Homogenization of Frenkel-Kontorova models and dislocation dynamics

Régis Monneau

Paris-Est University, Ecole des Ponts ParisTech, CERMICS

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Plan

1. Physical motivation

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2. Notion of hull function

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3. Homogenization : the hyperbolic rescaling

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4. Homogenization : the parabolic rescaling

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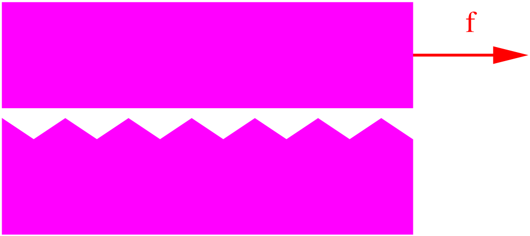
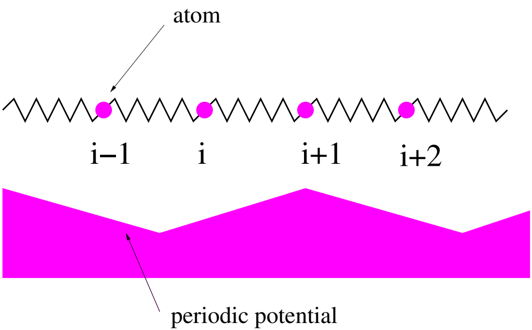
4. Homogenization : the parabolic rescaling
5. Dislocation dynamics

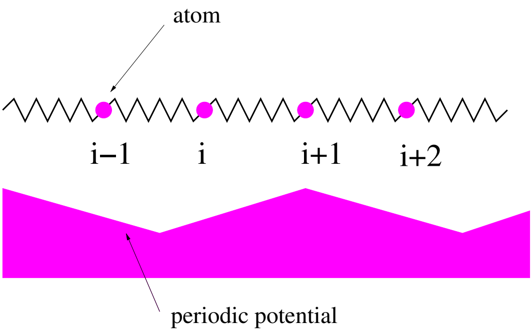
Physical motivation

Interfacial slip




atom
i−1
i
i+1
i+2
periodic potential

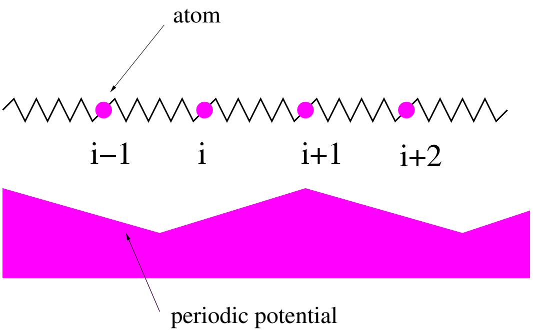
Frenkel-Kontorova model



$$m\frac{d^2U_i}{dt^2} + \gamma\frac{dU_i}{dt} = (U_{i+1} - U_i) + (U_{i-1} - U_i) + \sin(2\pi U_i) + f$$

damping constant

Frenkel-Kontorova model



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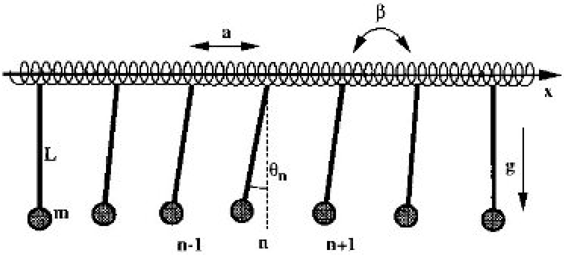
driving force

A mechanical model

Elastically coupled pendulums



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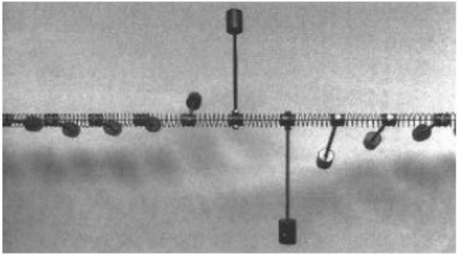

Other applications of the FK model

- propagation of defects in crystals (dislocations)
- adsorbed atomic layers
- magnetic chains
- DNA dynamics
- ...

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Book of [Braun, Kivshar]

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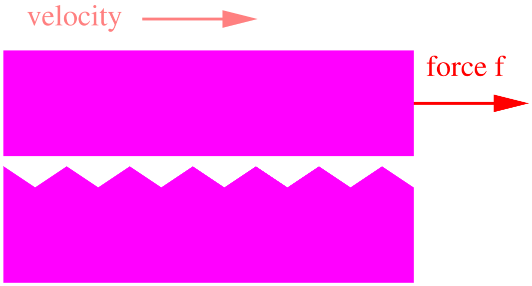
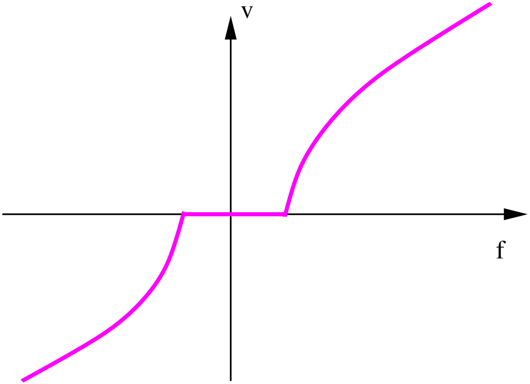
- related problem : traffic

Mean velocity



velocity versus force



Notion of hull function

Notion of hull function
introduced for stationary FK by [Aubry, 1983].

hull function h

$$m\frac{d^2U_i}{dt^2} + \frac{dU_i}{dt} = (U_{i+1} - U_i) + (U_{i-1} - U_i) + \sin(2\pi U_i) + f$$

- Look for particular solutions

$$U_i(t) = h\,(vt + iq)$$

hull function h

$$m\frac{d^2U_i}{dt^2}+\frac{dU_i}{dt}=(U_{i+1}-U_i)+(U_{i-1}-U_i)+\sin(2\pi U_i)+f$$

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$$U_i(t)=h\,(vt+iq)$$

hull funtion $= h$ with $h(z+1)=1+h(z)$

mean velocity $= v$

hull function h

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- Look for particular solutions

$$U_i(t)=h\,(vt+iq)$$

hull funtion $= h$ with $h(z+1)=1+h(z)$

mean velocity $= v$

mean density $= \frac{1}{q}$

$$\frac{U_{i+l}-U_i}{l}\longrightarrow q \quad \text{as} \quad l\to+\infty$$

equation of the hull function h

$$mv^2h''(z) + vh'(z) = h(z+q) + h(z-q) - 2h(z) + \sin(2\pi h(z)) + f$$

Thm 1 (Uniqueness of v), [Forcadel, Imbert, M.]

There exists a critical mass $m_c > 0$ such that for all $0 \leq m < m_c$, there exists a unique v such that there exists a hull function h.

But no uniqueness of the hull function in general.

Example for $m = 0, f = 0, q = 1$

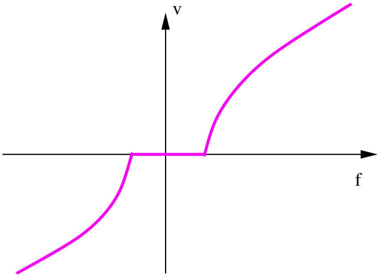
Then $v = 0$ and

$$h_1(z) = \lfloor z \rfloor \quad \text{and} \quad h_2(z) = \frac{1}{2} + \lfloor z \rfloor$$

are two discontinuous hull functions.

Thm 2 [Forcadel, Imbert, M.]

- **(Monotonicity)**
  v is non-decreasing in f
- **(Threshold effect)**
  Moreover if $q = 1$, then there exists $f_c > 0$ such that $v = 0$ for $|f| < f_c$



Construction of the hull function when $m = 0$

With n nearest neighbors (on the left and on the right)

$$\frac{dU_i}{dt} = F(U_{i-n}, ..., U_{i+n})$$

General dynamics

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$$\frac{dU_i}{dt} = F(U_{i-n}, ..., U_{i+n})$$

We assume for $V = (V_{-n}, ..., V_n)$ that F satisfies

1. **(Periodicity + Regularity)**

$$\begin{cases} F(1+V_{-n}, ..., 1+V_n) = F(V) \\ F \quad \text{is Lipschitz-continuous} \end{cases}$$

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$$\frac{\partial F}{\partial V_j} \geq 0 \quad \text{for} \quad 1 \leq |j| \leq n$$

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$\Longrightarrow$ allows to preserve the **ordering of particles** $U_i \leq U_{i+1}$.

Imbedding ODEs into a single PDE

$$\frac{dU_i}{dt} = F(U_{i-n}, ..., U_{i+n})$$

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- The function $u(t,x) = U_{\lfloor x \rfloor}(t)$ is a (discontinuous) viscosity solution of

$$u_t = F([u(t,\cdot)]_n(x)) \quad (1)$$

with

$$[w]_n(x) = (w(x-n), ..., w(x+n))$$

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- We have the comparison principle for equation (1).

Thm 3 (Hull function), [Forcadel, Imbert, M.]

For any $q > 0$, here exists a global solution of (1) on $\mathbb{R} \times \mathbb{R}$

$$u_\infty(t,x) = h(\lambda t + qx)$$

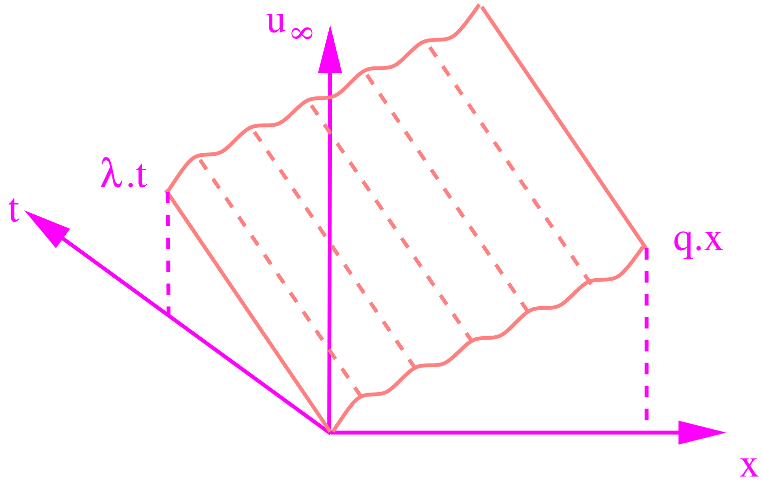
where the hull function satisfies

$$h(z+1) = 1+h(z)$$

Moreover $\lambda =: \bar{F}(q)$ is unique.

λ = generalized velocity

Graph of u_∞



Idea to build h

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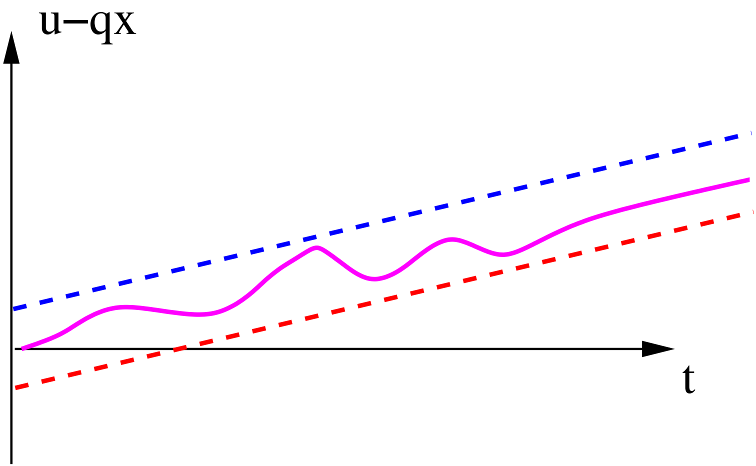
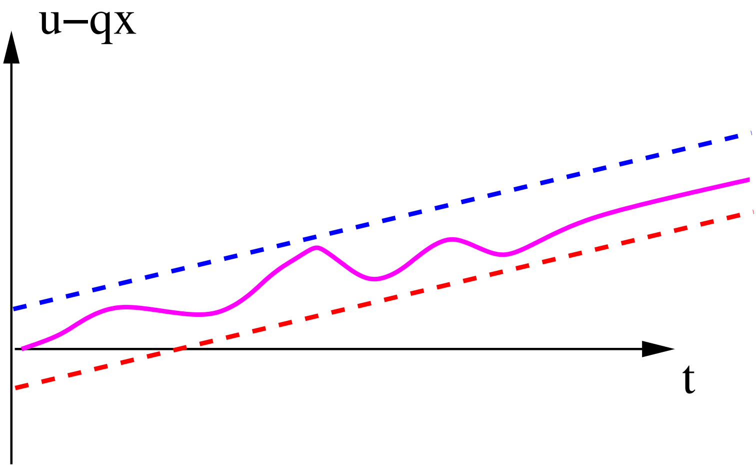
3. **(Like an ODE)**
The solution looks like the solution to an ODE : $u' \simeq F(u)$.

$$\frac{u(t)}{t} \to \lambda \quad \text{as} \quad t \to +\infty$$



(Global control on the solution)

$$|u(t,x) - (\lambda t + qx)| \leq C_2$$



This allows to build a global solution u_∞ which defines the hull function.

Homogenization : the hyperbolic rescaling

Set for $\varepsilon > 0$

$$\begin{cases} u^\varepsilon(t,x) = \varepsilon u\left(\dfrac{t}{\varepsilon}, \dfrac{x}{\varepsilon}\right), \\ u^\varepsilon(0,x) = u_0(x) \end{cases}$$

Homogenization

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Thm 4 (Homogenization), [Forcadel, Imbert, M.]

Under suitable assumptions on u_0, we have $u^\varepsilon \to u^0$ with

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The density of particles $\rho = \dfrac{1}{u^0_x}$ satisfies formally the conservation law

$$\rho_t = (\bar{H}(\rho))_x \quad \text{with} \quad \bar{H}(\rho) = -\rho \bar{F}(1/\rho)$$

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Local ansatz for the proof

$$u^\varepsilon(t,x) \simeq \varepsilon h\left(\frac{u^0(t,x)}{\varepsilon}\right)$$

To prove the homogenization result,
we need to build approximate Lipschitz supersolutions h^δ :

$$\lambda^\delta h_z^\delta(z) \geq F(h^\delta(z-nq), ..., h^\delta(z+nq))$$

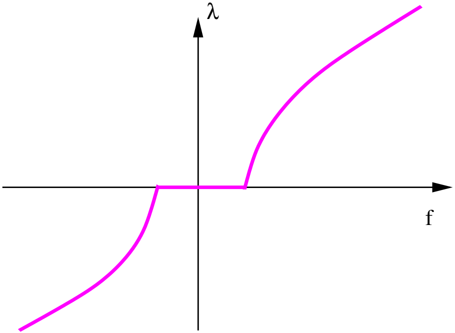
with

$$\begin{cases} \lambda^\delta \to \lambda \\ |h_z^\delta| \leq C/\delta \end{cases}$$

Regularity of the hull function versus plateau for the velocity

F independent on t

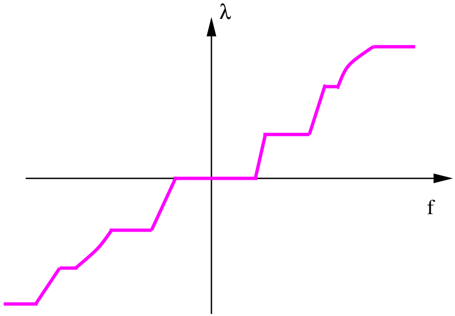
$$\frac{dU_i}{dt} = F(U_{i-n}, ..., U_{i+n}) + f$$



At most one plateau (at the level $\lambda = 0$).

F periodic in t

$$\frac{dU_i}{dt} = F(t, U_{i-n}, ..., U_{i+n}) + f$$



Several plateaux (physical hint in [Braun, Kivshar]),
Partial devil staircase ?

Thm 4 (Continuous hull function / no plateau), [Forcadel, Imbert, M.]

Assume that there exists a continuous hull function for the parameters (q, f_0). Then the map

$$f \mapsto \lambda = \overline{F}(q, f)$$

has no plateau at the level $\lambda_0 = \overline{F}(q, f_0)$.

An example

For

$$\frac{dU_i}{dt} = U_{i+1} + U_{i-1} - 2U_i + \beta \sin(2\pi U_i) + f$$

with

$$U_i(t) = h(\lambda t + iq)$$

(case $f = 0$)

- (Resonance case)
  For $q \in \mathbb{N} \setminus \{0\}$ or $|\beta| > 2$,
  then every hull function is discontinuous
  (and there is a 0-plateau).
- (KAM case ; [..., De La Llave])
  If q is diophantine, then there exists $\beta_0 = \beta_0(q) > 0$
  such that the hull function is analytic for $|\beta| < \beta_0$
  (and there is no 0-plateau).

The case $m > 0$ with acceleration

$$m\frac{d^2U_i}{dt^2} + \frac{dU_i}{dt} = F(t, U_{i-n}, ..., U_{i+n})$$

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- Setting $W_i = U_i + 2m\frac{dU_i}{dt}$, we get

$$\begin{cases} \dfrac{dU_i}{dt} = \dfrac{1}{2m}(W_i - U_i) \\ \\ \dfrac{dW_i}{dt} = \dfrac{1}{2m}(U_i - W_i) + 2F(t, U_{i-n}, ..., U_{i+n}) \end{cases}$$

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Monotone system if m is small enough s.t. for $V = (V_{-n}, ..., V_n)$

$$\frac{1}{2m} + 2\frac{\partial F}{\partial V_0} \geq 0$$

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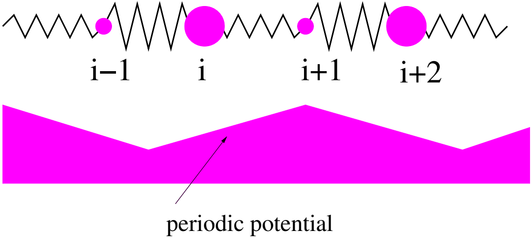
Simplification of an idea of [Baesens, MacKay, 2004].

Case of N types of particles



$$\begin{cases} m\dfrac{d^2U_i}{dt^2} + \dfrac{dU_i}{dt} = \beta_{i+1}(U_{i+1} - U_i) + \beta_i(U_{i-1} - U_i) + \sin(2\pi U_i) + f \\ \beta_1, ..., \beta_N > 0 \quad \text{with} \quad \beta_{i+N} = \beta_i \end{cases}$$

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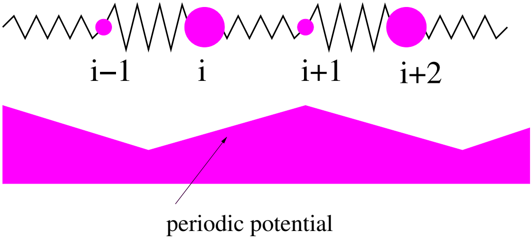

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$\Longrightarrow$ similar homogenization results

Homogenization : the parabolic rescaling

Case $f = 0$

$$\begin{cases} \dfrac{dU_i}{dt} = U_{i+1} + U_{i-1} - 2U_i + \varepsilon^{2(\alpha-1)} \sin(2\pi U_i) \\ \\ U_i(0) = \dfrac{1}{\varepsilon} u_0(i\varepsilon^{\alpha}) \end{cases}$$

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For $\alpha = 1$: hyperbolic rescaling

$$u^\varepsilon(t,x) = \varepsilon U_{\lfloor \frac{x}{\varepsilon} \rfloor}\left(\frac{t}{\varepsilon}\right) \longrightarrow u^0 \quad \text{with} \quad u^0_t = 0 = \bar{F}(u^0_x)$$

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For $\alpha > 2$: parabolic rescaling

$$u^\varepsilon(t,x) := \varepsilon U_{\lfloor \frac{x}{\varepsilon^\alpha} \rfloor} \left(\frac{t}{\varepsilon^{2\alpha}} \right)$$

high density $= \dfrac{1}{\varepsilon^{\alpha-1}(u_0)_x}$

small potential $\simeq$ (density)$^{-2}$

Thm (Diffusive limit), [Alibaud, Briani, M.]

If $\alpha > 2$, under suitable assumptions on u_0, we have $u^\varepsilon \to u^0$ with

$$\begin{cases} u^0_t = G(u^0_x)u^0_{xx} \\ u^0(0,x) = u_0(x) \end{cases}$$

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- Ansatz

$$u^\varepsilon \simeq \varepsilon h\left(\frac{\tilde{u}^\varepsilon}{\varepsilon}, u^0_x\right) \quad \text{with} \quad \tilde{u}^\varepsilon \simeq u^0 + \varepsilon^2 v\left(\frac{u^0}{\varepsilon}\right)$$

h = hull funcion

v = corrector

- Related to the homogenization of (see [Jerrard, 1997])

$$u_t = u_{xx} + \frac{1}{\varepsilon}\sin\left(\frac{2\pi u}{\varepsilon}\right)$$

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$$u_t = u_{xx} + \frac{1}{\varepsilon} \sin\left(\frac{2\pi u}{\varepsilon}\right)$$

- For $\alpha = 2$, new phenomenon from discretness

$$u_t^0 = b(u_x^0) + G(u_x^0) u_{xx}^0$$

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Example : $b \neq 0$ for certain non symmetric equations

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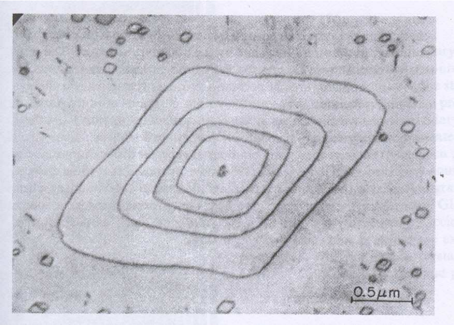
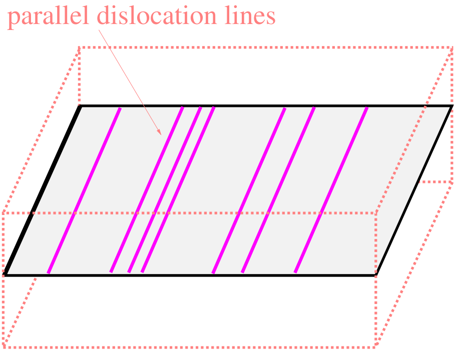
- Case $\alpha = 1$: completely open

Homogenization of dislocation dynamics

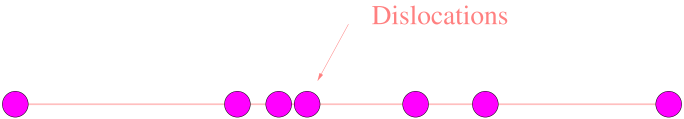
Curved dislocations in a crystal



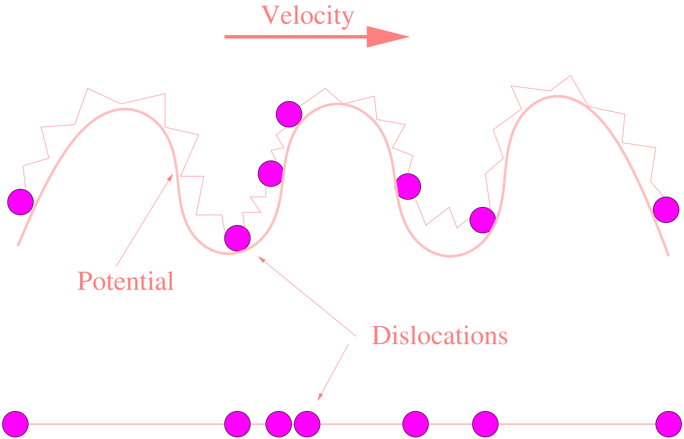
Straight dislocations lines



Points



Dynamics with interactions



The dislocation case

- Formal energy (case $n = +\infty$)

$$E = \sum_i V_0(U_i) + \frac{1}{2} \sum_{i \neq j} V(U_j - U_i)$$

- Gradient flow dynamics (case $m = 0$)

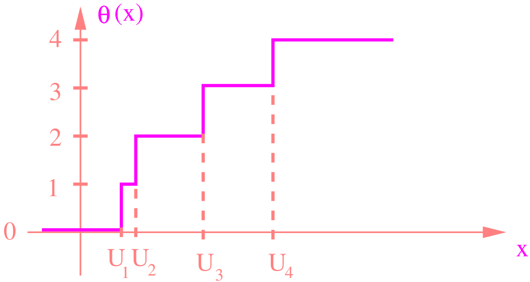
$$\frac{dU_i}{dt} = -\frac{\partial E}{\partial U_i} + f$$

Dislocation dynamics :

- two-body interactions
- $V(x) = -\ln |x|$
- $V_0(x+1) = V_0(x)$

Cumulative distribution

$$\theta(t,x) = \sum_i H(x - U_i(t)) \quad \text{with} \quad H = \text{Heaviside function}$$



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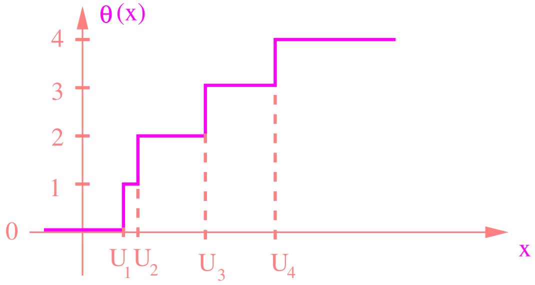
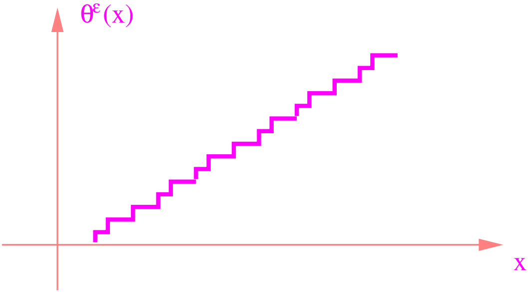


$$\theta_t = |\theta_x| \; c[\theta] \quad \text{with a non-local velocity} \quad c[\theta]$$

Rescaling

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



Thm 5 [Forcadel, Imbert, M.]

Under suitable assumptions, we have $\theta^\varepsilon \longrightarrow \theta^0$ with

$$\theta^0_t = \bar{H}(\theta^0_x, \mathcal{L}\theta^0)$$

with

$$\mathcal{L}w = -(-\Delta)^{\frac{1}{2}}w$$

Thm 5 [Forcadel, Imbert, M.]

Under suitable assumptions, we have $\theta^\varepsilon \longrightarrow \theta^0$ with

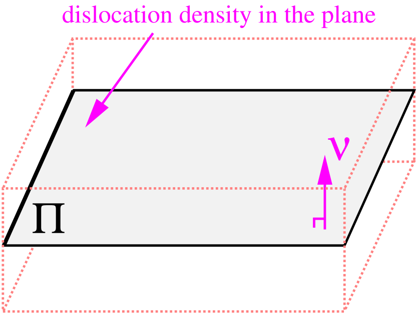
$$\theta^0_t = \bar{H}(\theta^0_x, \mathcal{L}\theta^0)$$

with

$$\mathcal{L}w = P.V.\frac{1}{x^2} \star w$$

$\mathcal{L}\theta^0$ = self-stress created by the dislocation density θ^0_x

Mechanical interpretation



$$\text{div}\, \underline{\underline{\sigma}} = 0 \quad \text{with} \quad [u] = b\theta^0 \quad \text{on} \quad \Pi$$

$\underline{\underline{\sigma}}$: stress, u : displacement, b : Burgers vector

$$\mathcal{L}\theta^0 = \nu \cdot \underline{\underline{\sigma}} \cdot b$$

Mechanical interpretation

$$\begin{cases} \mathcal{L}\theta^0 = \sigma & \text{stress} \\ \\ \theta^0_x = \rho & \text{dislocation density} \end{cases}$$

1. Orowan's law (plastic strain velocity)

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

Mechanical interpretation

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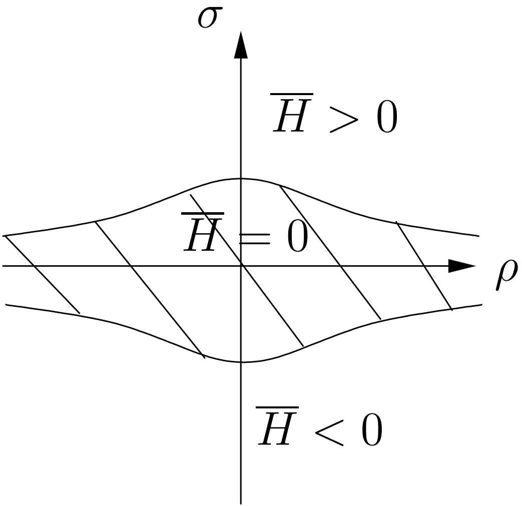
$$\dot{e}_p = \rho\sigma$$

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

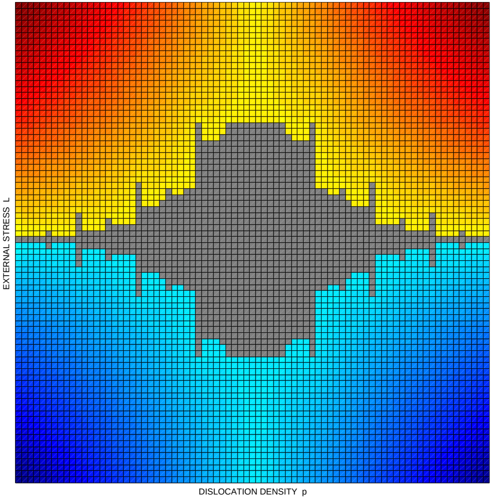
$$\dot{e}_p = C\text{sign}(\sigma)((|\sigma| - \sigma_c)^+)^m$$

3. By homogenization we find

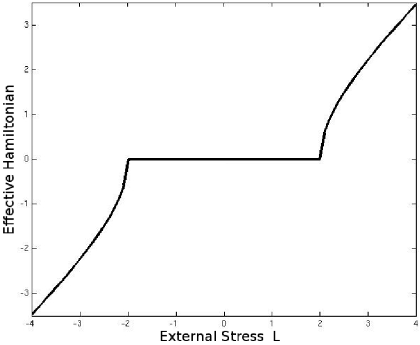
$$\dot{e}_p = \overline{H}(\rho, \sigma)$$


σ
$\overline{H} > 0$
$\overline{H} = 0$
ρ
$\overline{H} < 0$

Computation of $\bar{H}$ (done by S. Cacace)



Computation of $\sigma \mapsto \bar{H}(\rho, \sigma)$



Working on dislocations ...

N. Alibaud (Besançon Univ.)

G. Barles (Tours Univ.)

R. Benguria (Santiago Univ.)

A. Briani (Tours Univ.)

S. Cacace (Roma Univ.)

P. Cardaliaguet (Paris Dauphine Univ.)

E. Carlini (La Sapienza)

A. Chambolle (CMAP)

F. Da Lio (Padova Univ.)

J. Dolbeault (Paris Dauphine Univ.)

A. El Hajj (Compiègne Univ.)

Working on dislocations ...

M. Falcone (Roma Univ.)

A. Fino (Tripoli Univ.)

N. Forcadel (Paris Dauphine Univ.)

A. Ghorbel (Gafsa Univ.)

M. Gonzalez (UPC Barcelona Univ.)

P. Hoch (CEA)

H. Ibrahim (Beyrouth Univ.)

C. Imbert (Paris Dauphine Univ.)

O. Ley (Rennes Univ.)

Y. Le Bouar (ONERA)

S. Patrizi (Austin Univ.)

Thank you !