Semi-discrete models for planar disclinations and dislocations

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Outline of the talk

- Introduction
  - Equilibrium problems in intrinsic elasticity: compatible and incompatible kinematics
  - Equations for wedge disclinations and edge dislocations
  - Airy Stress function method
- Variational systematization of the Airy Stress Function method

Some references

– P.C., L. De Luca, M. Morandotti, to appear on SIAM SIMA, ArXiv: 2207.02511

– P.C, E. Fabbrini, M. Morandotti, in progress.

– C. Zhang and A. Acharya. On the relevance of generalized disclinations in defect mechanics. *Journal of the Mechanics and Physics of Solids, 119:188–223, 2018.*

– C. Zhang, A. Acharya, and S. Puri. Finite element approximation of the fields of bulk and interfacial line defects. *Journal of the Mechanics and Physics of Solids, 114:258–302, 2018.*

– H. S. Seung and D. R. Nelson. Defects in flexible membranes with crystalline order. *Physical Review A, 38:1005–1018, 1988.*

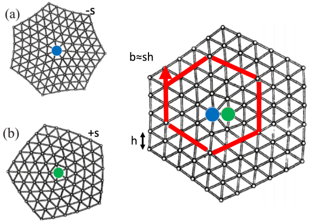
– P. Cordier, S. Demouchy, B. Beausir, V. Taupin, F. Barou, and C. Fressengeas, *Nature*, 507(7490):51–56, 2014. – C. Fressengeas, V. Taupin, and L. Capolungo, *Int. J. of Solids and Structures*, 48(25):3499–3509, 2011.

– V. Taupin, L. Capolungo, C. Fressengeas, M. Upadhyay, and B. Beausir, *Int. J. of Solids and Structures*, 71:277–290, 2015.

– P. Cermelli and G. Leoni, *SIAM J. Math. Anal. 37 (2005), 1131–1160.*

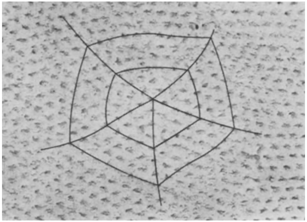
Outline of the talk

- Equilibrium equations for wedge disclinations with the Airy method (*regular* functionals): existence, uniqueness, regularity of minimizers.
- Equilibrium equations for edge dislocations with the Airy method (*singular* functionals)
  - Eshelby's *kinematical* characterization of an edge dislocation in terms of a disclination dipole
  - Proof of the *energetic* equivalence of an edge dislocation with a disclination dipole



Planar wedge disclinations

- Volterra, *Ann. Scient. Ecole Nor. Sup.*, 24:401–517, 1907.



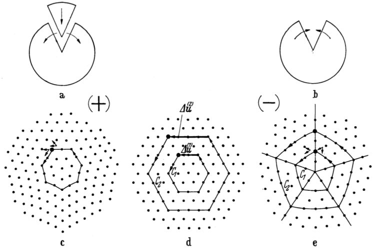


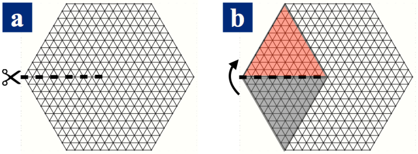
Fig. 1.

E. Kröner (ed.), *Mechanics of Generalized Continua*

- Type-2 superconductor.

Anthony et al., *Proceed. IUTAM '67*, (1968).
Träuble, H., and D. Essmann, *Phys. Stat. Sol.* 25, 373 (1968).
Essmann, D., and Träuble, H., *Phys. Letters* 24A, 526 (1967).

Disclinations on triangular lattice



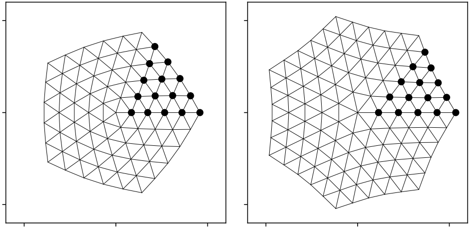
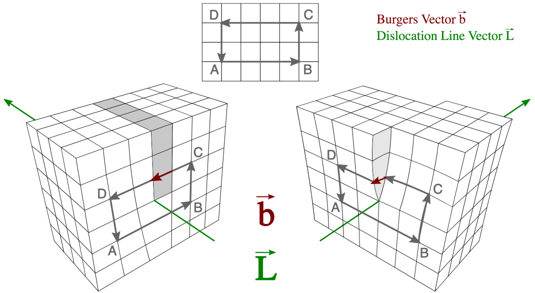


Figure: Positive $(+\frac{\pi}{3})$ and negative $(-\frac{\pi}{3})$ disclination.

P.C., P.Van Meurs, *ESAIM COCV*, 27(23), 2021

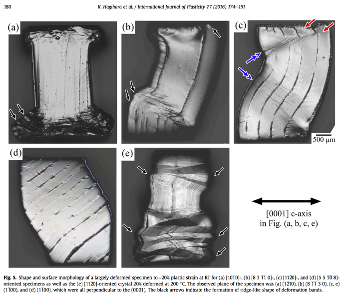
Dislocations

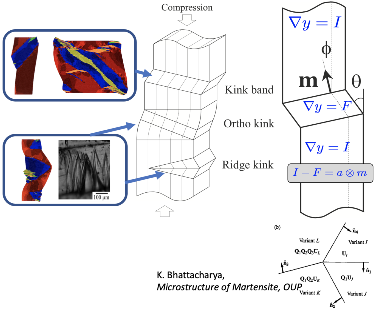


- Edge (left), screw (right) dislocations

M. Fleck, own work, CC BY-SA 4.0, `https://commons.wikimedia.org/w/index.php?curid=96858277`

Crystal plasticity: kinking





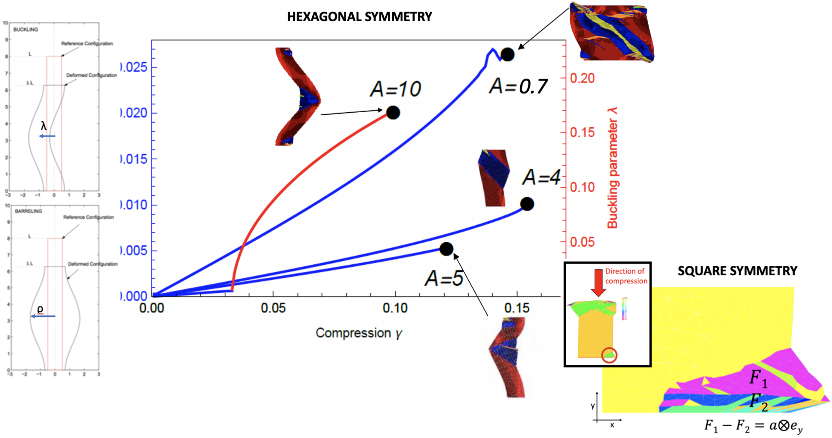
L: Hagihara et al., *Int. J. Plast.* 77 (2016); R: T. Inamura, *Acta Mat.* 173 (2019)

Numerical modeling work:

- E. Arbib, P. Biscari, et al., *IJP* 102728 (2020)
- R. Baggio, E. Arbib, P. Biscari, S. Conti, et al. *PRL*, 123 (2019)
- P.C., E. Arbib, G. Zanzotto, in progress.

Hexagonal lattice

- Material vs. structural instabilities: buckling vs. barrelling and emergence of ortho- vs. kink- bands



Linearized planar strain elasticity

- Linearized kinematics in plane strain regime
- $\Omega \subset \mathbb{R}^2$, $\Omega \ni x = (x_1, x_2)$
- $u : \Omega \to \mathbb{R}^2$ displacement
- $F = \nabla u$, displacement gradient
- $\epsilon : \Omega \to \mathbb{R}^{2\times 2}_{sym}$ strain, $\epsilon = (F + F^T)/2$
- $\sigma : \Omega \to \mathbb{R}^{2\times 2}_{sym}$ stress, $\sigma = \mathbb{C}\epsilon$
- $(\lambda, \mu), (E, \nu)$ elastic constants
- $b_j \in \mathbb{R}^2$ Burgers vectors; $s_i \in \mathbb{R}$ Frank angles.
- (n, t) normal and tangential vector to $\partial\Omega$

We characterize dislocations and disclinations as solutions to system of PDEs in incompatible elasticity.

Compatible elasticity:

$$\mathrm{Curl}\, F = 0 \text{ in } H^{-1}(\Omega, \mathbb{R}^{2\times 2}) \iff \exists u \in H^1(\Omega, \mathbb{R}^2) : \nabla u = F$$

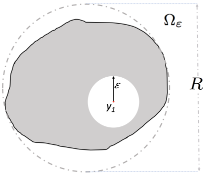
$$\mathrm{curlCurl}\epsilon = 0 \text{ in } H^{-2}(\Omega, \mathbb{R}^{2\times 2}_{sym}) \iff \exists u \in H^1(\Omega, \mathbb{R}^2) : \frac{\nabla u + \nabla^T u}{2} = \epsilon$$

(here we assume Ω simply connected)

Core-radius approach for edge dislocations

- $H : \Omega \to \mathbb{R}^{2\times 2}$, incompatible deformation gradient

$$\begin{cases} \operatorname{Curl} H = \sum_{j}^{J} b_j \delta\left(x - y_j\right) \text{ in } \Omega \\ \operatorname{Div} \mathbb{C}H = 0 \text{ in } \Omega \\ \mathbb{C}Hn = 0 \text{ on } \partial\Omega \end{cases} \tag{1}$$



- Characterized by singular displacements, energy and stresses.
- $\varepsilon > 0$ core radius regularized in the form

$$\min_{H \in \mathcal{H}} \frac{1}{2} \int_{\Omega_\varepsilon} \mathbb{C}H : H dx$$

$$\mathcal{H} := \left\{ H \in H\left(\operatorname{Curl}0; \Omega_\varepsilon\right) : \int_{\partial B_\varepsilon(y_j)} Ht dl = b_j, j = 1, \ldots, J \right\}$$

$$H\left(\operatorname{Curl}0; \Omega_\varepsilon\right) := \left\{ H \in L^2\left(\Omega_\varepsilon, \mathbb{R}^{2\times 2}\right) : \operatorname{Curl} H = 0 \right\}$$

- For general Ω, energy expansion as $\varepsilon \to 0$: self, interaction, elastic terms.
- Energy of a single edge dislocation placed in $(0,0)$ ($\Omega_\varepsilon = B_R(0) \setminus \overline{B_\varepsilon(0)}$)

$$\mathcal{E}_{disloc} = \frac{E}{1-\nu^2} \frac{|b|^2}{8\pi} \log \frac{R}{\varepsilon} \tag{2}$$

P. Cermelli and G. Leoni, *SIAM J. Math. Anal. 37 (2005), 1131–1160.*

Equilibrium equations for disclinations

$$\begin{cases} \operatorname{Div} \mathbb{C}\epsilon = & 0 & \text{in } H^{-1}(\Omega, \mathbb{R}^{2\times 2}_{sym}) \\ \operatorname{curlCurl}\epsilon = & -\sum_i^I s_i \delta(x - z_i) & \text{in } H^{-2}(\Omega) \\ \sigma n = & 0 & \text{on } \partial\Omega \end{cases} \tag{3}$$

- Energy of a single wedge disclination placed in $(0,0)$ $(\Omega = B(0,R))$

$$\mathcal{E}_{discl} = \frac{E}{1-\nu^2} \frac{s^2 R^2}{32\pi} \tag{4}$$

- Volterra, *Ann. Scient. Ecole Nor. Sup.*, 24:401–517, 1907.

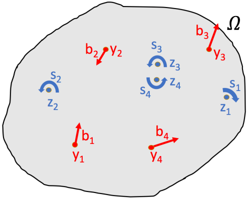
Equilibrium equations for disclinations and dislocations

1. s_i = Disclination angle; $b_j \in \mathbb{R}^2$ = Burgers vector
2. System of PDEs in intrinsic, incompatible elasticity

$$\begin{cases} \operatorname{Div} \mathbb{C}\epsilon = 0 & \text{in } H^{-1}(\Omega, \mathbb{R}^{2\times 2}_{sym}) \\ \operatorname{curl}\operatorname{Curl}\epsilon = \underbrace{-\sum_i^I s_i \delta(x - z_i)}_{\text{disclinations}} + \underbrace{\sum_j^J \operatorname{curl}(b^j \delta(x - y_j))}_{\text{dislocations}} & \text{in } \Omega \\ \sigma n = 0 & \text{on } \partial\Omega \end{cases}$$

Analytical issues, $\Omega \subset \mathbb{R}^2$

1. $\delta(x) \in H^{-2}(\Omega) \to$ disclinations are *weak* solutions (variational principle).
2. $\partial_{x_i}\delta(x) \notin H^{-2}(\Omega)$ dislocations are *distributional* solutions (no variational principle).



The Airy Stress Function method

1. A very very classical method in continuum mechanics and Civil Engineering
2. Volterra, 1907; Wientgarten 1906, Michell 1899, ...
3. in 2D linearized (and intrinsic) elasticity
4. $v : \Omega \to \mathbb{R}$ Airy Stress Function, defined via the identification

$$\mathcal{A}(v) := \begin{bmatrix} \dfrac{\partial^2 v}{\partial x_2^2} & -\dfrac{\partial^2 v}{\partial x_1 \partial x_2} \\ -\dfrac{\partial^2 v}{\partial x_1 \partial x_2} & \dfrac{\partial^2 v}{\partial x_1^2} \end{bmatrix} = \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{22} \end{bmatrix} = \sigma$$

5. We have

$$\begin{cases} \operatorname{Div} \mathbb{C}\epsilon = 0 & \text{in } \Omega \\ \operatorname{curl}\operatorname{Curl}\epsilon = \underbrace{-\sum_i^I s_i \delta(x - z_i)}_{\text{disclinations}} + \underbrace{\sum_j^J \operatorname{curl}(b^j \delta(x - y_j))}_{\text{dislocations}} & \text{in } \Omega \\ \sigma n = 0 & \text{on } \partial\Omega \end{cases}$$

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5. The problem now writes (at least formally)

$$\begin{cases} \cancel{\operatorname{Div} \mathbb{C}\epsilon \equiv} & \cancel{0} & \text{in } \Omega \\ \dfrac{1-\nu^2}{E} \Delta^2 v = & \underbrace{-\sum_i^I s_i \delta(x - z_i)}_{\text{disclinations}} + \underbrace{\sum_j^J \operatorname{curl}(b^j \delta(x - y_j))}_{\text{dislocations}} & \text{in } \Omega \\ \nabla^2 v t = & 0 & \text{on } \partial\Omega \end{cases}$$

Theorem (P.C., L. De Luca, M. Morandotti, SIAM SIMA 2024)

Let $\Omega \subset \mathbb{R}^2$ *open, bounded, simply connected with* $\partial\Omega \in C^4$*. Denote with* $v \in H^2_0(\Omega)$ *the unique weak solution to*

$$\begin{cases} \dfrac{1-\nu^2}{E}\Delta^2 v = -\displaystyle\sum_i^I s_i \delta(x - z_i) & \text{in } H^{-2}(\Omega) \\ v = \partial_n v = 0 & \text{on } \partial\Omega\,; \end{cases} \tag{5}$$

then $\epsilon = \epsilon[v] := \mathbb{C}^{-1}\mathcal{A}(v)$ *is a weak solution to*

$$\begin{cases} \operatorname{curl}\operatorname{CURL}\epsilon = -\displaystyle\sum_i^I s_i \delta(x - z_i) & \text{in } H^{-2}(\Omega) \\ \operatorname{Div}\mathbb{C}\epsilon = 0 & \text{in } H^{-1}(\Omega) \\ \mathbb{C}\epsilon\, n = 0 & \text{on } \partial\Omega\,. \end{cases} \tag{6}$$

Viceversa, if ϵ *is a weak solution to* (6)*, then* $\epsilon \in L^2(\Omega; \mathbb{R}^{2\times 2}_{sym})$ *and there exists a function* $v \in H^2_0(\Omega)$ *such that* $\epsilon = \mathbb{C}^{-1}\mathcal{A}(v)\,.$

Remark on the boundary regularity

- $\sigma n = 0$ is a *natural* BC; vice-versa $(\nabla^2 v)\, t = 0$ is a *constraint*.
- Theorem presented here requires $\partial\Omega \in C^4$
- Work in progress on Lipschitz case.

• Issue: how do we treat in general the non-standard BC?

$$\begin{cases} \dfrac{1-\nu^2}{E}\Delta^2 v = -\displaystyle\sum_i^I s_i \delta(x - z_i) & \text{in } H^{-2}(\Omega) \\ \nabla^2 v\, t = 0 & \text{on } \partial\Omega \end{cases} \tag{7}$$

• Here is the idea (in a toy model): we consider $\partial\Omega$ as a closed, C^2, Jordan curve. Then the two problems are equivalent:

$$\begin{cases} -\Delta u = 0 & \text{in } H^{-1}(\Omega) \\ u = const. & \text{on } \partial\Omega \end{cases} \iff \begin{cases} -\Delta u = 0 & \text{in } H^{-1}(\Omega) \\ \partial_t u = 0 & \text{on } \partial\Omega \end{cases} \tag{8}$$

Characterization of tangential boundary condition

Theorem

Let $\Omega \subset \mathbb{R}^2$ be an open and bounded set with boundary of class C^2. Let $v \in C^2(\overline{\Omega})$. Then, for every connected component Γ of $\partial\Omega$ we have that

$$\nabla^2 v\, t = 0 \ \text{on}\ \Gamma \qquad \Leftrightarrow \qquad v = a\,, \quad \partial_n v = \partial_n a \ \text{on}\ \Gamma\,, \tag{9}$$

for some affine function a.

The idea of the proof.

- Write $\nabla^2 v\, t \equiv \partial_t \nabla v$ in (t, n) (tangent, normal to $\partial\Omega$) basis.
- Implication: $\Leftarrow$ Obvious.
- Implication: $\Rightarrow$ use some Differential Geometry/ODEs.

Remark.
If Ω is simply connected, we can then choose $a(x, y) \equiv 0$ (or any other affine function).
Not so if Ω is not simply connected!

- Let $\gamma : [0,l] \to \mathbb{R}^2$ be the arc-length parameterization of $\partial\Omega$; $l = |\partial\Omega|$.
- $\gamma'(\xi) := (-\sin\vartheta(\xi)), \cos(\vartheta(\xi))$ with $\vartheta \in C^1$.
- Set $\varkappa(\xi) := \vartheta'(\xi)$ for every $\xi \in [0,\ell]$
- Let $g_D, g_N := [0,\ell] \to \mathbb{R}$ be the functions defined by $g_D := v \circ \gamma$ and $g_N := \partial_n v \circ \gamma$.

Then

$$\begin{cases} g_D''(\xi) = \langle \nabla^2 v(\gamma(\xi))\, \gamma'(\xi), \gamma'(\xi)\rangle - \varkappa(\xi) g_N(\xi) \\ g_N'(\xi) = \langle \nabla^2 v(\gamma(\xi))\, \gamma'(\xi), -(\gamma'(\xi))^\perp\rangle + \varkappa(\xi) g_D'(\xi) \end{cases} \quad \text{for every } \xi \in [0,\ell]\,. \tag{10}$$

Observe $0 = (\nabla^2 v\, t) \equiv ((\nabla^2 v\, t, t)t + (\nabla^2 v\, t, n)n) = 0$. Hence, (10) becomes

$$\begin{cases} g_D''(\xi) = -\varkappa(\xi) g_N(\xi) \\ g_N'(\xi) = \varkappa(\xi) g_D'(\xi) \end{cases} \quad \text{for every } \xi \in [0,\ell]\,. \tag{11}$$

or

$$\begin{cases} z'(\xi) = -\varkappa(\xi) g_N(\xi) \\ g_N'(\xi) = \varkappa(\xi) z(\xi) \\ z(\xi) = g_D'(\xi) \end{cases} \quad \text{for every } \xi \in [0,\ell]\,. \tag{12}$$

Solution: $(g_D'; g_N) = (-c_1 \sin\vartheta + c_2 \cos\vartheta; c_1 \cos\vartheta + c_2 \sin\vartheta)$,

$$g_D(\xi) = g_D(0) + \int_0^\xi \big(- c_1 \sin\vartheta(\zeta) + c_2 \cos\vartheta(\zeta)\big)\, \mathrm{d}\zeta = c_0 + \langle (c_1; c_2), \gamma(\xi)\rangle\,, \tag{13}$$

hence $v = a, \partial_n v = \partial_n a$ on Γ $\square$

- The unique solution to:

$$\begin{cases} \frac{1-\nu^2}{E}\Delta^2 v = -\sum_i^I s_i \delta(x - z_i) & \text{in } H^{-2}(\Omega) \\ v = \partial_n v = 0 & \text{on } \partial\Omega\,; \end{cases} \tag{14}$$

is the solution of

$$\min_{H_0^2(\Omega)} I(v),$$

with

$$I(v) := \frac{1}{2}\frac{1+\nu}{E}\int_\Omega \left(|\nabla^2 v| - \nu(\Delta v)^2\right) dx + \sum_i^I s_i v(x_i).$$

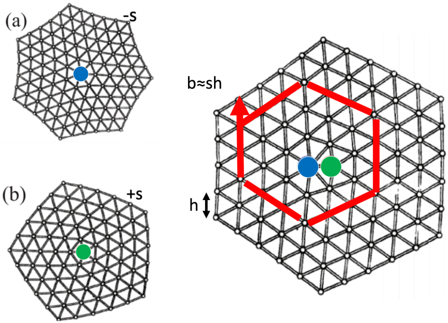
- The bulk term of I corresponding to the stored elastic energy; the linear term is the work done in order to remove/add material thus creating the disclination.
- Labelling $\overline{v}$ the solution of (14), we recognize

$$I(\overline{v}) := \underbrace{\frac{1}{2}\frac{1+\nu}{E}\int_\Omega |\nabla^2 \overline{v}|^2 - \nu(\Delta\overline{v})^2\, dx}_{\equiv \frac{1}{2}\int_\Omega [2\mu|\epsilon(u)|^2 + \lambda(\operatorname{div} u)^2] dx} + \sum_i^I s_i \langle \delta(x - x_i), \overline{v}\rangle$$

Kinematic characterization of dislocations (Eshelby)

- Modeling of dislocations (singular problems)

$$\frac{1-\nu^2}{E}\Delta^2 v = -\sum_{j}^{J} \operatorname{curl}(b^j \delta(x-y_j) \text{ in } \Omega$$



- The dipole of disclinations amounts to an edge dislocation corresponding to removing the half-plane of atoms singled out by sliding the wedge with $b = hs$. Eshelby, *Briy. J. App. Phys.* 17 (1966).

- We can do some heuristic argument in a ball
- Compute the Airy function for a single disclination centered in a ball.

For $\Omega = B(0, R)$ and for $I = 1$, $z_i = 0$, we have

$$v_p(x) := s\frac{E}{1-\nu^2}\frac{|x|^2}{16\pi}\log|x|^2$$

- Compute the Airy function for a dipole of disclinations centered in a ball.

$$v_h(x) := v_p\left(x + \left(\frac{h}{2}, 0\right)\right) - v_p\left(x - \left(\frac{h}{2}, 0\right)\right)$$

- Compute the Airy function for a single dislocation centered in a ball by repeating Eshelby's computation:

$$v_D(x) = \lim_{h\to 0}\frac{v_h}{h} = s\frac{E}{1-\nu^2}\frac{1}{8\pi}(x_1\log|x|^2 + x_1) \tag{15}$$

The (heuristic) idea

- Fix $b = (0, b)$; $h > 0$ lattice spacing. Heuristically,

$$\underbrace{\operatorname{curl}(b\delta(x))}_{\text{dislocation}} = -b\partial_{\frac{(b)^\perp}{|b|}}\delta(x) = -b\partial_{x_1}\delta(x) \approx \underbrace{b\frac{\delta(x_1 - \frac{h}{2}, 0) - \delta(x_1 + \frac{h}{2}, 0)}{h}}_{\text{disclination dipole}} \quad (16)$$

  dislocation of Burgers vector b is (kinematically) equivalent to a dipoles of disclinations of angle $\pm s$, where $|b| = sh$.

- In the limit $h \to 0$ we recover on the right hand side of (16)

$$\lim_{h\to 0} \frac{\delta(x_1 - \frac{h}{2}, 0) - \delta(x_1 + \frac{h}{2}, 0)}{h} = -\partial_{x_1}\delta(x)$$

- We replace the equilibrium problem for a dislocation with a disclination dipole (where $s = b/h$)

$$\begin{cases} \dfrac{1-\nu^2}{E}\Delta^2 v = b\dfrac{\delta(x_1 - \frac{h}{2}, 0) - \delta(x_1 + \frac{h}{2}, 0)}{h} \\ v \in H^2_0(\Omega) \end{cases} \xrightarrow{h\to 0} \begin{cases} \dfrac{1-\nu^2}{E}\Delta^2 v = -b\partial_{x_1}\delta(x) \\ v \in H^2_0(\Omega) \end{cases}$$

Energies on a ball

Take $\Omega = B(0,R)$.

1. Energy of a disclination (v_p)

$$\mathcal{E}_{discl} = \frac{1}{2}\frac{1+\nu}{E}\int_\Omega |\nabla^2 v_p|^2 - \nu(\Delta v_p)^2\,dx = \frac{E}{1-\nu^2}\frac{s^2R^2}{32\pi}$$

2. limit of energy of a disclination dipole, $v_h(\cdot) := v_p(\cdot + (\frac{h}{2},0)) - v_p(\cdot - (\frac{h}{2},0))$

$$\lim_{h\to 0^+} \frac{1}{h^2\log\frac{R}{h}}\frac{1}{2}\frac{1+\nu}{E}\int_\Omega |\nabla^2 v_h|^2 - \nu(\Delta v_h)^2\,dx = \frac{E}{1-\nu^2}\frac{s^2}{8\pi} \tag{17}$$

and, for $0 < h < \varepsilon << 1$,

$$\frac{1}{2}\frac{1+\nu}{E}\int_{\Omega\setminus\overline{B(0,\varepsilon)}} |\nabla^2 v_h|^2 - \nu(\Delta v_h)^2\,dx \approx \frac{E}{1-\nu^2}\frac{\overbrace{(sh)^2}^{b^2,\text{Burgers}}}{8\pi}\log\frac{R}{\varepsilon} \tag{18}$$

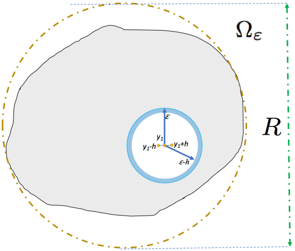
3. Recall, energy of a dislocation (v_D)

$$\mathcal{E}_{disloc} = \frac{1}{2}\frac{1+\nu}{E}\int_{\Omega\setminus\overline{B(0,\varepsilon)}} |\nabla^2 v_D|^2 - \nu(\Delta v_D)^2\,dx = \frac{E}{1-\nu^2}\frac{|b|^2}{8\pi}\log\frac{R}{\varepsilon}$$

4. Our asymptotic analysis in agreement at all orders with P. Cermelli and G. Leoni, *SIAM J. Math. Anal.* 37 (2005), 1131–1160.

Energetic equivalence of an edge dislocation with a disclination dipole

- $h > 0$ dipole arm
- $\varepsilon > 0$ core radius
- $0 < h < \varepsilon \ll R$
- $\Omega_\varepsilon := \Omega \backslash \overline{B_\varepsilon(y_1)}$



• **First step.** ε **fixed,** $h \to 0$. We discover the energy of a disclination dipole is $O(h^2)$ In fact we discover the energy behaves like:

$$h^2 \times \log \varepsilon \times Const.$$

(morally, the core-radius-regularized energy of a dislocation)

In this step the analysis is regular because limit energies are finite as they are regularized thanks to $\varepsilon > 0$.

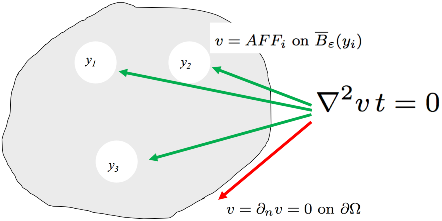
Energetic equivalence of an edge dislocation with a disclination dipole

• **Second step.** $\varepsilon \to 0$**.** Here the analysis for dislocations is singular. Therefore we cannot compute the limit of the energy as $\varepsilon \to 0$ as we would get $+\infty$. We follow the approach of Cermelli-Leoni and we compute the asymptotic expansion of energies in ε. In doing so,

- We identify all the classical terms of the expansion; self-energy, interaction energy etc.
- We obtain the expansion of Cermelli-Leoni for finite systems of dislocations by using the Airy variable.
- We show that Cermelli-Leoni's expansion coincides with ours at all terms.
- Therefore the limit system we have identified at Step 1 is precisely one of effective edge dislocations.

• **Third. Diagonal argument** $\varepsilon = \varepsilon(h)$**.**
We obtain all the results of energy expansion, classification of self/interaction/... energies directly for the disclination dipoles. We therefore extend Cermelli-Leoni's results from edge dislocations to dipoles of wedge disclinations.

ε, h-approximation



- Define the set

$$\mathscr{B}_{\varepsilon,R} := \left\{ w \in H_0^2(B_R(0)) : w = a \text{ in } B_\varepsilon(0) \text{ for some affine function } a \right\} \qquad (19)$$

- For $h < \varepsilon$, define the functional $\widetilde{\mathcal{J}}^s_{h,\varepsilon} : \mathscr{B}_{\varepsilon,R} \to \mathbb{R}$

$$\widetilde{\mathcal{J}}^s_{h,\varepsilon}(w^h) := \mathcal{G}(w^h; B_R(0)) + \frac{s}{2\pi(\varepsilon - h)} \int_{\partial B_{\varepsilon-h}(0)} \left[w^h\left(x + \frac{h}{2} e_1\right) - w^h\left(x - \frac{h}{2} e_1\right) \right] \mathrm{d}\mathcal{H}^1(x)$$

$$\mathcal{G}(v, B_R(0)) := \frac{1}{2} \frac{1+\nu}{E} \int_{B_R(0)} \left(|\nabla^2 v| - \nu(\Delta v)^2 \right) dx$$

- We assume $w^h = hw$ and write

$$\widetilde{\mathcal{J}}^s_{h,\varepsilon}(hw) = \mathcal{G}(hw; B_R(0)) + \frac{s}{2\pi(\varepsilon - h)} \int_{\partial B_{\varepsilon-h}(0)} \left[hw\Big(x + \frac{h}{2} e_1\Big) - hw\Big(x - \frac{h}{2} e_1\Big) \right] \mathrm{d}\mathcal{H}^1(x) \tag{20}$$

- We learn the regularized energy of a disclination dipole of finite charge s is of order $\mathrm{O}(h^2)$. In order to isolate the first non-zero contribution in the limit as $h \to 0$, we divide (20) by h^2 and we define the rescaled functional

$$\begin{aligned} \mathcal{J}^s_{h,\varepsilon}(w) &:= \frac{1}{h^2} \widetilde{\mathcal{J}}^s_{h,\varepsilon}(hw) \\ &= \mathcal{G}(w; B_R(0)) + \frac{s}{2\pi(\varepsilon - h)} \int_{\partial B_{\varepsilon-h}(0)} \frac{w(x + \frac{h}{2} e_1) - w(x - \frac{h}{2} e_1)}{h} \, \mathrm{d}\mathcal{H}^1(x) \, . \end{aligned} \tag{21}$$

- We are now ready to take the limits:

– as $h \to 0$ first, with $\varepsilon > 0$ fixed (disclination dipole $\to$ dislocation), Step 1.
– as $\varepsilon \to 0$ then (energy expansion for dislocation), Step 2.

We now show that the minimizers of $\mathcal{J}^s_{h,\varepsilon}$ in $\mathscr{B}_{\varepsilon,R}$ converge, as $h \to 0$, to the minimizers in $\mathscr{B}_{\varepsilon,R}$ of the functional $\mathcal{J}^s_{0,\varepsilon} : \mathscr{B}_{\varepsilon,R} \to \mathbb{R}$ defined by

$$\mathcal{J}^s_{0,\varepsilon}(w) := \mathcal{G}(w; B_R(0)) + \frac{s}{2\pi\varepsilon} \int_{\partial B_\varepsilon(0)} \partial_{x_1} w \, \mathrm{d}\mathcal{H}^1 \,. \tag{22}$$

• $\mathcal{J}^s_{0,\varepsilon}(w)$ is the equivalent -in the Airy world- of Cermelli-Leoni's model.
• Existence and uniqueness of minimizer for $\mathcal{J}^s_{0,\varepsilon}(w)$ in $\mathscr{B}_{\varepsilon,R}$ follows as in proof for $\mathcal{J}^s_{h,\varepsilon}(w)$ (actually, easier since there is no h-dependence).

Acknowledgments

References:

- P.C. L. De Luca, M. Morandotti, to appear on SIAM SIMA, ArXiv 2207.02511
- P.C. E. Fabbrini, M. Morandotti, in progress.

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Remarks

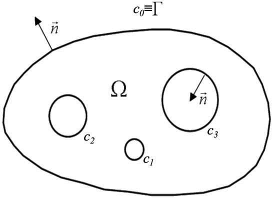
	Compatible elasticity	incompatible elasticity
Ω Simply connected	Classical[1]	ArXiv:2207.02511[2]
Ω non-simply connected	In progress[3]	In progress[3]

- [1] Classical, see P. G. Ciarlet. *Mathematical Elasticity, Volume II, 1997, Theorem 5.6-1(a)*; argument on page 397.
- [2] P.C., L. De Luca, M. Morandotti, to appear on SIAM SIMA, arXiv: 2207.02511
- [3] P.C., E. Fabbrini, M. Morandotti, in progress.

Mechanical equilibrium, domain with holes

First formulation: Selvadurai, *PDEs in Mechanics 2*, Thm. 8.8 .

$$\begin{cases} \Delta^2 v = 0, \text{ in } \Omega \\ \int_{c_i} \frac{\partial}{\partial n}(\Delta v)\, ds = 0, \\ \int_{c_i} \left(x \frac{\partial}{\partial n}(\Delta v) + y \frac{\partial}{\partial s}(\Delta v) \right) ds = -\frac{\xi_1^{(i)}}{1-\nu}, \\ \int_{c_i} \left(x \frac{\partial}{\partial s}(\Delta v) - y \frac{\partial}{\partial n}(\Delta v) \right) ds = -\frac{\xi_2^{(i)}}{1-\nu}, \end{cases} \tag{23}$$



with

$$\xi_1^{(i)} = \int_{c_i} (\sigma_{xx} n_x + \sigma_{xy} n_y)\, ds \qquad \xi_2^{(i)} = \int_{c_i} (\sigma_{xy} n_x + \sigma_{yy} n_y)\, ds$$

Second formulation: Angoshtari, A., Yavari, A. *The weak compatibility equations of nonlinear elasticity and the insufficiency of the Hadamard jump condition for non-simply connected bodies.* Continuum Mech. Thermodyn. 28, 1347–1359 (2016).

$$\begin{cases} \operatorname{div} \sigma = 0 & \text{in } \Omega, \\ \operatorname{curlCurl} \epsilon = 0 & \text{in } \Omega, \\ \int_{c_i} [\epsilon_{ab} - x^c(\epsilon_{ab,c} - \epsilon_{bc,a})]\, dx^b = 0 & \text{for } i = 1, \dots, \beta_1(\Omega), \\ \int_{c_i} (\epsilon_{ac,b} - \epsilon_{cb,a})\, dx^c = 0 & \text{for } i = 1, \dots, \beta_1(\Omega). \end{cases} \tag{24}$$

First formulation $\Longleftrightarrow$ Second formulation

Mechanical equilibrium, domain with holes

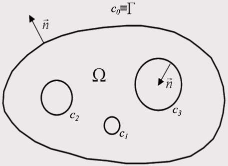
Theorem

Let
$$\mathcal{A} := \{u \in H^2(\Omega) \ s.t.\ \nabla^2 u\, t = 0 \ on\ \partial\Omega\}.$$

There exists a unique solution (up to an affine function) to

$$\min_{v \in \mathcal{A}} \frac{1}{2}\frac{1+\nu}{E}\int_\Omega [|\nabla^2 v|^2 - \nu(\Delta v)^2]\, dx$$

and such solution coincides with the solution to (23) *and* (24).



Idea of the proof.

- Existence follows from Direct Method.
- Characterize the minimizer $v \in \mathscr{A}$, with a general test function $\phi \in \mathscr{A}$

$$\begin{cases} \Delta^2 v = 0 \text{ in } \Omega \\ \displaystyle\int_{c_i} \Big(\frac{1-\nu^2}{E}\phi\, \partial_n(\Delta v) - \frac{1+\nu}{E}\langle \nabla^2 v\, n, \nabla\phi\rangle + \nu\frac{1+\nu}{E}\Delta v\, \partial_n \phi\Big)\, d\mathcal{H}^1 = 0, \quad i = 0, \dots, \beta_1(\Omega) \end{cases} \tag{25}$$

We characterize every element $\phi \in \mathscr{A}$

$$\begin{aligned} \phi\big|_{c_i}(\vartheta) &= d_0^i + (d_1^i \cos\vartheta + d_2^i \sin\vartheta)\,, \\ \partial_n \phi\big|_{c_i}(\vartheta) &= d_1^i \cos\vartheta + d_2^i \sin\vartheta\,, \qquad c_0^k, c_1^k, c_2^k \in \mathbb{R} \end{aligned} \tag{26}$$

Mechanical equilibrium, domain with holes

- In view of (26), the second equation of (25) reads as

$$\begin{cases} \dfrac{1-\nu^2}{E} \displaystyle\int_{c_i} \partial_n(\Delta v)\, d\mathcal{H}^1 = 0\,, \\ \dfrac{1+\nu}{E} \displaystyle\int_{c_i} [\big((1-\nu)\partial_n(\Delta v) + \nu\Delta v\big)\cos\vartheta - (\nabla^2 v\, n)_1] d\vartheta = 0\,, \\ \dfrac{1+\nu}{E} \displaystyle\int_{c_i} [\big((1-\nu)\partial_n(\Delta v) + \nu\Delta v\big)\sin\vartheta - (\nabla^2 v\, n)_2\,] d\vartheta = 0\,. \end{cases} \tag{27}$$

- One can verify that(27) $\iff$ **First formulation** (and hence $\iff$ **Second formulation**).