Forces on Dislocation Lines in Three Dimensions

Topics in the Calculus of Variations: Recent Advances and New Trends
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Outline

Introduction

Dislocations are crystallographic defects.

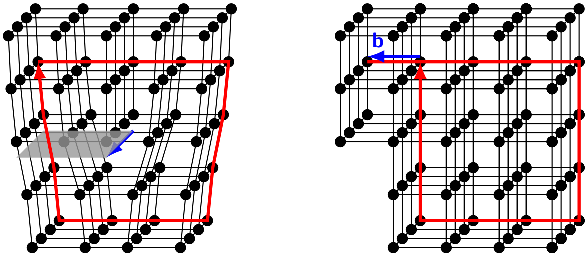

Figure: Sketch of an edge dislocation in a cubic lattice.

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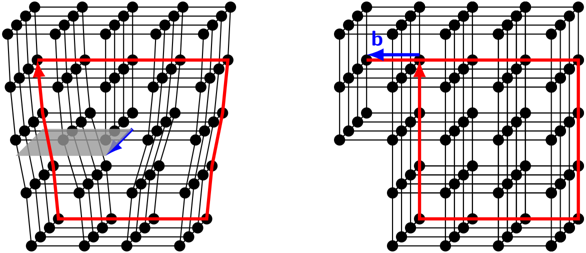


Figure: Sketch of an edge dislocation in a cubic lattice.

- The defect is concentrated on lines.
- The vector $b \in \mathcal{B}$ which characterizes the defect is called Burgers vector.

The Continuous Theory

In the continuous theory, one models dislocations as singularities of the elastic strain $\beta : \Omega \to \mathbb{R}^{3\times 3}$:

$$\operatorname{curl} \beta = b \otimes \tau \, d\mathcal{H}^1_{|\gamma},$$

where the γ is the dislocation curve, τ its tangent and b is the Burgers vector.

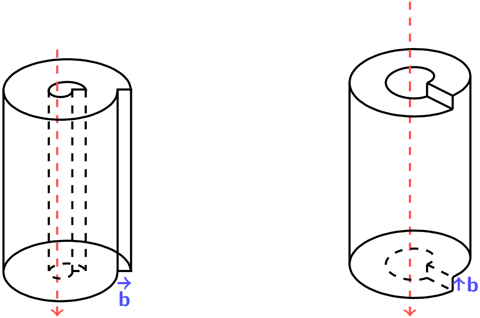
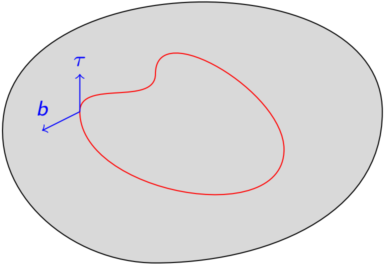


Figure: Sketch of an edge dislocation (left) and a screw dislocation (right) in a deformed cylinder. The dislocation line is the dashed, red line oriented downwards. The Burgers vector is drawn in blue.

Roadmap

- Understand the dynamics of curved dislocation lines.
- As a first step, study the asymptotic behavior of the induced elastic energy.
- Obtain the force as the variation of the effective energy.
- In a third step, we would like to solve the corresponding PDE (future work).



The Energy

For $\Omega \subseteq \mathbb{R}^3$, a fixed Burgers vector $b \in \mathbb{R}^3$ and a regular, closed curve $\gamma : [0, L] \to \Omega$, we define the corresponding dislocation density as

$$\mu = b \otimes \tau \, \mathcal{H}^1_{|\gamma},$$

where τ is the tangent of γ.
Moreover, we define the set of corresponding admissible strains to be

$$\mathcal{A}_\mu = \left\{ \beta \in L^1\left(\Omega; \mathbb{R}^{3\times 3}\right) : \operatorname{curl} \beta = \mu \text{ in } \mathcal{D}'(\Omega) \right\}.$$

The elastic energy is then

$$E_\varepsilon(\mu) = \inf_{\beta \in \mathcal{A}(\mu)} \int_{\Omega \setminus B_\varepsilon(\gamma)} \frac{1}{2} \mathcal{C}\beta : \beta \, dx.$$

Here, $\mathcal{C} \in \mathbb{R}^{3\times 3\times 3\times 3}$ is an isotropic elastic tensor i.e., $\mathcal{C}A = 2\mu A_{sym} + \lambda \operatorname{trace}(A) \, Id$ where μ, λ are such that $\mathcal{C}$ is positive definite on symmetric matrices.

The Energy II

Conti, Garroni, Ortiz '15: There exists a unique $K \in L^{\frac{3}{2}}(\mathbb{R}^3) \cap L^{\infty}_{loc}(\mathbb{R}^3 \setminus \gamma)$ such that

$$\begin{cases} \operatorname{div} \mathcal{C}K = 0, \\ \operatorname{curl} K = \mu_\gamma. \end{cases}$$

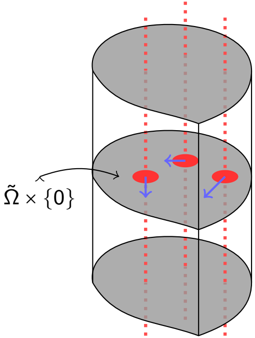
We use this solution to rewrite

$$E_\varepsilon(\mu_\gamma) = \int_{\Omega \setminus B_\varepsilon(\gamma)} \frac{1}{2} \mathcal{C}K : K \, dx + \inf_{u \in H^1(\Omega;\mathbb{R}^3)} I_\varepsilon(u),$$

where

$$I_\varepsilon(u) = \frac{1}{2} \int_{\Omega \setminus B_\varepsilon(\gamma)} \mathcal{C}\nabla u : \nabla u \, dx + \int_{\partial\Omega} u \cdot (\mathcal{C}K\nu) \, d\mathcal{H}^2 - \int_{\partial B_\varepsilon(\gamma)} u \cdot (\mathcal{C}K\nu_\varepsilon) \, d\mathcal{H}^2.$$

Results for Straight Parallel Dislocations



- cylindrical symmetry,
- straight, parallel dislocation edge/screw dislocations,
- reduction to an orthogonal slice,
- in-plane/out-of-plane components of the elastic strain satisfy β satisfy

$$\operatorname{curl} \beta = \sum_k b_k \delta_{x_k}$$

where b_k is an admissible Burger's vector.

Results for Straight Parallel Dislocations

$$I_\varepsilon(u) = \int_{\tilde{\Omega} \setminus \bigcup_k B_\varepsilon(x_k)} \frac{1}{2} \mathcal{C} \nabla u : \nabla u \, dx + \int_{\partial \tilde{\Omega}} u \cdot (\mathcal{C} K \nu) \, d\mathcal{H}^1 - \sum_k \int_{\partial B_\varepsilon(x_k)} u \cdot (\mathcal{C} K \nu_\varepsilon) \, d\mathcal{H}^1$$

Cermelli, Leoni '05 in the edge case and Blass, Morandotti '14 in the screw case:

- Existence of minimizers u_ε for I_ε for fixed ε.

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$$I_0(u) = \int_\Omega \frac{1}{2}\mathcal{C}\nabla u : \nabla u \, dx + \int_{\partial\Omega} u\cdot(\mathcal{C}K\nu)\, d\mathcal{H}^1.$$

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- This leads to

$$\begin{aligned} E_\varepsilon(\mu) &= \int_{\Omega\setminus\bigcup_k B_\varepsilon(x_k)} \frac{1}{2}\mathcal{C}K : K \, dx + I_0(u) + c + O(\varepsilon) \\ &= |\log\varepsilon| \sum_k \psi(b_k) + F(x_1,\dots,x_N) + c + O(\varepsilon). \end{aligned}$$

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- The force on the k-th dislocation is then given by (edge case)

$$\nabla_{x_k} F(x_1,\ldots,x_N) = -\int_{\partial B_r(x_k)} \left[\left(\frac{1}{2}\mathcal{C}\beta_0 : \beta_0\right)\mathbf{Id} - \beta_0^T\mathcal{C}\beta_0\right]\nu\, d\mathcal{H}^1,$$

  where $\beta_0 = K + \nabla u_0$ and $0 < r < \frac{1}{4}\min_{k\neq j}|x_k - x_j|$.
- In the screw case it simplifies even more.

Results for Curved Dislocation Lines in Three Dimensions

First we consider the toy case $\mathcal{C} = Id$.

$$I_\varepsilon(u) = \int_{\Omega \setminus B_\varepsilon(\gamma)} \frac{1}{2}|\nabla u|^2\,dx + \int_{\partial\Omega} u \cdot K\nu\,d\mathcal{H}^2 - \int_{\partial B_\varepsilon(\gamma)} u \cdot K\nu_\varepsilon\,d\mathcal{H}^2,$$

where K solves

$$\begin{cases} \operatorname{div} K = 0 \text{ in } \mathbb{R}^3, \\ \operatorname{curl} K = \mu_\gamma \text{ in } \mathbb{R}^3. \end{cases}$$

Existence of a minimizer u_ε for fixed $\varepsilon > 0$ is simple.

Theorem

Let u_ε be the minimizers for I_ε. Then there exists a a function $u_0 \in H^1(\Omega; \mathbb{R}^3)$ such that $u_\varepsilon \to u_0$ in $H^1_{loc}(\Omega \setminus \gamma)$ and

$$\lim_{\varepsilon \to 0} I_\varepsilon(u_\varepsilon) \to I_0(u_0),$$

where $I_0(u_0) = \int_\Omega \frac{1}{2}|\nabla u_0|^2\,dx + \int_{\partial\Omega} u_0 \cdot K\nu\,d\mathcal{H}^2$. Moreover, u_0 minimizes I_0.

Results for Curved Dislocation Lines in Three Dimensions

Sketch of proof:

- Standard estimates

$$\int_{\Omega\setminus B_\varepsilon(\gamma)} |\nabla u_\varepsilon|^2 - \int_{\partial B_\varepsilon(\gamma)} u_\varepsilon \cdot K\nu_\varepsilon \, d\mathcal{H}^2 - \int_{\partial\Omega} u_\varepsilon \cdot K\nu \, d\mathcal{H}^2$$
$$\geq \int_{\Omega\setminus B_\varepsilon(\gamma)} |\nabla u_\varepsilon|^2 - C_\varepsilon \|K\nu_\varepsilon\|_{L^2(\partial B_\varepsilon(\gamma))} \|u_\varepsilon\|_{H^1(\Omega\setminus B_\varepsilon(\gamma))} - C\|u_\varepsilon\|_{H^1(\Omega\setminus B_\varepsilon(\gamma))} \|K\nu\|_{L^2(\partial\Omega)}.$$

- By regularity of γ we can choose C_ε independent from ε.
- Typically $K \sim \frac{1}{\mathrm{dist}(x,\gamma)}$ but we can show $\|K\nu_\varepsilon\|_{L^2(\partial B_\varepsilon(\gamma))} \to 0$.
- Extend u_ε to Ω. Again constant does not depend on ε. $\Rightarrow$ Boundedness of extended u_ε.
- Hence, there exists $u_0 \in H^1(\Omega)$ and a subsequence such that $u_\varepsilon \rightharpoonup u_0$ in H^1.
- Lower semi-continuity: $\liminf_\varepsilon I_\varepsilon(u_\varepsilon) \geq I_0(u_0)$.
- Also, $I_0(u_0) \leftarrow I_\varepsilon(u_0) \geq I_\varepsilon(u_\varepsilon)$.
- This shows also $\int_{\Omega\setminus B_\varepsilon(\gamma)} |\nabla u_\varepsilon|^2 \, dx \to \int_\Omega |\nabla u_0|^2 \, dx$ which implies the strong convergence in $H^1_{loc}(\Omega \setminus \gamma)$.

Hence, the key is: $\|K\nu_\varepsilon\|_{L^2(\partial B_\varepsilon(\gamma))} \to 0$.

Asymptotics for the Strain

Question: How does $\|K\nu_\varepsilon\|_{L^2(\partial B_\varepsilon(\gamma))}$ behave?

We know that

$$\begin{cases} \operatorname{div} K = 0 \text{ in } \mathbb{R}^3, \\ \operatorname{curl} K = \mu_\gamma \text{ in } \mathbb{R}^3. \end{cases}$$

As $\operatorname{div} \mu_\gamma = 0$, we have

$$K = \operatorname{curl}(-\Delta)^{-1}\mu_\gamma = -b \otimes \int_\gamma \frac{x-y}{4\pi\,|x-y|^3} \times \tau(y)\, d\mathcal{H}^1(y).$$

Theorem

Let γ be a $C^{2,\alpha}$ curve. Then there exists $\varepsilon_0 = \varepsilon_0(\|\gamma\|_{C^{2,\alpha}}) > 0$ such that for all $0 < \varepsilon < \varepsilon_0$ and $x \in \partial B_\varepsilon(\gamma)$ it holds

$$K(x) = -b \otimes \left(\frac{1}{2\pi\,\varepsilon}\, \tau(\pi(x)) \times \nu_\varepsilon(x) + \frac{1}{2\pi}\,|\log(\varepsilon)|\, \tau(\pi(x)) \times H(\pi(x)) + O(1) \right).$$

Here, $\pi(x)$ is the point on γ closest to x, $\nu_\varepsilon(x)$ is the outer normal to $\partial B_\varepsilon(\gamma)$, and H is the curvature of γ. The $O(1)$-term is uniformly bounded for all γ such that $\|\gamma\|_{C^{2,\alpha}} \le M$.

In particular,

$$\|K\nu_\varepsilon\|_{L^2(\partial B_\varepsilon(\gamma))} \lesssim |\log \varepsilon|\varepsilon^{\frac{1}{2}} \to 0.$$

The Force on a Dislocation Line in Three Dimensions

Now, we derive the force on the dislocation as the variation with respect to the curve of the effective energy

$$F_\varepsilon(\mu_\gamma) = \int_{\Omega \setminus B_\varepsilon(\gamma)} \frac{1}{2}|K_\gamma|^2\,dx + \int_\Omega \frac{1}{2}|\nabla u_\gamma|^2\,dx + \int_{\partial\Omega} u_\gamma \cdot K_\gamma \nu\,d\mathcal{H}^2.$$

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Lemma

Let $\gamma \in C^{2,\alpha}([0,L];\Omega)$ be a closed curve and $\varphi \in C^{2,\alpha}\left([0,L];\mathbb{R}^3\right)$. Then there exists $\delta > 0$ such that the functions $K : (-\delta,\delta)\times\Omega\setminus B_\varepsilon(\gamma) \to \mathbb{R}^{3\times 3}$, $(t,x)\to K_{\gamma+t\varphi}(x)$ and $u : (-\delta,\delta)\times\Omega \to \mathbb{R}^3$, $(t,x)\to u_{\gamma+t\varphi}(x)$ are smooth.
Moreover, it holds

$$\frac{d}{dt}\bigg|_{t=0} K_{\gamma+t\varphi}(x) = -b\otimes\nabla_x \underbrace{\int_\gamma \left[\left(-\frac{x-y}{4\pi\,|x-y|^3}\times\tau(y)\right)\cdot\varphi(y)\right] d\mathcal{H}^1(y)}_{=:w_\gamma}.$$

and

$$\begin{cases} -\Delta\left(\frac{d}{dt}_{|t=0} u_{\gamma+t\varphi}\right) = 0 \text{ in } \Omega, \\ \nabla\left(\frac{d}{dt}_{|t=0} u_{\gamma+t\varphi}\right)\nu = -\left(\frac{d}{dt}_{|t=0} K_t\right)\nu \text{ on } \partial\Omega. \end{cases}$$

The Force on a Dislocation Line in Three Dimensions

Theorem

Under the same assumptions.

$$\left.\frac{dF_\varepsilon(\mu_{\gamma+t\varphi})}{dt}\right|_{t=0} = -\int_{\partial B_\varepsilon(\gamma)} \frac{1}{2}|K_\gamma|^2\,\varphi\cdot\nu + w_\gamma\, b\cdot(K_\gamma+\nabla u_\gamma)\nu - u_\gamma\cdot\dot{K}_\gamma\nu\, d\mathcal{H}^2$$
$$= \int_\gamma \left(-|b|^2\frac{|\log\varepsilon|}{2\pi}H + O(1)\right)\cdot\varphi\, d\mathcal{H}^1.$$

Again, the term $O(1)$ is uniformly bounded as long as $\|\gamma\|_{C^{2,\alpha}}$ is uniformly bounded.

This result is consistent with the fact that one can also use the asymptotics for K_γ to show that

$$F_\varepsilon(\mu_\gamma) = |b|^2\frac{|\log\varepsilon|}{2\pi}\mathcal{H}^1(\gamma) + O(1).$$

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The Force on a Dislocation Line in Three Dimensions

The corresponding results for the isotropic elasticity $\mathcal{C}A = 2\mu A_{sym} + \lambda trace(A)\, Id$ is:

Theorem

Under the same assumptions as before,

$$\left.\frac{dF_\varepsilon(\mu_{\gamma+t\varphi})}{dt}\right|_{t=0} = -\int_\gamma |\log\varepsilon| \left(\psi(\tau) H\cdot\varphi + \nabla\psi(\tau)\cdot H\,(\tau\cdot\varphi) + \nabla^2\psi H\cdot\varphi\right) + O(1)\varphi,$$

where $\psi(\tau) = \frac{\mu}{4\pi}(b\cdot\tau)^2 + \frac{\mu}{2\pi}\frac{\lambda+\mu}{2\mu+\lambda}|b-(b\cdot\tau)\tau|^2$ *is the line tension energy density per unit dislocation.*

To prove this we need again an asymptotic formula for the solution of

$$\begin{cases} \operatorname{div} \mathcal{C} K_\gamma = 0, \\ \operatorname{curl} K_\gamma = \mu_\gamma. \end{cases}$$

It can formally be written as

$$K_\gamma = \underbrace{\tilde{K}_\gamma}_{=\text{solution for } \mathcal{C}=Id} + N_{ijkl} * (\mu_\gamma)_{kl},$$

where $N_{ijkl} = -(\partial_j\partial_k\partial_p\varepsilon_{ilp} + \frac{\lambda}{2\mu+\lambda}\partial_j\partial_i\partial_p\varepsilon_{klp})\frac{|x|}{8\pi}$.

The Force on the Dislocation Line in Three Dimensions

Theorem

For a closed curve $\gamma \in C^{2,\alpha}$, *it holds for* $\varepsilon > 0$ *small enough and* $x \in \partial B_\varepsilon(\gamma)$

$$
\begin{aligned}
K_\gamma(x) = \frac{1}{\varepsilon}\Bigg(& \frac{b\cdot\nu}{4\pi}\left(\frac{4\mu+3\lambda}{2\mu+\lambda}\nu\otimes(\tau\times\nu)+\frac{\lambda}{2\mu+\lambda}(\tau\times\nu)\otimes\nu\right) \\
& +\frac{b\cdot(\tau\times\nu)}{4\pi}\,\frac{2\mu}{2\mu+\lambda}\left((\tau\times\nu)\otimes(\tau\times\nu)+\nu\otimes\nu\right)+\frac{b\cdot\tau}{2\pi}\tau\otimes(\tau\times\nu)+W\Bigg) \\
+|\log\varepsilon|\Bigg(& \frac{1}{4\pi}b\otimes(\tau\times H)-\frac{3(b\cdot\tau)}{8\pi}(H\times\tau)\otimes\tau+\frac{1}{4\pi}(H\times b)\otimes\tau+\frac{1}{8\pi}(\tau\times b)\otimes H \\
& -\frac{1}{8\pi}(\tau\times H)\otimes b+\frac{\lambda}{2\mu+\lambda}\Bigg(-\frac{3(b\cdot(H\times\tau))}{8\pi}\tau\otimes\tau+\frac{1}{8\pi}(b\times\tau)\otimes H \\
& +\frac{1}{8\pi}H\otimes(b\times\tau)+\frac{1}{4\pi}\tau\otimes(b\times H)+\frac{1}{4\pi}(b\times H)\otimes\tau+\frac{(\tau\times b)\cdot H}{8\pi}\delta_{ij}\Bigg)\Bigg) \\
+O(1).
\end{aligned}
$$

The Force on a Dislocation Line in Three Dimensions

This also shows that (c.f. also Conti, Garroni, Ortiz '15)

$$F_\varepsilon(\mu_\gamma) = |\log \varepsilon| \int_\gamma \psi(\tau)\, d\mathcal{H}^1 + O(1),$$

where $\psi(\tau) = \frac{\mu}{4\pi}(b\cdot\tau)^2 + \frac{\mu}{2\pi}\frac{\lambda+\mu}{2\mu+\lambda}|b-(b\cdot\tau)\tau|^2$ which is consistent with

$$\left.\frac{dF_\varepsilon(\mu_{\gamma+t\varphi})}{dt}\right|_{t=0} \approx |\log \varepsilon| \left.\frac{d\int_{\gamma+t\varphi}\psi(\tau)\, d\mathcal{H}^1}{dt}\right|_{t=0}.$$

Future Work on the Dynamics

- Again, first $\mathcal{C} = Id$, no restriction on the movement of the line, and rescale time by $|\log \varepsilon|$:

$$\gamma' = \frac{|b|^2}{2\pi} H + O(|\log \varepsilon|^{-1}).$$

- Abstract existence result for curve shortening flow in arbitrary dimensions available, Gage, Hamilton '86.
- Understand regularity of the $O(|\log \varepsilon|^{-1})$-term and use a fixed point argument to obtain existence.
- Study the limit $\varepsilon \to 0$.
- Dislocations cannot move in any direction.
- More realistic dynamics:

$$\gamma' = m(b,\tau) H,$$

  where $m(b,\tau)$ = projection into the plane spanned by b and τ (if $b \nparallel \tau$).
- Replace H by the variation of the anisotropic line tension energy.

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Thank you for your attention!