u>minimizing sequences</u> for I, given by $y(\cdot,t_n)$ as $t_n \to \infty$ [See [6]]

<u>The atomic/molecular structure of elastic materials</u>

This can vary widely, e.g.

metals

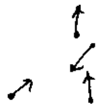


crystalline structure

polymers (e.g. rubber)

oscillating long chain molecules

air



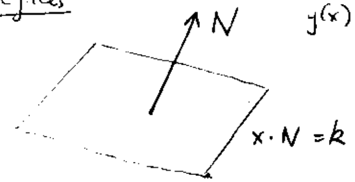
colliding molecules

This enters into the continuum theory in a very limited way — via the symmetry induced, for example, by a crystal lattice.

<u>How W influence the character of minimizers?</u>

For example, why do we see interfaces in crystals but not in rubber?

<u>Interfaces</u>



$y(x) = Ax + a \qquad x\cdot N > k$

$y(x) = Bx + b, \qquad x\cdot N < k$

y continuous $\iff (A-B)x + a - b = 0$ when $x\cdot N = k$

(exercise) $\iff \underline{B - A = d\otimes N}, \qquad a - b = kd$

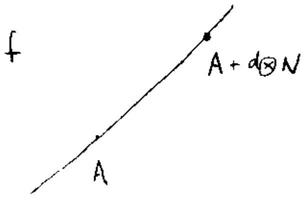
Hadamard's jump condition $\qquad d\otimes N = (d_i N_\alpha)$

<u>Rank-one convexity</u>

$W : M^{3\times 3} \to \mathbb{R}\cup\{+\infty\}$ is (strictly) <u>rank-one convex</u> if

$$t \longmapsto W(A + t\, d\otimes N)$$

is (strictly) convex for all $A \in M^{3\times3}$, $d, N \in \mathbb{R}^3$.



<u>Proposition</u>

W strictly rank-one convex $\Rightarrow$ no interfaces in minimizers.

<u>Pf</u> (Exercise, fill in the details) (For a converse see [7].)

Jump in stress across $x\cdot N = k$ is zero, i.e.

$$\frac{\partial W}{\partial A_{i\alpha}}(A + d\otimes N)\, N_\alpha = \frac{\partial W}{\partial A_{i\alpha}}(A)\, N_\alpha$$

Multiply by d_i. Then

$$\left\langle \frac{\partial W}{\partial A}(A + d\otimes N) - \frac{\partial W}{\partial A}(A),\; d\otimes N \right\rangle = 0$$

$$\Rightarrow \quad d\otimes N = 0 .$$

Lecture 2

Function spaces Let $1 \le p \le \infty$.

$$W^{1,p}(\Omega;\mathbb{R}^3) = \{ y:\Omega \to \mathbb{R}^3 : \|y\|_{L^p} + \|Dy\|_{L^p} < \infty \}$$

$$W_0^{1,p}(\Omega;\mathbb{R}^3) = \{ y \in W^{1,p}(\Omega;\mathbb{R}^3) : y|_{\partial\Omega} = 0 \}$$

We write these spaces as $W^{1,p}$, $W_0^{1,p}$ for short.

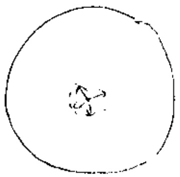
Examples of singular deformations

1. Piecewise affine maps $\in W^{1,\infty}$

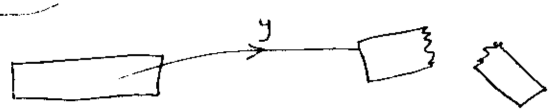
2. Let $\Omega = \{|x|<1\}$, y radial, i.e.

$$y(x) = \frac{r(R)}{R}x, \quad R=|x|, \quad r \in C^1([0,1]), \quad r(0) > 0$$

Then $y \in W^{1,p}$ iff $1 \le p < 3$.



cf. cavitation [8]

3. 

$y \notin W^{1,1}$

Linear boundary conditions.

Consider problem

$$\text{Minimize} \quad I(y) = \int_\Omega W(Dy)\,dx$$

$$y|_{\partial\Omega} = Ax, \qquad A \in M^{3\times 3}$$

An interesting construction (see [9])

Let $\bar{y} \in Ax + W_0^{1,p}$, $\bar{y}(x) \not\equiv Ax$. We construct ∞ly many other $y \in Ax + W_0^{1,p}$ having the same energy.

$$\text{Let} \quad \Omega = \underbrace{\bigcup_{i=1}^{\infty} (a_i + \varepsilon_i\Omega)}_{\text{disjoint}} \cup \underbrace{N}_{\text{meas } N = 0}, \quad a_i \in \mathbb{R}^3, \ \varepsilon_i > 0$$

Possible by Vitali's covering theorem in general, obvious if Ω is a cube.

$$\text{Let} \quad y(x) = Aa_i + \varepsilon_i \bar{y}\left(\frac{x-a_i}{\varepsilon_i}\right) \quad \text{if } x \in a_i + \varepsilon_i\Omega$$

Then $y \in Ax + W_0^{1,p}$ and

$$I(y) = \sum_i \int_{a_i+\varepsilon_i\Omega} W\left(D\bar{y}\left(\frac{x-a_i}{\varepsilon_i}\right)\right)dx \qquad z = \frac{x-a_i}{\varepsilon_i}$$

$$= \left(\sum_i \varepsilon_i^3\right) \int_\Omega W(D\bar{y})\,dz = I(\bar{y}).$$

A consequence If $\bar{y}$ minimizes I in $Ax + W_0^{1,p}$, $\bar{y}(x) \not\equiv Ax$, then

$\exists$ ∞ly many distinct minimizers.

Existence of minimizers

Consider for simplicity the problem

Minimize $\quad I(y) = \int_\Omega W(Dy)\,dx$

in $\mathcal{A} = \{ y \in W^{1,1} : y|_{\partial\Omega_1} = \bar{y} \}$.

The minimum exists if

1. W is polyconvex; i.e. $W(A) = g(A, \operatorname{cof} A, \det A)$ — g convex

2. $W(A) \geq c_0\left(|A|^p + |\operatorname{cof} A|^q\right) + c_1 , \qquad c_0 > 0, \quad p \geq 2, \quad q \geq \frac{p}{p-1}$

For the details see [1]. Example: the Mooney-Rivlin / Ogden models of rubber.

$$W \text{ polyconvex} \;\underset{\not\Leftarrow}{\Rightarrow}\; W \text{ quasiconvex} \;\underset{\not\Leftarrow\,?}{\Rightarrow}\; W \text{ rank-one convex}$$

$$\int_\Omega W(Dy)\,dx \geq \int_\Omega W(A)\,dx = (\operatorname{vol}\Omega)\, W(A) \qquad \forall\, y \in Ax + W_0^{1,\infty}$$

thus construction on previous page gives no new minimizers

Elastic crystals

General philosophy:

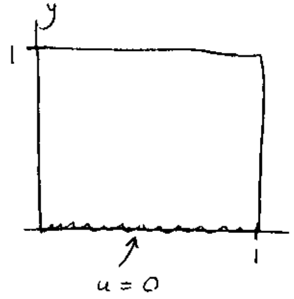
1. For crystals W is not rank-one convex; the Ince theorem does not apply, and in fact the minimum is not in general attained.

2. To get closer and closer to the lower bound for the energy, more and more microstructure is needed.

An artificial example

Minimize $\quad I(u) = \int_\square \left[(u_x^2 - 1)^2 + u_y^2 \right] dx\,dy$

subject to $\quad u|_{y=0} = 0$



Here $u = u(x,y)$ is a scalar.

Claim: $\inf I = 0$ but is not attained.

Proof

Define
$$\bar{u}(x,y) = \begin{cases} x\,\varphi(y) & 0 \leq x \leq \tfrac12 \\ (1-x)\,\varphi(y) & \tfrac12 \leq x \leq 1 \end{cases}$$

where $\varphi(y) = \begin{cases} y & 0 \leq y \leq 1 \\ 1 & y \geq 1 \end{cases}$,

and extend $\bar{u}$ as a 1-periodic function of x to all of $\mathbb{R} \times (0,\infty)$.

Let $u^{(j)}(x,y) = j^{-1}\bar{u}(jx, jy)$. Now

$Du^{(j)}(x,y) = (\bar{u}_x, \bar{u}_y)(jx, jy)$ and is uniformly bdd

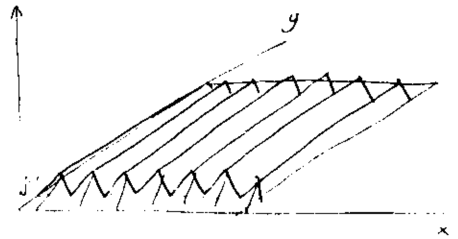
$= (\pm 1, 0)$ if $y > j^{-1}$

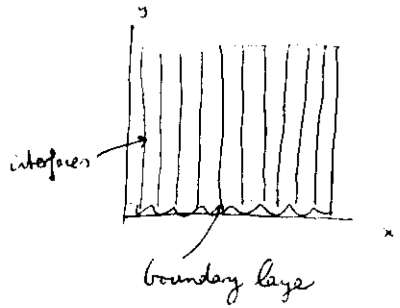
Hence
$$\lim_{j\to\infty} I(u^{(j)}) = \lim_{j\to\infty} \int_{\square \cap \{y > j^{-1}\}} \left[((u_x^{(j)})^2 - 1)^2 + (u_y^{(j)})^2 \right] dx\,dy = 0$$

$\Rightarrow \inf I = 0$

The inf is not attained, because $I(u) = 0,\ u|_{y=0} = 0 \Rightarrow u_y \equiv 0$

$\Rightarrow u(x,y) = u(x,0) + \int_0^y u_y(x,z)\,dz = 0 \Rightarrow u_x \equiv 0 \Rightarrow I(u) = 1$ Contradiction.





Notes: (a) For problems when one of the dimensions is one (domain or range) rank 1 convexity $\Leftrightarrow$ convexity. Here the integrand $(u_x^2-1)^2+u_y^2$ is not convex in (u_x, u_y).

(b) Note that $u^{(j)} \xrightarrow{*} 0$ in $W^{1,\infty}$, but that 0 is not a minimizer.

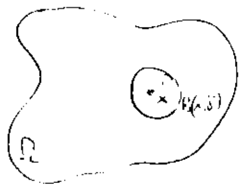
The Young measure A tool for describing microstructure.

Intuitive description: for precise statements see [10].

Let $z^{(j)}: \Omega \to \mathbb{R}^k$ be a sequence of measurable functions.
Fix $x \in \Omega$, j, $\delta > 0$. Let

$\nu^{(j)}_{x,\delta}$ = (prob. distribution of values of $z^{(j)}(y)$, y chosen uniformly (at random from $B(x,\delta)$)

Young measure $\nu_x = \lim_{\delta \to 0} \lim_{j \to \infty} \nu^{(j)}_{x,\delta}$ (2)



If $f \in C(\mathbb{R}^k)$ then

$$f(z^{(j)}) \xrightarrow{L^1} \langle \nu_x, f \rangle = \int_{\mathbb{R}^k} f(\lambda)\, d\nu_x(\lambda). \qquad (3)$$

[More precisely, if $z^{(j)}$ is bdd, e.g. in L^1, then $\exists$ a subsequence and a family $(\nu_x)_{x\in\Omega}$ of prob. measures on $\mathbb{R}^m$, such that (2) holds, and then (3) holds whenever $f(z^{(j)})$ is seq. weakly relatively compact in L^1]

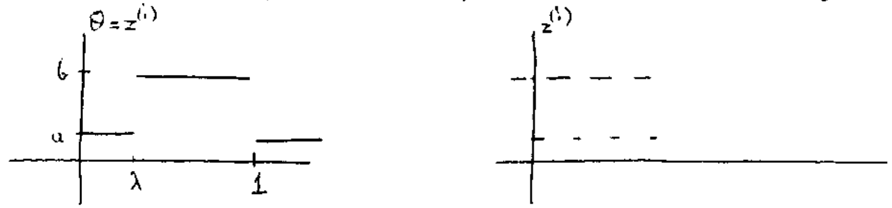
Lecture 3

Young measures contd.

Examples

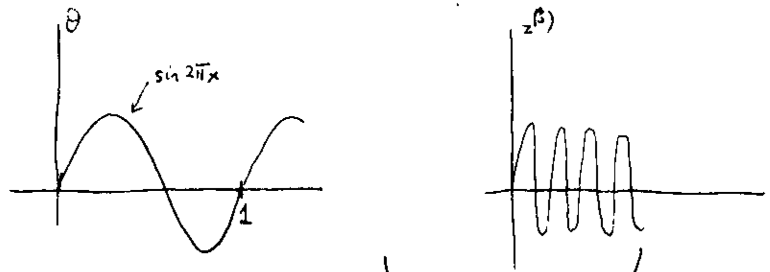
Let θ be a 1-periodic function on $\mathbb{R}$, and let $z^{(j)}(x) = \theta(jx)$

(i)

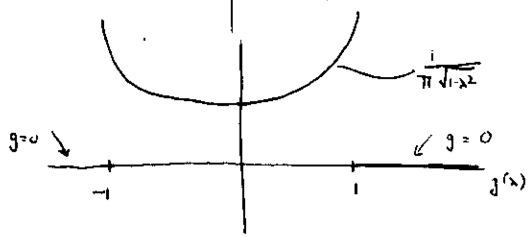


$$\nu_x = \lambda \delta_a + (1-\lambda)\delta_b \qquad (\text{independent of } x)$$

(ii)



$$d\nu_x(\lambda) = g(\lambda)\, d\lambda$$



Young measures of gradients

For example in lecture 2, the Young measure corresponding to the gradient $Du^{(j)}$ is

$$\nu_x = \frac{1}{2}\delta_{(1,0)} + \frac{1}{2}\delta_{(-1,0)}$$

More generally, let $y^{(j)} \to y$ in $W^{1,p}(\Omega, \mathbb{R}^3)$ ($p \geq 2$, or $Dy^{(j)}$ bdd in L^q, $q \geq p/(p-1)$). Consider the Young measure ν_x corresponding to (an appropriate subsequence) of $Dy^{(j)}$. Of course, for each x, ν_x is a probability measure on $M^{3\times 3}$.

Necessary conditions from weak continuity of Jacobians

$$\operatorname{cof}\langle \nu_x, A\rangle = \langle \nu_x, \operatorname{cof} A\rangle, \qquad \det\langle \nu_x, A\rangle = \langle \nu_x, \det A\rangle$$

$$\operatorname{cof}\left(\int_{M^{3\times3}} A\, d\nu_x(A)\right) = \int_{M^{3\times3}} \operatorname{cof} A\, d\nu_x(A)$$

Reshetnyak, Zhang

$$\operatorname{cof} Dy \qquad \qquad \text{wk lim } \operatorname{cof} Dy^{(j)}$$

A minimization problem for crystals

Minimize $\quad I(y) = \displaystyle\int_\Omega W(Dy(x))\,dx$

in $\quad \mathcal{A} = \{ y \in W^{1,1} : y|_{\partial\Omega} = \bar{y} \}$

(H1) $\quad W : M^{3\times3} \longrightarrow \mathbb{R} \cup \{+\infty\}$ is continuous, with
$W(A) < \infty \iff \det A > 0$.

(H2) $\quad W(A) \geq c_1 |A|^p + c_2 |\operatorname{cof} A|^q + c_3, \qquad \forall A$

$c_1, c_2 > 0, \quad p \geq 2, \quad q \geq \frac{p}{p-1}$

(H3) $\quad W(QA) = W(A) \qquad \forall A \in M^{3\times3}, \quad Q \in SO(3)$

N.B. no convexity hypotheses.

(H1), (H2) $\Rightarrow$ W attains a minimum on $M^{3\times3}$.
wlog we can suppose the minimum value $= 0$.

Let $\quad M = \{ A \in M^{3\times3} : W(A) = 0 \}$

By (H3), $\quad SO(3)M = M$.

Proposition

Let $y^{(j)}$ be a minimizing sequence for I in $\mathcal{A}$, and let $(\nu_x)_{x\in\Omega}$ be the Young measure corresponding to $Dy^{(j)}$. Then if $\inf_{\mathcal{A}} I = 0$,

$$\operatorname{supp} \nu_x \subset M \quad \text{for a.e. } x \in \Omega.$$

Proof.

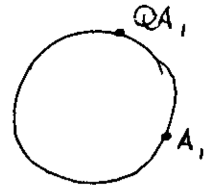
Let $\quad f(A) = \min(W(A), 1), \quad f$ is continuous

So

$$\int_\Omega f(Dy^{(j)})\,dx \longrightarrow \int_\Omega \underbrace{\int_{M^{3\times3}} f(A)\,d\nu_x(A)}_{=0 \text{ a.e.}}\,dx = 0$$

1-well problem

$M = SO(3)A_1, \quad A_1 \in M^{3\times3}_+$ given



Thm (following Kinderlehrer & Reshetnyak)

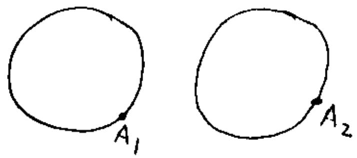
$\inf_{\mathcal{A}} I = 0 \iff$ the affine map $x \longmapsto Ax + a$ belongs to $\mathcal{A}$ for some $A \in M$, $a \in \mathbb{R}^3$.

In this case, every minimizing sequence $y^{(j)}$ has a subsequence $y^{(\mu)}$ such that
$Dy^{(\mu)} \longrightarrow A$ strongly in L^r $\forall r < p$
and some $A \in M$ (i.e. no microstructure

Pf uses Young measure in similar way to below.

2-well problem

$$M = SO(3)A_1 \cup SO(3)A_2$$



Suppose (i) $\det A_1 = \det A_2$
(ii) $\exists$ rank-one connection
$$RA_1 - A_2 = a \otimes n$$

By change of variables we can then reduce to case

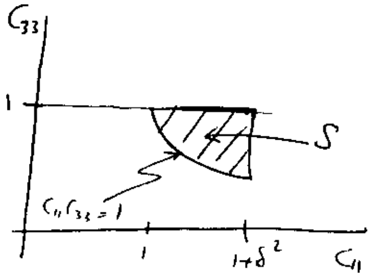
$$M = SO(3)S^+ \cup SO(3)S^-$$
$$S^\pm = 1 \pm \delta e_3 \otimes e_1, \quad \delta > 0$$

Occurs for orthorhombic $\to$ monoclinic transformation.

Theorem

Let $\inf_{\mathcal{A}} I = 0$, $y^{(j)}$ be a minimizing sequence, $y^{(j)} \rightharpoonup y$ in $W^{1,p}$. Then $\det Dy(x) = 1$, $Dy^T(x)Dy(x) \in \mathcal{R}$ a.e., where

$$\mathcal{R} = \left\{ \begin{pmatrix} C_{11} & 0 & C_{13} \\ 0 & 1 & 0 \\ C_{13} & 0 & C_{33} \end{pmatrix} : (C_{11}, C_{33}) \in S \right\}$$



Conversely, let $\bar{y}$ be smooth, $\det D\bar{y}(x) = 1$, $D\bar{y}(x)^T D\bar{y}(x) \in \mathcal{R}$ a.e. $x \in \Omega$. Then

$$\inf_{\mathcal{A}} I = 0.$$

Proof of necessity

$$\operatorname{supp} \nu_x \subset SO(3)S^+ \cup SO(3)S^-$$

Let $\nu_x^\pm = \nu_x \big|_{SO(3)S^\pm}$. Thus $\nu_x = \nu_x^+ + \nu_x^-$.

Let $\mu_x^\pm(E) = \nu_x^\pm(ES^\pm)$. Thus $\operatorname{supp} \mu_x^\pm \subset SO(3)$,

and

$$\langle \nu_x, f \rangle = \int_{SO(3)S^+} f(A)\, d\nu_x^+(A) + \int_{SO(3)S^-} f(A)\, d\nu_x^-(A)$$
$$= \int_{SO(3)} f(RS^+)\, d\mu_x^+(R) + \int_{SO(3)} f(RS^-)\, d\nu_x^-(R).$$

Fix x. Let $F = Dy(x)$. Then
$F = \langle \nu_x, A \rangle$, $\operatorname{cof} F = \langle \nu_x, \operatorname{cof} A \rangle$, $\det F = \langle \nu_x, \det A \rangle$.

$$Fe_2 = \langle \nu_x, A \rangle e_2 = \underbrace{\int_{SO(3)} R\, d(\mu_x^+ + \mu_x^-)}_{M} e_2$$

$$\det F = 1$$

$$(\operatorname{cof} F)e_2 = \langle \nu_x, \operatorname{cof} A \rangle e_2 = \left(\int_{SO(3)} R \operatorname{cof} S^+ d\mu_x^+ + \int_{SO(3)} R \operatorname{cof} S^- d\mu_x^- \right) e_2$$
$$= Me_2 = Fe_2.$$

So $C = F^TF$ satisfies $Ce_2 = e_2$, $\det C = 1 = C_{11}C_{33} - C_{13}^2$

But $\left.\begin{array}{l} (A^TA)_{11} = 1+\delta^2 \\ (A^TA)_{33} = 1 \end{array}\right\}$ for $A \in \operatorname{supp} \nu_x$

So
$$1+\delta^2 = \langle \nu_x, (A^TA)_{11} \rangle \geq [\langle \nu_x, A \rangle^T \langle \nu_x, A \rangle]_{11} = C_{11}$$
$$1 = \langle \nu_x, (A^TA)_{33} \rangle \geq [\langle \nu_x, A \rangle^T \langle \nu_x, A \rangle]_{33} = C_{33} \quad \square$$

Theorem (uniqueness)

Let $\mathcal{A} = \{ y : y|_{\partial\Omega} = Fx \}$, where $F = \lambda S^+ + (1-\lambda) S^-$, $0<\lambda<1$.

Then for any minimizing sequence,

$$\nu_x = \lambda \delta_{S^+} + (1-\lambda)\delta_{S^-} \qquad \text{a.e. } x \in \Omega .$$

In particular the min. is not attained.

Layers, layers within layers, experiments . . .

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