

# Homogenization of the dislocation dynamics

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Joint work with Cyril Imbert and Régis Monneau

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# Plan

- 1 Physical motivations
- 2 Homogenization of a particle system
- 3 Homogenization of the dynamics of dislocation lines
- 4 Qualitative properties of the effective Hamiltonian

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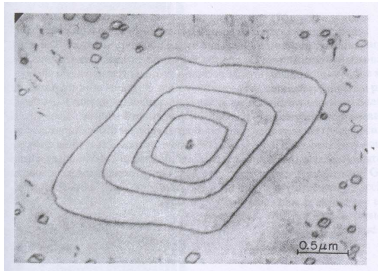
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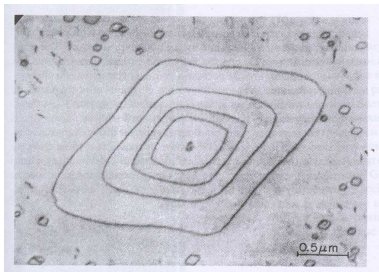
# Observation of dislocations



Definition : a dislocation is a line of crystal defects.

Goal: modeling of plastic behaviour of crystal.

# Observation of dislocations

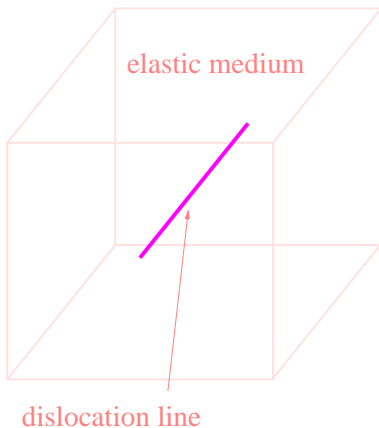


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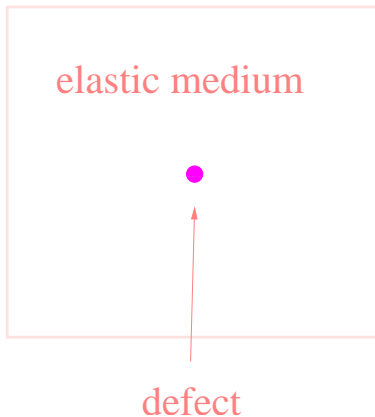
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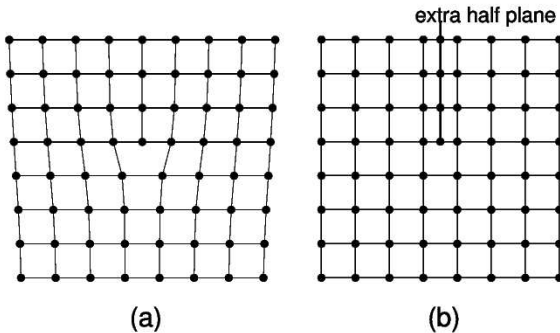
# Continuous 3D model



# Continuous 2D model

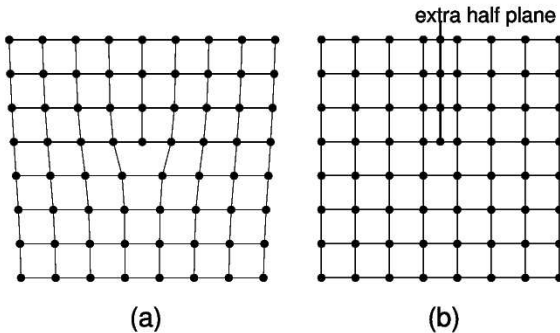


# Atomic structure of a dislocation



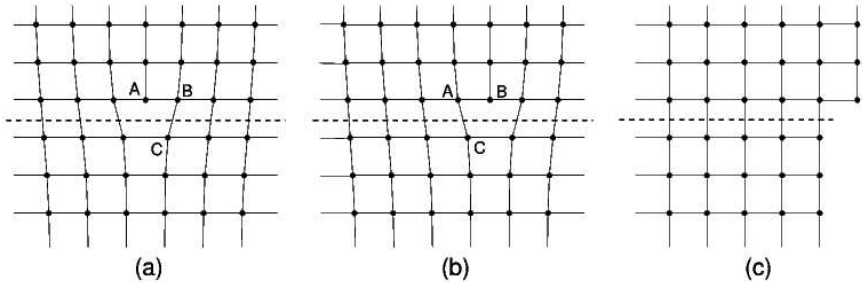
topological defect = dislocation

# Atomic structure of a dislocation



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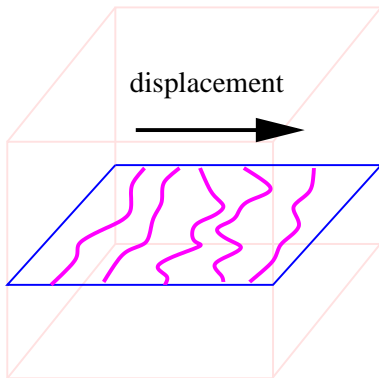
# Displacement of a dislocation



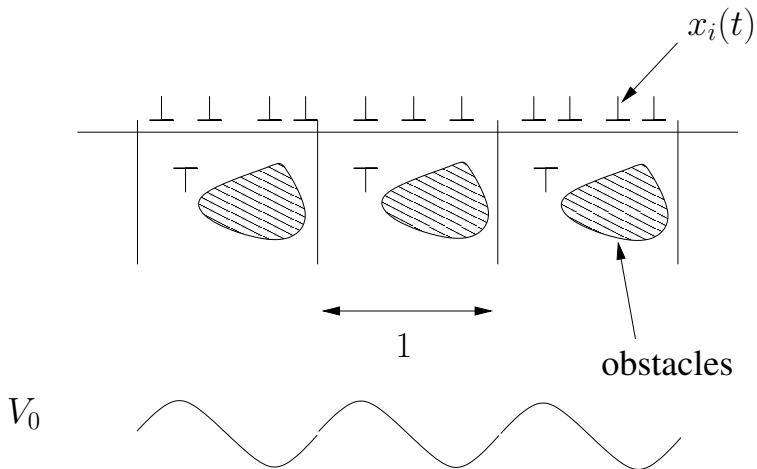
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# Homogenization

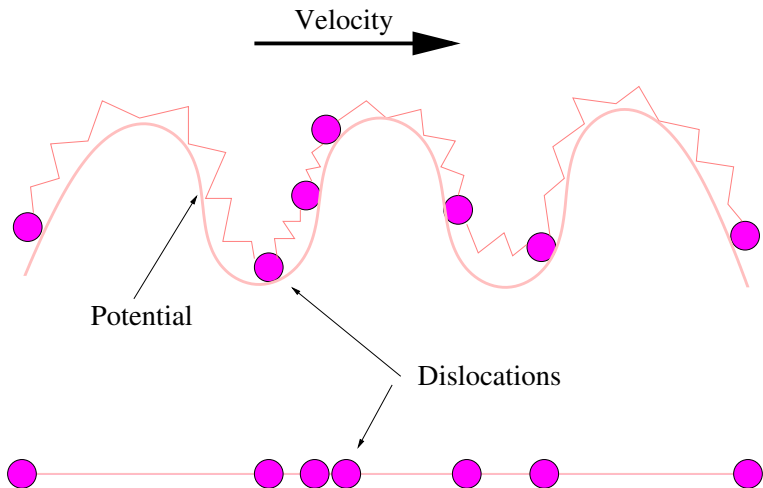


# Homogenization 1D





# Homogenization 1D



# Modelling

$$\dot{x}_i = -\nabla_{x_i} E$$

with

$$E = \sum_i V_0(x_i) + \sum_{i < j} V(x_i - x_j)$$

and

$$V_0(x + 1) = V_0(x)$$

$$V(x) = \ln |x|$$

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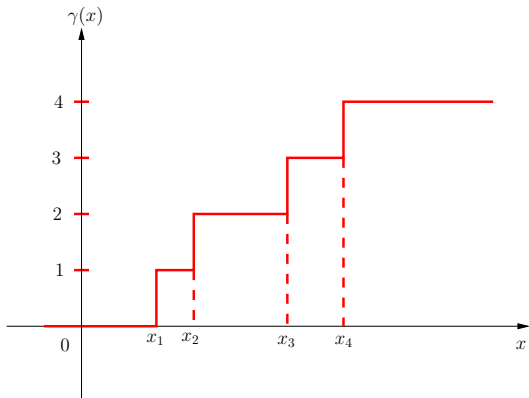
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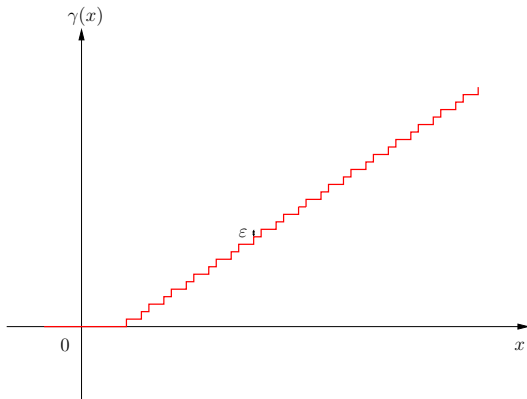
$$\dot{x}_i = -V_0(x_i) - \sum_{j \neq i} V'(x_i - x_j).$$

# Homogenization 1D



Plastic deformation:  $\gamma(x, t) = \sum_i H(x - x_i(t))$

# Rescaling



Plastic deformation:  $\gamma^\epsilon(x, t) = \epsilon \gamma\left(\frac{x}{\epsilon}, \frac{t}{\epsilon}\right)$

# Limit $\varepsilon = 0$ : Homogenization result

## Theorem ( NF,Imbert, Monneau)

Under certain assumptions on the initial data and on  $V_0$ , there exists  $\bar{H}$  such that  $\gamma^\varepsilon(x, t)$  converges to the solution  $u^0(x, t)$  of

$$\begin{cases} \frac{\partial u^0}{\partial t} = \bar{H}(\mathcal{I}_1[u^0(\cdot, t)], Du_0) \\ +I.C. \end{cases} \quad (1)$$

where

$$\mathcal{I}_1[U](x) = \int_{\mathbb{R}} (U(x+z) - U(x) - \nabla_x U(x) \cdot z 1_B(z)) \frac{1}{|z|^2} dz$$



# Idea of the proof

$\gamma^\varepsilon$  is a (discontinuous) solution of

$$\begin{cases} \frac{\partial \gamma^\varepsilon}{\partial t} = \left( c\left(\frac{x}{\varepsilon}\right) + M^\varepsilon \left[ \frac{\gamma^\varepsilon(\cdot, t)}{\varepsilon} \right] (x) \right) |D\gamma^\varepsilon| \\ + I.C. \end{cases} \quad (2)$$

where  $M^\varepsilon$  is a non-local operator of order 0 defined by

$$M^\varepsilon [U] (x) = \int_{\mathbb{R}} dz J(z) E (U(x + \varepsilon z) - U(x))$$

# Assumptions on $V$

We make the following assumptions on  $V$ :

- $V \in W_{\text{Loc}}^{1,\infty}(\mathbb{R})$  and  $V'' \in W^{1,1}(\mathbb{R} \setminus \{0\})$ ,
- $V$  is symmetric *i.e.*  $V(-y) = V(y)$ ,
- $V$  is non-increasing and convex on  $(0, +\infty)$ ,
- $V'(y) \rightarrow 0$  as  $|y| \rightarrow +\infty$ ,
- there exists a constant  $g_0$  such that  $V''(y)y^2 = g_0$  for  $|y| \geq 1$ .

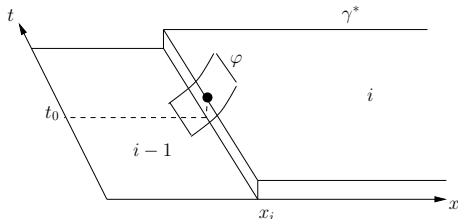
# Idea of the proof

## Lemma

We have

$$\sum_{j \neq i} V'(x_i - x_j) = J \star E(\gamma^*(\cdot) - \gamma^*(x_i))(x_i).$$

# Proof that $\gamma^*$ is a sub-solution



$t \mapsto \varphi(x_i(t), t)$  reaches a local minimum in  $t_0$

$$\implies \varphi_t(x_i(t_0), t_0) + \dot{x}_i(t_0) D\varphi(x_i(t_0), t_0) = 0.$$

$$\implies \varphi_t(x_i(t_0), t_0) = \left( J \star E(\gamma^*(\cdot) - \gamma^*(x_i))(x_i) + c(x) \right) |D\varphi(x_i(t_0), t_0)|.$$

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# Model

We consider the following model

$$\begin{cases} \frac{\partial u^\varepsilon}{\partial t} = \left( c\left(\frac{x}{\varepsilon}\right) + M^\varepsilon \left[ \frac{u^\varepsilon(\cdot, t)}{\varepsilon} \right] (x) \right) |Du^\varepsilon| & \text{in } \mathbb{R}^N \times [0, +\infty) \\ u^\varepsilon(\cdot, t=0) = u_0 & \text{on } \mathbb{R}^N \end{cases}$$

where  $M^\varepsilon$  is a non-local operator of order 0 defined by

$$M^\varepsilon [U] (x) = \int_{\mathbb{R}^N} dz J(z) E (U(x + \varepsilon z) - U(x))$$

# Assumptions on $J$

We make the following assumptions on  $J$ :

- $J \in W^{1,1}(\mathbb{R}^N)$  and  $J \geq 0$ ,
- $J$  is symmetric, *i.e.*  $J(-y) = J(y)$ ,
- there exists a function  $g \in C^0(\mathbf{S}^{N-1})$ ,  $g \geq 0$  such that
$$J(z) = \frac{1}{|z|^{N+1}} g\left(\frac{z}{|z|}\right) \text{ for } |z| \geq 1,$$

# Cell problem

- Cell problem:

$$\lambda = \left( c(y) + L + M_p[v(\tau, \cdot)](y) \right) |p + Dv| \quad (3)$$

where

$$M_p[U](y) = \int dz J(z) \{ E(U(y+z) - U(y) + p \cdot z) - p \cdot z \}.$$

- $\lambda = \overline{H}(L, p).$



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- $\lambda = \overline{H}(L, p).$

# Ergodicity

## Theorem (NF, Imbert, Monneau)

*Under certain assumptions on  $J$  and  $c$ , there exists a unique  $\lambda$  such that there exists a solution  $v$  of (3). Moreover, the oscillation of  $v$  is bounded.*

# Convergence result

## Theorem (NF, Imbert, Monneau)

*Under certain assumptions on  $J$ ,  $c$  and  $u_0$ ,  $u^\varepsilon$  converges to the unique viscosity solution  $u^0$  of*

$$\begin{cases} \frac{\partial u^0}{\partial t} = \overline{H}(\mathcal{I}_1[u^0(\cdot, t)], Du_0) \\ u^0(\cdot, t=0) = u_0 \end{cases} \quad (4)$$

where

$$\mathcal{I}_1[U](x) = \int_{\mathbb{R}^N} \frac{g\left(\frac{z}{|z|}\right)}{|z|^{N+1}} (U(x+z) - U(x) - \nabla_x U(x) \cdot z 1_B(z)) dz$$

# Some works on dislocation density dynamics

- [Groma, Balogh]
- [El Hajj]
- [Ibrahim]
- [Monneau]

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# Qualitative properties

## Theorem (NF, Imbert, Monneau)

We assume that  $N = 1$  and that  $\int c = 0$ . Then we have the following properties:

① If  $c \equiv 0$  then  $\overline{H}(L, p) = L|p|$

②  $L\overline{H}(L, p) \geq 0$ .

③ If  $c \not\equiv 0$  then

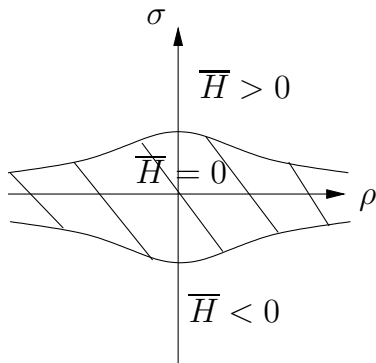
$$\overline{H}(L, p) = 0 \quad \text{for } (L, p) \in B_\delta(0).$$

④  $\overline{H}(L, p) = 0$  if  $L = 0$ .

⑤ For all  $L > 0$ ,

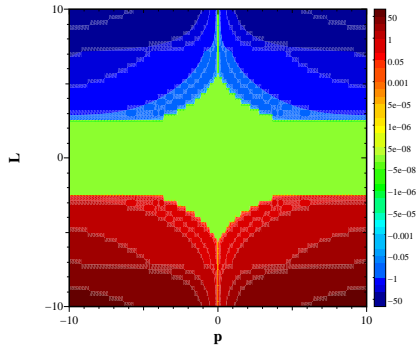
$$\overline{H}(L, p) > 0 \quad \text{for } p \text{ big enough}$$

# Schematic representation of the effective Hamiltonian



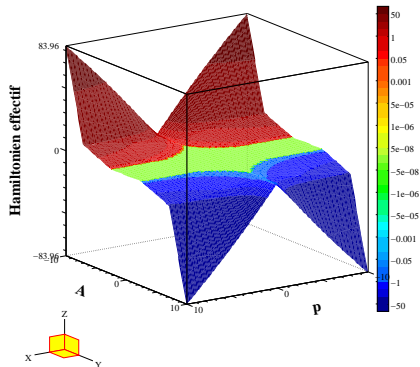
# Simulation of the effective Hamiltonian (Amin Ghorbel)

## Effective hamiltonian

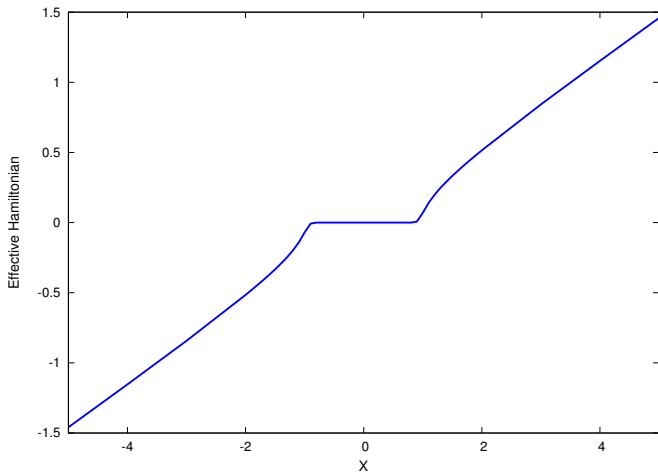




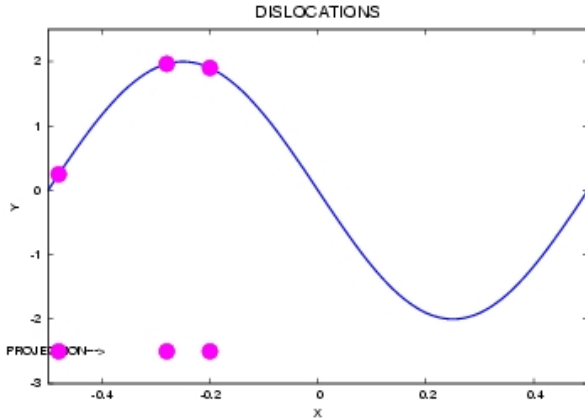
# Simulation of the effective Hamiltonian (Amin Ghorbel)



# Simulation de l'Hamiltonien effectif (Amin Ghorbel)



# Simulation of the dislocation dynamics



# Perspectives

- Homogenization of Frenkel-Kontorova model (joint work with C. Imbert and R. Monneau)
- Homogenization of more realistic models
- Numerical analysis