Viscosity solutions for particle systems and homogenization of dislocation dynamics

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Abstract

In this paper, we give a review of recent results about the homogenization of particle systems with applications to Frenkel-Kontorova models and dislocation dynamics of curves. We underline the main ideas which allow us to extend the nonlinear homogenization methods for viscosity solutions, to the present framework of particles in interactions, or moving fronts in interactions.

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1 Introduction

In this paper we are interested in the homogenization of dislocation dynamics. Dislocations are defects in crystals, that can move in the material when they are submitted to a shear stress. In this introduction we will explain how we can modelize the dynamics of those defects by the evolution of particle systems in dimension 1. We will moreover give a first homogenization result in this framework, for nearest neighbors interactions between particles. The limit equation is identified as a Hamilton-Jacobi equation. In Section 2, we will introduce more material, like the notion of hull function, and the Ansatz to explain the main ideas which allow to justify the homogenization. In Section 3, for the case of two-body interactions, we will introduce the notion of cumulative distribution function. In this case, the effective equation is a non-local Hamilton-Jacobi equation, involving a half-Laplacian which is related to the long range interaction forces which behave like $1/x$.

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A suitable notion of viscosity solution will be given and the notion of correctors will be presented. Qualitative properties of the effective Hamiltonian will be also given. Finally, in Section 4, we will introduce the modelling for the dynamics of dislocation curves, and we will also provide a homogenization result. Detailed proofs of the results presented in this paper can be found in [6, 7].

1.1 Modelling of dislocation dynamics by particle systems

Dislocations are curves defects in crystals that can move inside crystallographic planes of the material. In the simplest case, we can assume that theses curves are parallel straight lines (along the direction e_2) all moving in the same plane of basis (e_1, e_2). For this special geometry, the i-th line can be described by its first coordinate (along the direction e_1) that we denote by the real number U_i. We also assume that these positions of the dislocations are ordered, i.e. satisfy for all $i \in \mathbb{Z}$

$$U_i < U_{i+1}.$$

In particular, there is no "shock" between two particles. The typical evolution of the position U_i of the dislocation is given by the overdamped dynamics:

$$m_0 \frac{d^2 U_i}{d\tau^2} + k \frac{dU_i}{d\tau} = f_i, \quad i \in \mathbb{Z},$$

where τ is the time variable, $m_0 \geq 0$ is the effective mass of the dislocation, and $k > 0$ is the damping factor. Here f_i is the effective force acting on the i-th dislocation. We assume that the force f_i has two main contributions:

$$f_i = f_i^{per} + f_i^{int},$$

where f_i^{int} is the force created by the interaction between the i-th dislocation and its m nearest neighbors (m on the left and m on the right). This means that we can write this contribution as

$$f_i^{int} = - \sum_{j \in \{-m,...,m\} \setminus \{0\}} V'(U_i - U_{i+j}),$$

where V is the potential of pair interactions. On the one hand, the case $m = 1$ is the simplest case and corresponds to the interactions with the first nearest neighbors. On the other hand, the case $m = +\infty$ corresponds to considering all two-body interactions between dislocations. The other contribution f_i^{per} describes the interaction of the i-th dislocation with the other fixed defects of the crystal (like for instance fixed dislocations). To simplify the analysis, we simply assume that f_i^{per} is 1-periodic, and write it as

$$f_i^{per} = f - V_0'(U_i),$$

where V_0 is a 1-periodic potential and f is a constant effective force acting on the dislocation, that can be interpreted as the applied resolved shear stress in the material.

Our main goal is to describe the behaviour at large scales of this infinite system of particles, i.e. to perform the homogenization of this system. Even if under suitable assumptions, the homogenization can be done when the effective mass m_0 is small enough (see [8]), we will restrict our presentation to the case where $m_0 = 0$, i.e. the *fully overdamped dynamics*. Without loss of generality, we can take the damping factor $k = 1$, and we have

$$\begin{cases} \dfrac{dU_i}{d\tau} = F(U_{i-m}, ..., U_{i+m}), \quad i \in Z\,, \\[2mm] \text{with} \quad F(U_{i-m}, ..., U_{i+m}) = f - V_0'(U_i) - \displaystyle\sum_{j \in \{-m,...,m\}\setminus\{0\}} V'(U_i - U_{i+j})\,. \end{cases} \quad (1.1)$$

1.2 First assumptions and first homogenization result

Dislocation dynamics is described by this system for $m = +\infty$ and the special two-body interaction $V(x) = -\ln|x|$ (see Subsection 3.7 for the results in this case).

Nevertheless, we can study systems (1.1) for general m and potentials V, which describe the evolution of general systems of particles. In particular, when m is finite, observe that because of the ordering of the particles ($U_i < U_{i+1}$), the natural domain of definition of F is

$$\mathcal{D} = \left\{ (\overline{U}_{-m}, ..., \overline{U}_m) \in \mathbb{R}^{2m+1}, \quad \overline{U}_{-m} < \overline{U}_{-m+1} < \cdots < \overline{U}_m \right\}\,.$$

We then make the following basic assumptions:

(A) Assumptions on the potentials V_0 and V:

    $i)$**(Periodicity)** $V_0 \in C^2(\mathbb{R})$ and $V_0(x+1) = V_0(x)$,

    $ii)$**(Convexity)** V is convex on $[0, +\infty)$ and V is convex on $(-\infty, 0]$,

    $iii)$**(Regularity)** V'' is bounded on $(0, +\infty)$ and on $(-\infty, 0)\,.$

Let us make a few comments on these assumptions. In assumption Aii), the convexity of the potential implies on $\mathcal{D}$ that

$$F(\overline{U}_{-m}, ..., \overline{U}_m) \quad \text{is non-decreasing in each} \quad \overline{U}_i \quad \text{for} \quad 1 \leq |i| \leq m\,. \quad (1.2)$$

This property is essential to ensure a comparison principle for the system (1.1) and in particular to preserve the ordering of the particles. Remark also that condition Aii) allows the potential to be Lipschitz continuous but non convex at the origin.

The regularity of the potentials V_0 and V given respectively in assumptions Ai) and Aiii) are sufficient to ensure that the function F defined in (1.1) is globally Lipschitz continuous on $\mathcal{D}$.

A typical example of such a system is the classical Frenkel-Kontorova model (FK) with

$$m = 1, \quad V(x) = \frac{1}{2}x^2, \quad V_0(x) = \sin(2\pi x).$$

In this model, each particle U_i can be interpreted as the position of an atom, and this model has been used for instance to describe qualitatively the dynamics of a single dislocation in a lattice of atoms (see [10]). This model can also describe the friction between two materials. Indeed, this model was originally introduced in Kontorova, Frenkel [10] to describe the plasticity at a microscopic level. Such a model is sketched on figure 1.
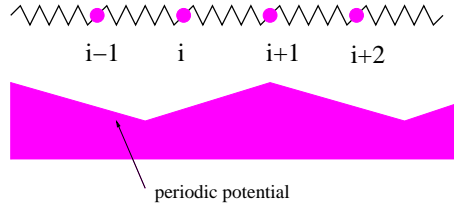

Figure 1: Sketch of the chain of particles for the classical FK model

In order to make precise the initial position of the particles, let us consider a Lipschitz continuous function $u_0(x)$ which satisfies the following assumption:

(I0) **Initial gradient bounded from above and below**

$$0 < 1/K_0 \leq (u_0)_x \leq K_0 \quad \text{on} \quad \mathbb{R},$$

for some fixed $K_0 > 0$. Let us now assume that

$$U_i(0) = \varepsilon^{-1} u_0(i\varepsilon),$$

with $\varepsilon > 0$.

It is then natural to ask what is the macroscopic behaviour of the solution $U = (U_i)_{i\in\mathbb{Z}}$ as ε goes to zero. To this end we define the following function which describes the rescaled positions of the particles

$$\overline{u}^\varepsilon(t,x) = \varepsilon U_{\lfloor \varepsilon^{-1}x \rfloor}(\varepsilon^{-1}t) \tag{1.3}$$

where $\lfloor \cdot \rfloor$ denotes the floor integer part and where the particles satisfy the following system of ODE's

$$\frac{dU_i}{d\tau} = U_{i+1} + U_{i-1} - 2U_i - 2\pi \cos(2\pi U_i), \quad i \in \mathbb{Z}.$$

4

In the limit $\varepsilon = 0$, we will see that the effective equation is the following Hamilton-Jacobi equation

$$\begin{cases} u_t^0 = \overline{F}(u_x^0) & \text{for} \quad (t,x) \in (0,+\infty) \times \mathbb{R}, \\[2mm] u^0(0,x) = u_0(x) & \text{for} \quad x \in \mathbb{R}, \end{cases} \tag{1.4}$$

where the function $\overline{F}$ will be identified later on.

More precisely, we have the following homogenization result:

Theorem 1.1. (Homogenization with m nearest neighbors interactions)
Under assumption (I0)-(A), there exists a continuous function $\overline{F} : \mathbb{R} \to \mathbb{R}$, such that the function $\overline{u}^\varepsilon$ converges uniformly on compact sets of $[0,+\infty) \times \mathbb{R}$ to the unique viscosity solution u^0 of (1.4).

2 Homogenization in the case of the m nearest neighbors interactions

One important remark is that we can imbed the ODE system (1.1) into a single PDE. To this end, for a given function $v(y)$ with $y \in \mathbb{R}$, we define

$$[v]_m(y) = (v(y-m), v(y-m+1), ..., v(y+m)).$$

Then we can look for solutions $u(\tau,y)$ to the following "finite differences-like" PDE

$$u_\tau = F([u(\tau,\cdot)]_m) \quad \text{for} \quad (\tau,y) \in (0,+\infty) \times \mathbb{R}. \tag{2.1}$$

In the present paper, we work with viscosity solutions, which are possibly discontinuous (see for instance [5] for a general introduction to the viscosity solution theory).

We see in particular that $U_i(\tau) = u(\tau,i)$ for $i \in \mathbb{Z}$. Then equation (2.1) can be interpreted as the evolution of a family of systems of ODE's indexed by a parameter $a \in [0,1)$. This parameter is the fractional part of the general coordinate $y = i + a$.

2.1 Effective Hamiltonian and notion of hull function

To study the solutions of (2.1), it is classical to introduce the so-called *hull function*, i.e. a function $h(z)$ such that $u(\tau,y) = h(py + \lambda\tau)$ is a solution of (2.1). We refer for instance to the pioneering work of Aubry [1], and Aubry, Le Daeron [2], where, in particular, they studied this notion in details in the stationary case.

More precisely we introduce the

Definition 2.1. (Hull function)
Under assumption (A) and given $p \in (0, +\infty)$ and a number $\lambda \in \mathbb{R}$, we say that $h(z)$ is a hull function for the problem (2.1), if and only if $h \in L^{\infty}_{loc}(\mathbb{R})$ and satisfies

$$\begin{cases} \lambda h_z = F(h(z - mp), ..., h(z + mp)) \\ \\ h(z + 1) = h(z) + 1 \\ \\ h_z(z) \geq 0 \end{cases} \quad \text{for all} \quad z \in \mathbb{R}. \qquad (2.2)$$

Then we have the following characterization of the effective Hamiltonian:

Theorem 2.2. (Effective Hamiltonian versus hull function)
Under assumption (A) and given $p \in (0, +\infty)$, there exists a unique real number λ such that there exists a hull function h (depending on p) satisfying (2.2). Moreover this real number λ is denoted by $\overline{F}(p)$ and it defines a continuous function $\overline{F} : (0, +\infty) \to \mathbb{R}$.

2.2   The general homogenization result

We now consider the following problem satisfied by $u^{\varepsilon}(t, x)$

$$\begin{cases} u_t^{\varepsilon} = F\left(\left[\dfrac{u^{\varepsilon}(t, \cdot)}{\varepsilon}\right]_m^{\varepsilon}\right) & \text{for} \quad (t, x) \in (0, +\infty) \times \mathbb{R}, \\ \\ u^{\varepsilon}(0, x) = u_0(x) & \text{for} \quad x \in \mathbb{R}, \end{cases} \qquad (2.3)$$

where, for some function $v(x)$, we set

$$[v]_m^{\varepsilon}(x) = (v(x - m\varepsilon), ..., v(x + m\varepsilon)) \ .$$

Then we have the following homogenization result

Theorem 2.3. (Homogenization)
Under assumptions (I0)-(A), the solution u^{ε} to (2.3) converges uniformly on compact sets of $[0, +\infty) \times \mathbb{R}$ to the unique viscosity solution u^0 of (1.4), where the effective Hamiltonian $\overline{F}$ is given in Theorem 2.2.

Remark 2.4. *Theorem 1.1 is a corollary of Theorem 2.3, because of the following inequality $u^{\varepsilon} - \varepsilon \lceil K_0 \rceil \leq \overline{u}^{\varepsilon} \leq u^{\varepsilon}$, which follows from the comparison principle.*

Let us also mention that our result can be seen as a natural generalization of corresponding homogenization results for Hamilton-Jacobi equations, whose literature is now huge. Let us simply cite the pioneering paper of Lions, Papanicolaou, Varadhan [11].

Concerning the homogenization of equations with periodic terms in u/ε (which is the case of the models considered in the present paper), only very few results exist. Let us mention the recent result of Imbert, Monneau [9] and the one of Barles [3]. We can also cite the work of Boccardo, Murat [4] on the homogenization of elliptic equations.

2.3   Ansatz for the proof of convergence

The proof follows the lines of the Evans' perturbed test function method, that we do not recall here. Let us only focus, at a formal level, on the additional difficulties raised by the dependence of the non-linearity F on the oscillating variable u/ϵ.

To simplify, let us assume that u^0 is C^1 and that

$$p = u_x^0(t_0, x_0), \quad \lambda = u_t^0(t_0, x_0) = \overline{F}(p).$$

Then the natural ansatz (which can be seen as the perturbed test function) is

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

where h is the hull function.

When h is smooth enough (i.e. C^1 here), then we can compute with $z = \dfrac{u^0(t, x)}{\varepsilon}$:

$$\hat{u}_t^\varepsilon(t, x) - F\left(\left[\frac{\hat{u}^\varepsilon(t, \cdot)}{\varepsilon}\right]_m^\varepsilon (x)\right)$$

$$= u_t^0 h_z(u^0/\varepsilon) - F\left(\left[h\left(\frac{u^0(t, \cdot)}{\varepsilon}\right)\right]_m^\varepsilon (x)\right)$$

$$= (u_t^0 - \lambda)\, h_z + F([h(\cdot)]_m^p(z)) - F\left(\left[h\left(\frac{u^0(t, \cdot)}{\varepsilon}\right)\right]_m^\varepsilon (x)\right)$$

$$= o(1) \quad \text{in a neighborhood of} \quad (t_0, x_0)$$

where we have used the equation satisfied by h to get the third line. For the fourth line, we have used the fact that $h(z)$ *is Lipschitz continuous in z* and that u^0 is C^1.
By perturbations, we understand that we can easily get sub and supersolutions in a small neighborhood of (t_0, x_0). This can then be used to justify the limit equation.

In the general case, we can not perform directly this computation. The difficulty is due to the fact that $h(z)$ may be discontinuous in the variable z. We can nevertheless

overcome this difficulty, by replacing the hull function h by a Lipschitz continuous supersolution or a Lipschitz continuous subsolution of the equation satisfied by the hull function.

2.4 Sketch of the construction of the hull function

Step 1: the Cauchy problem
We consider the following Cauchy problem

$$\begin{cases} w_\tau = F([w(\tau, \cdot)]_m) & \text{for} \quad (\tau, y) \in (0, +\infty) \times \mathbb{R}, \\ w(0, y) = py & \text{for} \quad y \in \mathbb{R}. \end{cases} \tag{2.4}$$

Because of the invariance of the problem by integer translations on w and the special form of the initial condition (look at its $\frac{1}{p} \cdot \mathbb{Z}$ translations in space), we see that

$$w(\tau, y + 1/p) = w(\tau, y) + 1. \tag{2.5}$$

Moreover, from the invariance by translations in y and the comparison principle, we can deduce that

$$w(\tau, y + y') \geq w(\tau, y) \quad \text{for any} \quad y' \geq 0. \tag{2.6}$$

Step 2: heuristics
The behaviour of $W(\tau, y) = w(\tau, y) - py$ can be essentially sketched by an ODE, obtained by neglecting the y variable. One way to charicature the situation is for instance to choose $p = 0$, which gives formally for $W(\tau, y) = W(\tau)$:

$$W_\tau = g(W) \quad \text{with} \quad g(W) = F(W, ..., W).$$

Here g is 1-periodic, and we can deduce that

$$|W(\tau) - \mu\tau| \leq C \quad \text{for some} \quad \mu \in \mathbb{R}. \tag{2.7}$$

Step 3: proof of the heuristics
In the general case, using the invariance by continuous translations in time, it is possible to deduce, from the comparison principle, the existence for any $p > 0$ of a real number λ such that

$$|w(\tau, y) - py - \lambda\tau| \leq C \tag{2.8}$$

with $C \in \mathbb{N}$ a universal constant (we can choose $C = 6$). Here inequality (2.8) appears to be a generalization of (2.7) for every $p > 0$.

Step 4: construction of global solutions
Then, up to consider translations in time

$$w_n(\tau, y) = w(n + \tau, y) - \lfloor \lambda n \rfloor$$

with $n \to +\infty$, we can build a global subsolution $\overline{w}_\infty$ and a global supersolution $\underline{w}_\infty$, defined as follows

$$\overline{w}_\infty = \limsup_{n \to +\infty}{}^* w_n, \quad \underline{w}_\infty = \liminf_{n \to +\infty}{}_* w_n$$

We can next apply the Perron's method in order to define a solution w_∞ as the smallest supersolution which is above $\overline{w}_\infty$ (and below $\underline{w}_\infty + 2C$). In particular w_∞ still satisfies (2.8) with the constant C replaced with another constant.

Step 5: identifying the hull function

We now simply define

$$\tilde{w}_\infty(\tau, y) = \inf_{\sigma \in \mathbb{R}} w_\infty(\tau + \sigma, y - \lambda \sigma / p).$$

By construction, $\tilde{w}_\infty$ is still a supersolution which satisfies

$$\overline{w}_\infty \leq \tilde{w}_\infty \leq w_\infty.$$

By definition of w_∞, we deduce that

$$w_\infty(\tau, y) = \tilde{w}_\infty(\tau, y) = h(py + \lambda \tau)$$

with $h(z) = \tilde{w}_\infty(0, z/p)$. Similarly, it is possible to deduce from (2.5)-(2.6) the properties of the hull function h.

3 Homogenization in the case of two-body interactions

In the case of two-body interactions, we are interested in solutions of (1.1) with $m = +\infty$ and in their collective behaviour as time goes to $+\infty$.

First, the potential V has to have a suitable behaviour at infinity in order to give a meaning to the sum of the interactions. Second, the system of ODE's can be transformed into a single PDE by the use of a cumulative distribution function. Then we can state the homogenization result for system of ODE's (Theorem 3.1 below). Next, we stress the link with the case of short range interactions (i.e. a finite number m of neighbours) studied above. We next explain how to get such a result. After making precise the notion of viscosity solution we use, we construct correctors and we give the general homogenization result (Theorem 3.6 below). We conclude this section by explaining how to extend these results to the physical (singular) case $V(X) = -\ln|X|$ and by giving the main qualitative properties of the effective non-linearity. The effective non-linearity is important from the point of view of applications since it governs the macroscopic behaviour of the material.

3.1 Assumptions

We will make the following additional assumption
(A') Additional assumptions on the potential V:
We assume (A) and moreover the following properties

i)**(Symmetry)** $\quad V(-x) = V(x)$

ii)**(Vanishing force at infinity)** $\quad V'(y) \to 0 \quad$ as $\quad |y| \to +\infty$

iii)**(Behaviour at infinity)** $\quad \exists R_0 > 0, g_0 \geq 0, \quad$ such that $\quad V''(y)y^2 = g_0 \quad$ for $\quad |y| \geq R_0$.

Let us make a few comments on these assumptions. Assumption A'ii) claims that the interaction vanishes at infinity, which is very natural. Assumption A'iii) on the behaviour of the potential at infinity will guarantee the convergence of the serie in (1.1). Finally assumption A'i) on the symmetry is also very natural for applications in physics, and will be very helpful in the analysis. For instance, let us consider the dynamics of a finite number N of particles. Then, using among other things assumption A'i), it is possible to show that the minimal distance $d(\tau)$ between any pair of particles satisfies

$$d(\tau) \geq d(0)e^{-\tau||V_0''||_{L^\infty(\mathbb{R})}}.$$

In particular, this property avoids any meeting of particles in finite time (even in the case of an infinite number of particles).

3.2 Homogenization in terms of the cumulative distribution function

Given the position of the particles with $U_i < U_{i+1}$, we will replace the function u of Section 2 with the following cumulative distribution function defined as follows

$$\rho(\tau, Y) = \sum_{i \geq 0} H(Y - U_i(\tau)) + \sum_{i < 0}(H(Y - U_i(\tau)) - 1), \tag{3.1}$$

where $H(Y) = 1_{\{Y \geq 0\}}$ is the Heaviside function. In Section 4, we will see that this function ρ can be used very easily to extend the model to the dynamics of curves.

In order to make precise the initial positions of the particles, let us consider a function ρ_0 which satisfies the following assumption:
(I0') Initial condition

$$\rho_0 \in W^{2,\infty}(\mathbb{R}) \quad \text{and} \quad \rho_0' \geq 0.$$

We point out that the $W^{2,\infty}$ regularity appears to be a technical assumption.

For $\varepsilon > 0$, we then define the initial positions U_i of (a finite number N_ε of) particles by considering

$$\rho(0, Y) = \lfloor \varepsilon^{-1} \rho_0(\varepsilon Y) \rfloor \,,$$

where $\lfloor \cdot \rfloor$ is the floor integer part. Obviously, for non constant initial data ρ_0, the number N_ε of particles goes to infinity as ε goes to zero.

We define the following function which describes the rescaled positions of the particles

$$\overline{\rho}^\varepsilon(t, X) = \varepsilon \rho \left(\varepsilon^{-1} t, \varepsilon^{-1} X \right) \,. \tag{3.2}$$

In the limit $\varepsilon = 0$, we will see that the effective equation is the following non-local Hamilton-Jacobi equation

$$\begin{cases} \rho_t^0 = \overline{H}(\rho_X^0, \pi g_0 I_1 \rho^0) & \text{for} \quad (t, X) \in (0, +\infty) \times \mathbb{R} \,, \\ \\ \rho^0(0, X) = \rho_0(X) & \text{for} \quad X \in \mathbb{R} \,, \end{cases} \tag{3.3}$$

where the function $\overline{H}$ will be defined later and I_1 is a singular integral operator (see below). Notice that ρ_X^0 can be interpreted as the macroscopic density of particles.

For any function $v(X)$, the operator I_1 is defined in the Fourier space by

$$\widehat{I_1 v}(\xi) = -|\xi| \widehat{v}(\xi) \,.$$

It can be seen as the half-Laplacian $I_1 = -(-\Delta)^{\frac{1}{2}}$. A notion of viscosity solution for equation (3.5) can be defined (see [6]), using the following Lévy-Khintchine expression of $I_1 w$ in the real space:

$$(I_1 w)(X) = \frac{1}{\pi} \int_{\mathbb{R}} \frac{dZ}{Z^2} \left\{ w(X + Z) - w(X) - w'(X) \, Z \, 1_{\{|Z| \leq 1\}} \right\} \,. \tag{3.4}$$

We have the following homogenization result:

Theorem 3.1. (Homogenization with two-body interactions)
Under assumption (I0')-(A'), there exists a continuous function $\overline{H}(q, L)$, which is non-decreasing in the variable L. Moreover the function $\overline{\rho}^\varepsilon$ converges uniformly on compact sets of $[0, +\infty) \times \mathbb{R}$ to the unique viscosity solution ρ^0 of (3.5).

3.3 Short range interactions and relation with the nearest neighbors case

The case of short range interactions corresponds to the case where $g_0 = 0$ in assumption A'iii). A simple example is for instance the case of a potential V with compact support.

In the general case of short range interactions, the effective equation (3.5) is local and can be written

$$\rho_t^0 = \overline{H}(\rho_X^0) \quad \text{with} \quad \overline{H}(q) = \overline{H}(q, 0).$$ (3.5)

Remark also that $\rho(\tau, U_i) = i$ and then (up to forget the particular conditions (I0) and (I0') that we imposed on the initial conditions), we see that

$$\overline{\rho}^\varepsilon(t, \overline{u}^\varepsilon(t, x)) = x \quad \text{for} \quad x = k\varepsilon \quad \text{with} \quad k \in \mathbb{Z}.$$

Therefore passing formally to the limit, we see that

$$\rho^0(t, u^0(t, x)) = x$$

which is a meaningful relation between the point of view of Section 2 and the one of the present section. Joint to the equation (1.4) satisfied by u^0, we deduce the following relation between the two effective Hamiltonians that we obtained

$$\overline{H}(q) = -q\overline{F}(1/q).$$

Remark 3.2. *If $\theta = \rho_X^0$ denotes the macroscopic dislocation density, we can see, by deriving equation (3.5), that it solves formally the following conservation law:*

$$\theta_t = (\overline{H}(\theta))_X.$$

3.4 Notion of viscosity solution

We start by writting the equation satisfied by the cumulative distribution function $\rho(\tau, Y)$. It is possible to see that ρ satisfies

$$\rho_\tau = |\nabla_Y \rho| \{c(Y) + M[\rho(\tau, \cdot)](Y)\} \quad \text{for} \quad (\tau, Y) \in (0, +\infty) \times \mathbb{R}$$ (3.6)

where for any function $w(Y)$, the non-local operator M is defined as

$$M[w](Y) = \int_{\mathbb{R}} dZ \, J(Z) E\left(w(Y + Z) - w(Y)\right)$$

and E is a variant of the floor integer part, defined as follows

$$E(\rho) = k - \frac{1}{2} \quad \text{if} \quad k \le \rho < k + 1 \quad \text{for} \quad k \in \mathbb{Z}.$$

Moreover we have

$$c(Y) = V_0'(Y) - f \quad \text{and} \quad J = V'' \quad \text{on} \quad \mathbb{R} \backslash \{0\}.$$ (3.7)

In order to prove the homogenization result (Theorem 3.1), we need a good notion of viscosity solution for equation (3.6). To this end, we need to introduce some notation.

Recall that for a function ρ, ρ^* denotes its upper semi-continuous envelope, and ρ_* denotes its lower semi-continuous envelope. Recall that by definition of E, we have $E^* = E$, while

$$E_*(\rho) = k - \frac{1}{2} \quad \text{if} \quad k < \rho \leq k+1 \quad \text{for} \quad k \in \mathbb{Z}.$$

Then, $M^* = M$ and M_* denotes the operator M with E replaced with E_*. Remark in particular that we may have $M^*[\rho(\tau, \cdot)](Y_0) > M_*[\rho(\tau, \cdot)](Y_0)$ if ρ is constant in a neighborhood of Y_0.

Definition 3.3. (Viscosity solution)

A upper semi-continuous (resp. lower semi-continuous) function $\rho : [0, +\infty) \times \mathbb{R} \to \mathbb{R}$ is a viscosity subsolution (resp. supersolution) of (3.6) if for any point $(t_0, Y_0) \in (0, +\infty) \times \mathbb{R}$ and any test function $\phi \in C^2([0, +\infty) \times \mathbb{R})$ such that $\rho - \phi$ attains a maximum (resp. a minimum) at the point (t_0, Y_0), then we have

$$\phi_t(t_0, Y_0) \leq |\nabla_Y \phi(t_0, Y_0)| \{c(Y_0) + M^*[\rho(t_0, \cdot)](Y_0)\}, \tag{3.8}$$

$$(\text{resp.} \quad \phi_t(t_0, Y_0) \geq |\nabla_Y \phi(t_0, Y_0)| \{c(Y_0) + M_*[\rho(t_0, \cdot)](Y_0)\} \quad). \tag{3.9}$$

A function ρ is a viscosity solution of (3.6), if ρ^* is a subsolution and ρ_* is a supersolution.

Remark that in this definition, we use the operator M^* for subsolutions and M_* for supersolutions. This definition is an adaptation of the definition introduced by Slepčev in [12], and allows us to get the stability (by passage to the limit) of the solutions. Indeed, loosely speaking, we can say that the viscosity inequalities (3.8) and (3.9) are the less restrictive ones we can require, because we always have $M_* \leq M^*$.

In particular, even if it is not completely straightforward, it is possible to check that the function ρ defined in (3.1) is indeed a discontinuous viscosity solution of (3.6).

3.5 The correctors

For any $q \in \mathbb{R}$ and $v : \mathbb{R} \to \mathbb{R}$, let us define

$$M_q[v](Y) = \int_{\mathbb{R}} dZ \ J(Z) \ \{E(v(Y + Z) - v(Y) + qZ) - qZ\}.$$

Definition 3.4. (Corrector)

Under assumption (A') and given $q, L \in \mathbb{R}$ and a number $\mu \in \mathbb{R}$, we say that $v : \mathbb{R} \to \mathbb{R}$

is a corrector, if and only if $v \in L^\infty(\mathbb{R})$ and satisfies

$$\begin{cases} \mu = |q + \nabla_Y v| \{c(Y) + L + M_q[v](Y)\} \\[2mm] v(Y+1) = v(Y) \\[2mm] q(q + (\nabla_Y v)(Y)) \geq 0 \end{cases} \qquad \text{for all} \quad Y \in \mathbb{R}. \qquad (3.10)$$

Then we have the following characterization of the effective Hamiltonian:

Theorem 3.5. (Effective Hamiltonian versus the corrector)
Under assumption (A') and given $q, L \in \mathbb{R}$, there exists a unique real number μ such that there exists a corrector (depending on q, L) satisfying (3.10). Moreover the real number μ is denoted by $\overline{H}(q, L)$ and this defines a continuous function $\overline{H} : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$, which is moreover non-decreasing with respect to its second variable L.

The construction of the corrector is similar to the one of the hull function (see Subsection 2.4). Remark also that the correctors may be discontinuous (in particular for $\mu = 0$ which corresponds to the case of the pinning of particles).

Interpretation of the corrector in terms of particles
Let us now consider the function

$$\rho(\tau, Y) = \mu \tau + qY + v(Y).$$

Assume for instance that $q > 0$. Then from the last inequality in (3.10), we know that $\rho(\tau, Y)$ is non-decreasing in Y. Assume moreover that $\mu \neq 0$. Then from the equation satisfied by the corrector, we deduce that $\rho(\tau, Y)$ is increasing in Y. We then define the particles of positions $U_i(\tau)$ by the relation

$$\rho(\tau, U_i(\tau)) = i.$$

Then we can check that these particles have the dynamics corresponding to the two-body interactions. Moreover, by construction, we have

$$U_i(\tau + 1/\mu) = U_{i-1}(\tau).$$

This means that the dynamics of those particles is $1/|\mu|$-periodic, and after one period, each particle takes the place of its nearest neighbor (on the left if $\mu > 0$ and on the right if $\mu < 0$). Remark also that for any irrational q, there is no reason to have any kind of spatial periodicity in the particle positions U_i.

3.6 The general homogenization result

We now consider the following problem satisfied by $\rho^\varepsilon(t, X)$:

$$\begin{cases} \rho_t^\varepsilon = |\nabla_X \rho^\varepsilon| \left\{ c(X/\varepsilon) + M^\varepsilon[\rho^\varepsilon(t, \cdot)](X) \right\} & \text{for} \quad (t, X) \in (0, +\infty) \times \mathbb{R}\,, \\ \rho^\varepsilon(0, x) = \rho_0(X) & \text{for} \quad X \in \mathbb{R}\,, \end{cases} \tag{3.11}$$

where, for some function $w(X)$, we set

$$M^\varepsilon[w](X) = \int_\mathbb{R} dZ J(Z) E \left(\frac{w(Y + \varepsilon Z) - w(Y)}{\varepsilon} \right)\,.$$

Then we have the following homogenization result:

Theorem 3.6. (Homogenization)
Under assumptions (I0')-(A'), the solution ρ^ε to (3.11) converges uniformly on compact sets of $[0, +\infty) \times \mathbb{R}$ to the unique viscosity solution ρ^0 of (3.5), where the effective Hamiltonian $\overline{H}$ is given in Theorem 3.5.

The proof of Theorem 3.6 can be done using the ansatz $\hat{\rho}^\varepsilon(t, X) = \rho^0(t, X) + \varepsilon v(X/\varepsilon)$ as a good approximation of ρ^ε. The main point is that the non-local term can be essentially split in two parts:

$$M^\varepsilon[\hat{\rho}^\varepsilon(t, \cdot)](X) \simeq L + M_p[v](X/\varepsilon)$$

with $p = \rho_X(t, X)$ and $L = \pi g_0 I_1[\rho^0(t, \cdot)](X)$. This essentially allows us to recover the cell equation for the corrector (see (3.10)).

Remark also that Theorem 3.1 can be seen as a corollary of Theorem 3.6 as in Remark 2.4.

3.7 Extension to the case $V(X) = -\ln|X|$

We have the following homogenization result:

Theorem 3.7. (Homogenization in the case $V(X) = -\ln|X|$)
Assume that $V(X) = -\ln|X|$ and V_0 satisfies Ai). Then there exists an effective Hamiltonian $\overline{H}(q, L)$. This is a continuous function which is moreover non-decreasing in L. Then, under the additional assumption (I0'), the function $\overline{\rho}^\varepsilon$ defined in (3.2) converges uniformly on compact sets of $[0, +\infty) \times \mathbb{R}$ to the unique viscosity solution ρ^0 of (3.5).

This result is the analogue of Theorem 3.1 in the more singular case of a logarithmic two-body potential. It can be proven that the effective Hamiltonian $\overline{H}$ is well-defined as the limit as δ goes to zero, of Hamiltonians $\overline{H}_\delta$ corresponding to approximations V_δ of V. These approximations V_δ are chosen in such a way that assumptions (A') are satisfied for any $\delta > 0$. Nevertheless, remark that we do not know if there exist correctors in the limit case $\delta = 0$.

Theorem 3.8. (Qualitative properties of $\overline{H}$)
Under the assumptions of Theorem 3.7 with $f = 0$, the function $\overline{H} : \mathbb{R}^2 \to \mathbb{R}$ satisfies the following properties:

1. **(Orowan law)** *If $V_0 \equiv 0$ then $\overline{H}(q, L) = qL$ for $q > 0$.*

2. **(Bound)** *We have*
$$\left| \frac{\overline{H}(q, L)}{|q|} - L \right| \leq \|V_0'\|_\infty \quad for \quad (q, L) \in (0, +\infty) \times \mathbb{R}.$$

3. **(0-plateau property)** *If $V_0' \not\equiv 0$, then there exists $r_0 > 0$ (only depending on $\|V_0'\|_\infty$) such that:*
$$\overline{H}(q, L) = 0 \quad for \quad (q, L) \in B_{r_0}(0) \cap (0, +\infty) \times \mathbb{R}.$$

The proofs of the previous properties are essentially based on the comparison principle applied at the approximate level $\overline{H}_\delta$ for $\delta > 0$. The Orowan law is well-known in the framework of the flow rule in elasto-visco-plasticity. The 0-plateau property shows us the existence of a threshold for the driving force f of the model. Basically, if this driving force is not large enough, then the dislocations are pinned in the material, and there is no macroscopic motion, i.e. $\overline{H} = 0$. The typical profile of $\overline{H}$ as a function of L is given on figure 2.

4 Extension to dislocation dynamics described by the motion of curves

4.1 The modelling

In the physical application to dislocation dynamics, the dislocations are general curves, not necessarily straight lines as in Subsection 1.1. In the special case where all these dislocation curves are contained in a single plane and have the same physical properties
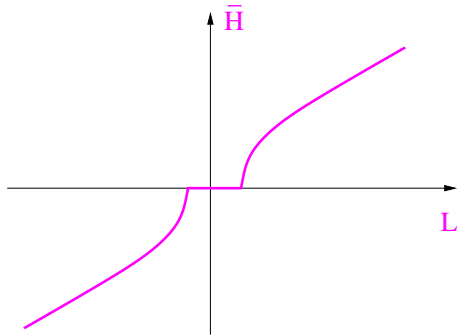
Figure 2: Sketch of the graph of the map $L \mapsto \overline{H}(q, L)$

(namely the same Burgers vector), then we can represent these curves $(\Gamma^k)_{k \in \mathbb{Z}}$ as level sets of a single function ρ:

$$\Gamma^k = \left\{ z \in \mathbb{R}^N, \quad \rho(z) = k \right\} .$$

For our physical application, we have $N = 2$, but we will write the model in all dimension N. Each dislocation Γ^k creates a stress field, whose resolved shear component (the resolved Peach-Koehler force) computed at the point $y \in \mathbb{R}^N$ can be written with a good approximation as:

$$\left\{ (J - \delta_0) \star 1_{\{\rho(\cdot) \geq k\}} \right\} (y) , \tag{4.1}$$

where the kernel J satisfies proper assumptions (see below). The typical profile of the stress given in (4.1) is represented on figure 3. We see that the (discontinuous) profile represented on figure 3 is a kind of regularization of the function $-1/x_1$.
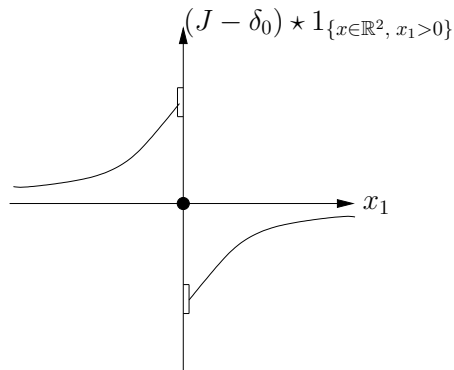

Figure 3: Typical profile for the Peach-Koeller force created by a dislocation straight line.

We make the following assumptions on the kernel J:

$$\begin{cases} J \in W^{1,1}(\mathbb{R}^N), \quad J(-z) = J(z) \geq 0, \quad \int_{\mathbb{R}^N} J = 1 \\[4mm] \exists\ R_0 > 0 \text{ and } \exists\ g \in C^0(\mathbf{S}^{N-1}),\ g > 0 \text{ such that } J(z) = \dfrac{1}{|z|^{N+1}}\ g\left(\dfrac{z}{|z|}\right) \text{ for } |z| \geq R_0. \end{cases}$$
$$(4.2)$$

On the one hand, the first line of (4.2) allows us to recover a profile as in figure 3. On the other hand, the second line of (4.2) is related to the long range interactions between curves. This can be seen as a generalization of the relation (3.7) under assumption A'iii).

Then, in the framework of linear elasticity, the total stress can be seen as the sum of the contributions of each dislocation Γ^k given in (4.1). It is possible to see that the sum of these contributions, computed at the point y, can be rewritten as follows

$$M[\rho](y) = \int_{\mathbb{R}} dz\, J(z) E\left(\rho(y+z) - \rho(y)\right).$$

We also assume that these dislocations are distributed in a periodic landscape with some obstacles. The effective stress field created by these obstacles is represented by a function $c(y)$ satisfying

$$c \quad \text{is Lipschitz continuous and } \mathbb{Z}^N\text{-periodic.}$$

Then the total stress at a point y can be expressed as

$$V_\nu(y) = c(y) + M[\rho](y).$$

Assuming that each dislocation curve Γ^k move with the *normal velocity* equal to the shear stress V_ν, we see that the evolution equation satisfied by the function $\rho(\tau, y)$, whose level sets represent the dislocations, can be written as follows (as a simple generalization of equation (3.6)):

$$\rho_\tau = |\nabla_y \rho|\left\{c(y) + M[\rho(\tau, \cdot)](y)\right\} \quad \text{for} \quad (\tau, y) \in (0, +\infty) \times \mathbb{R}^N. \qquad (4.3)$$

4.2 Homogenization of the dynamics of curves in interaction

We are interested in the behaviour at large scale of solutions of equation (4.3). This is equivalent to consider for small $\varepsilon > 0$ the function

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

Imposing for instance the following initial condition

$$\rho^\varepsilon(0, x) = \rho_0(x),$$

we will see, in the limit $\varepsilon \to 0$, that the effective equation is

$$\begin{cases} \partial_t \rho^0 = \overline{H}\left(\nabla \rho^0, \mathcal{I}_1[\rho^0(t, \cdot)]\right) & \text{in} \quad (0, +\infty) \times \mathbb{R}^N, \\ \rho^0(0, x) = \rho_0(x) & \text{on} \quad \mathbb{R}^N, \end{cases} \tag{4.4}$$

where $\overline{H}$ is a continuous function and $\mathcal{I}_1$ is an anisotropic Lévy operator of order 1 associated with the function g appearing in (4.2). It is defined for any function $w \in C_b^2(\mathbb{R}^N)$ by

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

which is a generalization of the half-Laplacian defined in (3.4). This Lévy operator $\mathcal{I}_1$ only keeps the memory of the long range interactions between dislocations, as the *effective Hamiltonian* $\overline{H}$ keeps the memory of the short range interactions.

Then we have the following result:

Theorem 4.1. (Homogenization of dislocation curves)
Under the previous assumptions, there exists a continuous function $\overline{H} : \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}$ such that $\overline{H}(q, L)$ is non-decreasing in L. If we assume moreover that $\rho_0 \in W^{2,\infty}(\mathbb{R}^N)$, then the function ρ^ε converges locally uniformly, as $\varepsilon \to 0$, to the unique viscosity solution ρ^0 of (4.4).

This result can be proven in the framework of viscosity solutions. The proof is similar to the one of Theorem 3.6 in the one-dimensional case.

Acknowledgements

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