Reduced ODE dynamics as formal relativistic asymptotics of a Peierls-Nabarro model

H. Ibrahim [†,‡], R. Monneau [*]

March 10, 2014

Abstract

In this paper, we consider a scalar Peierls-Nabarro model describing the motion of dislocations in the plane (x_1, x_2), along the line $x_2 = 0$. Each dislocation can be seen as a phase transition and creates a scalar displacement field in the plane. This displacement field solves a simplified elasto-dynamics equation which is simply the linear wave equation. The total displacement field creates a stress which makes move the dislocation themselves. By symmetry, we can reduce the system to the wave equation in the half plane $x_2 > 0$ coupled with an equation for the dynamics of dislocations on the boundary of the half plane, i.e. on $x_2 = 0$. Our goal is to understand the dynamics of well-separated dislocations in the limit when the distance between dislocations is very large of order $1/\varepsilon$. After rescaling, this corresponds to introduce a small parameter ε in the system. In the limit $\varepsilon \to 0$, we are formally able to identify a reduced ODE model describing the dynamics of relativistic dislocations, if a certain conjecture is assumed to be true.

AMS subject classifications: 70H40, 45M05, 35D30
Key words: Peierls-Nabarro model, dislocation dynamics, relativitic dymamics, formal asymptotics, reduced model.

1 Introduction

1.1 Setting of the problem

In this paper, we consider a scalar Peiels-Nabarro model describing the dynamics of dislocations in the plane (x_1, x_2), along the line $x_2 = 0$. This is a phase field model, where each dislocation can be seen as a phase transition essentially between two consecutive integers. We refer to [13] for an overview on the Peierls-Nabarro model. Our scalar Peiels-Nabarro model (see (1.1) below) can

[*]Université Paris-Est, Ecole des Ponts, CERMICS, 6 et 8 avenue Blaise Pascal, Cité Descartes Champs-sur-Marne, 77455 Marne-la-Vallée Cedex 2, France. E-mail: monneau@cermics.enpc.fr

[†]Lebanese University, Faculty of Sciences, Mathematics Department, Hadeth, Beirut, Lebanon.

[‡]School of arts and sciences, Mathematics Department, Lebanese International University (LIU), Beirut Campus, Al-Mouseitbeh, P.B. Box 14-6404, Beirut, Lebanon. Email: hassan.ibrahim@liu.edu.lb

be seen as a scalar simplification of the vectorial Peierls-Nabarro Galerkin model introduced in [3] (see also [4]).

A dislocation is a defect in a crystal and creates a stress field in the material (see [10]). The total stress field creates a force acting on each dislocation, and makes those dislocations move on the line $x_2 = 0$. The whole model can be seen as a coupling between a dynamics on the line $x_2 = 0$ and a dynamics outside the line $x_2 = 0$.

In the model that we consider, the phase field is a scalar quantity which can be identified to a scalar displacement of atoms in the crystal. This displacement satisfies a scalar elasto-dynamics equation, which is simply the linear wave equation in the plane, outside the line $x_2 = 0$. By symmetry, we can reduce the problem to the wave equation on the half plane $x_2 > 0$ coupled with a Peierls-Nabarro type dynamics on the boundary of the half plane, i.e. on $x_2 = 0$. We are interested in the dynamics of well-separated dislocations and in the limit when the distance between dislocations is very large, of order $1/\varepsilon$. After a suitable rescaling, it corresponds to introduce a small parameter $\varepsilon > 0$ in the model and then to study the limit $\varepsilon \to 0$. More precisely we consider a phase field $u^\varepsilon(x_1, x_2, t)$ which is a real function solution of the following system

$$\begin{cases} \Box u^\epsilon = 0, & x_2 > 0 \\ N_\varepsilon u^\varepsilon = 0, & x_2 = 0 \end{cases} \tag{1.1}$$

where the two operators $\Box$ and N_ε applied on a scalar function $u = u(x,t)$, $x = (x_1, x_2) \in \mathbb{R}^2$ are defined as follows:

$$\begin{cases} \Box u := \dfrac{1}{c_0^2} u_{tt} - \Delta u, & x_2 > 0, \\ N_\varepsilon u := \beta \left(\dfrac{1}{c_0^2} u_{tt} - \partial_{11} u \right) + k u_t - \dfrac{1}{\varepsilon} \left(\partial_2 u - \dfrac{1}{\varepsilon} W'(u) + \sigma(x_1, t) \right), & x_2 = 0, \\ \beta = m c_0^2, \end{cases} \tag{1.2}$$

where $c_0 \in (0, \infty)$ is the velocity of sound in the crystal, and $m, k \in [0, \infty)$ are parameters. The quantity m can be interpreted as a kind of mass of the dislocation and k can be seen as a damping factor that is classical for the evolution Peierls-Nabarro model (see for instance [9]). Here we use the notation $u_t = \dfrac{\partial u}{\partial t}$, $u_{tt} = \dfrac{\partial^2 u}{\partial t^2}$, $\partial_i u = \dfrac{\partial u}{\partial x_i}$, $\partial_{ii} u = \dfrac{\partial^2 u}{\partial x_i^2}$ for $i = 1, 2$ and $\Delta u = \partial_{11} u + \partial_{22} u$. In this model, the scalar-valued function W is a 1-periodic smooth potential mimicking the periodicity of the atoms in the crystal. We assume that W satisfies

$$\begin{cases} W(u+1) = W(u) \text{ for any } u \in \mathbb{R}, \\ W = 0 \text{ on } \mathbb{Z}, \\ W > 0 \text{ on } \mathbb{R} \setminus \mathbb{Z}, \\ \alpha_0 := W''(0) > 0. \end{cases}$$

A dislocation will be naturally seen as a phase transition between a two consecutive minima of W. In this model, we consider the presence of a given exterior scalar stress field $\sigma(x_1, t)$ which has a contribution to the force acting on the dislocations on $x_2 = 0$. This contribution is taken into account in the definition of the operator N_ε. The limit $\varepsilon \to 0$ has been studied rigorously in [9] in the particular case $\beta = 0$, $c_0 = +\infty$ and $k = 1$, which corresponds to a quasi-static approximation.

In the present paper our goal is to study formally the limit $\varepsilon \to 0$ for our more general model in the relativistic regime. In fact, contrary to [9, Theorem 1.1] where the passage to limit $\varepsilon \to 0$ took place via the stability theorem for viscosity solutions, we only provide heuristic asymptotic analysis when the term ε becomes negligible assuming that Conjecture (A) below is true. Note that all derivations made throughout the paper are only formally (absolutely not rigorously) justified.

For $\sigma \equiv 0$, the simplest situation is the case of a single and stationary dislocation

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

where ϕ is a normalized phase transition between 0 and 1, solution of the following system:

$$\begin{cases} \Delta\phi = 0, & x_2 > 0 \\ \beta\partial_{11}\phi + \partial_2\phi - W'(\phi) = 0, & x_2 = 0, \\ \phi(-\infty,0) = 0, \quad \phi(+\infty,0) = 1. \end{cases} \tag{1.3}$$

We are interested in the dynamics of $N \geq 1$ dislocations of positions $X_i(t) \in \mathbb{R}$ for $i = 1,...,N$ on the axis $x_2 = 0$. Because we are considering a relativistic regime, it is natural to introduce the following relativistic coefficient:

$$\gamma_i(t) = \frac{1}{\sqrt{1 - \left(\frac{X_i'(t)}{c_0}\right)^2}}, \tag{1.4}$$

where $(\ )'$ denotes the time derivative. This coefficient γ_i encodes the contraction of the fields in the x_1 direction. Then a natural ansatz for describing the phase transition associated to those dislocations is the following

$$\hat{u}^\varepsilon(x,t) = \left\{\sum_{i=1}^N \phi\left(\gamma_i(t)\left(\frac{x_1 - X_i(t)}{\varepsilon}\right), \frac{x_2}{\varepsilon}\right)\right\} + \varepsilon v^\varepsilon(x,t) \tag{1.5}$$

where v^ε appears to be a correction term that will be precised later. Such an ansatz is compatible with the dynamics (1.1) only for suitable correction terms v^ε (and Conjecture (A)) which impose the following asymptotical dynamics:

$$m_0(\gamma_i X_i')' + k_0\gamma_i X_i' = -\sigma(X_i,t) + \frac{1}{\pi}\sum_{j\neq i}\frac{1}{\gamma_j}\frac{1}{(X_i - X_j)}, \quad i = 1,...,N \tag{1.6}$$

where m_0, k_0 are parameters that will be precised later. Our ODE dynamics (1.6) is similar to equation (1) in [17].

The term $(\gamma_i X_i')' = \gamma_i^3 X_i''$ is the natural relativistic acceleration and $m_0\gamma_i^3$ is the effective mass of the dislocation, which is coherent with the one computed in [11] for screw dislocations (see also (3.12) in [15]).

The term $k_0\gamma_i X_i'$ can be seen as a friction term (viscous force) which will slow down the motion of the dislocations. This term is compatible with the one given in (2.21) and (2.18) in [15], for the Eshelby approximation [6]. We will see that the damping factor k_0 vanishes when the coefficient k vanishes in (1.2). The precise statement of our result is given in result 1.1.

1.2 Assumptions

We will choose

$$v^\varepsilon(x,t) = \frac{\sigma(x_1,t)}{W''(0)} - \sum_{i=1}^{N} \sum_{\alpha=1,2,3} a_i^\alpha(t)\psi^\alpha\left(\gamma_i(t)\left(\frac{x_1 - X_i(t)}{\varepsilon}\right), \frac{x_2}{\varepsilon}\right) \tag{1.7}$$

where the coefficients a_i^α are given by

$$a_i^1 := \frac{2\gamma_i' X_i'}{c_0^2}, \quad a_i^2 := \frac{\gamma_i' X_i' + (\gamma_i X_i')'}{c_0^2} \quad \text{and} \quad a_i^3 := k\gamma_i X_i' \quad \text{for} \quad i = 1, ..., N. \tag{1.8}$$

Here we assume the existence of corrector functions ψ^α, $\alpha = 1,2,3$ which satisfy:

$$\begin{cases} \Delta\psi^1 = x_1\partial_{11}\phi, & x_2 > 0 \\ A\psi^1 = \beta x_1 \partial_{11}\phi - \dfrac{\overline{\beta}_0}{2\alpha_0}(W''(\phi) - W''(0)), & x_2 = 0, \end{cases} \tag{1.9}$$

$$\begin{cases} \Delta\psi^2 = \partial_1\phi, & x_2 > 0 \\ A\psi^2 = \beta \partial_1\phi + \dfrac{\overline{\beta}_0}{\alpha_0}(W''(\phi) - W''(0)), & x_2 = 0, \end{cases} \tag{1.10}$$

and

$$\begin{cases} \Delta\psi^3 = 0, & x_2 > 0 \\ A\psi^3 = \partial_1\phi + \dfrac{\overline{k}_0}{\alpha_0}(W''(\phi) - W''(0)), & x_2 = 0, \end{cases} \tag{1.11}$$

where the linearized operator A is defined by:

$$A\psi := \beta\partial_{11}\psi + \partial_2\psi - W''(\phi)\psi. \tag{1.12}$$

The fact that the corrector ψ^3 has to solve equation (1.11) may be heuristically inferred from the computations in [9, Section 3.1] (see, in particular, formula (3.18) there). Similarly, it can be seen from the computations done later in the present paper, that the two other correctors ψ^1 and ψ^2 have to solve respectively equations (1.9) and (1.10). Although we have no proof of existence of such ψ^α, $\alpha = 1,2,3$ (see Conjecture (A)), it is possible to remark (see Formal Corollary 3.2) that those correctors can only exist with a certain decay at infinity, if they satisfy a compatibility condition which forces the following values of the parameters:

$$\overline{k}_0 = \int_{\{x_2=0\}} (\partial_1\phi)^2 \quad \text{and} \quad \overline{\beta}_0 = \int_{\{x_2>0\}} (\partial_1\phi)^2 + \int_{\{x_2=0\}} \beta(\partial_1\phi)^2. \tag{1.13}$$

We also define the following parameters

$$k_0 = \overline{k}_0 k \quad \text{and} \quad m_0 = \frac{\overline{\beta}_0}{c_0^2} = \frac{1}{c_0^2}\int_{\{x_2>0\}} (\partial_1\phi)^2 + m\int_{\{x_2=0\}} (\partial_1\phi)^2, \tag{1.14}$$

where m_0 can be interpreted as a kind of effective mass of the dislocation. For the simplicity of notation, we call $\psi^0 = \phi$ and set the Heaviside function $H(x_1) = \mathbf{1}_{[0,+\infty)}(x_1)$.

Inspired by [9, Theorems 3.1, 3.2], we consider the following.

Conjecture (A):
There exist profile functions ψ^α, $\alpha = 0,1,2,3$, *respectively solutions of (1.3), (1.9), (1.10), (1.11), which satisfy with* $\phi = \psi^0$*:*

$$\begin{cases} \begin{cases} |\nabla \psi^\alpha(x)| \le \dfrac{C}{1+|x_1|} & \alpha = 0,1,2,3, \\ |\partial_{11}\psi^\alpha(x)| \le \dfrac{C}{1+|x_1|^2} & \alpha = 0,1,2,3, \end{cases} \\ \\ |\psi^\alpha(x_1,0)| \le \dfrac{C}{1+|x_1|} \quad \alpha = 1,2,3, \\ \\ \left|\phi(x_1,0) - H(x_1) + \dfrac{1}{\alpha_0 \pi x_1}\right| \le \dfrac{C}{1+|x_1|^2} \quad \textit{if} \quad |x_1| \ge 1. \end{cases}$$

Conjecture (A) remains open in this paper and it is by no means justified in this work. We only give some comments on this conjecture in Subsection 3.1. Therefore it is essential to have an answer to the following question:

Open question 1. Do we have existence of profiles ψ^α, $\alpha = 0,1,2,3$ as in Conjecture (A)?

1.3 The main result

Before stating our main result, we again stress on the fact that all our derivations are formal and based on Conjecture (A).

Formal Result 1.1 ***(Reduced ODE dynamics as an asymptotic of the PN model)***
Let us consider the assumptions of Subsection 1.2, with W *and* σ *smooth enough. We assume in particular that Conjecture (A) holds true. Given* $T > 0$, *let us assume the existence of particles* $X_i = X_i(t)$ *for* $i = 1,2\ldots,N$, *satisfying*

$$\left.\begin{cases} X_{i+1}(t) - X_i(t) \ge 2\delta > 0 \\ |X_i'| \le c_0(1-\delta), \quad \delta > 0 \end{cases}\right| \quad \textit{for} \quad t \in [0,T], \tag{1.15}$$

solutions of the dynamics (1.6) for $t \in (0,T)$, *namely*

$$m_0(\gamma_i X_i')' + k_0 \gamma_i X_i' = -\sigma(X_i,t) + \frac{1}{\pi}\sum_{j\neq i} \frac{1}{\gamma_j}\frac{1}{(X_i - X_j)}, \quad i = 1,...,N$$

with γ_i *is given by* (1.4) *and the parameters* m_0, k_0 *are given in (1.14). Let us consider the ansatz function* $\hat{u}^\varepsilon$ *given by (1.5) and the correction term* v^ε *given by (1.7) with the coefficients* a_i^α *given by (1.8). Then for any fixed* $\delta > 0$, *we have as* $\varepsilon \to 0$

$$\begin{cases} \Box \hat{u}^\varepsilon = O_\delta(1) & \textit{uniformly in } L^\infty(\{x_2 > 0\} \times (0,T)) \\ N_\varepsilon \hat{u}^\varepsilon = O_\delta(1) & \textit{uniformly in } L^\infty(\{x_2 = 0\} \times (0,T)). \end{cases} \tag{1.16}$$

Here we only get $O_\delta(1)$ right hand sides of (1.16). Nevertheless this still means that the ansatz (1.5) is a good approximation of the solution because the operator N_ε involves $O(1/\varepsilon^2)$-terms and the boundary condition involving N_ε has consequences on the first PDE of (1.16). The important consequence of this result is the identification of the limit dynamics (1.6). It is then natural to raise the following questions:

Open question 2. Do we have long time existence of solutions of the reduced ODE dynamics (1.6)?

Open question 3. Can we have a more precise and rigorous justification of the limit dynamics (1.6) for solutions of (1.1)?

In the case of finite ε for the Peierls-Nabarro Galerkin models, the effective dislocation dynamics can reveal retardation effects. We refer the reader for instance to [14, 16, 18].

The interested reader can also consult [7] to see how the classical Peierls-Nabarro model can be rigorously derived from the Frenkel-Kontorova model at a smaller scale. We also refer the reader to [5, 12] for the relation between the Peierls-Nabarro model and other models at larger scales.

1.4 Organization of the paper

In Section 2, we recall the physical derivation of our Peierls-Nabarro type model (1.1). In Section 3, we give some simple properties on the correctors including compatibility conditions. In order to do the proof of our main result, we start with preliminary computations on our ansatz $\hat{u}^\varepsilon$ in Section 4. Finally in Section 5, we give the proof of our main result, namely result 1.1.

2 Physical derivation of the model

We consider a two-dimensional crystal and call $U(x_1, x_2, t)$ the horizontal displacement (along the axis x_1) of the atoms. A natural action of the system without dislocations describing waves of velocity c_0, is the following

$$\int_{\mathbb{R}^2\times(0,T)} \frac{1}{2}|\nabla U|^2 - \frac{1}{2c_0^2}(U_t)^2. \tag{2.1}$$

We now assume that dislocations are localized on the line $x_2 = 0$ and can only move along this line. We also assume the antisymmetry

$$U(x_1, -x_2, t) = -U(x_1, x_2, t)$$

but allow a jump of u when we cross the line $x_2 = 0$:

$$U(x_1, 0^+, t) - U(x_1, 0^-, t) =: \eta(x_1, t).$$

Then the function η can describe a dislocation as a phase transition between two integers (if we normalise to one unit the Burgers vector which is here a scalar quantity because U is itself scalar).

Then the action (2.1) has to be modified as follows

$$\mathcal{A}(U,\eta) := \int_{\mathbb{R}^2\times(0,T)} \left\{ \frac{1}{2}|\nabla U - \eta e_2 \delta_0(x_2)|^2 - \frac{1}{2c_0^2}(U_t)^2 \right\} + \int_{\{x_2=0\}\times(0,T)} \overline{W}(\eta).$$

Here (e_1, e_2) the standard orthonormal basis and we had to substract a Dirac mass in order to compensate the jump of u. The last integral is an energy term created by the misfit of the upper and lower half crystal created by the presence of the dislocation. In particular W is 1-periodic, non negative and vanishes on integers (the case $\eta \in \mathbb{Z}$ corresponding to the case of no misfit in the crystal). Then the natural Peierls model is the following

$$\left\{ \begin{array}{l} \mathcal{A}'_U = 0, \\ \overline{k}\eta_t = -\mathcal{A}'_\eta \end{array} \right.$$

where the first line is the first variation of the action with respect to u, and the second line is the gradient flow evolution of the field η where $\overline{k}$ is a damping factor. Then it is easy to check that

$$u(x_1,x_2,t) = \left\{ \begin{array}{lll} 2U(x_1,x_2,t) & \text{if} & x_2 > 0, \\ \eta(x_1,t) & \text{if} & x_2 = 0, \end{array} \right.$$

solves (1.1) for $\varepsilon = 1$, $\sigma = 0$, $\beta = 0$, $\overline{k} = \dfrac{k}{4}$ and $\overline{W} = \dfrac{1}{4}W$. More generally, we recover (1.1) if we consider the general action

$$\begin{aligned} \mathcal{A}(U,\eta) := \; & \frac{1}{\varepsilon}\int_{\mathbb{R}^2\times(0,T)} \left\{ \frac{1}{2}|\nabla U - \eta e_2 \delta_0(x_2)|^2 + (\nabla U - \eta e_2\delta_0(x_2))\cdot\Sigma - \frac{1}{2c_0^2}(U_t)^2 \right\} \\ & + \int_{\{x_2=0\}\times(0,T)} \left\{ \frac{1}{\varepsilon^2}\overline{W}(\eta) + \overline{\beta}\left(|\partial_1\eta|^2 - \frac{1}{c_0^2}(\eta_t)^2 \right) \right\} \end{aligned} \tag{2.2}$$

assuming that $\operatorname{div}\Sigma = 0$ and $\sigma(x_1,t) := 2e_2\cdot\Sigma(x_1,0,t)$ and $\overline{\beta} = \dfrac{\beta}{4}$. We have to emphasize the fact that model (2.2) in the special case $\overline{\beta} = 0$, is a simplified scalar version of a more general model called the Peierls-Nabarro Galerkin model [3], where the displacement U is vectorial.

3 Some remarks on the correctors

In this section, we discuss Conjecture (A) and give some necessary properties of the correctors.

3.1 Discussion on Conjecture (A)

The aim of this subsection is to convince the reader that Conjecture (A) sounds very reasonable. To this end, we indicate several arguments and a possible strategy to try to prove Conjecture (A), even if we prove no rigorous results in this direction. We discuss heuristically and successively the existence and the asymptotics for each profile function ψ^α for $\alpha = 0, 1, 2, 3$.

Case of $\psi^0 = \phi$

For the special case of $W'(u) = -\frac{1}{2\pi a} \sin\left\{2\pi(u - \frac{1}{2})\right\}$ for some $a > 0$, we recall (see [9]) that the solution ϕ_0 of (1.3) for $\beta = 0$ is

$$\phi_0(x) = \frac{1}{\pi} \arctan\left(\frac{x_1}{x_2 + a}\right) + \frac{1}{2}. \tag{3.1}$$

We also refer to [2] for properties of ϕ_0 in the case $\beta = 0$ for more general potentials W. In Section 5 of [9], we recall that we can see the map $\Phi = \phi(\cdot, 0) \mapsto L\Phi := \partial_2\phi(\cdot, 0)$ (with ϕ harmonic on the half plane $\{x_2 > 0\}$) can be seen as a half-Laplacian $L = -(-\Delta)^{\frac{1}{2}}$ with symbol $\hat{L} = -|\xi|$. Therefore, in equation (1.3), we can reformulate the differential operator as

$$\beta\partial_{11}\phi + \partial_2\phi = \beta\partial_{11}\phi - (-\Delta)^{\frac{1}{2}}\phi \quad \text{on} \quad \{x_2 = 0\}$$

First possible strategy

For $\beta = 0$, we know that the profile $\phi(x_1, 0)$ behaves like $\phi(\pm\infty, 0) \mp C/x_1$ at infinity, and $\partial_2\phi(x_1, 0) \simeq \mp C'/x_1$ as $x_1 \to \pm\infty$. Now for a general β, this indicates that the term $\beta\partial_{11}\phi(x_1, 0)$ is expected to behave like $1/x_1^3$ and then is neglectible at infinity with respect to $\partial_2\phi(x_1, 0)$. This suggests that the term $\beta\partial_{11}\phi$ should be seen (at least at infinity) as a small perturbation of the equation and this suggests to try to construct such solutions by a perturbation method.

Second possible strategy

Notice also that the operator

$$\beta\partial_{11}\Phi + \partial_2\Phi \tag{3.2}$$

enjoys a nice maximum principle for $\beta \geq 0$. Therefore, we could also try construct hull functions as in [8], and then traveling waves as in [1]. This alternative approach could give the existence of such profile ϕ.

Case of ψ^3

The construction of ψ^3 is given in [9] in the special case $\beta = 0$. For the case $\beta > 0$, we look for solutions ψ^3 of

$$\begin{cases} \Delta\psi^3 = 0 & \text{on} \quad \{x_2 > 0\}, \\ A\psi^3 = f_1 \quad \text{with} \quad f_1 := \partial_1\phi + \frac{\overline{k}_0}{\alpha_0}(W''(\phi) - W''(0)) & \text{on} \quad \{x_2 = 0\} \end{cases} \tag{3.3}$$

with the operator A defined in (1.12). Here the additional term $\beta\partial_{11}\phi$ contained in the operator A, has a good sign in all the estimates (and this is related to the fact that the operator given in (3.2) has a maximum principle). Therefore it seems reasonable to try to adapt the analysis carried out in [9], to the case $\beta > 0$, and to get the existence of correctors ψ^3.

In order to check the asymptotics of ψ^3, we could try to compare ψ^3 with some supersolution of the same equation, having in mind that f_1 behaves at most as $O(1/x_1)$ at infinity. Notice that ϕ is an approximate solution of the left hand side of (1.11). Looking at some function like $C\min(\phi(x_1, x_2), \phi(-x_1, x_2))$ for a constant C large enough, it should be possible to construct such a supersolution and to get some information on the decay at infinity of ψ^3 like $1/|x_1|$ as x_1 goes to infinity. Notice that another approach could be also to try to estimate directly the half Laplacian on functions behaving like $1/|x_1|$ at infinity. Then from the estimate on ψ^3, and from the elliptic regularity theory, we could also get some similar decay on $\nabla\psi^3$. Finally, since the decay of $\psi^3(x_1,0)$ is like $1/|x_1|$, it sounds reasonable to get a better decay on $\partial_{11}\psi^3(x_1,0)$, which is the claim in Conjecture (A).

Case of ψ^2

Step 1: an explicit computation and reduction of the problem

We first notice that

$$\theta_2 = \frac{x_1(\phi - 1/2)}{2},$$

solves

$$\Delta\theta_2 = \partial_1\phi.$$

We now define:

$$h(x_1,x_2) = \frac{1}{2}\int_0^{x_1}\left(\phi(y_1,x_2) - \frac{1}{2}\right)dy_1 - g(x_2) \quad \text{with} \quad g''(x_2) = \frac{1}{2}\partial_1\phi(0,x_2),$$

then $\Delta h = 0$. Therefore, if we set $\bar{\theta}_2 = \theta_2 - h$, we obtain

$$\Delta\bar{\theta}_2 = \partial_1\phi.$$

Recall that it sounds reasonable to have

$$\phi(x_1,0) - \frac{1}{2} = \pm\frac{1}{2} - \frac{C}{x_1} + O\left(\frac{1}{x_1^2}\right) \quad \text{as} \quad x_1 \to \pm\infty. \tag{3.4}$$

Then, we can see that

$$\bar{\theta}_2(x_1,0) = -\frac{C}{2}\ln(2+|x_1|) + C' + O\left(\frac{1}{x_1}\right) \quad \text{as} \quad |x_1| \to +\infty.$$

Therefore, setting for $x = (x_1,x_2)$

$$\bar{\bar{\theta}}_2(x) = \bar{\theta}_2(x) + \frac{C}{2}\ln|(x_1,x_2-1)| - C_0$$

for a suitable constant C_0, we see (because the logarithm function is harmonic in 2D oustide its singularity) that $\bar{\bar{\theta}}_2$ satisfies

$$\begin{cases} \Delta\bar{\bar{\theta}}_2 = \partial_1\phi & \text{in} \quad \{x_2 > 0\}, \\ \bar{\bar{\theta}}_2(x_1,0) = O\left(\dfrac{1}{x_1}\right) & \text{as} \quad |x_1| \to +\infty. \end{cases} \tag{3.5}$$

This shows that we are looking for a solution ψ^2 such that

$$\bar{\psi}^2 = \psi^2 - \bar{\bar{\theta}}_2$$

solves

$$\begin{cases} \Delta\bar{\psi}^2 = 0 & \text{on} \quad \{x_2 > 0\}, \\ \\ A\bar{\psi}^2 = f_2 \quad \text{with} \quad f_2 := -A\bar{\bar{\theta}}_2 + \beta\partial_1\phi + \dfrac{\overline{\beta}_0}{\alpha_0}(W''(\phi) - W''(0)) & \text{on} \quad \{x_2 = 0\} \end{cases}$$

where it is reasonable to expect that $A\bar{\bar{\theta}}_2$ behaves at most like $O(1/x_1)$ at infinity, because of (3.5). Therefore f_2 should also behave at most like $O(1/x_1)$ at infinity.

Step 2: conclusion

We now see that the problem reduces exactly to the problem studied in the construction of ψ^3 (see (3.3)). The approach proposed there should allow to conclude to the existence of a suitable corrector $\bar{\psi}^2$ (and then ψ^2) with the expected asymptotics.

Case of ψ^1

We notice that

$$\theta_1 = \frac{x_1^2\partial_1\phi}{4} - \frac{\theta_2}{2} \quad \text{where we recall that} \quad \theta_2 = \frac{x_1(\phi - \frac{1}{2})}{2}$$

solves

$$\Delta\theta_1 = x_1\partial_{11}\phi.$$

If we have the analogue of (3.4), but for the derivatives, i.e.

$$\partial_1\phi(x_1, 0) = \frac{C}{x_1^2} + O\left(\frac{1}{x_1^3}\right) \quad \text{as} \quad x_1 \to \pm\infty$$

then we deduce that

$$\frac{x_1^2\partial_1\phi}{4} = C + O(1/x_1) \quad \text{for} \quad x_2 = 0.$$

Therefore, proceeding exactly as in the case of ψ^2, we can try to get a profile ψ^1.

3.2 Properties of the correctors

Let us consider a function Ψ solution of

$$\begin{cases} \Delta\Psi = F & \text{on} \quad \Omega := \{x_2 > 0\}, \\ A\Psi = G & \text{on} \quad \partial\Omega = \{x_2 = 0\}. \end{cases} \tag{3.6}$$

Formal Lemma 3.1 (Compatibility condition)

If Ψ solves (3.6) with sufficient decay at infinity, then we have

$$\int_\Omega F\zeta + \int_{\partial\Omega} G\zeta = 0 \quad \text{with} \quad \zeta = \partial_1\phi \tag{3.7}$$

where ϕ is the solution of (1.3).

Proof of Formal Lemma 3.1
Step 1: self-adjoint property
For (F,G) and $(\hat{F},\hat{G})$, let us define the scalar product as

$$\int_\Omega F\hat{F} + \int_{\partial\Omega} G\hat{G}.$$

Then a simple computation (by integration by parts) shows that the operator $\Psi \mapsto (\Delta\Psi, A\Psi)$ is self-adjoint for this scalar product, i.e. for any Ψ, Φ, we have

$$\int_\Omega (\Delta\Psi)\Phi + \int_{\partial\Omega} (A\Psi)\Phi = \int_\Omega \Psi(\Delta\Phi) + \int_{\partial\Omega} \Psi(A\Phi). \tag{3.8}$$

Step 2: consequence
Because ϕ solves (1.3), we deduce that $\zeta = \partial_1\phi$ solves the linearized equation, i.e.

$$\begin{cases} \Delta\zeta = 0 & \text{on} \quad \Omega, \\ A\zeta = 0 & \text{on} \quad \partial\Omega \end{cases}$$

Using (3.8), this implies immediately (3.7). □

Formal Corollary 3.2 (Values of the parameters for the correctors)
If ψ^1, ψ^2, ψ^2 solve respectively (1.9), (1.10), (1.11), then the values of the parameters $\overline{k}_0$ and $\overline{\beta}_0$ are given by (1.13).

Proof of Formal Corollary 3.2
Applying Formal Lemma 3.1 for $\Psi = \psi^1$ and using equation (1.9), we get

$$\begin{aligned} 0 &= \int_\Omega x_1(\partial_{11}\phi)\partial_1\phi + \int_{\partial\Omega} (\partial_1\phi)\left\{\beta x_1\partial_{11}\phi - \frac{\overline{\beta}_0}{2\alpha_0}(W''(\phi) - W''(0))\right\} \\ &= \int_\Omega -\frac{(\partial_1\phi)^2}{2} + \int_{\partial\Omega} -\frac{\beta(\partial_1\phi)^2}{2} + \frac{\overline{\beta}_0}{2}. \end{aligned}$$

where we have used integration by parts and the fact that $\phi(-\infty,0) = 0$, $\phi(+\infty,0) = 1$, $W'(0) = W'(1)$ and $\alpha_0 = W''(0)$. This identifies the value of $\overline{\beta}_0$. The reasoning is similar when dealing with ψ^2 and ψ^3. □

4 Preliminary computations

The goal of this section is to prove two technical results, namely Formal Lemmata 4.1 and 4.2, that will be used in the next section to do the proof of our main result.

In order to simplify the presention, we will use the following notations.

Abridged notations:

- $\xi_i^1 = \gamma_i(t)\left(\dfrac{x_1 - X_i(t)}{\varepsilon}\right)$,

- $\xi_i^2 = \dfrac{x_2}{\varepsilon}$,
- $\xi_i = (\xi_i^1, \xi_i^2)$,
- $\phi_i = \phi(\xi_i), \quad \psi_i^\alpha = \psi^\alpha(\xi_i), \quad \tilde{\phi}_i = \phi_i - H(\xi_i^1)$,
- $\partial_p \phi_i = (\partial_p \phi)(\xi_i), \quad \partial_{pq}\phi_i = (\partial_{pq}\phi)(\xi_i), \quad p, q = 1, 2$,
- $\partial_p \psi_i^\alpha = (\partial_p \psi^\alpha)(\xi_i), \quad \partial_{pq}\psi_i^\alpha = (\partial_{pq}\psi^\alpha)(\xi_i), \quad p, q = 1, 2$,
- $\partial_t \psi_i^\alpha = \dfrac{d}{dt}[\psi^\alpha(\xi_i)], \quad \partial_{tt}\psi_i^\alpha = \dfrac{d^2}{dt^2}[\psi^\alpha(\xi_i)]$.

Remark that in regards of the above notations, the function $\hat{u}^\varepsilon$ can be simply written

$$\hat{u}^\varepsilon = \sum_i \phi_i + \varepsilon \left\{ \frac{\sigma}{\alpha_0} - \sum_{i=1,..,N} \sum_{\alpha=1,2,3} a_i^\alpha \psi_i^\alpha \right\}. \tag{4.1}$$

Then we have the following result:

Formal Lemma 4.1 (Computation of $W'(\hat{u}^\varepsilon)$)
Assume (1.15) for some $\delta > 0$ and assume W smooth enough. Given the point $(x_1, t) \in \mathbb{R} \times [0, T]$, there exists $i_0 = i_0(x_1, t) \in \{1, 2, \ldots, N\}$ such that we have with the previous abridged notations for $x_2 = 0$ and for ε small enough (depending on δ):

$$W'(\hat{u}^\varepsilon(x_1, 0, t)) = W'(\tilde{\phi}_{i_0}) + \varepsilon W''(\tilde{\phi}_{i_0}) \left\{ \frac{\sigma(x_1, t)}{\alpha_0} - \sum_{\alpha=1,2,3} a_{i_0}^\alpha(t)\psi_{i_0}^\alpha - \frac{1}{\varepsilon} \sum_{i \in \{1,\ldots,N\} \setminus \{i_0\}} \frac{1}{\alpha_0 \pi \xi_i^1} \right\} + O_\delta(\varepsilon^2). \tag{4.2}$$

Proof of Formal Lemma 4.1
Using the expression (4.3) of $\hat{u}^\varepsilon$ and the periodicity of W', we can write

$$W'(\hat{u}^\varepsilon) \quad = \quad W'\left(\left(\sum_i \tilde{\phi}_i \right) + \varepsilon \left(\frac{\sigma}{\alpha_0} - \sum_i \sum_\alpha a_i^\alpha \psi_i^\alpha \right) \right).$$

We recall from (1.15) that the values of the $X_i(t)$ are well separated, i.e.

$$X_{i+1}(t) - X_i(t) \geq 2\delta > 0.$$

Then there exists an index $i_0 = i_0(x_1 t)$ (possibly non unique) such that

$$|x_1 - X_{i_0}(t)| = \inf_i |x_1 - X_i(t)|.$$

Step 1: computations for $i \neq i_0$
We have $|x_1 - X_i(t)| \geq \delta > 0$, which implies $|\xi_i^1| \geq \dfrac{\delta}{\varepsilon}$, and we deduce from the last line of conjecture (A) that

$$\phi_i - H(\xi_i^1) + \frac{1}{\alpha_0 \pi \xi_i^1} = O\left(\frac{1}{1 + (\delta/\varepsilon)^2} \right) = O_\delta(\varepsilon^2),$$

which shows that

$$\tilde{\phi}_i + \frac{1}{\alpha_0 \pi \xi_i^1} = O_\delta(\varepsilon^2). \tag{4.3}$$

Similarly, from the third line of (A), we deduce for $\alpha = 1, 2, 3$

$$|\psi_i^\alpha| \leq \frac{C}{1 + |\xi_i^1|} \leq \frac{C}{1 + \delta/\varepsilon} = O_\delta(\varepsilon). \tag{4.4}$$

Step 2: conclusion
From (4.3) and (4.4), we obtain

$$\left(\sum_i \tilde{\phi}_i\right) + \varepsilon\left(\frac{\sigma}{\alpha_0} - \sum_i \sum_\alpha a_i^\alpha \psi_i^\alpha\right) = \tilde{\phi}_{i_0} + \varepsilon\left(\frac{\sigma}{\alpha_0} - \sum_\alpha a_{i_0}^\alpha \psi_{i_0}^\alpha\right) + O_\delta(\varepsilon^2) - \sum_{i \neq i_0} \frac{1}{\alpha_0 \pi \xi_i^1},$$

that yields

$$W'(\hat{u}^\varepsilon) = W'(\tilde{\phi}_{i_0}) + W''(\tilde{\phi}_{i_0})\left\{\varepsilon\left[\frac{\sigma}{\alpha_0} - \sum_\alpha a_{i_0}^\alpha \psi_{i_0}^\alpha\right] - \sum_{i \neq i_0} \frac{1}{\alpha_0 \pi \xi_i^1}\right\} + O_\delta(\varepsilon^2),$$

where we have used a second order expansion of W' and the fact that $\frac{1}{\alpha_0 \pi \xi_i^1} = O_\delta(\varepsilon)$ for $i \neq i_0$. This is exactly (4.2). □

We also have the following result:

Formal Lemma 4.2 (Derivatives of the profile functions)
We recall that $\psi^0 = \phi$, and for $\alpha = 0, 1, 2, 3$, we set

$$\Psi_i^\alpha(x,t) := \psi^\alpha\left(\gamma_i(t)\left(\frac{x_1 - X_i(t)}{\varepsilon}\right), \frac{x_2}{\varepsilon}\right).$$

Under the assumptions and notations of Formal Lemma 4.1, the following holds for $(x,t) \in \mathbb{R} \times \mathbb{R}^+ \times [0,T]$

$$\begin{cases} \partial_1 \Psi_{i_0}^\alpha = \dfrac{\gamma_{i_0}}{\varepsilon} \partial_1 \psi_{i_0}^\alpha & \textit{and} \quad \partial_1 \Psi_i^\alpha = O_\delta(1) \ \textit{ if } i \neq i_0, \\ \partial_2 \Psi_{i_0}^\alpha = \dfrac{1}{\varepsilon} \partial_2 \psi_{i_0}^\alpha & \textit{and} \quad \partial_2 \Psi_i^\alpha = O_\delta(1) \ \textit{ if } i \neq i_0, \\ \partial_t \Psi_{i_0}^\alpha = -\dfrac{\gamma_{i_0} X'_{i_0}}{\varepsilon} \partial_1 \psi_{i_0}^\alpha + O(1) & \textit{and} \quad \partial_t \Psi_i^\alpha = O_\delta(1) \ \textit{ if } i \neq i_0, \\ \partial_{11} \Psi_{i_0}^\alpha = \dfrac{\gamma_{i_0}^2}{\varepsilon^2} \partial_{11} \psi_{i_0}^\alpha & \textit{and} \quad \partial_{11} \Psi_i^\alpha = O_\delta(1) \ \textit{ if } i \neq i_0, \end{cases} \tag{4.5}$$

and for all $i = 1, ..., N$

$$\begin{cases} \partial_{22} \Psi_i^\alpha = \dfrac{1}{\varepsilon^2} \partial_{22} \psi_i^\alpha \\ \partial_{tt} \Psi_i^\alpha = \dfrac{1}{\varepsilon^2} (\gamma_i X'_i)^2 \partial_{11} \psi_i^\alpha + \dfrac{J_i^\alpha}{\varepsilon} + O(1) \quad \textit{with} \quad J_i^\alpha := -2\gamma'_i X'_i \ \xi_i^1 \partial_{11} \psi_i^\alpha - (\gamma'_i X'_i + (\gamma_i X'_i)') \partial_1 \psi_i^\alpha \end{cases} \tag{4.6}$$

with

$$J^\alpha_{i_0} = O_\delta(1) \quad \textit{and} \quad J^\alpha_i = O_\delta(\varepsilon) \quad \textit{if} \quad i \neq i_0. \tag{4.7}$$

Proof of Formal Lemma 4.2
The computation of the space derivatives for $i = i_0$ are straightforward. For $i \neq i_0$, the estimates like $O_\delta(1)$ of the space derivatives $\partial_p \Psi^\alpha_i$ for $p = 1, 2$ and $\partial_{11}\Psi^\alpha_i$ follow from Conjecture (A).

We have

$$\partial_t \Psi^\alpha_i = \left(-\frac{\gamma_i X'_i}{\varepsilon} + \frac{\gamma'_i}{\gamma_i}\xi^1_i\right)\partial_1\psi^\alpha_i$$

and

$$\partial_{tt}\Psi^\alpha_i = \left(-\frac{\gamma_i X'_i}{\varepsilon} + \frac{\gamma'_i}{\gamma_i}\xi^1_i\right)^2 \partial_{11}\psi^\alpha_i + \left[-\frac{(\gamma_i X'_i)'}{\varepsilon} + \left(\frac{\gamma'_i}{\gamma_i}\right)'\xi^1_i + \frac{\gamma'_i}{\gamma_i}\left\{-\frac{\gamma_i X'_i}{\varepsilon} + \frac{\gamma'_i}{\gamma_i}\xi^1_i\right\}\right]\partial_1\psi^\alpha_i.$$

We first notice that the second line of (1.15) implies that γ_i is bounded, and then γ'_i is also bounded as a consequence of (1.6). Using again Conjecture (A), we immediately obtain the desired estimates for $\partial_t \Psi^\alpha_i$ and $\partial_{tt}\Psi^\alpha_i$ in each case $i = i_0$ and $i \neq i_0$. □

5 Proof of 1.1

The main result of this section is Formal Proposition 5.1 below which will imply Formal Result 1.1.

Formal Proposition 5.1 (Plugging the ansatz in the equations)
Let $\hat{u}^\varepsilon$ given by (1.5) with v^ε defined in (1.7) for general coefficients $a^\alpha_i(t)$ and for ϕ solution of (1.3) and for general $\psi^\alpha, \alpha = 1, 2, 3$ such that Conjecture (A) holds. We assume moreover that

$$|\Delta\psi^\alpha(x)| \leq \frac{C}{1 + |x_1|} \quad \textit{for} \quad \alpha = 1, 2, 3. \tag{5.1}$$

We assume (1.15) and also that W, σ are smooth enough. Then for any $(x, t) \in \mathbb{R} \times \mathbb{R}^+ \times [0, T]$, we have the following estimates with the index $i_0 = i_0(x_1, t)$ defined in Formal Lemma 4.1:

$$\begin{cases} \Box \hat{u}^\varepsilon = O_\delta(1) + \dfrac{1}{\varepsilon} I^1_{i_0}, \\ N_\varepsilon \hat{u}^\varepsilon = O_\delta(1) + \dfrac{1}{\varepsilon} I^2_{i_0}, \end{cases} \tag{5.2}$$

where

$$\begin{cases} I^1_i &= -\dfrac{1}{c_0^2}\left\{2\gamma'_i X'_i\ \xi^1_i \partial_{11}\phi_i + (\gamma'_i X'_i + (\gamma_i X'_i)')\partial_1\phi_i\right\} + \displaystyle\sum_{\alpha=1,2,3} a^\alpha_i(t)\Delta\psi^\alpha_i, \\ \\ I^2_i &= \dfrac{1}{\alpha_0}\left(-\sigma(X_i, t) + \dfrac{1}{\pi}\displaystyle\sum_{j\neq i}\dfrac{1}{\gamma_j(X_i - X_j)}\right)(W''(0) - W''(\phi_i)) \\ & \quad - \left\{2m\gamma'_i X'_i\ \xi^1_i \partial_{11}\phi_i + \left\{k\gamma_i X'_i + m(\gamma'_i X'_i + (\gamma_i X'_i)')\right\}\partial_1\phi_i\right\} + \displaystyle\sum_{\alpha=1,2,3} a^\alpha_i(t) A\psi^\alpha_i. \end{cases}$$

with

$$\left\{\begin{array}{l} \Delta\psi_i^\alpha := \partial_{11}\psi_i^\alpha + \partial_{22}\psi_i^\alpha, \\ A\psi_i^\alpha = \beta\partial_{11}\psi_i^\alpha + \partial_2\psi_i^\alpha - W''(\phi_i)\psi_i^\alpha. \end{array}\right.$$

Proof of Formal Result 1.1
Fom equations (1.9), (1.10) and (1.11) and Conjecture (A), we deduce that (5.1) holds. The same three equations also yield

$$\left\{\begin{array}{ll} \displaystyle\sum_{\alpha=1,2,3} a_i^\alpha \Delta\psi^\alpha = a_i^1 x_1 \partial_{11}\phi + a_i^2\partial_1\phi, & x_2 > 0, \\ \displaystyle\sum_{\alpha=1,2,3} a_i^\alpha A\psi^\alpha = \frac{f}{\alpha_0}(W''(\phi) - W''(0)) + \beta a_i^1 x_1\partial_{11}\phi + (\beta a_i^2 + a_i^3)\partial_1\phi, & x_2 = 0, \end{array}\right. \tag{5.3}$$

with

$$f := \overline{\beta}_0\left(-\frac{a_i^1}{2} + a_i^2\right) + \overline{k}_0 a_i^3.$$

Then we see that $I_i^1 = 0$ if and only if

$$\left\{\begin{array}{l} a_i^1 = \dfrac{2\gamma_i' X_i}{c_0^2}, \\ a_i^2 = \dfrac{\gamma_i' X_i' + (\gamma_i X_i')'}{c_0^2}, \end{array}\right. \tag{5.4}$$

and $I_i^2 = 0$ if and only if

$$\left\{\begin{array}{l} f = -\sigma(X_i,t) + \dfrac{1}{\pi}\displaystyle\sum_{j\neq i}\frac{1}{\gamma_j(X_i - X_j)}, \\ \beta a_i^1 = 2m\gamma_i' X_i', \\ \beta a_i^2 + a_i^3 = k\gamma_i X_i' + m(\gamma_i' X_i' + (\gamma_i X_i')'). \end{array}\right. \tag{5.5}$$

We therefore see that (5.4) and (5.5) are satisfied if and only if $\beta = mc_0^2$, the coefficients a_i^α are given by (1.8) and the ODE dynamics (1.6) for the coefficients m_0, k_0 given by (1.14). □

We now turn to the proof of Formal Proposition 5.1.

Proof of Formal Proposition 5.1
The proof is made in several steps.

Step 1: computation of $\Box\hat{u}^\varepsilon$
Using Formal Lemma 4.2 (precisely we use (4.6) and the fourth line of (4.5)), we get

$$\Box\hat{u}^\varepsilon = O_\delta(1) + \sum_i \left\{\frac{1}{\varepsilon^2}\left(A_1\phi_i + \varepsilon\frac{J_i^0}{c_0^2}\right) - \frac{1}{\varepsilon}\left\{\sum_{\alpha=1,2,3} a_i^\alpha(t)\left(A_1\psi_i^\alpha + \varepsilon\frac{J_i^\alpha}{c_0^2}\right)\right\}\right\},$$

where for $\alpha = 0, 1, 2, 3$

$$A_1\psi_i^\alpha := \left\{ \left(\frac{\gamma_i X_i'}{c_0}\right)^2 \partial_{11}\psi_i^\alpha - \gamma_i^2 \partial_{11}\psi_i^\alpha - \partial_{22}\psi_i^\alpha \right\} = -\Delta\psi_i^\alpha$$

which reads explicitly for $\alpha = 0$:

$$A_1\phi_i = -\Delta\phi_i = 0.$$

Using moreover (4.7) and (5.1), we get

$$\Box\hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon}\left\{ \frac{J_{i_0}^0}{c_0^2} - \sum_{\alpha=1,2,3} a_{i_0}^\alpha(t) A_1\psi_{i_0}^\alpha \right\} = O_\delta(1) + \frac{1}{\varepsilon} I_{i_0}^1.$$

Step 2: computation of $N_\varepsilon \hat{u}^\varepsilon$

Step 2.1: computation
Using Formal Lemma 4.2, we get

$$\begin{aligned} N_\varepsilon\hat{u}^\varepsilon = \;& O_\delta(1) + \frac{W'(\hat{u}^\varepsilon)}{\varepsilon^2} - \frac{\sigma}{\varepsilon} \\ & + \sum_i \left\{ \frac{1}{\varepsilon^2}(A_2\phi_i + \varepsilon m J_i^0 - \varepsilon k \gamma_i X_i' \partial_1\phi_i) - \frac{1}{\varepsilon} \sum_{\alpha=1,2,3} a_i^\alpha (A_2\psi_i^\alpha + \varepsilon m J_i^\alpha - \varepsilon k\gamma_i X_i'\partial_1\psi_i^\alpha) \right\} \end{aligned}$$

with for $\alpha = 0, 1, 2, 3$

$$A_2\psi_i^\alpha := \beta\left(\frac{(\gamma_i X_i')^2}{c_0^2}\partial_{11}\psi_i^\alpha - \gamma_i^2\partial_{11}\psi_i^\alpha \right) - \partial_2\psi_i^\alpha = -\beta\partial_{11}\psi_i^\alpha - \partial_2\psi_i^\alpha.$$

Using (4.7) and Conjecture (A), we deduce

$$N_\varepsilon\hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon^2}\left(W'(\hat{u}^\varepsilon) + A_2\phi_{i_0}\right) + \frac{1}{\varepsilon}\left\{ -\sigma + \frac{1}{\varepsilon}\sum_{i\neq i_0} A_2\phi_i + mJ_{i_0}^0 - k\gamma_{i_0}X_{i_0}'\partial_1\phi_{i_0} - \sum_{\alpha=1,2,3} a_{i_0}^\alpha A_2\psi_{i_0}^\alpha \right\}.$$

From equation (1.3) we have, for all $i = 1, ..., N$

$$A_2\phi_i = -W'(\phi_i) = -W'(\tilde{\phi}_i).$$

From Conjecture (A) we deduce that for $i \neq i_0$,

$$A_2\phi_i = -W''(0)\tilde{\phi}_i + O(\tilde{\phi}_i^2) = \frac{1}{\pi\xi_i^1} + O_\delta(\varepsilon^2),$$

then

$$N_\varepsilon\hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon^2}\Big(W'(\hat{u}^\varepsilon) - W'(\tilde{\phi}_{i_0})\Big) + \frac{1}{\varepsilon}\left\{ -\sigma + \sum_{i\neq i_0}\frac{1}{\pi\varepsilon\xi_i^1} + mJ_{i_0}^0 - k\gamma_{i_0}X_{i_0}'\partial_1\phi_{i_0} - \sum_{\alpha=1,2,3} a_{i_0}^\alpha A_2\psi_{i_0}^\alpha \right\}.$$

Using now Formal Lemma 4.1, we get

$$N_\varepsilon \hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon}\left\{ \begin{array}{l} W''(\tilde{\phi}_{i_0})\left\{\dfrac{\sigma}{\alpha_0} - \displaystyle\sum_{\alpha=1,2,3} a_{i_0}^\alpha \psi_{i_0}^\alpha - \sum_{i\neq i_0} \frac{1}{\alpha_0 \pi \varepsilon \xi_i^1}\right\} + \displaystyle\sum_{i\neq i_0}\frac{1}{\pi\varepsilon\xi_i^1} \\ -\sigma + mJ_{i_0}^0 - k\gamma_{i_0} X'_{i_0}\partial_1\phi_{i_0} - \displaystyle\sum_{\alpha=1,2,3} a_{i_0}^\alpha A_2 \psi_{i_0}^\alpha \end{array}\right\}.$$

Using the fact that

$$A_2\psi_{i_0}^\alpha = -A\psi_{i_0}^\alpha - W''(\phi_{i_0})\psi_{i_0}^\alpha$$

we get

$$N_\varepsilon \hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon}\left\{ \begin{array}{l} (W''(\tilde{\phi}_{i_0}) - W''(0))\left\{\dfrac{\sigma}{\alpha_0} - \displaystyle\sum_{i\neq i_0} \frac{1}{\alpha_0 \pi \varepsilon \xi_i^1}\right\} \\ +mJ_{i_0}^0 - k\gamma_{i_0} X'_{i_0}\partial_1\phi_{i_0} + \displaystyle\sum_{\alpha=1,2,3} a_{i_0}^\alpha A \psi_{i_0}^\alpha \end{array}\right\}. \tag{5.6}$$

Step 2.2: evaluation
We now write $\varepsilon\xi_i^1 = \gamma_i(X_{i_0} - X_i) + \dfrac{\gamma_i}{\gamma_{i_0}}\varepsilon\xi_{i_0}^1$ to obtain for $i \neq i_0$:

$$\frac{1}{\alpha_0\pi\varepsilon\xi_i^1} = \frac{1}{\alpha_0\pi\gamma_i(X_{i_0} - X_i)} + O_\delta(\varepsilon\xi_{i_0}^1),$$

where we have used assumption (1.15). Therefore

$$\frac{1}{\varepsilon}(W''(\tilde{\phi}_{i_0}) - W''(0))\sum_{i\neq i_0}\frac{1}{\alpha_0\pi\varepsilon\xi_i^1} \;=\; \frac{1}{\varepsilon}(W''(\tilde{\phi}_{i_0}) - W''(0))\sum_{i\neq i_0}\frac{1}{\alpha_0\pi\gamma_i(X_{i_0} - X_i)} + O_\delta(\xi_{i_0}^1\tilde{\phi}_{i_0}).$$

Finally, by plugging this relation into (5.6) and using Conjecture (A) to see that $O_\delta(\xi_{i_0}^1\tilde{\phi}_{i_0}) = O_\delta(1)$, we obtain the second equation of (5.2). □

Acknowledgments
The authors would like to thank an anonymous referee for his/her valuable remarks improving strongly the manuscript.

References

[1] M. Al Haj, N. Forcadel, R. Monneau, *Existence and uniqueness of traveling waves for fully overdamped Frenkel-Kontorova models*, Archive for Rational Mechanics and Analysis 210 (1) (2013), 45-99.

[2] X. Cabré and J. Solà-Morales *Layer solutions in a half-space for boundary reactions*, Comm. Pure Appl. Math., 58 (12): 1678-1732, 2005.

[3] C. Denoual, *Dynamic dislocation modeling by combining Peierls-Nabarro and Galerkin methods*, Physical Review B 70, 024106 (2004).

[4] C. Denoual, *Modeling dislocation by coupling Peierls-Nabarro and element-free Galerkin methods*, Comput. Methods Appl. Mech. Engrg. 196 (2007) 1915-192.

[5] A. El Hajj, H. Ibrahim and R. Monneau, *Dislocation dynamics: from microscopic models to macroscopic crystal plasticity*, Continuum Mech. Thermodyn. (2009) 21: 109123.

[6] J. D. Eshelby, *Uniformly moving dislocations*, Proc. Phys. Soc. A, 62, 307-314.

[7] A. Fino, H. Ibrahim and R. Monneau, *The Peierls-Nabarro model as a limit of a Frenkel-Kontorova model*, J. Differential Equations 252 (2012) 258-293.

[8] N. Forcadel, C. Imbert, R. Monneau, *Homogenization of fully overdamped Frenkel-Kontorova models*, Journal of Differential Equations 246 (3) (2009), 1057-1097.

[9] M. Gonzalez and R. Monneau, *Slow motion of particle systems as a limit of a reaction-diffusion equation with half-Laplacian in dimension one*, DCDS-A 32 (4) (2012), 1255-1286.

[10] J. R. Hirth and L. Lothe, *Theory of dislocations*, Second Edition. Malabar, Florida: Krieger, 1992.

[11] J. R. Hirth, H. M. Zbib and L. Lothe, *Forces on high velocity dislocations*, Model. Simul. Mater. Sci. Eng, 6 (2), 165-169.

[12] R. Monneau and S. Patrizi, *Homogenization of the Peierls-Nabarro model for dislocation dynamics*, J. Differential Equations 253 (7) (2012), 2064-2105.

[13] F. R. N. Nabarro, *Fifty-year study of the Peierls-Nabarro stress*, Material Science and Engineering A 234-236, p. 67-76, 1997.

[14] Y. P. Pellegrini, *Dynamic Peierls-Nabarro equations for elastically isotropic crystals*, Phys. Rev. B 81, 024101 (2010).

[15] L. Pillon, *Modélisations du mouvement instationnaire et des interactions de dislocations*, PhD thesis, Pierre et Marie Curie University, Paris, France, (2008).

[16] L. Pillon and C. Denoual, *Inertial and retardation effects for dislocation interactions*, Philosophical Magazine - Vol. 89 - Issue 2 - 2009 - pp. 127-141.

[17] L. Pillon, C. Denoual, R. Madec and Y. P. Pellegrini, *Influence of inertia on the formation of dislocation dipoles*, Journal de Physique IV (Proceedings), Volume 134, Issue 1, August 2006, pp.49-54.

[18] L. Pillon, C. Denoual and Y. P. Pellegrini, *Equation of motion for dislocations with inertial effects*, Phys. Rev. B 76, 224105 (2007).