On the Mechanics of Crystalline Solids with a Continuous Distribution of Dislocations

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Workshop Analytical Aspects of Mathematical Physics
Zurich, May 28th, 2013

Outline

Motivation

- importance of understanding the mechanics of elastic materials, not only perfect crystals
- classical description using a relaxed reference state is *not* valid in the presence of dislocations
- complete dislocation theory only in linear approximation (Kröner, Nabarro), nonlinear concepts are missing

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- importance of understanding the mechanics of elastic materials, not only perfect crystals
- classical description using a relaxed reference state is *not* valid in the presence of dislocations
- complete dislocation theory only in linear approximation (Kröner, Nabarro), nonlinear concepts are missing
- **goal:** configurations of minimal energy for crystalline solids with a uniform distribution of elementary dislocations

References

[CK] D. Christodoulou and I. Kaelin, *On the mechanics of crystalline solids with a continuous distribution of dislocations*. http://arxiv.org/abs/1212.5125, to appear in Advances in Theoretical and Mathematical Physics (ATMP).

[C1] D. Christodoulou, *On the geometry and dynamics of crystalline continua*. Ann. Inst. Henri Poincaré **69** (1998), 335-358.

The General Setting

- introduce the basic concepts to describe a crystalline solid containing dislocations as in **[C1]**
- uniform distribution of elementary dislocations and Lie group structure
- examples of the two elementary dislocations: edge and screw dislocations in 2 and 3 dimensions, respectively
- thermodynamic state space and state function

Basic Definitions

- $\mathcal{N}$: **material manifold** (oriented, n-dimensional)
- **evaluation map**

$$\begin{array}{rcl} \epsilon_y : \chi(\mathcal{N}) & \to & T_y\mathcal{N} \\ X & \mapsto & \epsilon_y(X) = X(y) \end{array}$$

$\chi(\mathcal{N})$: C^∞-vectorfields on $\mathcal{N}$

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Definition

A **crystalline structure** on $\mathcal{N}$: linear subspace $\mathcal{V} \subset \chi(\mathcal{N})$ such that $\epsilon_y|_{\mathcal{V}}$ is an isomorphism for each $y \in \mathcal{N}$.

Remark

$\mathcal{V}$ on $\mathcal{N}$ is **complete** *if each $X \in \mathcal{V}$ is complete.*

Basic Concepts

Definition

Given a complete crystalline structure $\mathcal{V}$ on $\mathcal{N}$, we define the **dislocation density** Λ by:

$$\Lambda(y)(X, Y) = \epsilon_y^{-1}\left([X, Y](y)\right) \in \mathcal{V}\,, \ \forall y \in \mathcal{N}, X, Y \in \mathcal{V}\,.$$

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Remark

If Λ is constant on $\mathcal{N}$ then, for all $X, Y \in \mathcal{V}$, there is a $Z \in \mathcal{V}$ such that

$$[X, Y] = Z\,.$$

Thus $\mathcal{V}$ is a **Lie algebra** *and $\mathcal{N}$ is the corresponding* **Lie group**.

Examples

i) Edge Dislocation

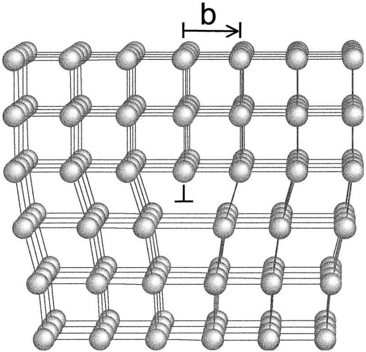

Figure 1: Elementary edge dislocation in a two dimensional crystal lattice. Burger's vector *b* points in the direction of the 1st axis. (Sonde Atomique et Microstructures, Université de Rouen)

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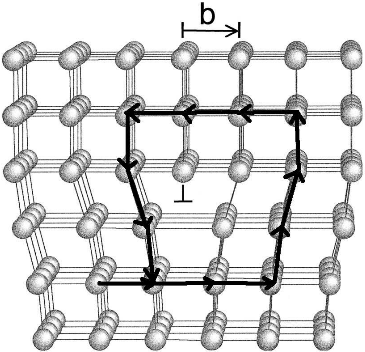

Figure 1: Elementary edge dislocation in a two dimensional crystal lattice. Burger's vector *b* points in the direction of the 1st axis.
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Edge Dislocation

- in the continuum limit, this phenomenon is mathematically represented by the commutation relation

$$[E_1, E_2] = E_1 \,, \tag{1}$$

where E_1, E_2 are the vectorfields along the coordinate axes

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- **affine group**: characterized by transformations of $\mathbb{R}$

$$x \mapsto e^{y^1} x + y^2,$$

generated by $E_1 = \frac{\partial}{\partial y^1}, E_2 = e^{y^1} \frac{\partial}{\partial y^2}$, satisfying (1)

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- corresponding metric

$$\overset{\circ}{n} = (\omega^1)^2 + (\omega^2)^2 = (dy^1)^2 + e^{-2y^1} (dy^2)^2 \,,$$

$\{E_1, E_2\}$ basis of $\mathcal{V}$, dual basis $\{\omega^1, \omega^2\}$ for $\mathcal{V}^*$

- $(\mathcal{N}, \overset{\circ}{n})$ is isometric to the **hyperbolic plane** $\mathcal{H}$

Examples

ii) Screw Dislocation

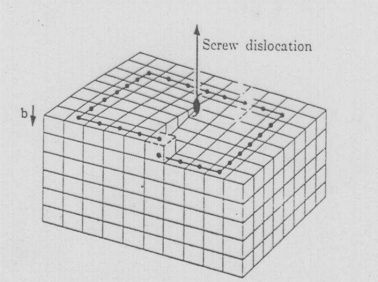

Figure 2: Elementary screw dislocation in a crystal lattice. Burger's vector b in the direction of the 3rd axis.
(Sonde Atomique et Microstructures, Université de Rouen)

Screw Dislocation

- in the continuum limit, this phenomenon is mathematically represented by the commutation relations

$$[E_1, E_2] = E_3\,,\ [E_1, E_3] = 0\,,\ [E_2, E_3] = 0\,, \tag{2}$$

where E_1, E_2, E_3 are the vectorfields along the coordinate axes

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- **Heisenberg group**: characterized by unitary transformations of $L^2(\mathbb{R}, \mathbb{C})$

$$\Psi(x) \mapsto \Psi'(x) = e^{i(y^2 x + y^3)}\Psi(x + y^1),$$

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- corresponding metric (homogeneous space)

$$\overset{\circ}{n} = (\omega^1)^2 + (\omega^2)^2 + (\omega^3)^2 = (dy^1)^2 + (dy^2)^2 + (dy^3 - y^1 dy^2)^2\,,$$

$\{E_1, E_2, E_3\}$ basis of $\mathcal{V}$, dual basis $\{\omega^1, \omega^2, \omega^3\}$ for $\mathcal{V}^*$

Thermodynamic State Space

- $S_2^+(\mathcal{V})$: inner products on $\mathcal{V}$
- **thermodynamic state space**: $S_2^+(\mathcal{V}) \times \mathbb{R}^+ \ni (\gamma, \sigma)$
- $\gamma \in S_2^+(\mathcal{V})$: **thermodynamic configuration**
- $\sigma \in \mathbb{R}^+$: **entropy per particle**
- $V(\gamma)$: **thermodynamic volume** corresponding to γ
- a **thermodynamic state function** κ is a real-valued function on the thermodynamic state space

Thermodynamic Variables

- **thermodynamic stress** corresponding to (γ, σ) is $\pi(\gamma, \sigma) \in (S_2(\mathcal{V}))^*$ defined by

$$-\frac{1}{2}\pi(\gamma, \sigma) V(\gamma) = \frac{\partial\left(\kappa(\gamma, \sigma) V(\gamma)\right)}{\partial \gamma}$$

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- **thermodynamic temperature** corresponding to (γ, σ) is $\vartheta(\gamma, \sigma) \in \mathbb{R}$ given by

$$\vartheta(\gamma, \sigma) = \frac{\partial\left(\kappa(\gamma, \sigma) V(\gamma)\right)}{\partial \sigma},$$

  with $\vartheta(\gamma, \sigma) \searrow 0$, for $\sigma \to 0$

Static Case

- $\mathcal{N} = \Omega \overset{\text{cpt.}}{\subset} \mathbb{R}^n$, $\mathcal{M} = \mathcal{E}^n$ Euclidean space ($n = 2, 3$)
- **material picture**

$$\begin{aligned} \phi : \mathcal{N} &\to \mathcal{M} \\ y &\mapsto \phi(y) = x \end{aligned}$$

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$$\gamma(y) = i^*_{\phi,y} g \,,$$

where $i_{\phi,y} = d\phi(y) \circ \epsilon_y : \mathcal{V} \to T_x\mathcal{M}$

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  where $i_{\phi,y} = d\phi(y) \circ \epsilon_y : \mathcal{V} \to T_x\mathcal{M}$
- **energy per particle** $e(\gamma)$ (a state function) defines the **thermodynamic stress** π

$$-\frac{1}{2}\pi V = \frac{\partial e}{\partial \gamma}$$

Static Case

- given a volume form ω on $\mathcal{V}$, pick a basis $E_1, \ldots, E_n$ of $\mathcal{V}$ s.t. $\omega(E_1, \ldots, E_n) = 1$. Dual basis $\omega^1, \ldots, \omega^n$,

$$\omega^A E_B = \delta^A_B \,, \quad A, B = 1, \ldots, n$$

- m_{ab} metric induced on $\mathcal{N}$ by the Euclidean metric g on $\mathcal{M}$, $m = \phi^* g$,

$$\begin{aligned} m_{ab} &= g_{ij} \frac{\partial x^i}{\partial y^a} \frac{\partial x^j}{\partial y^b} \qquad [x^i = \phi^i(y)] \,, \\ \gamma_{AB} &= E^a_A E^b_B m_{ab} \end{aligned}$$

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- thermodynamic stresses S on $\mathcal{N}$ and $T = \phi_* S$ on $\mathcal{M}$
$$\begin{aligned} S^{ab} &= \pi^{AB} E^a_A E^b_B \,, \\ T^{ij} &= S^{ab} \frac{\partial x^i}{\partial y^a} \frac{\partial x^j}{\partial y^b} \end{aligned}$$

Euler-Lagrange Equations

- **total energy** of a domain Ω in the material manifold $\mathcal{N}$

$$E = \int_{\Omega} e(\gamma) d\mu_\omega \,, \tag{3}$$

where $d\mu_\omega$ is the volume form on $\mathcal{N}$ induced by ω

- first variation of the energy (3) is

$$\dot{E} = \frac{\partial}{\partial \lambda}\bigg|_{\lambda=0} E(\gamma + \lambda \dot{\gamma}) = \int_{\Omega} \frac{\partial e(\gamma)}{\partial \gamma} \cdot \dot{\gamma} \, d\mu_\omega$$

- by definition of the thermodynamic stress,

$$\dot{E} = -\int_{\Omega} \frac{1}{2} \pi^{AB} \dot{\gamma}_{AB} \sqrt{\det \gamma} \det \omega(y) \; d^n y$$

Boundary Value Problem

Finally, the **Euler-Lagrange equations** for the static case read

$$\overset{m}{\nabla}_a S^{ab} = 0 \quad \text{in } \Omega\,,$$

a *system of elliptic PDE*. Or, equivalently, ($T = \phi_* S$ and $m = \phi^* g$)

$$\overset{g}{\nabla}_i T^{ij} = 0 \quad \text{in } \phi(\Omega)\,.$$

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The (free) **boundary conditions** are

$$S^{ab} M_b = 0 \quad \text{on } \partial\Omega\,,$$

where $M_b Y^b = 0$ for all $Y \in T_y \partial\Omega$. Or, equivalently,

$$T^{ij} N_j = 0 \quad \text{on } \partial\phi(\Omega)\,,$$

where $N_j X^j = 0$ for all $X \in T_{\phi(y)} \phi(\partial\Omega)$.

Assumptions

Postulate

We stipulate that e has a strict minimum at a certain inner product $\mathring{\gamma}$.

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Choose $(E_1, \dots, E_n)$ to be an orthonormal basis relative to $\mathring{\gamma}$, so $\mathring{\gamma}_{AB} = \delta_{AB}$. $\mathring{\gamma}$ induces a metric $\mathring{n}$ on $\mathcal{N}$ by

$$\mathring{n} = \sum_{A,B=1}^{n} \mathring{\gamma}_{AB}\, \omega^A \otimes \omega^B = \sum_{A=1}^{n} \omega^A \otimes \omega^A$$

In the following, we make use of the volume form ω_0 on $\mathcal{V}$ corresponding to $\mathring{\gamma}$, $\omega_0(E_1, \dots, E_n) = 1$.

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Remark

$\overset{\circ}{n}$ has curvature except when $\mathcal{V}$ is Abelian (no dislocations). On the other hand, m is flat, being the pullback of the flat Euclidean metric. Thus, unless $\mathcal{V}$ is Abelian, $\overset{\circ}{n}$ is not isometric to m.

The Analysis of Equilibrium Configurations

Uniform Distribution of Dislocations

- choice of **isotropic energy** and elimination of the crystalline structure
- setup of the boundary value problem (in 2d)
- method of the solution for the 2-dimensional case
- strategy for the 3-dimensional case

Toy Energy

Note that $\overset{\circ}{n}$ and $m = \phi^* g$ (g: the Euclidean metric on $\mathcal{M}$) on $\mathcal{N}$ relate to $\overset{\circ}{\gamma}$ and γ via:

$$\overset{\circ}{\gamma} = \epsilon_y^* \left. \overset{\circ}{n} \right|_{T_y \mathcal{N}} \quad , \quad \gamma = \epsilon_y^* \left. m \right|_{T_y \mathcal{N}} \ .$$

Proposition

The eigenvalues $\lambda_i : i = 1, \ldots, n$ of γ relative to $\overset{\circ}{\gamma}$ coincide with the eigenvalues of m relative to $\overset{\circ}{n}$.

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Remark

If our energy per particle were to depend only on the eigenvalues of γ relative to $\overset{\circ}{\gamma}$, then the crystalline structure $\mathcal{V}$ on $\mathcal{N}$ would be eliminated in favor of the Riemannian metric $\overset{\circ}{n}$.

Toy Energy

- **isotropic energy density**: e is a symmetric function of the eigenvalues λ_k of γ relative to $\overset{\circ}{\gamma}$ (or m relative to $\overset{\circ}{n}$),

$$e(\gamma) = e(\lambda_1, \ldots, \lambda_n)$$

- basic choice:

$$e(\gamma) = e(\lambda_1, \ldots, \lambda_n) = \frac{1}{2} \sum_{k=1}^{n} (\lambda_k - 1)^2 \geq 0 \,,$$

that satisfies $e(\lambda_1 = 1, \ldots, \lambda_n = 1) = 0$, strict minimum of the energy density at $\gamma = \overset{\circ}{\gamma}$, $\overset{\circ}{\gamma}_{AB} = \delta_{AB}$

- finally,

$$e(\gamma) = \frac{1}{2} \sum_{k=1}^{n} \left(\lambda_k^2 - 2\lambda_k + 1\right) = \frac{1}{2} \mathrm{tr}\, \gamma^2 - \mathrm{tr}\, \gamma + \frac{n}{2}$$

Stress Tensor

- from the definition of the thermodynamic stress on $\mathcal{V}$

$$\sqrt{\frac{\det m}{\det \overset{\circ}{n}}} S^{ab} = -2\frac{\partial e}{\partial m_{ab}}$$

- according to our choice of energy ($h = \overset{\circ}{n}$)

$$\begin{aligned} e(\lambda_1, \lambda_2) &= \frac{1}{2}\left((\lambda_1 - 1)^2 + (\lambda_2 - 1)^2\right) = \frac{1}{2}\mathrm{tr}_h(m^2) - \mathrm{tr}_h m + 1 \\ &= \frac{1}{2}\left(h^{-1}\right)^{ac}\left(h^{-1}\right)^{bd} m_{ab} m_{cd} - \left(h^{-1}\right)^{ab} m_{ab} + 1 \end{aligned}$$

- therefore,

$$S^{ab} = 2\sqrt{\frac{\det h}{\det m}}\left(h^{-1}\right)^{ac}\left(h^{-1}\right)^{bd}\left(h_{cd} - m_{cd}\right) \qquad (4)$$

- S is nonzero even for $m = \delta$ (i.e. for $\phi = id$), which reflects the fact that there are internal stresses due to dislocations

Setup and Method in 2d

- $\mathcal{N} = \mathcal{H}_\varepsilon$: hyperbolic plane (curvature: $-\varepsilon^2$).
- expansion of the hyperbolic metric h in terms of the curvature:

$$h_{ab} = \delta_{ab} + \varepsilon^2 f_{ab}\,,$$

where f_{ab} are analytic functions in (y^1, y^2) and ε^2

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  where f_{ab} are analytic functions in (y^1, y^2) and ε^2
- Consider mappings

$$\phi : \mathcal{H}_\varepsilon \to \mathcal{E}\,,$$

  where $\mathcal{E}$ is Euclidean space
- identity map

$$\begin{array}{rcl} id : \mathcal{H}_\varepsilon & \to & \mathcal{E} \\ (y^1, y^2) & \mapsto & (x^1, x^2) = (y^1, y^2) \end{array}$$

  (y^1, y^2): Riemannian normal coordinates in $\mathcal{H}_\varepsilon$,
  (x^1, x^2): rectangular coordinates in $\mathcal{E}$.

Boundary Value Problem in 2d

- fix a smooth bounded domain Ω in $\mathcal{N}$ containing 0.
- identity map $id : \mathcal{H}_0 = \mathcal{E}^2 \to \mathcal{E}^2$ is *unique* minimizer of our toy energy for parameter $\varepsilon = 0$
- restriction to ensure uniqueness of *id*
  - **i)** $0 \in \mathcal{H}_\varepsilon \mapsto 0 \in \mathcal{E}$,
  - **ii)** $\frac{\partial}{\partial y^1}\Big|_0 \mapsto d\phi \cdot \frac{\partial}{\partial y^1}\Big|_0 = l \, \frac{\partial}{\partial x^1}\big|_0 \quad , \; l > 0.$

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  i) $0 \in \mathcal{H}_\varepsilon \mapsto 0 \in \mathcal{E}$,
  ii) $\frac{\partial}{\partial y^1}\Big|_0 \mapsto d\phi \cdot \frac{\partial}{\partial y^1}\Big|_0 = l \, \frac{\partial}{\partial x^1}\big|_0 \quad , \, l > 0.$
- boundary value problem (static equations):

$$F_\varepsilon[\phi] = \begin{pmatrix} \overset{m}{\nabla}_b S^{ab} \\ S^{ab} M_b \end{pmatrix} = 0 \quad \begin{pmatrix} \text{in } \Omega \\ \text{on } \partial\Omega \end{pmatrix}, \tag{5}$$

a system of **elliptic** PDEs with free boundary conditions

Method of the Solution (in 2d)

Step 0: linearization of (5) at the identity $\phi = id + \psi$,

$$F_\varepsilon\,[\phi] = F_\varepsilon\,[id] + D_{id}F_\varepsilon \cdot \psi + N_\varepsilon(\psi) = 0\,,$$

where $N_\varepsilon(\psi) \sim \psi^2 + O(\psi^3)$

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Step 1: solution of the linear problem (Lax-Milgram)

Step 2: iteration scheme for solution of the nonlinear problem (for ε sufficiently small)

Step 3: scaling argument yields solution of the actual problem with curvature -1 and rescaled (smaller) domain

Step 1: Linear Problem

- iteration starting at $\psi_0 = 0$ corresponding to the linearized problem
$$L_0 \cdot \psi_1 = -F_\varepsilon\,[id]\ ,$$
L_ε: linearized operator $D_{id}F_\varepsilon$
- $S^{ab}(id) = 2\varepsilon^2\, f_{ab}|_{\varepsilon=0} + O(\varepsilon^4) \quad \Rightarrow \quad \psi_1 = O(\varepsilon^2)$

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- linearizing m at the trivial solution, $\phi^i = y^i + \psi^i$ for nonlinear ψ

$$m_{ab} = \delta_{ab} + \dot{m}_{ab} + O(\psi^2) \quad , \text{where} \quad \dot{m}_{ab} = \left(\frac{\partial \psi^b}{\partial y^a} + \frac{\partial \psi^a}{\partial y^b}\right)$$

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$$m_{ab} = \delta_{ab} + \dot{m}_{ab} + O(\psi^2) \quad , \text{where} \quad \dot{m}_{ab} = \left(\frac{\partial \psi^b}{\partial y^a} + \frac{\partial \psi^a}{\partial y^b}\right)$$
- linear boundary value problem $L_0 \cdot \psi + F_\varepsilon\left[id\right] = 0$
$$\begin{cases} \frac{\partial}{\partial y^b}\left(\dot{m}^{ab} - \varepsilon^2 I^{ab}\right) & = 0 \quad : \quad \text{in} \quad \Omega\,, \\ \left(\dot{m}^{ab} - \varepsilon^2 I^{ab}\right) M_b & = 0 \quad : \quad \text{on} \quad \partial\Omega \end{cases}$$
$$\dot{m}^{ab} = \left(h^{-1}\right)^{ac}\left(h^{-1}\right)^{bd}\dot{m}_{cd},\; I^{ab} = \left(h^{-1}\right)^{ac}\left(h^{-1}\right)^{bd}\left. f_{cd}\right|_{\varepsilon=0}.$$

Generalized Linear Problem

(M, g) a compact Riemannian manifold with boundary ∂M and X a vectorfield on M. Set

$$\pi = \mathcal{L}_X g \quad , \quad \pi_{ij} = \nabla_i X_j + \nabla_j X_i = \pi_{ji} \quad , \quad X_i = g_{ij} X^j \, ,$$

Lie derivative of the metric g along X.

- action integral

$$A = \int_M \left(\frac{1}{4} |\pi|_g^2 + \rho^i X_i \right) d\mu_g - \int_{\partial M} \tau^i X_i \; d\mu_g|_{\partial M}$$

- Euler-Lagrange equations $\dot{A} = 0$ and boundary conditions read

$$\begin{cases} \nabla_j \pi^{ij} &= \rho^i \qquad : \text{in } M \\ \pi^{ij} N_j &= \tau^i \qquad : \text{on } \partial M \end{cases} \tag{6}$$

- identification: $(\Omega, \dot{m}, id^* \delta)$ with (M, π, g)

Generalized Linear Problem

- $\sigma = \mathcal{L}_Y g$, i.e. $\sigma_{ij} = \nabla_i Y_j + \nabla_j Y_i = \sigma_{ji}, \quad Y_i = g_{ij} Y^j$
- suppose now that Y is a Killing field, i.e. $\sigma = \mathcal{L}_Y g = 0$
  $\Rightarrow$ integrability condition

$$\int_M Y_i \rho^i = \int_{\partial M} Y_i \tau^i$$

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  guarantees existence of a solution X for the boundary value problem (6) (Lax-Milgram)
- estimate ($p = 2$):
  $||X||_{H^s(M)} \leq C \left(||\rho||_{H^s(M)} + ||\tau||_{H^{s-1/2}(\partial M)} \right)$
- two solutions differ by a Killing field (uniqueness up to rotation and translation), elimination of Euclidean **Killing fields** by fixing a point and a direction

Step 2: Nonlinear Case

- solution of $F_\varepsilon[\phi] = 0$ provided ε is sufficiently small
- **Strategy**: iteration scheme for $\psi_n = \phi_n - id$, where the first step is the linearized problem
- **Iteration**: $L_0 \cdot \psi_{n+1} = -(L_\varepsilon - L_0) \cdot \psi_n - F_\varepsilon[id] - N_\varepsilon[\psi_n]$ requires integrability condition, satisfied by applying a doping technique

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- coordinates y^a on Ω, and π denoting the linearized metric $\dot{m}$

$$(AP)\begin{cases} \frac{\partial \pi^{ab}_{n+1}}{\partial y^b} = \rho^a_n & : \quad \text{in} \quad \Omega\,, \\ \left(\pi^{ab}_{n+1} - \sigma^{ab}_n\right) M_b = 0 & : \quad \text{on} \quad \partial\Omega\,, \end{cases} \tag{7}$$

where $\pi^{ab}_{n+1} = \frac{\partial \psi^b_{n+1}}{\partial y^a} + \frac{\partial \psi^a_{n+1}}{\partial y^b}$.

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- integrability condition

$$\int_\Omega \xi^a \rho^a_n - \int_{\partial\Omega} \xi^a \sigma^{ab}_n M_b = 0\,,$$

for every Killing field $\xi^a = \alpha^a_b y^b + \beta^a$, $\alpha^a_b = -\alpha^b_a$ of a background Euclidean metric $id^*\delta$.

Doping Technique

- $N = \frac{n(n+1)}{2}$ Killing fields ξ_A $(A : 1, \dots, N)$ in Euclidean space
- Doping (Kapouleas 1990): replace ρ by

$$\rho' = \rho + \sum_A c_A \xi_A$$

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- Integrability condition

$$\int_\Omega \xi_A \cdot \rho' = \int_{\partial\Omega} \xi_A \cdot \sigma_M \,,$$

where $\sigma_M = \sigma^{ab} M_b$.
- reformulate problem (7) using $\psi^a_{n+1} = X^a$

$$(AP) \begin{cases} \frac{\partial}{\partial y^b}\left(\frac{\partial X^b}{\partial y^a} + \frac{\partial X^a}{\partial y^b}\right) & = \rho'^a = \rho'^a_n \quad : \quad \text{in} \quad \Omega \,, \\ \left(\frac{\partial X^b}{\partial y^a} + \frac{\partial X^a}{\partial y^b}\right) M_b & = \tau^a = \sigma^{ab}_n M_b \quad : \quad \text{on} \quad \partial\Omega \,, \end{cases} \tag{8}$$

System in the limit $n \to \infty$

- estimate:

$$||X||_{H^{s+2}(\Omega)} \leq C(\Omega)\left(||\rho'||_{H^s(\Omega)} + ||\tau||_{H^{s+1/2}(\partial\Omega)}\right)$$

- Apply to (8)(n) with $\varepsilon \ll 1$ we prove contraction of ψ_n in $H^{s+2}(\Omega)$ for $s > \frac{n}{2}$, therefore limits $n \to \infty$ can be taken in the corresponding Sobolev spaces
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Proposition

For $\rho' = \rho + \sum_A c_A \xi_A$, where $c_A = \sum_B \left(M^{-1}\right)_{AB} \sigma_B$ we have

$$X^a := \sum_A c_A \xi_A^a \stackrel{!}{=} 0 \quad , (a = 1, \dots, n)$$

for ε sufficiently small.

Step 3: Scaling

$$\tilde{\phi}(y) = l\phi\left(\frac{y}{l}\right) \quad , \quad l > 0\,.$$

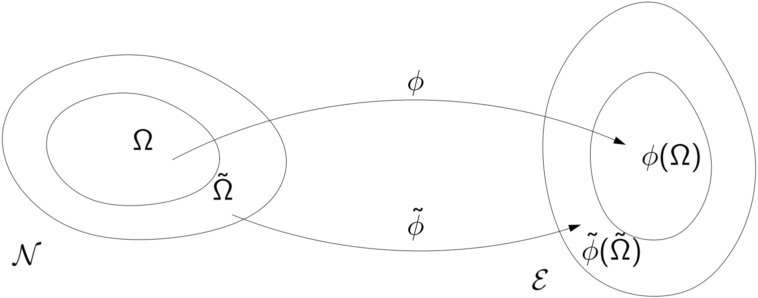

Figure 3: Mapping ϕ from Ω to $\phi(\Omega)$ and scaled version $\tilde{\phi} : \tilde{\Omega} = l\Omega \to \tilde{\phi}(\tilde{\Omega}) = l\phi(\Omega)$.

Isotropic Case

- metrics (*not* isometric, different curvatures)

$$\tilde{m}_{ab}(y) = m_{ab}\left(\frac{y}{l}\right) \quad , \quad \tilde{h}_{ab}(y) = h_{ab}\left(\frac{y}{l}\right)$$

- stresses

$$\tilde{S}^{ab}(y) = S^{ab}\left(\frac{y}{l}\right) \quad , \quad T^{ij}\left(\phi(y)\right) = T^{ij}\left(\phi\left(\frac{y}{l}\right)\right)$$

- equations

$$\overset{\tilde{m}}{\nabla}_b \tilde{S}^{ab}(y) = \frac{1}{l}\left(\overset{m}{\nabla}_b S^{ab}\right)\left(\frac{y}{l}\right)$$

$\Rightarrow$ If $\tilde{\phi}$ is a solution relative to $(\tilde{h}, \tilde{\Omega})$ then ϕ is a solution relative to (h, Ω).

Strategy for the 3d case: choice of anisotropic energy

- preferred direction of dislocations lines breaks isotropy
  $\Rightarrow$ crystalline structure $\mathcal{V}$ enters the problem
- $\gamma \in S_2^+(\mathcal{V})$,

$$\gamma = \begin{pmatrix} \bar{\gamma}_{AB} & \theta_A \\ \theta_A^T & \rho \end{pmatrix}$$

- **anisotropic energy** (O: rotation around dislocation line)

$$e(\bar{\gamma}, \theta, \rho) = e(O\bar{\gamma}\widetilde{O}, O\theta, \rho)\,,$$

  $\Rightarrow$ invariants $\operatorname{tr}\bar{\gamma}\,,\ \operatorname{tr}\bar{\gamma}^2\,,\ |\theta|^2\,,\ \rho$
- choice of anisotropic energy

$$e = \frac{1}{2}\left((\mu_1 - 1)^2 + (\mu_2 - 1)^2\right) + \frac{\alpha}{2}|\theta|^2 + \frac{\beta}{2}(\rho - 1)^2\,,$$

  where $\mu_{1,2}$ are the eigenvalues of $\bar{\gamma}_{AB}$ with respect to $\mathring{\bar{\gamma}}$.

Strategy for the 3d case: choice of coordinates

- left-invariant metric on Heisenberg group (homogeneous space, not isotropic, $\beta \in \mathbb{R}$)

$$\overset{\circ}{n} \equiv h = dx^2 + dy^2 + e^{2\beta}(dz - xdy)^2$$

- h with respect to $E_1 = X, E_2 = Y, E_3 = e^{-\beta} Z$ is orthonormal $h = \sum_{A=1}^{3} \omega^A \otimes \omega^A$
- local coordinate system $(y^a : a = 1, 2, 3)$ on $\mathcal{N}$ (origin: given point)
- change to Riemannian normal coordinates on $\mathcal{N}$ satisfying $h_{ab}(y) = \delta_{ab} + O(|y|^2)$
- show that

$$\gamma_{AB}(y) = \delta_{AB} + O(|y|^2)$$

and the same arguments apply as in the case of a uniform distribution of edge dislocations
- main difference to the 2-dimensional case: stress is more complicated due to anisotropic energy

Outlook

- generalization to isotropic energy of the type ($|b| < a$, $a > 0$)

$$e(\lambda_1, \lambda_2) \;=\; \frac{a}{2}\left((\lambda_1 - 1)^2 + (\lambda_2 - 1)^2\right) + b(\lambda_1 - 1)(\lambda_2 - 1)$$
$$+ O((\lambda_{1,2} - 1)^3)$$

- confront theory with experiments, e.g. scaling properties, internal stress distribution, predict nonlinear phenomena
- static solution for general energy, arbitrary dislocation density
- piezoelectric effect: internal stresses due to electric field

Thank you!

Legendre-Hadamard Conditions

- part of the hyperbolicity condition discussed in **[C2]**
- formulated in terms of $\frac{\partial \phi^i}{\partial y^a}(y) = v^i_a$
- requires for $\xi_a, \xi_b \in T^*_y\mathcal{N}, \eta^i, \eta^j \in T_{\phi(y)}\mathcal{M}$

$$\frac{1}{4}\frac{\partial^2 e}{\partial v^i_a \partial v^j_b}\xi_a\xi_b\eta^i\eta^j \quad : \quad \text{positive for } \xi, \eta \neq 0$$

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- Legendre-Hadamard condition in the static case reads:

$$\frac{\partial^2 e}{\partial \gamma_{AB} \partial \gamma_{CD}} \eta_C \eta_A \xi_B \xi_D + \frac{1}{2}\frac{\partial e}{\partial \gamma_{AB}} |\eta|^2 \xi_A \xi_B > 0 \quad (\eta, \xi \neq 0)$$

where $\xi_A = E_A^a \xi_a$ and $\eta_C = E_C^c v_c^l g_{li} \eta^i$.

Equivalences

Definition

Two crystalline structures $\mathcal{V}$ and $\mathcal{V}'$ on $\mathcal{N}$ are equivalent if there is a diffeomorphism ψ of $\mathcal{N}$ onto itself such that ψ_* induces an isomorphism of $\mathcal{V}$ onto $\mathcal{V}'$.

$A : \mathcal{V} \to \mathcal{V}'$: linear isomorphism, $A^* : S_2^+(\mathcal{V}') \to S_2^+(\mathcal{V})$ induced isomorphism defined by $\gamma = A^*\gamma'$, where

$$\gamma(X, Y) = \gamma'(AX, AY) \quad , \forall X, Y \in \mathcal{V} \, .$$

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Corresponding energy functions on $S_2^+(\mathcal{V})$ and $S_2^+(\mathcal{V}')$ denoted by e and e'

Definition

Two materials are said to be mechanically equivalent if $e'(\gamma') = e(\gamma)$, where $\gamma = A^*\gamma'$.

Equivalences

To capture the same substance in the same phase, we must have the same equilibrium mass density. e is defined on $S_2^+(\mathcal{V})$ and has a strict minimum at $\mathring{\gamma}$. Denote by $\omega_{\mathring{\gamma}}$ its corresponding volume form on $\mathcal{V}$. Pick a positive basis $(E_1, \ldots, E_n)$ for $\mathcal{V}$ which is orthonormal relative to $\mathring{\gamma}$. Then

$$\omega_{\mathring{\gamma}}(E_1, \ldots, E_n) = 1 \, .$$

Equilibrium mass density μ_0 (of small portions)

$$\omega(E_1, \ldots, E_n) = \mu_0 > 0 \quad , \quad \omega = \mu_0 \omega_{\mathring{\gamma}} \, ,$$

and $\mu_0' = \mu_0$.