Lecture 3:
Dislocation dynamics:
from microscopic models to macroscopic crystal plasticity

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Plan of the talk : Hierarchy of scales

(1) Frenkel-Kontorova (atomic)

$\Downarrow \quad (\varepsilon_1 \to 0)$

(2) Peierls-Nabarro (micro)

$\Downarrow \quad (\varepsilon_2 \to 0)$

(3) Dynamics of dislocations (meso)

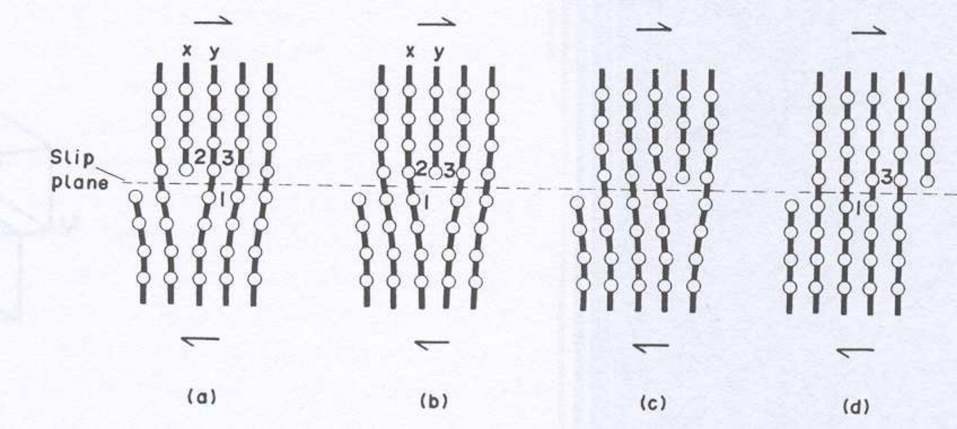
$\Downarrow \quad (\varepsilon_3 \to 0)$

(4) Crystal plasticity (macro)

2D Frenkel-Kontorova model

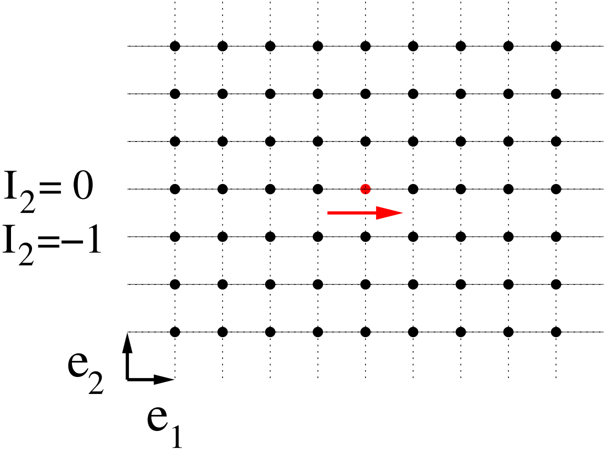
$$(\varepsilon = \varepsilon_1)$$

Motion of a dislocation



2D Frenkel-Kontorova

Points only move on the horizontal axis with $I = (I_1, I_2) \in \mathbb{Z}^2$



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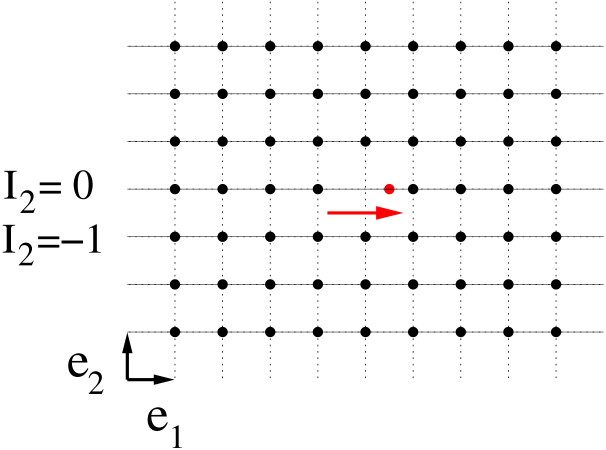
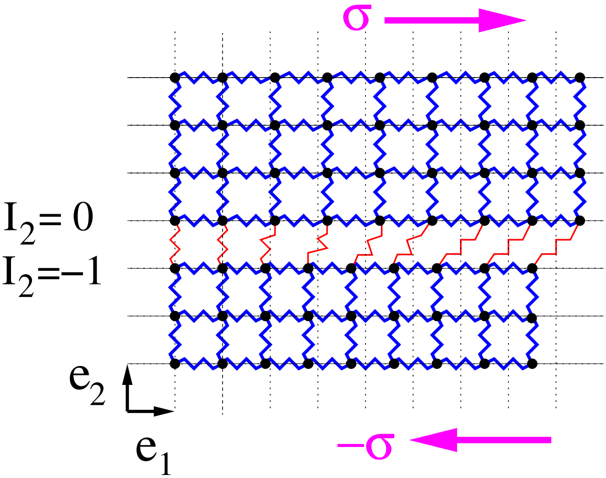


2D Frenkel-Kontorova

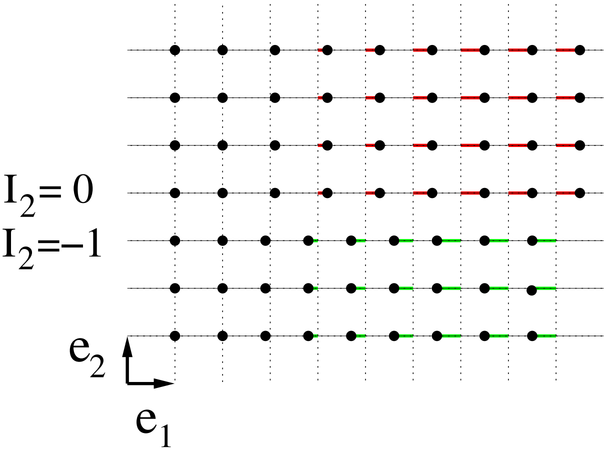
strong springs / weak springs, stress σ



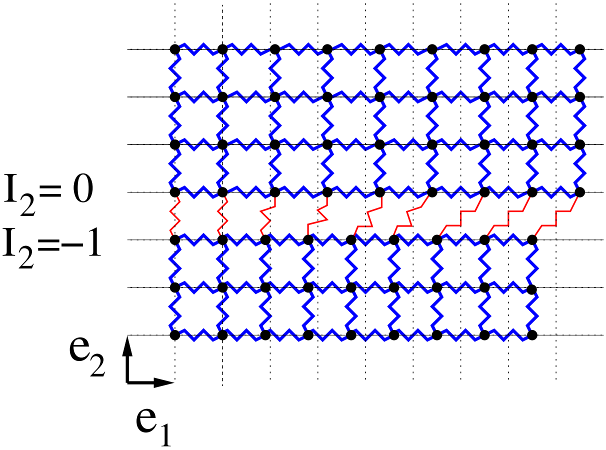
2D Frenkel-Kontorova

Assumption : antisymmetric horizontal displacement

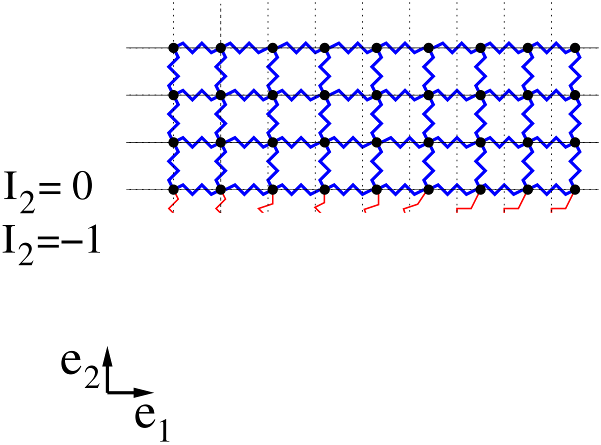
$$U_{(I_1,I_2)} = -U_{(I_1,-I_2-1)}$$



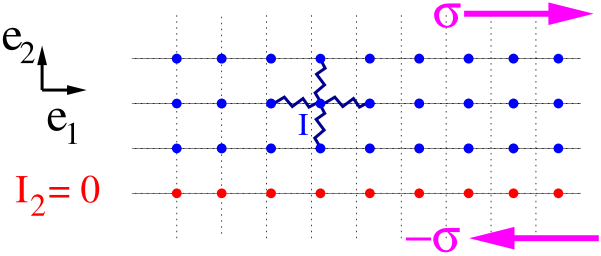
2D Frenkel-Kontorova



Half plane



Equilibrium of the blue points

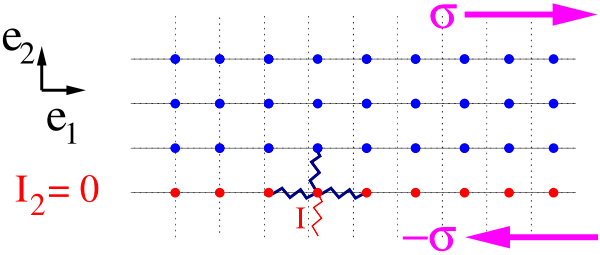


For $I = (I_1, I_2)$ with $I_2 \geq 1$

$$\sum_{J \in \mathbb{Z}^2,\ |J-I|=1} (U_J - U_I) = 0$$

(harmonic blue springs)

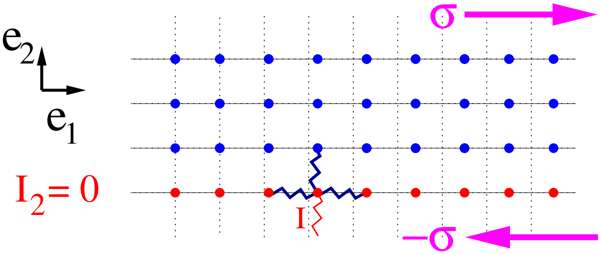
Dynamics of the red points



For $I = (I_1, I_2)$ with $I_2 = 0$

$$\frac{d}{dt}U_I = \quad -\varepsilon W'(U_I) + \sum_{\substack{J \in \mathbb{Z}^2,\ J_2 \geq 0, \\ |J-I|=1}} (U_J - U_I)$$

Dynamics of the red points



For $I = (I_1, I_2)$ with $I_2 = 0$

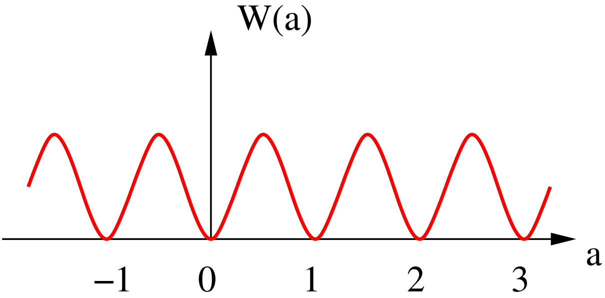
$$\frac{d}{dt}U_I = \varepsilon\varepsilon_2\sigma - \varepsilon W'(U_I) + \sum_{\substack{J\in\mathbb{Z}^2,\ J_2\geq 0,\\ |J-I|=1}} (U_J - U_I)$$

The full 2D Frenkel-Kontorova

$$\left\{\begin{array}{ll} \displaystyle\sum_{J\in\mathbb{Z}^2,\ |J-I|=1} (U_J - U_I) = 0 & \text{for} \quad I_2 \geq 1 \\[2em] \displaystyle\frac{d}{dt}U_I = \varepsilon\varepsilon_2\sigma - \varepsilon W'(U_I) + \sum_{\substack{J\in\mathbb{Z}^2,\ J_2\geq 0,\\ |J-I|=1}} (U_J - U_I) & \text{for} \quad I_2 = 0 \end{array}\right. \tag{1}$$

Potential W

smooth periodic potential $W(a+1) = W(a)$



W describes the misfit between the two half planes.

Homogenization of 1D FK models

- Fully overdamped FK
  [Forcadel, Imbert, M., (2009)]
- FK with acceleration
  [Forcadel, Imbert, M., (preprint 2010)]
- FK with parabolic rescaling
  [Alibaud, Briani, M. (2010)]

Convergence to the Peierls-Nabarro model

$(\varepsilon = \varepsilon_1 \to 0)$

Hyperbolic rescaling

$$u^{\varepsilon}(X,t) = U_{\frac{X}{\varepsilon}}\left(\frac{t}{\varepsilon}\right) \quad \text{for} \quad X = (X_1, X_2) \in (\varepsilon\mathbb{Z}) \times (\varepsilon\mathbb{N})$$

Convergence $\varepsilon \longrightarrow 0$

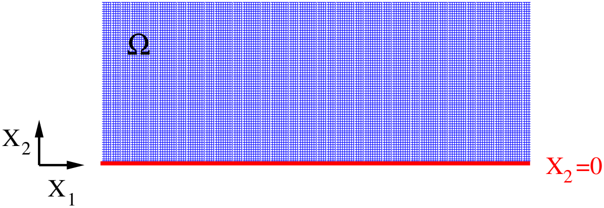
Baby Thm 1 (Formal convergence FK $\longrightarrow$ PN) [Fino, Ibrahim, M.]

As $\varepsilon \longrightarrow 0$, we have formally

$$u^\varepsilon \longrightarrow u^0$$

with u^0 solution of the PN model.

Peierls-Nabarro model



For $u^0(X_1, X_2, t)$:

$$\begin{cases} 0 = \Delta u^0 & \text{on} \quad \Omega = \{X_2 > 0\} \\ u^0_t = \varepsilon_2 \sigma - W'(u^0) + \dfrac{\partial u^0}{\partial X_2} & \text{for} \quad \partial\Omega = \{X_2 = 0\} \end{cases}$$

Reformulation of the PN model

$$\begin{cases} 0 = \Delta u^0 & \text{on} \quad \Omega \\ u_t^0 = \varepsilon_2 \sigma - W'(u^0) + \dfrac{\partial u^0}{\partial X_2} & \text{on} \quad \partial\Omega \end{cases}$$

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$$\Longrightarrow \quad V(x,t) = u^0(x,0,t) \quad \text{satisfies with } \varepsilon = \varepsilon_2$$

$$V_t = \varepsilon \sigma - W'(V) + I[V(\cdot,t)] \quad \text{for} \quad x \in \mathbb{R} \tag{2}$$

with the Lévy-Khintchine formula

$$I[w](x) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{dz}{z^2} \left(w(x+z) - w(x) - z w'(x) 1_{\{|z| \le 1\}} \right)$$

$$V_t = \varepsilon\sigma - W'(V) + I[V(\cdot,t)] \quad \text{for} \quad x \in \mathbb{R}$$

Rescaled to (anisotropic) mean curvature motion on $\mathbb{R}^N$
[Imbert, Souganidis (2009)]

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Rescaled to a line tension model on $\mathbb{R}^N$ (variational approach)
[Garroni, Müller (2006)]

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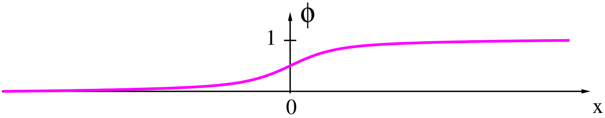
Homogenization of PN model on $\mathbb{R}^N$
[M., Patrizi (preprint 2010)]

The layer solution

[Cabré, Solà-Morales, (2005)]



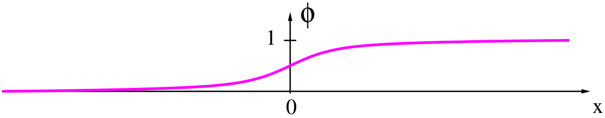
$$\begin{cases} 0 = -W'(\phi) + I[\phi] \quad \text{on} \quad \mathbb{R} \\ \phi' > 0, \quad \phi(-\infty) = 0, \quad \phi(+\infty) = 1, \quad \phi(0) = \dfrac{1}{2} \end{cases}$$

assuming

$$W''(0) > 0$$

The layer solution

[Cabré, Solà-Morales, (2005)]



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assuming

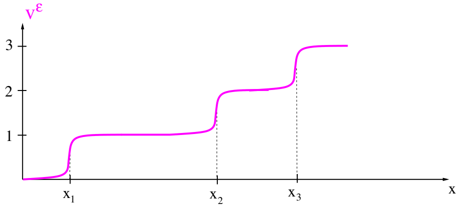
$$W''(0) = 1$$

Convergence to Dislocation points dynamics

$$(\varepsilon = \varepsilon_2 \to 0)$$

Parabolic rescaling

$$v^{\varepsilon}(x,t) = V\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon^2}\right) \quad \text{for} \quad x \in \mathbb{R}$$



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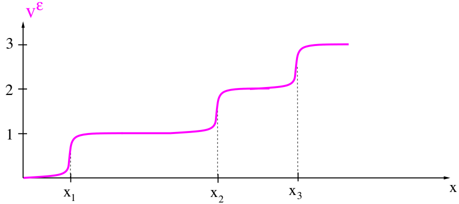


Well-prepared initial data

$$\begin{cases} x_1^0 < x_2^0 < \ldots < x_N^0 \\ \\ v_0^{\varepsilon}(x) = \varepsilon\sigma + \displaystyle\sum_{i=1}^{N} \phi\left(\frac{x - x_i^0}{\varepsilon}\right) \end{cases}$$

Convergence $\varepsilon \longrightarrow 0$

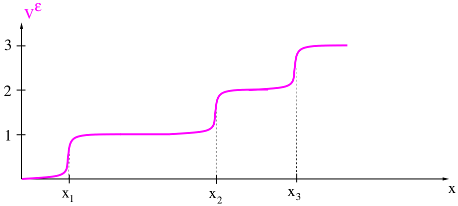
Thm 2 (Convergence PN $\longrightarrow$ DP) [Gonzalez, M. (preprint 2010)]

As $\varepsilon \longrightarrow 0$, we have

$$v^\varepsilon \longrightarrow v^0 \quad \text{in} \quad L^1_{loc}(\mathbb{R} \times [0,+\infty))$$

with

$$v^0(x,t) = \sum_{i=1}^{N} H(x - x_i(t)), \qquad (H = \text{Heaviside function})$$



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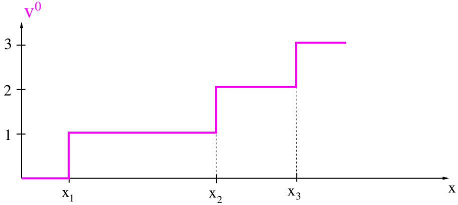

Dislocation points dynamics

$$\left\{\begin{array}{l} \dfrac{dx_i}{dt} = -\gamma\left(\sigma + \displaystyle\sum_{j\neq i} V'(x_i - x_j)\right) \\ \\ x_i(0) = x_i^0 \end{array}\right. \quad \Bigg| \quad \text{for} \quad i = 1, ..., N$$

with

$$\left\{\begin{array}{l} \gamma = \left(\displaystyle\int_{\mathbb{R}} (\phi')^2\right)^{-1} \\ \\ V(x) = -\dfrac{1}{\pi}\ln|x| \end{array}\right.$$

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$$\phi(x) - H(x) \sim -\frac{1}{\pi x} \quad \text{as} \quad |x| \to +\infty$$

Ansatz for the proof

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$$\tilde{v}^{\varepsilon}(x,t) = \varepsilon\sigma + \sum_{i=1}^{N} \left\{ \phi\left(\frac{x - x_i(t)}{\varepsilon}\right) \qquad\qquad\qquad\qquad \right\}$$

Ansatz for the proof

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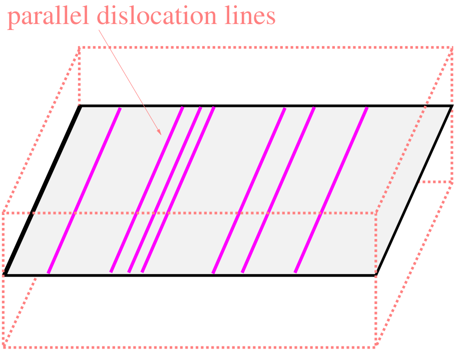
$$\tilde{v}^{\varepsilon}(x,t) = \varepsilon\sigma + \sum_{i=1}^{N} \left\{ \phi\left(\frac{x - x_i(t)}{\varepsilon}\right) - \varepsilon \dot{x}_i(t) \psi\left(\frac{x - x_i(t)}{\varepsilon}\right) \right\}$$

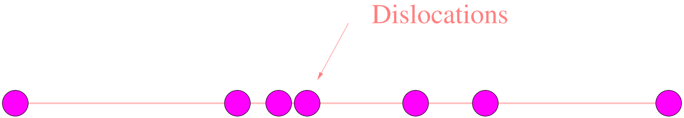
with the corrector ψ solving

$$I[\psi] - W''(\phi)\psi = \phi' + \gamma^{-1}(W''(\phi) - W''(0))$$

Straight dislocations lines



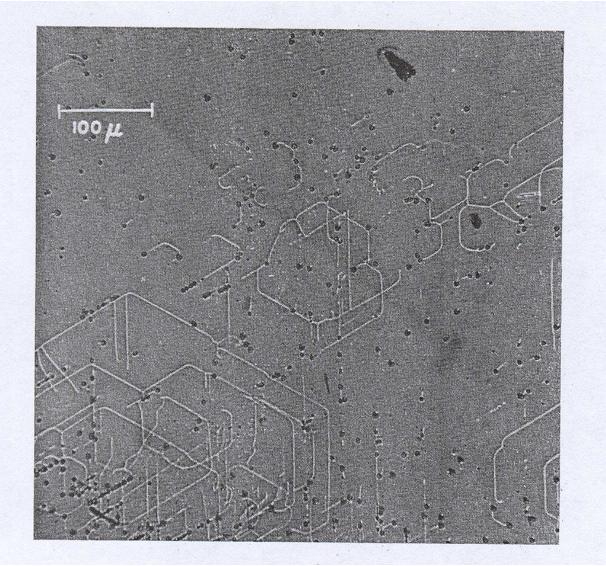
Points



Dislocation points dynamics with periodic obstacles

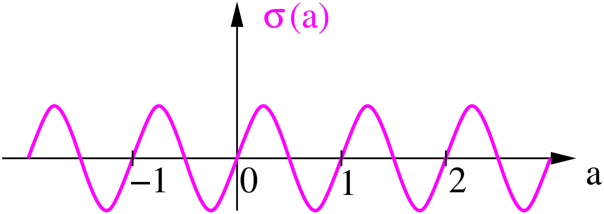
$(\varepsilon = \varepsilon_3)$

Precipitates = obstacles



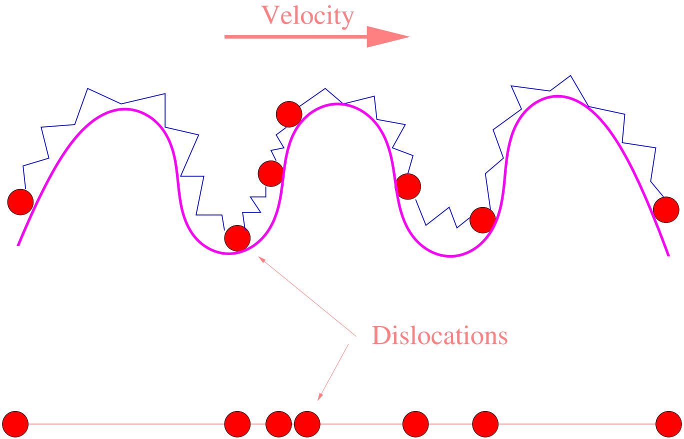
Stress σ

smooth periodic stress $\quad \sigma(a+1) = \sigma(a)$



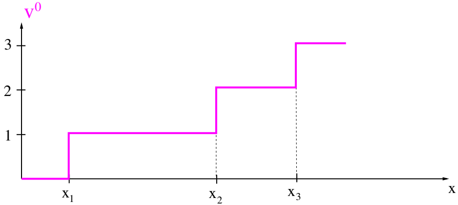
σ describes the obstacles to the motion of dislocations

Dynamics with two-body interactions



$$\begin{cases} N_\varepsilon \quad \text{dislocations} \quad x_1^0 < \ldots < x_{N_\varepsilon}^0 \\ \dfrac{dx_i}{dt} = -\gamma \left(\sigma(x_i) + \displaystyle\sum_{j \neq i} V'(x_i - x_j) \right) \\ x_i(0) = x_i^0 \end{cases} \tag{3}$$

$$v^0(x,t) = \sum_{i=1}^{N_\varepsilon} H(x - x_i(t))$$



Convergence to crystal plasticity

$(\varepsilon = \varepsilon_3 \to 0)$

Hyperbolic rescaling

$$w^{\varepsilon}(x,t) = \varepsilon v^0\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\right)$$

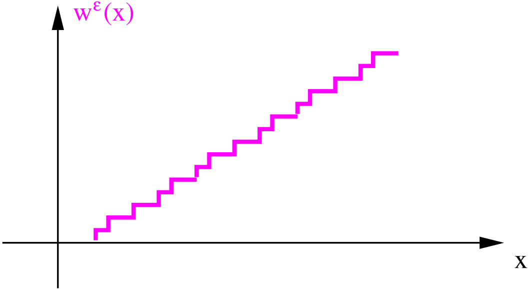
Convergence $\varepsilon \longrightarrow 0$

Thm 3 (Convergence DP → CP) [Forcadel, Imbert, M. (2009)]

As $\varepsilon \longrightarrow 0$, we have

$$w^\varepsilon \longrightarrow w^0 \quad \text{in} \quad L^\infty_{loc}(\mathbb{R}\times[0,+\infty))$$

where w^0 is a solution to the crystal plasticity model.



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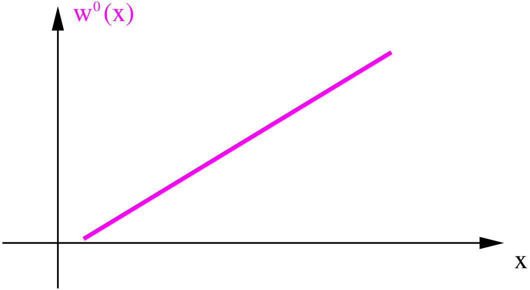

Dynamics for densities of dislocations

Crystal (elasto-visco-) plasticity

$$w^0_t = \bar{H}(w^0_x, I[w^0]) \tag{4}$$

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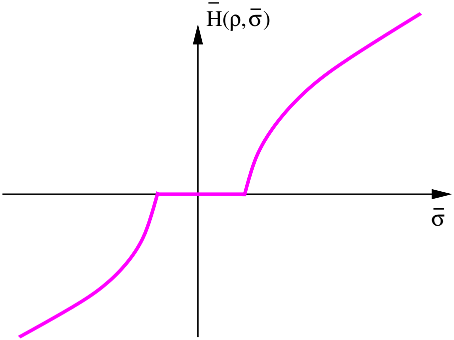
Mechanical interpretation

$$\begin{cases} w^0 & = \text{plastic strain} \\ w^0_t & = \text{plastic strain velocity} \\ w^0_x & = \text{density of dislocations} \\ I[w^0] & = \text{self-stress created by the density of dislocations} \\ w^0_t & = \bar{H}(w^0_x, I[w^0]) \quad \text{is the visco-plastic law} \end{cases}$$

Dynamics for densities of dislocations

Crystal (elasto-visco-) plasticity

$$w_t^0 = \bar{H}(w_x^0, I[w^0])$$



Dynamics for densities of dislocations

Crystal (elasto-visco-) plasticity

$$w^0_t = \bar{H}(w^0_x, I[w^0])$$

with the Orowan's law

$$\bar{H}(\rho, \bar{\sigma}) = \gamma \rho \bar{\sigma} \quad \text{if} \quad \sigma = 0 \quad \text{and} \quad \rho \geq 0$$

Study of self-similar solutions of $w_t = (I[w])|w_x|$
[Biler, Karch, M. (2010)]

Mechanical interpretation

$$\begin{cases} I[w^0] = \bar{\sigma} & \text{stress} \\ \\ w^0_x = \rho & \text{dislocation density} \end{cases}$$

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1. Orowan's law (plastic strain velocity)

$$\dot{e}_p = \bar{\sigma}|\rho|$$

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2. Norton law with threshold (elasto-visco-plasticity)

$$\dot{e}_p = C\text{sign}(\bar{\sigma})((|\bar{\sigma}| - \bar{\sigma}_c)^+)^m$$

Mechanical interpretation

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2. Norton law with threshold (elasto-visco-plasticity)

$$\dot{e}_p = C\text{sign}(\bar{\sigma})((|\bar{\sigma}| - \bar{\sigma}_c)^+)^m$$

3. By homogenization, we find

$$\dot{e}_p = \overline{H}(\rho, \bar{\sigma})$$

Crystal (elasto-visco-) plasticity

$$w_t^0 = \bar{H}(w_x^0, I[w^0])$$

conservation law for $\rho = w_x^0$ and $\bar{\sigma} = I[w^0]$

$$\rho_t = (\bar{H}(\rho, \bar{\sigma}))_x$$

How to compute $\bar{H}$?

In the case $I[w^0] = 0$, dislocation density $\rho = w^0_x$

- Look for particular solutions

$$x_j(t+T) = x_{j+1}(t)$$

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$$\Longrightarrow$$

$$x_j(t) = h\left(vt + \frac{j}{\rho}\right) \quad \text{with} \quad \left\{ \begin{array}{l} h = \text{ hull function} \\ h(a+1) = 1 + h(a) \end{array} \right.$$

$\Longrightarrow$ uniqueness of the velocity v

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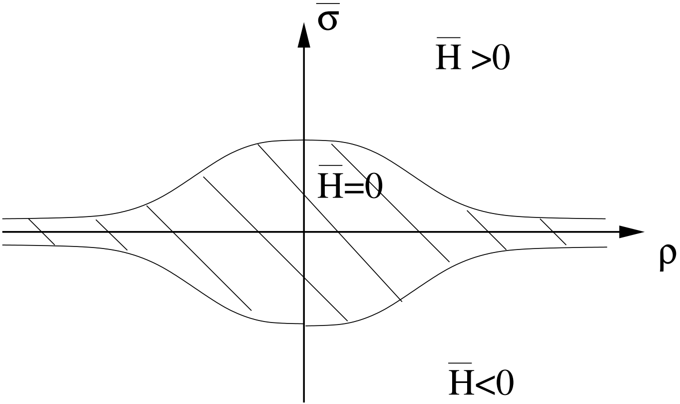
$$\Longrightarrow \quad \text{uniqueness of the velocity} \quad v$$

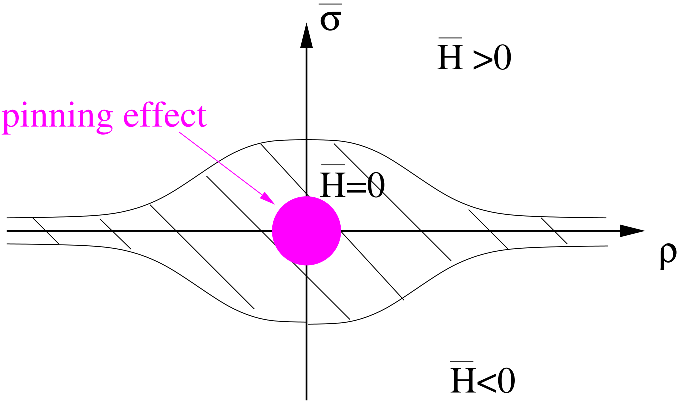
- Set

$$\bar{H}(\rho, 0) = -v\rho$$

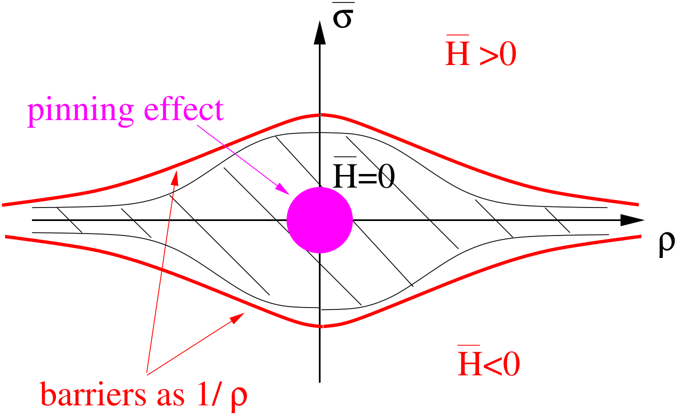
Effective Hamiltonian $\bar{H}(\rho, \bar{\sigma})$

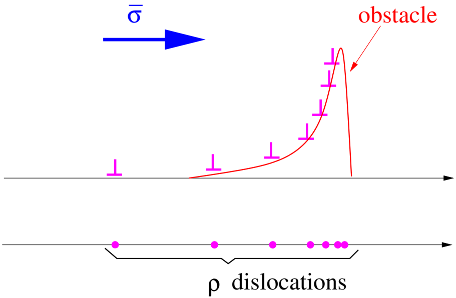


Pinning effect if $\int_{[0,1)} \sigma = 0$



Barriers for smooth enough interactions



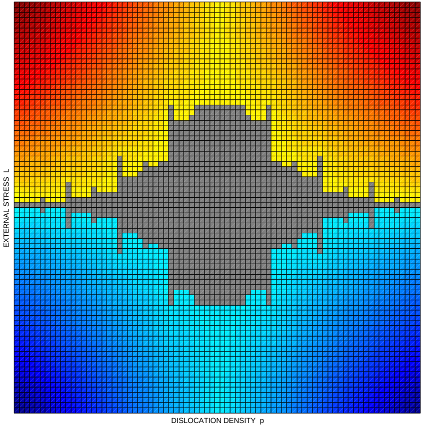


$$\overline{\sigma} = \frac{\sigma^{\text{obst}}}{\rho}$$

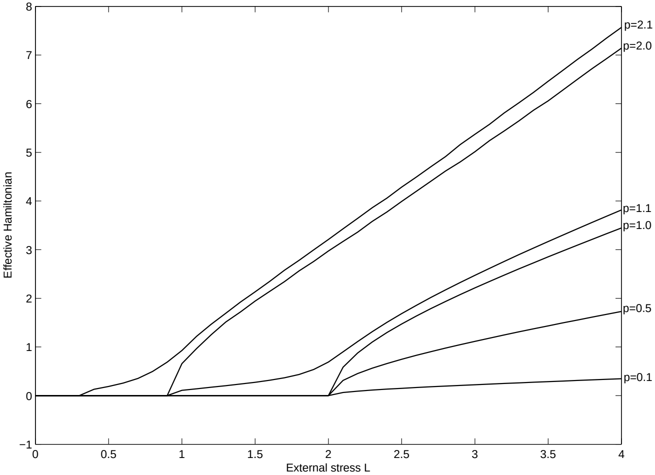
[Hirth, Lothe (1992), p. 766]

Effective Hamiltonian $\bar{H}(\rho, \bar{\sigma})$ (Numerics)

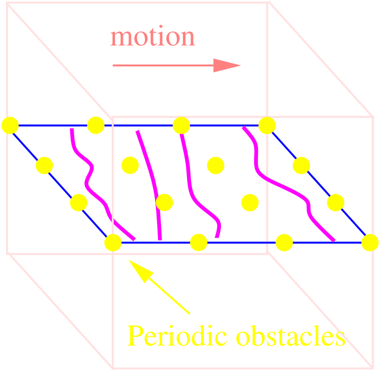
[Cacace, Chambolle, M. (preprint 2010)]



Effective Hamiltonian $\bar{\sigma} \mapsto \overline{H}(\rho, \bar{\sigma})$

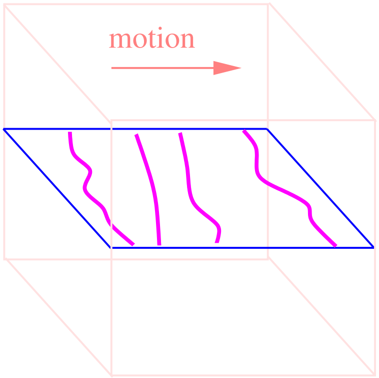


Homogenization of dislocation curves



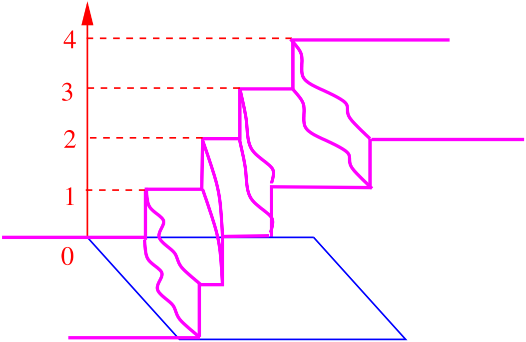
Limit for density of dislocations ?

Homogenization for curves



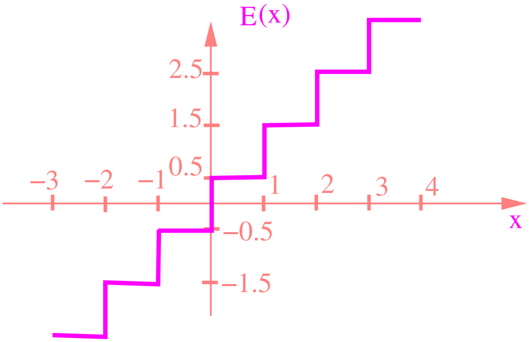
A single plane and a single Burgers vector

Plastic displacement



Odd integer part

$$E(w) = l + \frac{1}{2} \quad \text{for} \quad l \le w < l+1, \quad l \in \mathbb{Z}$$



We consider solutions $w(x,t)$ of

$$\begin{cases} w_t = |\nabla w| \ \{J \star E\{w(\cdot,t) - w(x,t)\}(x) + c(x)\} & \text{on} \quad \mathbb{R}^N \times (0,+\infty) \\ w(\cdot,0) = \frac{1}{\varepsilon} w_0(\varepsilon x) & \text{at} \quad t = 0 \end{cases}$$

Here $c(x)$ represents the stress field created by the obstacles (precipitates, other fixed dsilocations, ...) that are assumed to be periodic :

$$c(x+k) = c(x) \quad \text{for all} \quad k \in \mathbb{Z}^N$$

and

$$0 \leq J(z) = \frac{g(z/|z|)}{|z|^{N+1}} \cdot 1_{\{|z| \geq \delta\}} \quad \text{with} \quad \delta \quad \text{fixed}$$

with

$$g(-z) = g(z) \geq 0 \quad \text{and} \quad g \in C(\mathbb{S}^{N-1}; \mathbb{R})$$

Let

$$w^{\varepsilon}(x,t) = \varepsilon w\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\right)$$

Thm 3' (Convergence DD → CP) [Forcadel, Imbert, M. (2009)]

Assume $w_0 \in W^{2,\infty}(\mathbb{R}^N)$ and the technical condition :

$$g > 0 \quad \text{if} \quad N \geq 2$$

Then we have

$$w^{\varepsilon} \to w^0 \quad \text{in} \quad L^{\infty}_{loc}((0,+\infty) \times \mathbb{R}^N)$$

where w^0 is the solution of the limit equation for some suitable function $\bar{H}$

The limit equation

$$\begin{cases} w^0_t = \bar{H}(\nabla w^0, I[w^0(\cdot,t)]) & \text{on} \quad \mathbb{R}^N \times (0,+\infty) \\ w^0(\cdot,0) = w_0 & \text{at} \quad t = 0 \end{cases}$$

with

$$I[w](x) = \int_{\mathbb{R}^N} dz \, \frac{g(z/|z|)}{|z|^{N+1}} \left\{ w(x+z) - w(x) - z \cdot \nabla w(x) \cdot 1_{\{|z|<1\}} \right\}$$

Formal proposition (the cell problem)

If $w^\varepsilon \to w^0$ *and*

$$w^\varepsilon(t,x) \simeq w^0(t,x) + \varepsilon v\left(\frac{x}{\varepsilon}\right) \quad \textit{locally}$$

then $v(y)$ *is called the corrector and is assymptotically a solution of the following cell problem :*

$$\begin{cases} \lambda = |p + \nabla v(y)| \cdot \{c(y) + \bar\sigma + M_p[v](y)\} \quad \textit{on} \quad \mathbb{R}^N \\ \\ v(y+k) = v(y) \quad \textit{for all} \quad k \in \mathbb{Z}^N \end{cases}$$

with

$$\begin{cases} p = \nabla w^0(x,t) \\ \bar\sigma = I[w^0(\cdot,t)](x) \quad \textit{(Long range)} \\ \lambda = w^0_t(x,t) = \bar H(p,\bar\sigma) \\ M_p[v](y) = \displaystyle\int_{\mathbb{R}^N} dz\ J(z)\left\{E\left\{v(y+z) - v(y) + p\cdot z\right\} - p\cdot z\right\} \end{cases}$$

Main idea = splitting of interactions

Interactions = Short range + Long range

Conclusion

Hierarchy of scales

(1) Frenkel-Kontorova (atomic)

$\Downarrow \quad (\varepsilon_1 \to 0)$

(2) Peierls-Nabarro (micro)

$\Downarrow \quad (\varepsilon_2 \to 0)$

(3) Dynamics of dislocations (meso)

$\Downarrow \quad (\varepsilon_3 \to 0)$

(4) Crystal plasticity (macro)