

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

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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 a linear wave equation. The total displacement field creates a stress which makes move the dislocation itself. By symmetry, we can reduce the system to a 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. For the limit $\varepsilon \rightarrow 0$, we are formally able to identify a reduced ordinary differential equation model describing the dynamics of relativistic dislocations if a certain conjecture is assumed to be true.

Key words: Peierls–Nabarro model; Dislocation dynamics; Relativistic dynamics; Formal asymptotics; Reduced model

1 Introduction

1.1 Setting of the problem

In this paper, we consider a scalar Peierls–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 Peierls–Nabarro model (see (1.1) below) can 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 these dislocations move on the line $x_2 = 0$. The whole model can be seen as a coupling between the dynamics on the line $x_2 = 0$ and the dynamics outside the line $x_2 = 0$.

In the model that we consider, the phase field is a scalar quantity which can be identified with the scalar displacement of atoms in the crystal. This displacement satisfies a scalar elasto-dynamics equation, which is simply a linear wave equation in the plane outside the line $x_2 = 0$. By symmetry, we can reduce the problem to the wave equation in the half plane $x_2 > 0$ coupled with the 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 $\varepsilon \rightarrow 0$. More precisely, we consider a phase field $u^\varepsilon(x_1, x_2, t)$, which is a real function solution of the following system:

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

where the two operators \square 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:

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

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 dislocation and k can be seen as a damping factor that is classical for the evolution of the Peierls–Nabarro model (see, for instance, [9]). Here we use the notations $u_t = \frac{\partial u}{\partial t}$, $u_{tt} = \frac{\partial^2 u}{\partial t^2}$, $\partial_i u = \frac{\partial u}{\partial x_i}$, $\partial_{ii} u = \frac{\partial^2 u}{\partial x_i^2}$ 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 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 operator N_ε . The limit $\varepsilon \rightarrow 0$ has been studied rigorously in [9] in a particular case of $\beta = 0$, $c_0 = +\infty$ and $k = 1$, which corresponds to a quasi-static approximation.

In the present paper, our goal is to study formally the limit $\varepsilon \rightarrow 0$ for our more general model in the relativistic regime. In fact, contrary to [9, Theorem 1.1], where the passage to limit $\varepsilon \rightarrow 0$ 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) 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 $i = 1, \dots, N$ 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 with those dislocations is as follows,

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

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:

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

where m_0, k_0 are parameters that will be precised later. Our ordinary differential equation (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 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) that will slow down the motion of 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

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

where the coefficients a_i^α are given as

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

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

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

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

and

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

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)]. 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 the compatibility condition that forces the following values of the parameters:

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

We also define the following parameters:

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

where m_0 can be interpreted as a kind of effective mass of 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 as solutions for (1.3), (1.9), (1.10), (1.11), which satisfy with $\phi = \psi^0$:

$$\left\{ \begin{array}{l} |\nabla\psi^\alpha(x)| \leq \frac{C}{1 + |x_1|} \quad \alpha = 0, 1, 2, 3, \\ |\partial_{11}\psi^\alpha(x)| \leq \frac{C}{1 + |x_1|^2} \quad \alpha = 0, 1, 2, 3, \\ |\psi^\alpha(x_1, 0)| \leq \frac{C}{1 + |x_1|} \quad \alpha = 1, 2, 3, \\ \left| \phi(x_1, 0) - H(x_1) + \frac{1}{\alpha_0\pi x_1} \right| \leq \frac{C}{1 + |x_1|^2} \quad \text{if } |x_1| \geq 1. \end{array} \right.$$

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 Section 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 Peierls–Nabarro model)

Let us consider the assumptions of Section 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 $i = 1, 2, \dots, N$, satisfying

$$\left\{ \begin{array}{l} X_{i+1}(t) - X_i(t) \geq 2\delta > 0 \\ |X'_i| \leq c_0(1 - \delta), \quad \delta > 0 \end{array} \right\} \quad \text{for } t \in [0, T], \tag{1.15}$$

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

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

with γ_i as given by (1.4) and the parameters m_0, k_0 as given in (1.14). Let us consider the ansatz function \hat{u}^ε given by (1.5) and the correction term v^ε given by (1.7) with the

coefficients a_i^ε given by (1.8). Then for any fixed $\delta > 0$, we have $\varepsilon \rightarrow 0$,

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

Here we only get $O_\delta(1)$ on 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 partial differential equation of (1.16). An 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 a 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 the 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}^ε 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 as follows:

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

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) is the standard orthonormal basis and we had to subtract a Dirac mass in order to compensate the jump of u . The last integral is an energy term created by the misfit of upper and lower half crystal created by the presence of 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 following is the natural Peierls model:

$$\begin{cases} \mathcal{A}'_U = 0, \\ \bar{k} \eta_t = -\mathcal{A}'_\eta, \end{cases}$$

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 \bar{k} is a damping factor. Then it is easy to check that

$$u(x_1, x_2, t) = \begin{cases} 2U(x_1, x_2, t) & \text{if } x_2 > 0, \\ \eta(x_1, t) & \text{if } x_2 = 0, \end{cases}$$

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

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

assuming that $\text{div } \Sigma = 0$ and $\sigma(x_1, t) := 2e_2 \cdot \Sigma(x_1, 0, t)$ and $\bar{\beta} = \frac{\beta}{4}$. We have to emphasize the fact that model (2.2) in the special case $\bar{\beta} = 0$ 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 section 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 asymptotics for each profile function ψ^α for $\alpha = 0, 1, 2, 3$.

Case of $\psi^0 = \phi$

For the special case of $W'(u) = -\frac{1}{2\pi a} \sin \{2\pi(u - \frac{1}{2})\}$ 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 the 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 $x_1 \rightarrow \pm\infty$. 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 is neglectable 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

Note 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 to construct hull functions as in [8], and then travelling 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

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

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 corrector 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. Note that ϕ is an approximate solution of the left-hand side of (1.11). Looking at some function such as $C \min(\phi(x_1, x_2), \phi(-x_1, x_2))$ for a constant C large enough, it could be possible to construct such a supersolution and to get some information on the decay at infinity of ψ^3 such as $1/|x_1|$ as x_1 goes to infinity. Note 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 note 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

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

Then we can see that

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

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

outside its singularity) that $\bar{\theta}_2$ satisfies

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

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

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

solves

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

where it is reasonable to expect that $A\bar{\theta}_2$ 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 expected asymptotics.

Case of ψ^1

We note that

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

solves

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

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

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

then we deduce that

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

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

3.2 Properties of the correctors

Let us consider a function Ψ solution of

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

Formal Lemma 3.1 (Compatibility condition)

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

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

where ϕ is a 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.

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

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

Formal Corollary 3.2 (Values of the parameters of correctors)

If ψ^1, ψ^2, ψ^3 solve respectively (1.9), (1.10), (1.11), then the values of the parameters \bar{k}_0 and $\bar{\beta}_0$ 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

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

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 $\bar{\beta}_0$. 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, which will be used in the next section to do the proof of our main result.

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

Abridged notations:

- $\xi_i^1 = \gamma_i(t) \left(\frac{x_1 - X_i(t)}{\varepsilon} \right),$
- $\xi_i^2 = \frac{x_2}{\varepsilon},$
- $\xi_i = (\xi_i^1, \xi_i^2),$
- $\phi_i = \phi(\xi_i), \quad \psi_i^\alpha = \psi^\alpha(\xi_i), \quad \tilde{\phi}_i = \phi_i - H(\xi_i^1),$
- $\partial_p \phi_i = (\partial_p \phi)(\xi_i), \quad \partial_{pq} \phi_i = (\partial_{pq} \phi)(\xi_i), \quad p, q = 1, 2,$
- $\partial_p \psi_i^\alpha = (\partial_p \psi^\alpha)(\xi_i), \quad \partial_{pq} \psi_i^\alpha = (\partial_{pq} \psi^\alpha)(\xi_i), \quad p, q = 1, 2,$
- $\partial_t \psi_i^\alpha = \frac{d}{dt} [\psi^\alpha(\xi_i)], \quad \partial_{tt} \psi_i^\alpha = \frac{d^2}{dt^2} [\psi^\alpha(\xi_i)].$

Remark that with regard of the above notations, the function \hat{u}^ε can be simply written as

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

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 to be smooth enough. Given the point $(x_1, t) \in \mathbb{R} \times [0, T]$, there exists $i_0 = i_0(x_1, t) \in \{1, 2, \dots, N\}$ such that we have with the previous abridged notations for $x_2 = 0$ and for ε small enough (depending on δ):

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

Proof of Formal Lemma 4.1

Using the expression (4.3) of \hat{u}^ε and the periodicity of W' , we can write

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

We recall from (1.15) that the values of $X_i(t)$ 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 $|\xi_i^1| \geq \frac{\delta}{\varepsilon}$, 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 Conjecture (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

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

which 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 profile functions)

We recall that $\psi^0 = \phi$, and for $\alpha = 0, 1, 2, 3$, we set

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

Under the assumptions and notations of Formal Lemma 4.1, the following holds for $(x, t) \in$

$\mathbb{R} \times \mathbb{R}^+ \times [0, T]$

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

and for all $i = 1, \dots, N$

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

with

$$J_{i_0}^\alpha = O_\delta(1) \quad \text{and} \quad J_i^\alpha = O_\delta(\varepsilon) \quad \text{if } i \neq i_0. \tag{4.7}$$

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 such as $O_\delta(1)$ of the space derivatives $\partial_p \Psi_i^\alpha$ for $p = 1, 2$ and $\partial_{11} \Psi_i^\alpha$ follow from Conjecture (A).

We have

$$\partial_t \Psi_i^\alpha = \left(-\frac{\gamma_i X'_i}{\varepsilon} + \frac{\gamma'_i \xi_i^1}{\gamma_i} \right) \partial_1 \psi_i^\alpha$$

and

$$\partial_{tt} \Psi_i^\alpha = \left(-\frac{\gamma_i X'_i}{\varepsilon} + \frac{\gamma'_i \xi_i^1}{\gamma_i} \right)^2 \partial_{11} \psi_i^\alpha + \left[-\frac{(\gamma_i X'_i)'}{\varepsilon} + \left(\frac{\gamma'_i}{\gamma_i} \right)' \xi_i^1 + \frac{\gamma'_i}{\gamma_i} \left\{ -\frac{\gamma_i X'_i}{\varepsilon} + \frac{\gamma'_i \xi_i^1}{\gamma_i} \right\} \right] \partial_1 \psi_i^\alpha.$$

We first note 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 $\partial_t \Psi_i^\alpha$ and $\partial_{tt} \Psi_i^\alpha$, in each case $i = i_0$ and $i \neq i_0$. □

5 Proof of 1.1

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

Formal Proposition 5.1 (Plugging ansatz in equations)

Let \hat{u}^ε is given by (1.5) with v^ε as defined in (1.7) for general coefficients $a_i^\alpha(t)$ and for ϕ solution of (1.3) and for general $\psi^\alpha, \alpha = 1, 2, 3$, such that Conjecture (A) holds. Moreover,

we assume that

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

We assume that (1.15) and also 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:

$$\begin{cases} \square \hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon} I_{i_0}^1, \\ N_\varepsilon \hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon} I_{i_0}^2, \end{cases} \tag{5.2}$$

where

$$\begin{cases} I_i^1 = -\frac{1}{c_0^2} \{2\gamma'_i X'_i \xi_i^1 \partial_{11} \phi_i + (\gamma'_i X'_i + (\gamma_i X'_i)') \partial_1 \phi_i\} + \sum_{\alpha=1,2,3} a_i^\alpha(t) \Delta \psi_i^\alpha, \\ I_i^2 = \frac{1}{\alpha_0} \left(-\sigma(X_i, t) + \frac{1}{\pi} \sum_{j \neq i} \frac{1}{\gamma_j(X_i - X_j)} \right) (W''(0) - W''(\phi_i)) \\ \quad - \{2m\gamma'_i X'_i \xi_i^1 \partial_{11} \phi_i + \{k\gamma_i X'_i + m(\gamma'_i X'_i + (\gamma_i X'_i)')\} \partial_1 \phi_i\} + \sum_{\alpha=1,2,3} a_i^\alpha(t) A \psi_i^\alpha. \end{cases}$$

with

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

Proof of Formal Result 1.1

From equations (1.9), (1.10) and (1.11) and Conjecture (A), we deduce that (5.1) holds. The same three equations also yield

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

with

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

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

$$\begin{cases} a_i^1 = \frac{2\gamma'_i X_i}{c_0^2}, \\ a_i^2 = \frac{\gamma'_i X'_i + (\gamma_i X'_i)'}{c_0^2}, \end{cases} \tag{5.4}$$

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

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

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 is 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 $\square \hat{u}^\varepsilon$

Using Formal Lemma 4.2 (precisely we use (4.6) and the fourth line of (4.5)), we get

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

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 $\alpha = 0$:

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

Moreover, using (4.7) and (5.1), we get

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

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

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

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 $i = 1, \dots, N$,

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

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

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

then

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

Using now Formal Lemma 4.1, we get

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

Using the fact that

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

we get

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

Step 2.2: Evaluation

We now write $\varepsilon \xi_i^1 = \gamma_i(X_{i_0} - X_i) + \frac{\gamma_i}{\gamma_{i_0}} \varepsilon \xi_{i_0}^1$ 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,

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

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

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References

- [1] AL HAJ, M., FORCADEL, N. & MONNEAU, R. (2013) Existence and uniqueness of traveling waves for fully overdamped Frenkel-Kontorova models. *Arch. Ration. Mech. Anal.* **210**(1), 45–99.
- [2] CABRÉ, X. & SOLÀ-MORALES, J. (2005) Layer solutions in a half-space for boundary reactions. *Comm. Pure Appl. Math.* **58**(12), 1678–1732.
- [3] DENOUAL, C. (2004) Dynamic dislocation modeling by combining Peierls-Nabarro and Galerkin methods. *Phys. Rev. B* **70**, 024106.
- [4] DENOUAL, C. (2007) Modeling dislocation by coupling Peierls-Nabarro and element-free Galerkin methods. *Comput. Methods Appl. Mech. Eng.* **196**, 1915–1923.
- [5] EL HAJJ, A., IBRAHIM, H. & MONNEAU, R. (2009) Dislocation dynamics: From microscopic models to macroscopic crystal plasticity. *Contin. Mech. Thermodyn.* **21**, 109–123.
- [6] ESHELBY, J. D. (1949) Uniformly moving dislocations. *Proc. Phys. Soc. A* **62**, 307–314.
- [7] FINO, A., IBRAHIM, H. & MONNEAU, R. (2012) The Peierls-Nabarro model as a limit of a Frenkel-Kontorova model. *J. Differ. Equ.* **252**, 258–293.
- [8] FORCADEL, N., IMBERT, C. & MONNEAU, R. (2009) Homogenization of fully overdamped Frenkel-Kontorova models. *J. Differ. Equ.* **246**(3), 1057–1097.
- [9] GONZALEZ, M. & MONNEAU, R. (2012) Slow motion of particle systems as a limit of a reaction-diffusion equation with half-Laplacian in dimension one. *Discrete Contin. Dyn. Syst. A* **32**(4), 1255–1286.
- [10] HIRTH, J. R. & LOTHE, L. (1992) *Theory of Dislocations*, 2nd ed. Krieger, Malabar, FL.
- [11] HIRTH, J. R., ZBIB, H. M. & LOTHE, L. (1998) Forces on high velocity dislocations. *Model. Simul. Mater. Sci. Eng.* **6**(2), 165–169.
- [12] MONNEAU, R. & PATRIZI, S. (2012) Homogenization of the Peierls-Nabarro model for dislocation dynamics. *J. Differ. Equ.* **253**(7), 2064–2105.
- [13] NABARRO, F. R. N. (1997) Fifty-year study of the Peierls-Nabarro stress. *Mater. Sci. Eng. A* **234–236**, 67–76.

- [14] PELLEGRINI, Y. P. (2010) Dynamic Peierls-Nabarro equations for elastically isotropic crystals. *Phys. Rev. B* **81**, 024101.
- [15] PILLON, L. (2008) *Modélisations du Mouvement Instationnaire et des Interactions de Dislocations*, PhD thesis, Pierre et Marie Curie University, Paris, France.
- [16] PILLON, L. & DENOVAL, C. (2009) Inertial and retardation effects for dislocation interactions. *Phil. Mag.* **89**(2), 127–141.
- [17] PILLON, L., DENOVAL, C., MADEC, R. & PELLEGRINI, Y. P. (August 2006) Influence of inertia on the formation of dislocation dipoles. *J. Phys. IV (Proc.)* **134**(1), 49–54.
- [18] PILLON, L., DENOVAL, C. & PELLEGRINI, Y. P. (2007) Equation of motion for dislocations with inertial effects. *Phys. Rev. B* **76**, 224105.