Dislocations dynamics: from microscopic models to macroscopic crystal plasticity

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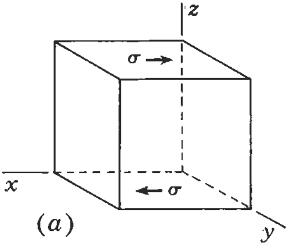
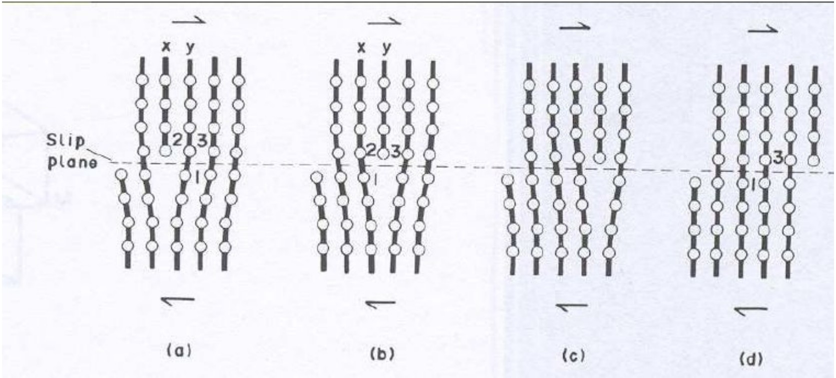
- S. P. and E. Valdinoci, Relaxation times for atom dislocations in crystals, *preprint*
- S. P. and E. Valdinoci, Crystal dislocations with different orientations and collisions, to appear in *Arch. Rational Mech. Anal.*
- S. P. and E. Valdinoci, Homogenization and Orowan's law for anisotropic fractional operators of any order, *Nonlinear Analysis: Theory, Methods and Applications*, Available online 27 August 2014

Dislocations are defect lines in crystalline solids whose motion is directly responsible for the plastic deformation of these materials. Their typical length is of order of $10^{-6}m$ with thickness of order of $10^{-9}m$.

Geometry of an edge dislocation



Motion of a dislocation line



Dislocations can be described at several scales by different models:

1. atomic scale (Frenkel-Kontorova model)
2. microscopic scale (Peierls-Nabarro model)
3. mesoscopic scale (Discrete dislocation dynamics)
4. macroscopic scale (elasto-visco-plasticity with density of dislocations)

Peierls-Nabarro model

$$\Big\Downarrow (\epsilon \to 0)$$

Discrete dislocation dynamics

The Peierls-Nabarro model

We consider a straight dislocation line parallel to e_3.

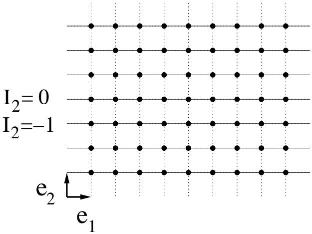


Figure 1: Perfect crystal

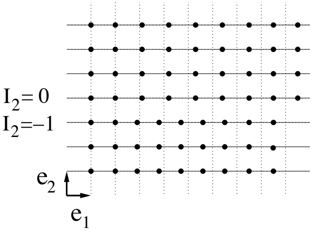


Figure 2: Schematic view of a edge dislocation in the crystal

Assumptions

- the dislocation defects are described by the mismatch between the two planes $I_2 = 0$ and $I_2 = -1$
- the displacement of the crystal is antysimmetric wrt the plane $e_1 e_3$
- any atoms move only in the direction e_1
- the displacement is independent of e_3

The Peierls-Nabarro model

The P-N model is a *continuous* model where a dislocation is described by means of a scalar phase field defined over the slip plane.

The medium will be $\mathbb{R}^2$, endowed with coordinates (x, y).

The disregistry of the upper half crystal $\{y > 0\}$ relative to the lower half $\{y < 0\}$ is given by $v(x)$, which is a transition between 0 and 1:

$$\begin{cases} v(-\infty) = 0, \quad v(+\infty) = 1 \\ v' > 0. \end{cases}$$

The total energy is given by

$$\mathcal{E} = \underbrace{\frac{1}{2}\int_{(\mathbb{R}^2)^+} |\nabla V(x,y)|^2 dxdy}_{\text{elastic energy}} + \underbrace{\int_{\mathbb{R}} W(V(x,0))dx}_{\text{misfit energy}}$$

where $V : (\mathbb{R}^2)^+ \to \mathbb{R}$ represents (twice) the (scalar) displacement and it is such that

$$V(x,0) = v(x).$$

The potential W satisfies

- $W(u+1) = W(u) \quad \forall u \in \mathbb{R}$ (periodicity)
- $W(\mathbb{Z}) = 0 < W(u) \quad \forall u \in \mathbb{R} \setminus \mathbb{Z}$ (minimum property)

The Peierls-Nabarro model

A critical point of the energy satisfies

$$\begin{cases} \Delta V(x,y) = 0 & (x,y) \in (\mathbb{R}^2)^+ \\ \partial_y V(x,0) = W'(V(x,0)) & x \in \mathbb{R} \end{cases}$$

The Peierls-Nabarro model

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$$\begin{cases} \Delta V(x,y) = 0 & (x,y) \in (\mathbb{R}^2)^+ \\ \partial_y V(x,0) = W'(V(x,0)) & x \in \mathbb{R} \end{cases}$$

The system can be rewritten for

$$v(x) = V(x,0)$$

as follows

$$-(-\Delta)^{\frac{1}{2}} v = W'(v) \quad \text{in } \mathbb{R}$$

where

$$(-\Delta)^{\frac{1}{2}} v = \mathcal{F}^{-1}(|\xi| v) \quad \text{for any } v \in S(\mathbb{R}^n)$$

and $\mathcal{F}$ is the Fourier transform.

The Peierls-Nabarro model

The phase transition v therefore satisfies

$$\begin{cases} -(-\Delta)^{\frac{1}{2}} v = W'(v) \quad \text{in } \mathbb{R} \\ v' > 0 \\ v(-\infty) = 0, \quad v(+\infty) = 1, \quad v(0) = \frac{1}{2} \end{cases}$$

The Peierls-Nabarro model

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In the original PN model:

$$W(v) = \frac{1}{4\pi^2}(1 - \cos(2\pi v))$$

and

$$v(x) = \frac{1}{2} + \frac{1}{\pi}\arctan(2x)$$

The Peierls-Nabarro model

More in general, we consider the layer function v solution of, for $s \in (0,1)$

$$\begin{cases} -(-\Delta)^s v = W'(v) & \text{in } \mathbb{R} \\ v' > 0 \\ v(-\infty) = 0, \quad v(+\infty) = 1, \quad v(0) = \frac{1}{2} \end{cases} \tag{1}$$

where for $\varphi \in C^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$

$$\mathcal{I}_s[\varphi](x) := -(-\Delta)^s \varphi(x) = c(n,s)\, PV \int_{\mathbb{R}^n} \frac{\varphi(x+y) - \varphi(x)}{|y|^{n+2s}} dy.$$

The Peierls-Nabarro model

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Under additional assumptions on the potential W, the *existence of a unique solution* of (1) was proven by Cabré-Sire and Palatucci-Savin-Valdinoci

Asymptotic estimates have been proved by Dipierro, Figalli, Monneau, Palatucci, Savin, Valdinoci in different papers.

We consider the evolutive version of the PN model:

$$\partial_t v = \mathcal{I}_s v - W'(v) + \sigma_\epsilon(t,x) \quad \text{in } \mathbb{R} \times \mathbb{R}^+$$

where

$$\sigma_\epsilon(t,x) = \epsilon^{2s}\sigma(\epsilon^{2s+1}t, \epsilon x)$$

is an exterior stress acting on the material and ϵ is a small positive parameter. Then we consider the following rescaling:

$$v_\epsilon(t,x) := v\left(\frac{t}{\epsilon^{1+2s}}, \frac{x}{\epsilon}\right)$$

and we look at the equation satisfied by the rescaled function v_ϵ

$$(PN)_\epsilon \begin{cases} (v_\epsilon)_t = \frac{1}{\epsilon}\left(\mathcal{I}_s v_\epsilon - \frac{1}{\epsilon^{2s}} W'(v_\epsilon) + \sigma(t,x)\right) & \text{in } (0,+\infty)\times\mathbb{R} \\ v_\epsilon(0,\cdot) = v_\epsilon^0 & \text{on } \mathbb{R}, \end{cases}$$

On W and σ we assume:

$$\begin{cases} W \in C^{3,\alpha}(\mathbb{R}) & \text{for some } 0<\alpha<1 \\ W(v+1) = W(v) & \text{for any } v\in\mathbb{R} \\ W = 0 \text{ on } \mathbb{Z}, \quad W>0 \text{ on } \mathbb{R}\setminus\mathbb{Z} \\ W''(0) > 0. \end{cases}$$

$$\begin{cases} \sigma \in BUC([0,+\infty)\times\mathbb{R}) \\ \|\sigma_x\|_{L^\infty([0,+\infty)\times\mathbb{R})} + \|\sigma_t\|_{L^\infty([0,+\infty)\times\mathbb{R})} \le M \\ |\sigma_x(t,x+h) - \sigma_x(t,x)| \le M|h|^\alpha, \quad x,h\in\mathbb{R}, t>0\ \alpha\in(s,1). \end{cases}$$

Let v be the layer solution.

Definition

Given $x_0 \in \mathbb{R}$, we say that the function

$$v\left(\frac{x - x_0}{\epsilon}\right)$$

is a transition layer centered at x_0 and positively oriented and

$$v\left(\frac{x_0 - x}{\epsilon}\right) - 1$$

is a transition layer centered at x_0 and negatively oriented.

From PN to DDD

We consider as initial condition the state obtained by superposing N copies of the transition layer, centered at $x_1^0, ..., x_N^0$, $N - K$ of them positively oriented and the remaining K negatively oriented, that is

$$v_\epsilon^0(x) = \frac{\epsilon^{2s}}{\beta}\sigma(0, x) + \sum_{i=1}^{N} v\left(\zeta_i \frac{x - x_i^0}{\epsilon}\right) - K,$$

where $\zeta_1, ..., \zeta_N \in \{-1, 1\}$, $\sum_{i=1}^{N}(\zeta_i)^- = K$, $0 \leq K \leq N$ and

$$\beta := W''(0) > 0.$$

Let us introduce the solution $(x_i(t))_{i=1,\ldots,N}$ to the system

$$(DDD)\begin{cases}\dot{x}_i = \gamma\left(\sum_{j\neq i}\zeta_i\zeta_j\frac{x_i - x_j}{2s|x_i - x_j|^{1+2s}} - \zeta_i\sigma(t,x_i)\right) & \text{in } (0,T_c)\\ x_i(0) = x_i^0, \end{cases}$$

where $\gamma := 1/\int_{\mathbb{R}}(v'(x))^2 dx$,

From PN to DDD

Let us introduce the solution $(x_i(t))_{i=1,...,N}$ to the system

$$(DDD) \begin{cases} \dot{x}_i = \gamma \left(\sum_{j \neq i} \zeta_i \zeta_j \frac{x_i - x_j}{2s|x_i - x_j|^{1+2s}} - \zeta_i \sigma(t, x_i) \right) & \text{in } (0, T_c) \\ x_i(0) = x_i^0, \end{cases}$$

where $\gamma := 1/\int_{\mathbb{R}} (v'(x))^2 dx$,

$0 < T_c \leq +\infty$ is the first time when a collision between two particles occurs:

$$x_i(t) < x_{i+i}(t), \text{ for any } t \in [0, T_c) \text{ and any } i$$

$$\exists\ i_0 \text{ such that } x_{i_0}(T_c) = x_{i_0+1}(T_c)$$

From PN to DDD

Theorem (S. P., E. Valdinoci)

Let

$$v_0(t,x) = \sum_{i=1}^{N} H(\zeta_i(x - x_i(t))) - K,$$

where H is the Heaviside function and $(x_i(t))_{i=1,\dots,N}$ *is the solution to (DDD).*
Then, for every $\epsilon > 0$ *there exists a unique solution* v_ϵ *to* $(PN)_\epsilon$*.*
Furthermore, as $\epsilon \to 0^+$

$$\limsup_{\substack{(t',x')\to(t,x)\\ \epsilon\to 0^+}} v_\epsilon(t',x') \le (v_0)^*(t,x)$$

$$\liminf_{\substack{(t',x')\to(t,x)\\ \epsilon\to 0^+}} v_\epsilon(t',x') \ge (v_0)_*(t,x),$$

for any $(t,x) \in [0, T_c) \times \mathbb{R}$*.*

The case $K = 0$, i.e., the case in which the dislocations have *all the same orientation* and therefore

$$T_c = +\infty,$$

was already studied by:

- Gonzales, Monneau: $s = \frac{1}{2}$
- Dipierro, Palatucci, Valdinoci: $s \in \left(\frac{1}{2}, 1\right)$
- Dipierro, Figalli, Valdinoci: $s \in \left(0, \frac{1}{2}\right)$

We have (optimal) estimates for T_c in the following situations:

- 2 particles (+-):
  - $T_c < +\infty$ if either $\sigma \leq 0$ or $\theta_0 < \left(\frac{1}{2s\|\sigma\|_\infty}\right)^{\frac{1}{2s}}$

$$T_c \leq \frac{s\theta_0^{1+2s}}{(2s+1)\gamma(1-2s\theta_0^{2s}\|\sigma\|_\infty)}$$

  - if $\theta_0 \geq \left(\frac{1}{2s\|\sigma\|_\infty}\right)^{\frac{1}{2s}}$ it may happen that $T_c = +\infty$.
- 3 particles (+-+)
- N alternates particles
- N particles, two of which sufficiently close each other

What happens for $t \geq T_c$?

What happens for $t \geq T_c$?

Suppose that there are two particles with different orientation and that a collision occurs at a time $0 < T_c < +\infty$, and

$$x_1(T_c) = x_2(T_c) = x_c$$

Theorem

Assume $N = 2$ and $K = 1$. Let v_ϵ be the solution to $(PN)_\epsilon$, then

$$\lim_{t \to T_c^-} \lim_{\epsilon \to 0^+} v_\epsilon(t, x) = 0 \quad \textit{for any } x \neq x_c$$

$$\limsup_{\substack{t \to T_c^- \\ \epsilon \to 0^+}} v_\epsilon(t, x_c) \geq 1.$$

From PN to DDD

Theorem (S. P., E. Valdinoci)

Assume $N = 2$ *and* $K = 1$ *and let* v_ϵ *the solution of* $(PN)_\epsilon$*. Then there exists* $\epsilon_0 > 0$ *such that for any* $\epsilon < \epsilon_0$ *there exist* $T_\epsilon,\ \varrho_\epsilon > 0$ *such that*

$$T_\epsilon = T_c + o(1), \quad \varrho_\epsilon = o(1) \quad \text{as } \epsilon \to 0,$$

$$v_\epsilon(T_\epsilon, x) \le \varrho_\epsilon \quad \text{for any } x \in \mathbb{R}.$$

From PN to DDD

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$$v_\epsilon(T_\epsilon, x) \leq \varrho_\epsilon \quad \text{for any } x \in \mathbb{R}.$$

Theorem (S. P., E. Valdinoci)

Assume in addition $\sigma \equiv 0$*. Then there exist* $\epsilon_0 > 0$ *and* $c > 0$ *such that for any* $\epsilon < \epsilon_0$ *we have*

$$|v_\epsilon(t, x)| \leq \varrho_\epsilon e^{c\frac{T_\epsilon - t}{\epsilon^{2s+1}}}, \quad \text{for any } x \in \mathbb{R} \text{ and } t \geq T_\epsilon.$$

From PN to DDD

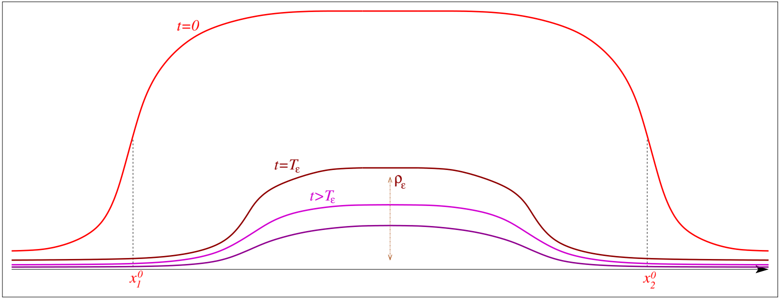

Figure 1: Evolution of the dislocation function in case of two particles.

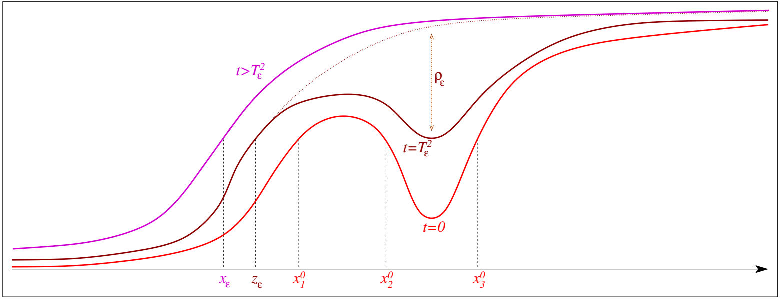

Figure 2: Evolution of the dislocation function in case of three particles.

Peierls-Nabarro model

$$\Big\Downarrow (\epsilon \to 0)$$

Dislocation density model

From PN to DDD

Let us go back to the evolutive PN model in dimension n:

$$\partial_t u = \mathcal{I}_1[u(t,\cdot)] - W'(u) + \sigma(t,x) \quad \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n$$

where for $\varphi \in C^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$

$$\mathcal{I}_1[\varphi](x) := PV \int_{\mathbb{R}^N} (\varphi(x+z) - \varphi(x)) \frac{1}{|z|^{n+1}} g\left(\frac{z}{|z|}\right) dz.$$

We assume:

- $g \in C(\mathbf{S}^{n-1})$, $g > 0$, g even;
- $W \in C^{1,1}(\mathbb{R})$ and $W(v+1) = W(v)$ for any $v \in \mathbb{R}$;
- $\sigma \in C^{0,1}(\mathbb{R}^+ \times \mathbb{R}^n)$ and $\sigma(t+1,x) = \sigma(t,x)$, $\sigma(t,x+k) = \sigma(t,x)$ for any $k \in \mathbb{Z}^n$ and $(t,x) \in \mathbb{R}^+ \times \mathbb{R}^n$.

$$\partial_t u = \mathcal{I}_1[u(t,\cdot)] - W'(u) + \sigma(t,x) \quad \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n$$

We consider the following initial condition: for $\epsilon > 0$

$$u(0,x) = \frac{1}{\epsilon} u_0(\epsilon x) \quad \text{on } \mathbb{R}^n,$$

where $u_0 \in W^{2,\infty}(\mathbb{R}^n)$.

The parameter ϵ takes into account the fact that the number of dislocations is increasing of order $1/\epsilon$.

$$\partial_t u = \mathcal{I}_1[u(t,\cdot)] - W'(u) + \sigma(t,x) \quad \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n$$

We consider the following initial condition: for $\epsilon > 0$

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where $u_0 \in W^{2,\infty}(\mathbb{R}^n)$.

The parameter ϵ takes into account the fact that the number of dislocations is increasing of order $1/\epsilon$.

We want to identify at large scale an evolution model for the dynamics of a density of dislocations (DD)

$$\begin{cases} \partial_t u = \mathcal{I}_1[u(t,\cdot)] - W'(u) + \sigma(t,x) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n \\ u(0,x) = \frac{1}{\epsilon} u_0(\epsilon x) & \text{on } \mathbb{R}^n \end{cases}$$

$$\Downarrow$$

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

$$\Downarrow$$

Homogenization problem:

$$\begin{cases} \partial_t u^\epsilon = \mathcal{I}_1[u^\epsilon(t,\cdot)] - W'\left(\frac{u^\epsilon}{\epsilon}\right) + \sigma\left(\frac{t}{\epsilon}, \frac{x}{\epsilon}\right) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n \\ u^\epsilon(0,x) = u_0(x) & \text{on} \quad \mathbb{R}^n \end{cases}$$

Theorem (R. Monneau, S. P.)

The solution u^ϵ converges towards the solution u^0 of the following homogenized problem:

$$\begin{cases} \partial_t u = \overline{H}(\nabla u, \mathcal{I}_1[u(t,\cdot)]) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n \\ u(0,x) = u_0(x) & \text{on} \quad \mathbb{R}^n, \end{cases}$$

locally uniformly in (t,x), for some effective Hamiltonian $\overline{H}$ such that

- *for any $(p,L) \in \mathbb{R}^n \times \mathbb{R}$, $\overline{H}(p,L)$ is defined through the so called cell-problem;*
- *$\overline{H} : R^n \times \mathbb{R} \to \mathbb{R}$ is continuous;*
- *$\overline{H}(p,\cdot)$ is non-decreasing for any $p \in \mathbb{R}^n$.*

Mechanical interpretation of the homogenization result: the homogenized equation

$$\begin{cases} \partial_t u = \overline{H}(\nabla u, \mathcal{I}_1[u(t,\cdot)]) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^N \\ u(0,x) = u_0(x) & \text{on} \quad \mathbb{R}^N, \end{cases}$$

can be interpreted as the plastic flow rule in a model for macroscopic crystal plasticity. In the equation:

- u^0 is the plastic strain;
- $\partial_t u^0$ is the plastic strain velocity;
- ∇u^0 is the dislocation density;
- $\mathcal{I}_1[u^0]$ is the internal stress created by the density of dislocations contained in a slip plane.

Assume:

- $n = 1$
- $\sigma \equiv 0$
- $\mathcal{I}_1 = -(-\Delta)^{\frac{1}{2}}$
- $W \in C^{4,\beta}(\mathbb{R})$, $0 < \beta < 1$; $W(v+1) = W(v)$, $\forall v \in \mathbb{R}$; $W > 0$ on $\mathbb{R} \setminus \mathbb{Z}$; $W''(0) > 0$.

Orowan's law:

$$\overline{H}(p, L) \sim c_0 |p| L$$

for small p and L, where $c_0 > 0$

Theorem (R. Monneau, S. P.)

Let $p_0,\ L_0 \in \mathbb{R}$. Then there exists $c_0 > 0$ such that

$$\frac{\overline{H}(\delta p_0, \delta L_0)}{\delta^2} \to c_0 |p_0| L_0 \quad \text{as } \delta \to 0^+.$$

For $s > \frac{1}{2}$:

$$\begin{cases} \partial_t u^\epsilon = \epsilon^{2s-1}\mathcal{I}_s[u^\epsilon(t,\cdot)] - W'\left(\frac{u^\epsilon}{\epsilon}\right) + \sigma\left(\frac{t}{\epsilon}, \frac{x}{\epsilon}\right) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n \\ u^\epsilon(0,x) = u_0(x) & \text{on} \quad \mathbb{R}^n. \end{cases}$$

For $s < \frac{1}{2}$:

$$\begin{cases} \partial_t u^\epsilon = \mathcal{I}_s[u^\epsilon(t,\cdot)] - W'\left(\frac{u^\epsilon}{\epsilon^{2s}}\right) + \sigma\left(\frac{t}{\epsilon^{2s}}, \frac{x}{\epsilon}\right) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^n \\ u^\epsilon(0,x) = u_0(x) & \text{on} \quad \mathbb{R}^n. \end{cases}$$

From PN to DD

Theorem (S.P., E. Valdinoci)

- *For $s > \frac{1}{2}$, $u^\epsilon \to u^0$ converges locally uniformly in (t,x) towards the solution u^0 of*

$$\begin{cases} \partial_t u = \overline{H}_1(\nabla_x u) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^N \\ u(0,x) = u_0(x) & \text{on} \quad \mathbb{R}^N, \end{cases}$$

- *For $s < \frac{1}{2}$, the solution u^ϵ converges locally uniformly in (t,x) towards the solution u^0 of*

$$\begin{cases} \partial_t u = \overline{H}_2(\mathcal{I}_1[u]) & \text{in} \quad \mathbb{R}^+ \times \mathbb{R}^N \\ u(0,x) = u_0(x) & \text{on} \quad \mathbb{R}^N, \end{cases}$$

where the effective Hamiltonians $\overline{H}_1(p)$and $\overline{H}_2(L)$ are defined through a cell-problem.

From PN to DD

Assume:

- $n = 1$
- $\sigma \equiv 0$
- $\mathcal{I}_s = -(-\Delta)^s$
- $W \in C^{4,\beta}(\mathbb{R})$, $0 < \beta < 1$; $W(v+1) = W(v)$, $\forall v \in \mathbb{R}$; $W > 0$ on $\mathbb{R} \setminus \mathbb{Z}$; $W''(0) > 0$.

Theorem (S.P., E. Valdinoci)

Let $p_0, L_0 \in \mathbb{R}$ with $p_0 \neq 0$. Then there exists $c_0 > 0$ such that

$$\frac{\overline{H}(\delta p_0, \delta^{2s} L_0)}{\delta^{1+2s}} \to c_0 |p_0| L_0 \quad \text{as } \delta \to 0^+.$$