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

H. IBRAHIM ^{†,‡}, R. MONNEAU ^{*}

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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 $\varepsilon \rightarrow 0$, we are formally able to identify a reduced ODE model describing the dynamics of relativistic dislocations.

AMS subject classifications: 70H40, 45M05, 35D30

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 [11] for an overview on the Peierls-Nabarro model. Our scalar Peierls-Nabarro model (see (1.1) below) can

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be seen as a scalar simplification of the vectorial Peierls-Nabarro Galerkin model introduced in [2] (see also [3]).

A dislocation is a defect in a crystal and creates a stress field in the material (see [8]). 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 $\varepsilon \rightarrow 0$. More precisely we consider a phase field $u^\varepsilon(x_1, x_2, t)$ which is a real function solution of the following system

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

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:

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

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 [7]). Here we use the notation $u_t = \frac{\partial u}{\partial t}$, $u_{tt} = \frac{\partial^2 u}{\partial t^2}$, $\partial_i u = \frac{\partial u}{\partial x_i}$, $\partial_{ii} u = \frac{\partial^2 u}{\partial x_i^2}$ 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 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 $\varepsilon \rightarrow 0$ has been studied rigorously in [7] in the particular case $\beta = 0$, $c_0 = +\infty$ and $k = 1$, which corresponds to a quasistatic 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.

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:

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

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:

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

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

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

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 which impose the following asymptotical dynamics:

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

where m_0, k_0 are parameters that will be precised later. Our ODE dynamics (1.6) is similar to equation (1) in [15].

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 [9] for screw dislocations (see also (3.12) in [13]).

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 [13], for the Eshelby approximation [5]. 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 Theorem 1.1.

1.2 Assumptions

We will choose

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

where the coefficients a_i^α are given by

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

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

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

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

and

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

where the linearized operator A is defined by:

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

It is possible to see (see Corollary 3.2) that those correctors can only exist if they satisfy a compatibility condition which forces the following values of the parameters:

$$\bar{k}_0 = \int_{\{x_2=0\}} (\partial_1 \phi)^2 \quad \text{and} \quad \bar{\beta}_0 = \int_{\{x_2>0\}} (\partial_1 \phi)^2 + \int_{\{x_2=0\}} \beta (\partial_1 \phi)^2. \quad (1.12)$$

We also define the following parameters

$$k_0 = \bar{k}_0 k \quad \text{and} \quad m_0 = \frac{\bar{\beta}_0}{c_0^2} = \frac{1}{c_0^2} \int_{\{x_2>0\}} (\partial_1 \phi)^2 + m \int_{\{x_2=0\}} (\partial_1 \phi)^2, \quad (1.13)$$

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 $H(x_1) = \mathbf{1}_{[0,+\infty)}(x_1)$. We consider the

following assumptions on the *profile functions* ψ^α , $\alpha = 0, 1, 2, 3$,

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

1.3 The main result

We show the following theorem:

Theorem 1.1 (*Reduced ODE dynamics as an asymptotic of the PN model*)

Let us consider the assumptions of Subsection 1.2, and assume W and σ smooth enough. For $i = 1, 2, \dots, N$, let us consider particles $X_i = X_i(t)$ satisfying

$$\left\{ \begin{array}{l} X_{i+1}(t) - X_i(t) \geq 2\delta > 0 \\ |X'_i| \leq c_0(1 - \delta), \quad \delta > 0 \end{array} \right\} \quad \text{for } t \in [0, T], \quad (1.14)$$

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

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

with γ_i is given by (1.4) and the parameters m_0, k_0 are given in (1.13). 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^α given by (1.8). Then for any fixed $\delta > 0$, we have as $\varepsilon \rightarrow 0$

$$\left\{ \begin{array}{l} \square \hat{u}^\varepsilon = O_\delta(1) \quad \text{uniformly in } L^\infty(\{x_2 > 0\} \times (0, T)) \\ N_\varepsilon \hat{u}^\varepsilon = O_\delta(1) \quad \text{uniformly in } L^\infty(\{x_2 = 0\} \times (0, T)). \end{array} \right. \quad (1.15)$$

Here we only get $O_\delta(1)$ right hand sides of (1.15). 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 (1.15). The important consequence of this result is the identification of the limit dynamics (1.6). We leave open the rigorous justification of this limit dynamics. The question of long time existence of solutions of the reduced ODE dynamics (1.6) is also open.

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 [12, 14, 16].

The interested reader can also consult [6] 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 [4, 10] 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 Theorem 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

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

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) 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 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

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

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 $\bar{W} = \frac{1}{4}W$. More generally, we recover (1.1) if we consider the general action

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

assuming that $\operatorname{div} \Sigma = 0$ 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 [2], where the displacement U is vectorial.

3 Some remarks on the correctors

For the special case of $W'(u) = -\frac{1}{2\pi a} \sin \left\{ 2\pi \left(u - \frac{1}{2} \right) \right\}$ for some $a > 0$, we recall (see [7]) that the solution ϕ_0 of (1.3) for $\beta = 0$ is

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

We also refer to [1] for properties of ϕ_0 in the case $\beta = 0$ for more general potentials W . From expression (3.1), it can be seen that assumption (A) on the profile functions, sounds reasonable (even if we have no proof of it, and the goal of the present paper is not to prove any rigorous results in this direction).

Let us consider a function Ψ solution of

$$\begin{cases} \Delta \Psi = F & \text{on } \Omega := \{x_2 > 0\}, \\ A\Psi = G & \text{on } \partial\Omega = \{x_2 = 0\}. \end{cases} \quad (3.2)$$

Lemma 3.1 (Compatibility condition)

If Ψ solves (3.2) with sufficient decay at infinity, then we have

$$\int_{\Omega} F\zeta + \int_{\partial\Omega} G\zeta = 0 \quad \text{with } \zeta = \partial_1 \phi \quad (3.3)$$

where ϕ is the solution of (1.3).

Proof of 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

$$\int_{\Omega} (\Delta\Psi)\Phi + \int_{\partial\Omega} (A\Psi)\Phi = \int_{\Omega} \Psi(\Delta\Phi) + \int_{\partial\Omega} \Psi(A\Phi). \quad (3.4)$$

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 (3.4), this implies immediately (3.3). □

Corollary 3.2 (Values of the parameters for the 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 (1.12).

Proof of Corollary 3.2

Applying 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 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 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 in regards of the above notations, the function \hat{u}^ε can be simply written

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

Then we have the following result:

Lemma 4.1 (Computation of $W'(\hat{u}^\varepsilon)$)

Assume (1.14) for some $\delta > 0$ and assume W smooth enough. Given the point $(x_1, t) \in \mathbb{R} \times [0, T]$, there exists $i_0 = i_0(x_1, t) \in \{1, 2, \dots, N\}$ such that we have with the previous abridged notations for $x_2 = 0$ and for ε small enough (depending on δ):

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

Proof of 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 (1.14) 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 $|\xi_i^1| \geq \frac{\delta}{\varepsilon}$, and we deduce from the last line of assumption (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

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

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

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

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). \square

We also have the following result:

Lemma 4.2 (Derivatives of the profile functions)

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

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

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

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

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

$$\left\{ \begin{array}{l} \partial_{22} \Psi_i^\alpha = \frac{1}{\varepsilon^2} \partial_{22} \psi_i^\alpha \\ \partial_{tt} \Psi_i^\alpha = \frac{1}{\varepsilon^2} (\gamma_i X'_i)^2 \partial_{11} \psi_i^\alpha + \frac{J_i^\alpha}{\varepsilon} + O(1) \end{array} \right. \quad \text{with } J_i^\alpha := -2\gamma'_i X'_i \xi_i^1 \partial_{11} \psi_i^\alpha - (\gamma'_i X'_i + (\gamma_i X'_i)') \partial_1 \psi_i^\alpha \quad (4.6)$$

with

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

Proof of 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 $\partial_p \Psi_i^\alpha$ for $p = 1, 2$ and $\partial_{11} \Psi_i^\alpha$ follow from assumption (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 notice that the second line of (1.14) implies that γ_i is bounded, and then γ_i' is also bounded as a consequence of (1.6). Using again assumptions (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 $i \neq i_0$. \square

5 Proof of Theorem 1.1

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

Proposition 5.1 (Plugging the ansatz in the equations)

Let \hat{u}^ε given by (1.5) with v^ε 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 assumption (A) holds. We assume moreover that

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

We assume (1.14) 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 Lemma 4.1:

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

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 Theorem 1.1

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

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

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

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

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

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

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 (1.13). \square

We now turn to the proof of Proposition 5.1.

Proof of Proposition 5.1

The proof is made in several steps.

Step 1: computation of $\square \hat{u}^\varepsilon$

Using 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 $\alpha = 0$:

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

Using moreover (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 Lemma 4.2, we get

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

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 assumption (A), we deduce

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

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

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

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

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

then

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

Using now Lemma 4.1, we get

$$N_\varepsilon\hat{u}^\varepsilon = O_\delta(1) + \frac{1}{\varepsilon} \left\{ W''(\tilde{\phi}_{i_0}) \left\{ \frac{\sigma}{\alpha_0} - \sum_{\alpha=1,2,3} a_{i_0}^\alpha \psi_{i_0}^\alpha - \sum_{i \neq i_0} \frac{1}{\alpha_0 \pi \varepsilon \xi_i^1} \right\} + \sum_{i \neq i_0} \frac{1}{\pi \varepsilon \xi_i^1} \right\}.$$

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

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

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 (1.14). 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 assumption (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). \square

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