R. Benguria · J. Dolbeault ·
R. Monneau

Harnack inequalities and discrete – continuum error estimates for a chain of atoms with two – body interactions

March 26, 2008

Abstract We consider deformations in $\mathbb{R}^3$ of an infinite linear chain of atoms where each atom interacts with all others through a two-body potential. We compute the effect of an external force applied to the chain. At equilibrium, the positions of the particles satisfy an Euler-Lagrange equation. For large classes of potentials, we prove that every solution is well approximated by the solution of a continuous model. We establish an error estimate between the discrete and the continuous solution based on a Harnack lemma of independent interest. Finally we apply our results to some Lennard–Jones potentials.

Keywords Two-body interactions · nonlinear elasticity · discrete-continuum · error estimates · Cauchy-Born rule · Harnack inequality · thermodynamic limit.

Mathematics Subject Classification (2000) 35J15 · 49M25 · 65L70 · 74A60 · 74G15

1 Introduction

In this paper, we are interested in the elastic behavior of a chain of atoms with two-body interactions. We consider in $\mathbb{R}^3$ and more generally in $\mathbb{R}^d$,

R. Benguria
Departamento de Fisica, Pontificia Universidad Católica de Chile, Casilla 306, Santiago 22, Chile. E-mail: rbenguri@puc.cl

J. Dolbeault
Ceremade (UMR CNRS no. 7534), Université Paris-Dauphine, Place de Lattre de Tassigny, 75775 Paris Cédex 16, France. E-mail: dolbeaul@ceremade.dauphine.fr

R. Monneau
CERMICS, Ecole nationale des Ponts et Chaussées, 6 et 8 avenue Blaise Pascal, Cité Descartes, Champs-sur-Marne, 77455 Marne-la-Vallée Cedex 2, France. E-mail: monneau@cermics.enpc.fr

$d \geq 1$, deformations of an infinite chain of atoms which are initially aligned with constant inter-atomic spacing.

The Cauchy-Born rule states that, when submitted to a small strain, the positions of the atoms follow the displacement of the material at macroscopic level. Our main result, see Theorem 1, is that the Cauchy-Born rule applies, up to a small error that we estimate in terms of the two-body potential of interaction.

From a mathematical point of view, the key tool is *an estimate of Harnack type,* which constitutes our second main result. This estimate is of its own interest for the understanding of thermodynamical limits, which correspond here to the case when the number of atoms in the chain per unit length tends to infinity.

1.1 Setting of the problem

Denote by V_0 the two–body potential as a function of the distance between the atoms, and define

$$V(L) = V_0(|L|) \quad \text{for every } L \in \mathbb{R}^d\,.$$

For any vector $L \in \mathbb{R}^d$, we define the energy per atom of the perfect lattice $\{k\,L\}_{k\in\mathbb{Z}}$ by

$$W(L) = W_0(|L|) \quad \text{where} \quad W_0(r) = \sum_{k\in\mathbb{N}\setminus\{0\}} V_0(|k|\,r)\,.$$

By *perfect lattice,* we mean a lattice for which, for some $L^* \in \mathbb{R}^d$, $X_k^* = k\,L^*$ for any $k \in \mathbb{Z}$. Since it is one-dimensional, we shall also call it a *perfect chain* of atoms. We assume that the two–body potential V_0 decays sufficiently fast to zero at infinity in order that the series converges.

The macroscopic description

Let us now consider a map $\Phi : \mathbb{R} \longmapsto \mathbb{R}^d$ satisfying the following macroscopic "linear + periodic" condition

$$\Phi(x+k) = \Phi(x) + k\,L^0 \quad \text{for any } k \in \mathbb{Z}\,,\ x \in \mathbb{R}\,, \tag{1.1}$$

for some given vector $L_0 \in \mathbb{R}^d$. This periodicity condition provides us with some suitable compactness properties, which simplify the presentation and the proof of the results. We are interested in the following macroscopic equation of the equilibrium of the material in nonlinear elasticity

$$\big(\nabla W(\Phi')\big)' = f \quad \text{on } \mathbb{R}\,, \tag{1.2}$$

for some force $f : \mathbb{R} \to \mathbb{R}^d$ which is 1-periodic,

$$f(x+k) = f(x) \quad \text{for any } k \in \mathbb{Z}\,,\ x \in \mathbb{R}\,,$$

and satisfies the compatibility assumption

$$\int_{\mathbb{R}/\mathbb{Z}} f\,dx = 0\,.$$

The microscopic description

The heuristic idea is that the sequence $\big(\Phi(k\,\varepsilon)\big)_{k\in\mathbb{Z}}$ is a good approximation of the positions X_k^ε of the atoms of the chain, with interdistances of the order of ε, small. After the rescaling

$$X_k = \frac{1}{\varepsilon}\, X_k^\varepsilon\,,$$

the positions of the atoms of the chain are described by the map

$$\begin{aligned} X : \mathbb{Z} \;&\rightarrow\; \mathbb{R}^d,\\ k \;&\longmapsto\; X_k\,. \end{aligned}$$

We introduce the formal, infinite energy

$$E(X) = \frac{1}{2} \sum_{\substack{j,k\,\in\,\mathbb{Z},\\ j\neq k}} V(X_j - X_k) + \sum_{j\in\mathbb{Z}} X_j\cdot f_j\,,$$

where each $f_k \in \mathbb{R}^d$ represents the force acting on the atom at position X_k. Although the energy is not well–defined, the Euler–Lagrange equation makes sense under suitable assumptions on the two–body potential V and on the lattice X. We get

$$f_j + \sum_{k\in\mathbb{Z}\setminus\{j\}} \nabla V(X_j - X_k) = 0 \quad \text{for all } j\in\mathbb{Z}\,. \tag{1.3}$$

We now consider any integer N_ε large enough, assume that $\varepsilon = 1/N_\varepsilon$, and require that the positions of the atoms satisfy the following microscopic "linear + periodic" condition

$$X_{k+N_\varepsilon\, j} = X_k + N_\varepsilon\, j\, L^0 \quad \text{for any } j,\, k\in\mathbb{Z}\,. \tag{1.4}$$

We shall assume that the force acting on the k^{th} atom is given by

$$f_k = \int_{\varepsilon(k-\frac{1}{2})}^{\varepsilon(k+\frac{1}{2})} f(x)\, dx \quad \text{for any } k\in\mathbb{Z}\,, \tag{1.5}$$

which satisfies in particular the microscopic periodicity condition

$$f_{k+N_\varepsilon\, j} = f_k \quad \text{for any } j,\, k\in\mathbb{Z}$$

and the compatibility condition

$$\sum_{i=1}^{N_\varepsilon} f_i = 0\,.$$

Our goal is to give an error estimate between the interdistance of the atoms $X_{k+1} - X_k$ corresponding to (1.3)-(1.4) and the macroscopic deformation $\Phi'(k\,\varepsilon)$ of the continuous solution to the equations of nonlinear elasticity, (1.1)-(1.2). To this end we need some natural assumptions on the potentials.

1.2 Invertibility assumptions

Invertibility assumption at macroscopic level

First we assume that there exists $L^* \in \mathbb{R}^d$ with $L^* \neq 0$, such that

$$A_{ij} := \frac{\partial^2 W}{\partial L^i \, \partial L^j (L^*)} \quad \text{for any } i,\, j = 1,\, 2,\, \dots\, d$$

satisfies the following non-degeneracy assumption.

Assumption (A1)

The matrix $A = (A_{ij})$ is invertible.

Let us remark that by construction we have for the potential W_0:

$$W(L) = W_0(|L|) \quad \text{for any } L \in \mathbb{R}^d\,.$$

In particular, this implies that for $d \geq 2$

$$A = W_0''(|L^*|)\,\frac{L^*}{|L^*|} \otimes \frac{L^*}{|L^*|} + \frac{W_0'(|L^*|)}{|L^*|}\left(\mathrm{Id} - \frac{L^*}{|L^*|} \otimes \frac{L^*}{|L^*|}\right),$$

while for $d = 1$, we only have

$$A = W_0''(|L^*|)\,.$$

Invertibility assumption at microscopic level

To establish the stability of the lattice generated by the vector L^*, we consider the formal Hessian of the energy, which for $X_k^* = k\,L^*$ is defined by

$$E''(X^*) \cdot (Y, Y) := \sum_{i \in \mathbb{Z}} Y_i \cdot (B * Y)_i\,,$$

with

$$(B * Y)_i := \sum_{j \in \mathbb{Z}} B_{i-j} \cdot Y_j \quad \text{where } B_l = \begin{cases} \displaystyle\sum_{k \in \mathbb{Z}\setminus\{0\}} H_k^* & \text{if } l = 0\,, \\ -H_l^* & \text{if } l \neq 0\,, \end{cases} \tag{1.6}$$

and

$$H_k^* := D^2 V(k\,L^*)\,. \tag{1.7}$$

By construction, we see that the perfect chains, that is $Y = (Y_k)_{k \in \mathbb{Z}}$ with $Y_k = Y_0$ for any $k \in \mathbb{Z}$, are in the kernel of B, which is natural because of the invariance under translations of the problem. Let us call E_0 the energy E in the special case of zero forces, $f_k = 0$ for any $k \in \mathbb{Z}$, and set

$$\big(E_0'(X)\big)_j = \sum_{k \in \mathbb{Z}\setminus\{j\}} \nabla V(X_j - X_k)\,.$$

Let X^* be a perfect lattice. We see that for any $M \in \mathbb{R}^{d\times d}$, the lattice $(\mathrm{Id} + t\,M)X^*$ is also a perfect lattice, and then satisfies the equation of equilibrium (1.3) with zero forces:

$$E_0'\big((\mathrm{Id} + t\,M)\,X^*\big) = 0\,.$$

Here by $M\,X^*$, we denote the lattice made of the points kML^*, $k \in \mathbb{Z}$. Differentiating the equation with respect to t at $t = 0$, we get

$$E_0''(X^*) \cdot (MX) = 0\,,$$

which gives

$$B \cdot MX^* = 0\,.$$

We shall assume that the kernel of B is generated by the image of X^* by all translations and linear transforms based as above on a matrix in $\mathbb{R}^d \times \mathbb{R}^d$. More precisely, we make the following invertibility/stability–type assumption:

Assumption (A2)

There exists a positive constant C such that

$$\Big(|Y_{k+1} + Y_{k-1} - 2Y_k| \le C \quad \textit{and} \quad B\cdot Y = 0\Big) \\ \Longrightarrow \qquad Y = MX^* + b \quad \textit{for some } M \in \mathbb{R}^{d\times d},\ b \in \mathbb{R}^d\,.$$

If there was another element Y^* of this type in the kernel of B, this would mean that there is a deformation of the crystal (different from the above transforms) which does not change the energy up to the second order. In other words, the crystal would then have a possible instability in the direction Y^*. The true instability property (or possibly the stability) of the crystal should then be studied by the mean of an analysis of the higher order terms in the expansion of the energy.

1.3 Main results

In order to state our main results, we need some regularity and decay properties of the potential.

Assumption (A3)

$$W_0 \in C^3(0,+\infty)\,, \quad V_0 \in C^2 \cap W^{3,\infty}_{\mathrm{loc}}(0,+\infty)\,,$$

and for some $p > 1$, we assume that

$$\sup_{r\ge 1}\, r^p \left[|V_0(r) + r\,|V_0'(r)| + r^2\,|V_0''(r)| + r^3\,|V_0'''(r)|\right] < \infty\,.$$

For a given crystal lattice X, we can define its local distance to the perfect lattice $X^*_k = k\,L^*$ by

$$D_k(X, L^*) := \sup_{e \in Q_1} |X_{k+e} - X_k - e\,L^*| \,,$$

where for $n \in \mathbb{N} \setminus \{0\}$ we set the box

$$Q_n := \{e \in \mathbb{Z} \;:\; |e| \leq n\} \;.$$

Theorem 1 (Discrete–continuum error estimate)
Assume that (A1)–(A2)–(A3) hold and that f is bounded, periodic. Then there exists $\varepsilon_0 > 0$, such that, if

$$\sup_{x \in \mathbb{R}} |f(x)| \leq \varepsilon_0 \,, \quad |L^0 - L^*| \leq \varepsilon_0 \,, \quad \sup_{k \in \mathbb{Z}} |D_k(X, L^*)| \leq \varepsilon_0 \,,$$

then there exists a constant $C_0 > 0$ such that we have the following error estimate between any discrete solution X of (1.3)-(1.4)-(1.5) and the continuous solution Φ of (1.1)-(1.2),

$$|X_{k+1} - X_k - \Phi'(k\,\varepsilon)| \leq C_0\, \varepsilon^{\frac{p-1}{p+3}} \quad \forall\, \varepsilon \in (0, \varepsilon_0) \,.$$

Hence, when considering small perturbations of a stable perfect lattice, the deformed lattice still satisfies the Cauchy–Born rule with a good approximation (see for instance [28, 11] for interesting related works).

The proof of Theorem 1 is based on a new "Harnack–type" estimate, see Theorem 2, which is the core of our method. It would be natural and very interesting to generalize this result for m-dimensional lattices, with $m > 1$, under appropriate assumptions on the two-body potential, but this still an open question.

Remark 1 With our method, it is also possible to get estimates in the case of potentials with exponential decay at infinity, with a sharp estimate of the error.

Remark 2 In Theorem 1, we do not assume the uniqueness of the solution X to (1.3)-(1.4)-(1.5), but only its existence.

1.4 A brief review of the literature

Related to our study is the fundamental question of the periodic or non–periodic nature of an array of atoms interacting through two–body interactions, when minimizing its energy. In dimension 1, this question has been addressed in [12] for Lennard-Jones potentials. It has been proved that the ground state is unique and approaches uniform spacing in the thermodynamical limit. This has also been done in one dimension for other potentials in [17, 19] and generalized to two dimensions for very special potentials in [13, 16]. See the review paper [18]. In [25–27], the authors show that the periodic configuration has the minimal energy per particle for some potentials which are more general than the Lennard-Jones potential; they actually give a necessary condition on the Fourier transform of the potential so that the property is true, and some counter–examples for particular potentials when the condition is not satisfied.

In [1,24], continuum mechanics models are derived for systems with two–body potentials, assuming that the macroscopic displacement is equal to the microscopic one, that is when the Cauchy-Born rule applies. In [3], similar results are obtained up to higher order correction terms (and for other molecular models as well). Also see [10]. The problem of identifying the macroscopic equivalent of a microscopic state, and the conditions which allow to do that, are very close to the spirit of the Quasi–Continum Method (QCM), as presented in [20–23]. A particular model with first nearest neighbors interactions is for instance studied in [2]. Also see [7,8] for studies on the dynamics. In a stronger regularity framework, E and Ming have recently shown in [9] that there is a unique local minimizer which satisfies the Cauchy-Born rule using energy estimates. See references therein for a list of papers in preparation in this direction. Results based on Γ–convergence have been achieved in [5,6].

In the present paper, we prove that the Cauchy-Born rule applies and give a uniform error estimate, hence proving that the macroscopic displacement is equal to the microscopic one up to first order.

1.5 Organization of the paper

In Section 2, we prove a key "Harnack–type" estimate. Section 3 is independent of the rest of the paper and devoted to an extended "Harnack–type" estimate which gives a boundary layer estimate. In Section 4, we prove our main result, Theorem 1. In Section 5, we show some general properties of the potentials, which will be used in Section 6 to state some sufficient conditions such that the microscopic invertibility Assumption (A2) is satisfied by Lennard–Jones potentials, for a chain of atoms under compression.

2 A "Harnack-type" estimate

We shall say that a subset $K \subset \mathbb{Z}$ of indices is a *box,* or a discrete interval, if and only if it is the intersection of $\mathbb{Z}$ with an interval. For such a box K, let us define the semi–norm (inspired by [14,15], also see [4])

$$\mathcal{N}_K(X) := \sup_{k\in K} \inf_{L\in\mathbb{R}^d} D_k(X,L)\,.$$

For a given $\rho \in \mathbb{R}\setminus\{0\}$, let us set

$$K_\rho := K + Q_\rho\,,$$

where $Q_\rho := \{e \in \mathbb{Z}, \text{ such that } |e| \leq \rho\}$. Then we have the following generalization of Harnack–type estimates to discrete equations.

Theorem 2 ("Harnack-type" estimate)
Under Assumptions (A2)–(A3), there exists $\delta_0 > 0$, $\mu \in (0,1)$, C_1, $C_2 > 0$ such that, for every solution X of (1.3) satisfying

$$\sup_{k\in\mathbb{Z}} D_k(X, L^*) \le \delta_0 \tag{2.1}$$

and for any box $K \subset \mathbb{Z}$, we have

$$\mathcal{N}_K(X) \;\le\; \mu\, \mathcal{N}_{K_\rho}(X) + C_1 \sup_{k\in K_\rho} |f_k| \tag{2.2}$$

with

$$\rho^p = \frac{C_2}{\mathcal{N}_K(X)}\,. \tag{2.3}$$

Remark 3 In Theorem 2, we do not assume that $(f_k)_{k\in\mathbb{Z}}$ is uniformly bounded. Indeed in the proof of the Theorem, we only use the fact that f_k is finite for each $k \in \mathbb{Z}$.

Remark 4 Intuitively, the Euler–Lagrange equation satisfied by X in case $f_k = 0$ for any $k \in \mathbb{Z}$ can be thought of as an equation of the type

$$\frac{\partial^2 X}{\partial x^2} = 0 \quad \text{for any } x \in \mathbb{R}\,. \tag{2.4}$$

More generally, if we take $k \in \mathbb{Z}^m$ with $m > 1$, the equation for X becomes a system, which is similar to

$$\Delta X = 0 \quad \text{for any } x \in \mathbb{R}^m\,.$$

The set of harmonic polynomial solutions is much larger than the set of solutions of Equation (2.4). This is one of the difficulties that one would have to tackle for extending the results of this paper to dimensions $m > 1$.

By applying Theorem 2 with $K = \mathbb{Z}$, we get the following result.

Corollary 1 (Liouville result)
Under Assumptions (A2)–(A3), there exists $\delta_0 > 0$ such that, if $X = (X_k)_{k\in\mathbb{Z}}$ is a solution of (1.3) with zero forces, i.e., $f_k = 0$ for any $k \in \mathbb{Z}$, and satisfies

$$\sup_{k\in\mathbb{Z}} D_k(X, L^*) \le \delta_0\,,$$

then there exists $L \in \mathbb{R}^d$ such that

$$X_k = X_0 + k\,L \quad \textit{for any } k \in \mathbb{Z}\,.$$

Proof of Theorem 2.

Let us assume that the estimate is false. By taking appropriate sequences and passing to the limit, we are going to find a non perfect lattice Y such that $B * Y = 0$, a contradiction with (A2).

Step 1: Construction of sequences

Theorem 2 claims the existence of $\delta_0 > 0, \mu \in (0,1), C_1, C_2 > 0$ such that for every X satisfying (2.1) and for any box K, then (2.2) holds with the definition (2.3) of ρ and for $(f_k)_{k\in\mathbb{Z}}$ related to X by equation (1.3).

Assume by contradiction that the statement of Theorem 2 is false. This means that for every $\delta_0 > 0, \mu \in (0,1), C_1, C_2 > 0$, there exists X satisfying (1.3) with forces $(f_k)_{k\in\mathbb{Z}}$ and (2.1), and there exists a box K such that (2.2) is false with the definition (2.3) of ρ. Because we can choose $\delta_0 > 0$, $\mu \in (0,1)$, C_1, $C_2 > 0$ as we want, we can take sequences $(\delta_0^n)_{n\in\mathbb{N}}$, $(\mu^n)_{n\in\mathbb{N}}$, $(C_1^n)_{n\in\mathbb{N}}$, $(C_2^n)_{n\in\mathbb{N}}$, such that

$$\begin{cases} \delta_0^n \to 0\,, \\ \mu^n \to 1\,, \\ C_1^n\,,\ C_2^n \to +\infty\,, \end{cases}$$

and assume the existence of corresponding sequences $(X^n)_{n\in\mathbb{N}}$, $(K^n)_{n\in\mathbb{N}}$, $(\rho^n)_{n\in\mathbb{N}}$, $(f^n)_{n\in\mathbb{N}}$ such that

$$\begin{cases} \sup\limits_{k\in\mathbb{Z}} D_k(X^n, L^*) \le \delta_0^n \to 0\,, \\ (\rho^n)^p = \dfrac{C_2^n}{\mathcal{N}_{K^n}(X^n)} \to +\infty\,, \\ \mathcal{N}_{K^n}(X^n) \quad > \quad \mu^n \mathcal{N}_{K^n_{\rho^n}}(X^n) + C_1^n \sup\limits_{k\in K^n_{\rho^n}} |f_k^n|\,, \\ X^n \quad \text{satisfies (1.3) with forces} \quad f^n\,. \end{cases} \tag{2.5}$$

Then we set

$$\varepsilon^n := \mathcal{N}_{K^n}(X^n)\,,$$

which goes to zero because $\mathcal{N}_{K^n}(X^n) \le \sup\limits_{k\in\mathbb{Z}} D_k(X^n, L^*) \le \delta_0^n \to 0$.

When K^n is bounded, we can define $k^n \in K^n$ and $L^n \in \mathbb{R}^d$ such that

$$\mathcal{N}_{K^n}(X^n) = \inf_{L\in\mathbb{R}^d} D_{k^n}(X^n, L) = D_{k^n}(X^n, L^n)\,. \tag{2.6}$$

If K^n is unbounded, it may happen that the infimum is not reached. In that case we can choose an approximate minimizer k^n and some associated L^n such that we still have $\inf_{L\in\mathbb{R}^d} D_{k^n}(X^n, L) = D_{k^n}(X^n, L^n)$ and moreover

$$\frac{\mathcal{N}_{K^n}(X^n) - \inf_{L\in\mathbb{R}^d} D_{k^n}(X^n, L)}{\varepsilon^n} \to 0\,.$$

The proof can be easily adapted in that case. To simplify the presentation we will only do the proof when (2.6) holds.

There exists $e^n \in Q_1 \backslash \{0\} = \{\pm 1\}$ such that

$$|X^n_{k^n+e^n} - X^n_{k^n} - e^n L^n| = \varepsilon^n\,.$$

On the other hand we have

$$|X^n_{k^n+e^n} - X^n_{k^n} - e^n L^*| \le \delta^n_0 \,,$$

from which we get

$$|L^n - L^*| \le \varepsilon^n + \delta^n_0 \,. \tag{2.7}$$

Let us define

$$Y^n_k := \frac{X^n_{k^n+k} - X^n_{k^n} - k\, L^n}{\varepsilon^n}$$

and observe that, with $e = \pm 1$,

$$\varepsilon^n\, |Y^n_{k+e} - Y^n_k - e\, L| = |X^n_{k^n+k+e} - X^n_{k^n+k} - e\, L| \,,$$

$$D_k(Y^n, L) = \frac{1}{\varepsilon^n}\, D_{k+k^n}(X^n, L) \,.$$

Hence we obtain

$$\frac{1}{\mu^n} \ge \sup_{k\in K^n_{\rho^n}-k^n} \inf_{L\in\mathbb{R}^d} D_k(Y^n, L) \ge 1 = \inf_{L\in\mathbb{R}^d} D_0(Y^n, L) \quad \text{and} \quad Y^n_0 = 0 \,. \tag{2.8}$$

We will get some a priori bounds on the Y^n_k. To this end, we first need to control the variations of the lattice spacing.

Step 2: Control on the variations of the lattice spacing

We choose $\overline{L}^n_k \in \mathbb{R}^d$ such that for $k \in K^n_{\rho^n} - k^n$ we have

$$\inf_{L\in\mathbb{R}^d} D_k(Y^n, L) = D_k(Y^n, \overline{L}^n_k) \,.$$

In particular, we can take $\overline{L}^n_0 = 0$. By definition of $\overline{L}^n_k$, we deduce that

$$|Y^n_{k+1} - Y^n_k - \overline{L}^n_k| \le D_k(Y^n, \overline{L}^n_k) \quad \text{and} \quad |Y^n_k - Y^n_{k+1} + \overline{L}^n_{k+1}| \le D_{k+1}(Y^n, \overline{L}^n_{k+1}) \,.$$

Therefore, if $k, k+1 \in K^n_{\rho^n} - k^n$, we get

$$|\overline{L}^n_k - \overline{L}^n_{k+1}| \le D_k(Y^n, \overline{L}^n_k) + D_{k+1}(Y^n, \overline{L}^n_{k+1}) \le \frac{2}{\mu^n}$$

and then, if $k, k' \in K^n_{\rho^n} - k^n$, we deduce the following estimate

$$|\overline{L}^n_k - \overline{L}^n_{k'}| \le 2\frac{|k-k'|}{\mu^n} \,. \tag{2.9}$$

Similarly, from the fact that

$$\max\Big(|Y^n_{k+1} - Y^n_k - \overline{L}^n_k|,\ |Y^n_{k-1} - Y^n_k + \overline{L}^n_k|\Big) \le D_k(Y^n, \overline{L}^n_k) \le \frac{1}{\mu^n} \,, \tag{2.10}$$

we deduce that

$$|Y^n_{k+1} + Y^n_{k-1} - 2Y^n_k| \le \frac{2}{\mu^n} \quad \text{for every } k \in K^n_{\rho^n} - k^n \,. \tag{2.11}$$

Step 3: Quadratic bound on Y_k^n

Assume that $k \in K^n_{\rho^n} - k^n$ and let us assume to simplify that $k > 0$ (the other case $k < 0$ is similar). Then we have

$$|Y^n_{j+1} - Y^n_j - \overline{L}^n_j| \le D_j(Y^n, \overline{L}^n_j) \le \frac{1}{\mu^n}\,.$$

Using the fact that $\overline{L}^n_0 = 0$, we get

$$\begin{aligned}
|Y^n_k| &= \left| \sum_{j=0}^{k-1} \left\{ Y^n_{j+1} - Y^n_j - \overline{L}^n_j - (\overline{L}^n_0 - \overline{L}^n_j) \right\} \right| \\
&\le \sum_{j=0}^{k-1} \left\{ D_j(Y^n, \overline{L}^n_j) + \left| \overline{L}^n_j - \overline{L}^n_0 \right| \right\} \\
&\le \frac{k}{\mu^n} + \frac{2}{\mu^n} \sum_{j=0}^{k-1} j \\
&\le \frac{k^2}{\mu^n}
\end{aligned}$$

and from $Q_{\rho^n} \subset K^n_{\rho^n} - k^n$, we deduce that

$$|Y^n_k| \le \frac{k^2}{\mu^n} \quad \text{for all } k \in Q_{\rho^n}\,. \tag{2.12}$$

Step 4: Passing to the limit and getting a contradiction

Let us define

$$g^n_k := \frac{f^n_{k^n+k}}{\varepsilon^n} \quad \forall\, k \in K^n_{\rho^n} - k^n\,.$$

Then g^n_k satisfies

$$|g^n_k| \le \frac{1}{C^n_1} \to 0 \quad \text{as } n \to +\infty \tag{2.13}$$

because of (2.5). From (1.3) we deduce for all $j \in \mathbb{Z}$

$$\varepsilon^n g^n_j + \sum_{k \in \mathbb{Z}\setminus\{j\}} \nabla V\big((j-k)\,L^n + \varepsilon^n(Y^n_j - Y^n_k)\big) = 0\,,$$

i.e.,

$$g^n_j + \sum_{k \in \mathbb{Z}\setminus\{j\}} \int_0^1 dt\ (Y^n_j - Y^n_k)\cdot B^n_{jk}(t) = 0\,, \tag{2.14}$$

with

$$B^n_{jk}(t) = D^2 V\big((j-k)\,L^n + t\,\varepsilon^n(Y^n_j - Y^n_k)\big)\,.$$

Up to extraction of convergent subsequences, by (2.6), (2.12) and (2.13), we can assume that

$$\begin{cases} Y_k^n \to Y_k^\infty\,, \\ g_k^n \to 0\,, \\ L^n \to L^*\,, \\ B_{jk}^n(t) \to B_{jk}^\infty = D^2V\big(L^*(j-k)\big) = H_{j-k}^*\,. \end{cases}$$

Passing to the limit in (2.8) and (2.11), we get in particular

$$\inf_{L\in\mathbb{R}^d} D_0(Y^\infty, L) = 1 \tag{2.15}$$

and

$$|Y_{k+1}^\infty + Y_{k-1}^\infty - 2Y_k^\infty| \le 2 \quad \text{for every } k\in\mathbb{Z}\,. \tag{2.16}$$

We now want to pass to the limit in (2.14). To this end, we will estimate for any fixed $j \in Q_{\rho^n/2}$ separately

$$S_j^n = \sum_{k\in(j+Q_{\rho^n/2})\setminus\{j\}} \int_0^1 dt\ (Y_j^n - Y_k^n)\cdot B_{jk}^n(t)$$

and

$$F_j^n = \sum_{k\in\mathbb{Z}\setminus(j+Q_{\rho^n/2})} \int_0^1 dt\ (Y_j^n - Y_k^n)\cdot B_{jk}^n(t)$$

with S for the "short" distance contribution and F for the "far" away contribution.

For the short distances contribution, using (2.9)–(2.10), we get

$$|Y_j^n - Y_k^n| \le C_3\,(1+|j-k|^2) \quad \text{for every } k\in j+Q_{\rho^n/2} \tag{2.17}$$

with some constant $C_3 = C_3(j) > 0$. For the far away contribution, we have

$$|Y_j^n - Y_k^n| = \frac{1}{\varepsilon^n}\left|X_{k^n+j}^n - X_{k^n+k}^n - L^n(j-k)\right| \le C_4\,\frac{|j-k|}{\varepsilon^n} \tag{2.18}$$

for some constant $C_4 > 0$, where we have used the fact that

$$\sup_{k\in\mathbb{Z}} D_k(X^n, L^*) \le \delta_0^n \quad \text{with } \delta_0^n \text{ small enough}\,. \tag{2.19}$$

We claim that there exists a constant $C_5 > 0$ such that for n large enough, we have

$$|B_{jk}^n(t)| \le \frac{C_5}{(1+|j-k|)^{p+2}} \quad \text{for all } j,\,k\in\mathbb{Z}\,. \tag{2.20}$$

This will be proven in Step 5. On the one hand, from (2.20), (2.17) and the dominated convergence theorem, we deduce that

$$S_j^n \to S_j^\infty = (B^\infty\cdot Y^\infty)_j\,.$$

On the other hand, from (2.20), (2.18) and

$$\varepsilon^n \ (\rho^n)^p = C_2^n \to +\infty \, , \tag{2.21}$$

we deduce that there exists a constant $C_6 > 0$ such that

$$|F_j^n| \leq \frac{C_6}{\varepsilon^n \ (\rho^n)^p} = \frac{C_6}{C_2^n} \to 0 \, .$$

Therefore, we can pass to the limit in (2.14), and get that $S_j^\infty = 0$ for any $j \in \mathbb{Z}$, i.e.,

$$B^\infty \cdot Y^\infty = 0 \, .$$

Applying Assumption (A2) with estimate (2.16), we deduce that there exists $L \in \mathbb{R}^d$ such that

$$Y_k^\infty = Y_0^\infty + k \, L \, ,$$

which gives a contradiction with (2.15).

Step 5: Proof of (2.20)

We can write

$$B_{jk}^n(t) = D^2 V \left(Z_j^n(t) - Z_k^n(t) \right) \quad \text{with } Z_k^n(t) := (1-t) \, k \, L^n + t \, X_{k^n+k}^n \, .$$

We observe that

$$Z_j^n(t) - Z_k^n(t) - (j-k) \, L^* \\ = (1-t)(j-k)(L^n - L^*) + t \sum_{l=k}^{j-1} \left(X_{k^n+l+1}^n - X_{k^n+l}^n - L^* \right) .$$

Since $t \in [0,1]$, from (2.7) and (2.19) we deduce that

$$|Z_j^n(t) - Z_k^n(t)| \geq |j-k| \big(|L^*| - (\varepsilon^n + \delta_0^n) \big) \quad \text{for every } j, \, k \in \mathbb{Z} \, .$$

Finally Assumption (A3) on the decay at infinity on the potential V implies (2.20). This ends the proof of Theorem 2. □

Remark 5 As can be checked from the proof, Theorem 2 is still true with ρ chosen such that

$$\rho^p = \frac{C_2}{\mathcal{N}_{K_\rho}(X)} \, .$$

The proof is similar to the one of Theorem 2, if ρ^n in (2.5) and relation (2.21) are replaced respectively by

$$(\rho^n)^p = \frac{C_2^n}{\mathcal{N}_{K^n_{\rho^n}}(X^n)} \to +\infty$$

and

$$\varepsilon^n \ (\rho^n)^p > \mu^n \, C_2^n \to +\infty \, .$$

3 A boundary layer estimate

In this section, we will give a boundary layer estimate. To this end, one has to consider continuous extensions of the discrete norms and the corresponding Harnack–type estimate.

Let I be any interval and $K = I \cap \mathbb{Z}$. Recall that for any $j \in \mathbb{N}$, we set

$$K_j = K + Q_j \quad \text{with } Q_j = \{-j, -j+1, \ldots, j\} \ .$$

We extend the definitions given for integers to real numbers. Let

$$\widetilde{\mathcal{N}}_{I_r}(X) := (1-\alpha)\mathcal{N}_{K_k}(X) + \alpha \mathcal{N}_{K_{k+1}}(X)$$

for any $r = k + \alpha$, $k \in \mathbb{N}$, $\alpha \in [0, 1)$, and

$$\|f\|_{L^\infty(I_r)} = (1-\alpha) \sup_{j \in K_k} |f_j| + \alpha \sup_{j \in K_{k+1}} |f_j| \,.$$

Reciprocally, remark that if $K = \{k_-, k_+\}$, then it is natural to set $I = [k_-, k_+]$ and define

$$I_r := [k_- - r, k_+ + r] \tag{3.1}$$

As a consequence, we have the counterpart of Theorem 2 (same proof).

Theorem 3 (Extended "Harnack–type" estimate)
Under Assumptions (A2)–(A3), there exists $\delta_0 > 0$, $\mu \in (0, 1)$, C_1, $C_2 > 0$ such that for every solution X of (1.3) satisfying

$$\sup_{k \in \mathbb{Z}} D_k(X, L^*) \leq \delta_0 \,,$$

we have, for any interval I and any $r \in [0, +\infty)$,

$$\widetilde{\mathcal{N}}_{I_r}(X) \quad \leq \quad \mu\, \widetilde{\mathcal{N}}_{I_{r+\rho}}(X) + C_1 \|f\|_{L^\infty(I_{r+\rho})}$$

with

$$\rho^p = \frac{C_2}{\widetilde{\mathcal{N}}_{I_{r+\rho}}(X)} \,. \tag{3.2}$$

Remark 6 Theorem 3 is still true with the following choice of ρ:

$$\rho^p = \frac{C_2}{\widetilde{\mathcal{N}}_{I_r}(X)} \,.$$

An interesting corollary of this extended estimate is the following boundary layer estimate which gives a decay rate for the perturbation of a perfect chain of atoms.

Corollary 2 (Discrete boundary layer estimate)
Under Assumptions (A2)–(A3), there exist constants $\delta_0 > 0$ and $C_0 > 0$, such that, if $X = (X_k)_{k\in\mathbb{Z}}$ satisfies

$$\sup_{k\in\mathbb{Z}} D_k(X, L^*) \leq \delta_0 \tag{3.3}$$

and is a solution of (1.3) with forces satisfying

$$f_k = 0 \quad \text{for any } k \in \mathbb{N}\,,$$

then there exists $\overline{L} \in \mathbb{R}^d$ and $C_0 = C_0(\mu, C_2, p) > 0$ such that

$$D_k(X, \overline{L}) \leq C_0\, k^{-(p-1)} \quad \text{for any } k \in \mathbb{N}\,.$$

Proof. For any $k \in \mathbb{N}$, let us define

$$\mathbb{N}_k := \{j \in \mathbb{N} \,:\, j \geq k\}\,.$$

For any nonnegative real $r = k + \beta$ with $k \in \mathbb{N}$, $\beta \in (0, 1]$, we have

$$\widetilde{\mathcal{N}}_{[r,+\infty)}(X) = (1-\beta)\,\mathcal{N}_{\mathbb{N}_k}(X) + \beta\,\mathcal{N}_{\mathbb{N}_{k+1}}(X)\,,$$

where we use the fact that $[r, +\infty) = [k + 1, +\infty)_{1-\beta}$. By definition, the map $r \mapsto \widetilde{\mathcal{N}}_{[r,+\infty)}(X)$ is non–increasing. Consider the sequences $(M_k)_{k\in\mathbb{N}}$ and $(r_k)_{k\in\mathbb{N}}$ such that

$$M_0 := \widetilde{\mathcal{N}}_{[0,+\infty)}(X) = \mathcal{N}_{\mathbb{N}}(X) \quad \text{and} \quad r_0 := 0\,,$$

$$M_{k+1} := \mu\, M_k \quad \text{and} \quad r_{k+1} := \inf\left\{r \geq 0 \,:\, \widetilde{\mathcal{N}}_{[r,+\infty)}(X) \leq M_{k+1}\right\}$$

with $\mu \in (0, 1)$ defined in Theorem 3. We observe that $\widetilde{\mathcal{N}}_{[r_k,+\infty)}(X) = M_k$. We have nothing to prove if $M_0 = 0$, so we shall assume that $M_0 > 0$.

Step 1: The sequences are well–defined for any k

We only have to show that

$$\widetilde{\mathcal{N}}_{[r,+\infty)}(X) \to 0 \quad \text{as } r \to +\infty\,. \tag{3.4}$$

If (3.4) was not true, then there would exist $\delta_1 > 0$ and a sequence of integers $k_n \to +\infty$ such that

$$\inf_{L\in\mathbb{R}^d} D_{k_n}(X, L) \geq \delta_1 > 0\,.$$

Let us define X^n by $X^n_k := X_{k+k_n} - X_{k_n}$. Because of (3.3), we can extract a subsequence which converges to a limit X^∞ which satisfies (1.3) with zero forces and

$$\inf_{L\in\mathbb{R}^d} D_0(X^\infty, L) \geq \delta_1 > 0\,.$$

Applying Corollary 1 to X^∞, we get a contradiction. This proves (3.4).

Step 2: We have $\widetilde{\mathcal{N}}_{[r,+\infty)}(X) \le \frac{\tilde{C}_2}{r^p}$ for some constant $\tilde{C}_2 = \tilde{C}_2(\mu, C_2, p) > 0$.

We consider the extended "Harnack–type" estimate of Theorem 3 with the choice (3.2). Let $I_r = [r, +\infty)$ and $(I_r)_\rho = I_{r-\rho} = [r-\rho, +\infty)$ with the notation (3.1). With $\rho = \rho_k$ and $r = r_k + \rho_k$, we have

$$r_{k+1} - r_k \le \rho_k \quad \text{with} \quad \rho_k^p = \frac{C_2}{M_k}\,,$$

By definition of M_k, we have

$$\rho_k = \left(\frac{C_2}{M_k}\right)^{\frac{1}{p}} = \gamma^k \left(\frac{C_2}{M_0}\right)^{\frac{1}{p}} \quad \text{with} \quad \gamma = \mu^{-\frac{1}{p}}$$

and then

$$0 \le r_k \le \left(\frac{C_2}{M_0}\right)^{\frac{1}{p}} \sum_{i=0}^{k-1} \gamma^i \le \tilde{C}_0\, \gamma^k \quad \text{with} \quad \tilde{C}_0 = \frac{1}{\gamma - 1} \left(\frac{C_2}{M_0}\right)^{\frac{1}{p}},$$

so that

$$\widetilde{\mathcal{N}}_{[r_k,+\infty)}(X) = M_k = \mu^k\, M_0 \le M_0 \left(\frac{\tilde{C}_0}{r_k}\right)^p.$$

Let us define the map $h : [0, +\infty) \to [0, +\infty)$ by

$$h(r) := \widetilde{\mathcal{N}}_{[r,+\infty)}(X)\,.$$

The function h is non-increasing and satisfies

$$h(r_k) = \mu^k\, M_0 \le \frac{\tilde{C}_1}{r_k^p} \quad \text{with} \quad \tilde{C}_1 = M_0\, \tilde{C}_0^p = \frac{C_2}{(\gamma - 1)^p}\,.$$

If $r \in (r_k, r_{k+1})$, then we have

$$h(r) \le h(r_k) = \frac{h(r_{k+1})}{\mu} \le \frac{1}{\mu} \frac{\tilde{C}_1}{r_{k+1}^p} \le \frac{\tilde{C}_2}{r^p} \quad \text{with} \quad \tilde{C}_2 = \frac{\tilde{C}_1}{\mu}\,.$$

This proves that $\widetilde{\mathcal{N}}_{[r,+\infty)}(X) \le \tilde{C}_2 / r^p$ for any $r \ge 0$.

Step 3: Conclusion

For each $k \in \mathbb{N}$, let us choose $L_k \in \mathbb{R}^d$ such that

$$D_k(X, L_k) = \inf_{L \in \mathbb{R}^d} D_k(X, L)\,.$$

From Step 2, we have

$$D_k(X, L_k) \le \frac{\tilde{C}_2}{k^p}\,.$$

As in Step 2 of the proof of Theorem 2, we have

$$|L_{k+1} - L_k| \leq D_k(X, L_k) + D_{k+1}(X, L_{k+1}) \leq 2\,\frac{\tilde{C}_2}{k^p}\,.$$

Because $p > 1$, we see that the sequence $(L_k)_{k\in\mathbb{N}}$ converges to some limit $\overline{L} = \lim_{k\to+\infty} L_k$ such that

$$|\overline{L} - L_k| \leq 2\,\tilde{C}_2 \sum_{j\geq k} \frac{1}{j^p}\,.$$

Using the fact that $D_k(X, \overline{L}) \leq D_k(X, L_k) + |\overline{L} - L_k|$, we get

$$D_k(X, \overline{L}) \leq 2\,\tilde{C}_2 \left(\frac{3}{2\,k^p} + \sum_{j\geq k+1} \frac{1}{j^p} \right) \leq 2\,\tilde{C}_2 \left(\frac{3}{2\,k^p} + \frac{1}{(p-1)}\frac{1}{k^{p-1}} \right) \leq \frac{C_0}{k^{p-1}}\,,$$

with $C_0 := 2\,\tilde{C}_2 \left(\frac{3}{2} + \frac{1}{p-1}\right)$. □

4 Proof of Theorem 1

Step 1: A priori estimate

We apply the "Harnack–type" estimate of Theorem 2 with $K = \mathbb{Z}$ and get

$$\mathcal{N}_{\mathbb{Z}}(X) \quad \leq \quad \frac{C_1}{1-\mu} \sup_{k\in\mathbb{Z}} |f_k| \quad \leq \quad C_7\,\varepsilon \tag{4.1}$$

for some constant $C_7 > 0$, where we have used the relation (1.5) and the L^∞ bound on the force $f(x)$. Let us define

$$L_k := X_{k+1} - X_k\,.$$

There exists $\tilde{L}_k \in \mathbb{R}^d$ such that

$$\max\Big(|X_{k+1} - X_k - \tilde{L}_k|\,,\ |X_{k-1} - X_k + \tilde{L}_k| \Big) \leq D_k(X, \tilde{L}_k) = \inf_{L\in\mathbb{R}^d} D_k(X, L)\,.$$

This implies that

$$|L_{k+1} - L_k| \leq 2\,\mathcal{N}_{\mathbb{Z}}(X)\,.$$

As a consequence, for any $\rho \geq 1$ we have

$$\sup_{k\in Q_\rho} D_k(X, L_0) \leq (1 + 2\rho)\,\mathcal{N}_{\mathbb{Z}}(X)\,,$$

and for any $k \in Q_\rho$,

$$|X_k - X_0 - k\,L_0| \leq \rho\,(1 + 2\rho)\,\mathcal{N}_{\mathbb{Z}}(X)\,.$$

Therefore, and more generally for any $i \in \mathbb{Z}$, we get, for any $\rho \geq 1$,

$$|X_k - X_j - (k-j)\,L_i| \leq C_8\,\varepsilon\,\rho^2 \quad \text{for any } j,\, k \in i + Q_\rho\,, \tag{4.2}$$

for some constant $C_8 > 0$.

Step 2: The line tension formulation

Let us define the line tension of the chain by

$$T_i := \sum_{j,\,k\geq 0} \nabla V(X_{i+1+j} - X_{i-k})\,.$$

Using the fact that $\nabla V(-L) = -\nabla V(L)$, we can easily check that

$$T_i - T_{i-1} = - \sum_{k\in\mathbb{Z}\setminus\{i\}} \nabla V(X_i - X_k)\,. \tag{4.3}$$

By (1.3), this means $T_i - T_{i-1} = f_i$ and thus

$$T_i = T_0 + \sum_{j=1}^{i} f_j \quad \forall\, i \geq 1\,. \tag{4.4}$$

Step 3: Error estimate on the line tension

As in Step 4 of the proof of Theorem 2, we can split the term T_i in a "short distance" contribution

$$S_i = \sum_{(j,\,k)\in\Lambda_\rho} \nabla V(X_{i+1+j} - X_{i-k})\,,$$

with

$$\Lambda_\rho = \left\{(j,\,k) \in \mathbb{N}^2 \;:\; k \leq \rho \text{ and } j \leq \rho - 1\right\}\,,$$

and a "far away" contribution

$$F_i = \sum_{(j,\,k)\in\mathbb{N}^2\setminus\Lambda_\rho} \nabla V(X_{i+1+j} - X_{i-k})\,.$$

We deduce from Assumption (A3) that there exists a positive constant C_9 such that

$$|F_i| \leq C_9\, \rho^{-(p-1)}\,, \tag{4.5}$$

and similarly

$$\left| \sum_{(j,\,k)\in\mathbb{N}^2\setminus\Lambda_\rho} \nabla V\big((1+j+k)\, L_i\big) \right| \leq C_9\, \rho^{-(p-1)}\,. \tag{4.6}$$

On the other hand, we have

$$\left| S_i - \sum_{(j,\,k)\in\Lambda_\rho} \nabla V\big((1+j+k)\, L_i\big) \right| \leq C_{10} \sum_{(j,\,k)\in\Lambda_\rho} |X_{i+1+j} - X_{i-k} - (1+j+k)\, L_i|\,,$$

for some constant C_{10} which bounds the second derivatives of the potential $V(L)$ for $|L| \geq |L^*| - \delta_0$. Using (4.2), (4.3), (4.5) and (4.6), this implies that

$$\left| T_i - \sum_{j,\, k \geq 0} \nabla V\big((1+j+k)\, L_i\big) \right| \leq C_{11} \left(\varepsilon\, \rho^4 + \rho^{-(p-1)} \right)$$

for some constant $C_{11} > 0$. With the choice $\varepsilon\, \rho^{p+3} = 1$, which is optimal up to a numerical constant, the right hand side becomes $2\, C_{11}\, \varepsilon^{\frac{p-1}{p+3}}$ and we get

$$|T_i - \nabla W(L_i)| \leq C_{12}\, \varepsilon^{\frac{p-1}{p+3}} \tag{4.7}$$

for some constant $C_{12} > 0$.

Step 4: Existence of the solution Φ

Let us recall the continuous Euler-Lagrange equation (1.2), namely

$$\big(\nabla W(\Phi')\big)' = f \quad \text{on } \mathbb{R}\,. \tag{4.8}$$

Without loss of generality, we can moreover assume that

$$\Phi(0) = 0\,.$$

Then let us define

$$\mathcal{V}_1 := \left\{ \Phi \in W^{2,\infty}(\mathbb{R};\mathbb{R}^d) \;:\; \Phi(x+1) - \Phi(x) = L^0 \quad \text{and} \quad \Phi(0) = 0 \right\}\,,$$

$$\mathcal{V}_2 := \left\{ f \in L^{\infty}(\mathbb{R};\mathbb{R}^d) \;:\; f(x+1) = f(x) \quad \text{and} \quad \int_{\mathbb{R}/\mathbb{Z}} f = 0 \right\}\,,$$

and consider the map

$$\begin{array}{rcl} \Psi : \mathcal{V}_1 & \longrightarrow & \mathcal{V}_2 \\ \Phi & \longmapsto & \big(\nabla W(\Phi')\big)'\,. \end{array}$$

Let us remark that Ψ is C^1. Moreover, because of Assumption (A1), we know that $A = D^2W(L^*)$ is invertible, and then $D^2W(L^0)$ is also invertible for $|L^0 - L^*| \leq \varepsilon_0$ with ε_0 small enough. It is easy to check that $D\Psi(\Phi_0)$ is invertible for $\Phi_0(x) = x\, L^0$. From the Inverse Function Theorem, we deduce that there exists ε_0 small enough such that for any $f \in \mathcal{V}_2$ satisfying $\|f\|_{L^\infty(\mathbb{R})} \leq \varepsilon_0$, there exists a unique solution $\Phi \in \mathcal{V}_1$ solution of (4.8), with Φ in a neighborhood of Φ_0 in $\mathcal{V}_1$.

Step 5: Conclusion

From (4.8), we see that there exists a constant $\sigma_0 \in \mathbb{R}^d$ such that

$$\nabla W(\Phi'(x)) = \sigma_0 + \int_0^x f(y)\, dy\,.$$

From (1.5), (4.4) and (4.7), we deduce that

$$\left| T_0 + \int_{\frac{\varepsilon}{2}}^{(i+\frac{1}{2})\varepsilon} f(y)\, dy - \nabla W(L_i) \right| \le C_{12}\, \varepsilon^{\frac{p-1}{p+3}}\,. \tag{4.9}$$

Let us introduce an approximation of Φ by setting

$$\tilde{\Phi}'(x) := (1-t)\, L_i + t\, L_{i+1}$$

with $t = (x - i\,\varepsilon)/\varepsilon$ if $i\,\varepsilon \le x \le (i+1)\,\varepsilon$. Recall that $|L_{i+1} - L_i| \le 2\, C_7\, \varepsilon$ by (4.1). Now, using the L^∞ bound on the force f, we deduce from (4.9) that

$$\left| \Sigma_0 + \nabla W(\Phi'(x)) - \nabla W(\tilde{\Phi}'(x)) \right| \le C_{13}\, \varepsilon^{\frac{p-1}{p+3}} \tag{4.10}$$

with $\Sigma_0 = T_0 - \sigma_0$. On the other hand, because of the N_ε-periodicity of the L_i, we have

$$\begin{aligned} \int_0^1 \tilde{\Phi}'(x)\, dx &= \varepsilon \sum_{i=0}^{N_\varepsilon - 1} \Big(L_i + \frac{1}{2}\,(L_{i+1} - L_i) \Big) \\ &= \frac{\varepsilon}{2} \sum_{i=0}^{N_\varepsilon - 1} (L_{i+1} + L_i) = L^0\,, \end{aligned}$$

where we have used the fact that $L_i = X_{i+1} - X_i$ and (1.4). By (1.1), we have therefore

$$\int_0^1 \tilde{\Phi}'(x)\, dx = \int_0^1 \Phi'(x)\, dx\,. \tag{4.11}$$

Our goal is to use (4.11) to control Σ_0 in (4.10). To this end, we consider the Taylor expansion

$$\nabla W(\tilde{\Phi}') = \nabla W(\Phi') + D^2 W(\Phi') \cdot (\tilde{\Phi}' - \Phi') + O\big(|\tilde{\Phi}' - \Phi'|^2\big)\,.$$

Taking into account the invertibility of $D^2(\Phi')$, which follows from Assumption (A1) and the construction of Step 4, we deduce that

$$\left| \tilde{\Phi}'(x) - \Phi'(x) - \big(D^2(\Phi'(x))\big)^{-1}(\Sigma_0) \right| \le C_{14}\, \varepsilon^{\frac{p-1}{p+3}} + O\big(|\tilde{\Phi}'(x) - \Phi'(x)|^2\big) \tag{4.12}$$

and, as a consequence,

$$\begin{aligned} &\left| \tilde{\Phi}'(x) - \Phi'(x) - \big(D^2(L^0)\big)^{-1}(\Sigma_0) \right| \\ &\qquad \le C_{15} \left(\varepsilon^{\frac{p-1}{p+3}} + \|\tilde{\Phi}' - \Phi'\|^2_{L^\infty(\mathbb{R})} + |\Sigma_0|\, \|\phi' - L^0\|_{L^\infty(\mathbb{R})} \right). \end{aligned}$$

Now integrating on the interval $(0,1)$ and using (4.11), we get that

$$\left|\left(D^2(L^0)\right)^{-1}(\Sigma_0)\right| \le C_{15}\,\left(\varepsilon^{\frac{p-1}{p+3}} + \|\tilde{\Phi}' - \Phi'\|^2_{L^\infty(\mathbb{R})} + |\Sigma_0|\,\|\phi' - L^0\|_{L^\infty(\mathbb{R})}\right)$$

and then

$$|\Sigma_0| \le C_{16}\left(\varepsilon^{\frac{p-1}{p+3}} + \|\tilde{\Phi}' - \Phi'\|^2_{L^\infty(\mathbb{R})}\right).$$

Hence (4.12) implies

$$\|\tilde{\Phi}' - \Phi'\|_{L^\infty(\mathbb{R})} \le C_{17}\,\varepsilon^{\frac{p-1}{p+3}}\,.$$

where we have used the fact that $\|\tilde{\Phi}' - \Phi'\|_{L^\infty(\mathbb{R})}$ is small because Φ' and $\tilde{\Phi}'$ are both close to L^0. For any $i \in \mathbb{Z}$, we have

$$|L_i - \Phi'(i\,\varepsilon)| \le C_{17}\,\varepsilon^{\frac{p-1}{p+3}}\,,$$

which gives the result with $L_i = X_{i+1} - X_i$. This ends the proof of the Theorem. □

Remark 7 With suitable assumptions, we could also consider the equilibrium of a ring with a large number of atoms instead of a chain of aligned atoms with "linear + periodic" conditions.

5 Further general results on the potentials

Inspired by the line tension argument as of Step 2 of the proof of Theorem 1, let us state first a general result.

Proposition 1 (Sufficient conditions for Assumption (A2))
Let

$$P_j := \sum_{k\ge 1} k\, D^2V\left((k+|j|)\,L^*\right).$$

If we decompose P_j into P_j^1 and P_j^2 such that

$$P_j = P_j^1 \frac{L^*}{|L^*|} \otimes \frac{L^*}{|L^*|} + P_j^2\left(\mathrm{Id} - \frac{L^*}{|L^*|} \otimes \frac{L^*}{|L^*|}\right)$$

and if

$$\begin{cases} P_j^1 \le 0 \quad \text{for any } j \in \mathbb{Z}\setminus\{0\} \quad \text{and} \quad \displaystyle\sum_{j\in\mathbb{Z}} P_j^1 > 0\,, \\ -P_j^2 \le 0 \quad \text{for any } j \in \mathbb{Z}\setminus\{0\} \quad \text{and} \quad \displaystyle\sum_{j\in\mathbb{Z}} -P_j^2 > 0\,, \end{cases} \tag{5.1}$$

then Assumption (A2) is satisfied.

Proof. For any Y satisfying $|Y_{k+1}+Y_{k-1}-2Y_k|\le C$, let us set

$$(P*L)_i=\sum_{j\in\mathbb{Z}} P_{i-j}\,L_j \quad \text{with } L_j=Y_{j+1}-Y_j\,.$$

With $J_l := P_{l+1}-P_l$, we get

$$(P*L)_{i+1}-(P*L)_i=\sum_{j\in\mathbb{Z}} J_{i-j}\,L_j=(J*L)_i\,,$$

where

$$J_l=\sum_{m\ge 1} m\left\{D^2V\big((m+|l+1|)\,L^*\big)-D^2V\big((m+|l|)\,L^*\big)\right\}$$

$$=\begin{cases} -\displaystyle\sum_{h\ge l+1} D^2V(h\,L^*) & \text{if } l\ge 0\,,\\[2ex] \displaystyle\sum_{h\ge |l+1|+1} D^2V(h\,L^*) & \text{if } l\le -1\,.\end{cases}$$

Hence, with the notations introduced in (1.6)-(1.7) and using $D^2V(-h\,L^*)=D^2V(h\,L^*)$ for any $h\ge 0$, we get

$$(J*L)_i=\sum_{j\in\mathbb{Z}} Y_j\,(-J_{i-j}+J_{i-j+1})=-\sum_{j\in\mathbb{Z}} Y_j\,B_{i-j+1}=-\,(B*Y)_{i-1}=0\,.$$

Consequently, if we assume that $B*Y=0$, then $0=(J*L)_i=(P*L)_{i+1}-(P*L)_i$ means that

$$(P*L)_i=(P*L)_0 \quad \text{for any } i\in\mathbb{Z}\,,$$

and then $G_k=L_{k+1}-L_k$ satisfies

$$P*G=0\,.$$

We can project this equality along $\dfrac{L^*}{|L^*|}$ or $\left(\dfrac{L^*}{|L^*|}\right)^{\perp}$, and get

$$P^1*G^1=0 \quad \text{with} \quad G^1_k=\frac{L^*}{|L^*|}\cdot G_k\,, \tag{5.2}$$

$$P^2*G^2=0 \quad \text{with} \quad G^2_k=\left(\mathrm{Id}-\frac{L^*}{|L^*|}\otimes\frac{L^*}{|L^*|}\right)\cdot G_k\in\left(\frac{L^*}{|L^*|}\right)^{\perp}.$$

Consider the maximum of $(G^1_k)_{k\in\mathbb{Z}}$. If it is achieved at some k^1, we get from (5.2) that

$$P^1_0\,G^1_{k^1}=-\sum_{k\in\mathbb{Z}\setminus\{0\}} P^1_k\,G^1_{k^1-k}\le-\left(\sum_{k\in\mathbb{Z}\setminus\{0\}} P^1_k\right)G^1_{k^1}\,.$$

Then (5.1) implies

$$\sup_{k\in\mathbb{Z}} G^1_k \leq 0\,.$$

When the suppremum is reached at infinity, it is possible (up to translations at infinity) to see that the result is still true. Similarly, we get that

$$\inf_{k\in\mathbb{Z}} G^1_k \geq 0\,,$$

and then

$$G^1 = 0\ .$$

Now for any constant vector $\xi \in (L^*)^\perp$, let us set $G^\xi = \xi \cdot G^2$. Then we have

$$P^2 * G^\xi = 0\,,$$

which, as above, implies $G^\xi = 0$. Because this is true for any $\xi \in (L^*)^\perp$, this implies that

$$G^2 = 0\,.$$

Finally this gives that $G = 0$ and then

$$L_k = L_0 \quad \text{for any } k \in \mathbb{Z}\,,$$

which proves that $(Y_k)_{k\in\mathbb{Z}}$ is a perfect chain. □

From (1.7), we have

$$H^*_k = V_0''(|k\,L^*|)\frac{L^*}{|L^*|}\otimes\frac{L^*}{|L^*|} + \frac{V_0'(|k\,L^*|)}{|k\,L^*|}\left(\mathrm{Id} - \frac{L^*}{|L^*|}\otimes\frac{L^*}{|L^*|}\right)\,,$$

and by definition of P^1_j and P^2_j (see Proposition 1), we obtain

$$P^1_j(r) = \sum_{k\geq 1} k\,V_0''\big((k+|j|)\,r\big) \quad \text{and} \quad P^2_j(r) = \sum_{k\geq 1} k\,\frac{V_0'\big((k+|j|)\,r\big)}{(k+|j|)\,r}\,.$$

In Section 6 and under some assumptions on the potentials and on the range of r, we will check that the operators P^1 and P^2 satisfy Assumption (5.1).

Lemma 1 *With the notations of Proposition 1,*

$$\sum_{j\in\mathbb{Z}} P^1_j(r) = W_0''(r) \quad \textit{and} \quad r\sum_{j\in\mathbb{Z}} P^2_j(r) = W_0'(r)\,.$$

Proof. The result relies on the following computation.

$$\begin{aligned}\sum_{j\in\mathbb{Z}} P^1_j(r) &= \sum_{j\in\mathbb{Z}}\sum_{k\geq 1} k\,V_0''\big((k+|j|)\,r\big)\\ &= \sum_{k\geq 1} k\,V_0''(k\,r) + 2\sum_{j\geq 1}\sum_{k\geq 1} k\,V_0''\big((k+j)\,r\big)\\ &= \sum_{h\geq 1} h^2\,V_0''(h\,r) = W_0''(r)\,.\end{aligned}$$

The result for $P^2(r)$ follows from a similar computation which gives

$$\sum_{j\in\mathbb{Z}} P_j^2(r) = \sum_{h\geq 1} h^2\,\frac{V_0'(h\,r)}{h\,r} = \frac{1}{r}\sum_{h\geq 1} h\,V_0'(h\,r) = \frac{1}{r}\,W_0'(r)\,.$$

□

6 Applications to Lennard–Jones type potentials

Let us now consider potentials of Lennard–Jones type, i.e., for $r > 0$

$$V_0(r) = r^{-q} - r^{-p} \quad \text{with } 1 < p < q$$

and

$$W_0(r) = s_q\,r^{-q} - s_p\,r^{-p} \quad \text{with} \quad s_q = \sum_{k\in\mathbb{N}\setminus\{0\}} |k|^{-q} = \zeta(q) < s_p = \zeta(p)\,,$$

where ζ denotes the Rieman Zeta function. Then we define $r_1, r_2, \overline{r}_1, \overline{r}_2 > 0$ such that

$$0 = V_0'(r_1) = V_0''(r_2) = W_0'(\overline{r}_1) = W_0''(\overline{r}_2)$$

and find

$$r_1 := \left(\frac{q}{p}\right)^{\frac{1}{q-p}} \quad \text{and} \quad r_2 := \left(\frac{q(q+1)}{p(p+1)}\right)^{\frac{1}{q-p}} > r_1\,,$$

$$\overline{r}_1 := \left(\frac{s_q q}{s_p p}\right)^{\frac{1}{q-p}} < r_1 \quad \text{and} \quad \overline{r}_2 := \left(\frac{s_q q(q+1)}{s_p p(p+1)}\right)^{\frac{1}{q-p}} \in (\overline{r}_1, r_2)\,.$$

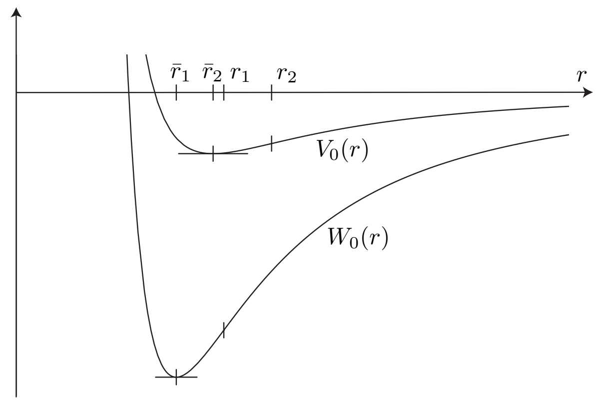

Fig. 1 *Van der Waals forces: plot of V_0 and W_0 with $p = 2.25$ and $q = 3.5$. Condition* (6.2) *(see below) is satisfied since $r_2/2 \approx 0.923723 < \bar{r}_1 \approx 1.15726$.*

Lemma 2 (Sufficient conditions for Lennard-Jones type potentials)

i) *The operator* $P^1(r)$ *satisfies Assumption (5.1) if* $r \in (r_2/2, \overline{r}_2)$, *which is possible if*

$$\left(\frac{s_q}{s_p}\right)^{\frac{1}{q-p}} > \frac{1}{2}\,. \tag{6.1}$$

ii) *The operator* $P^2(r)$ *satisfies Assumption (5.1) if* $r \in (r_1/2, \overline{r}_1)$, *which is possible if (6.1) is satisfied.*

iii) $P^1(r)$ *and* $P^2(r)$ *satisfy Assumption (5.1) simultaneously if* $r \in (r_2/2, \overline{r}_1)$ *which is possible if*

$$\left(\frac{s_q}{s_p}\right)^{\frac{1}{q-p}} > \frac{1}{2}\left(\frac{q+1}{p+1}\right)^{\frac{1}{q-p}}\,. \tag{6.2}$$

Proof. If $r \geq r_2/2$, then $P_j^1(r) < 0$ if $j \neq 0$. Similarly, if $r \geq r_1/2$, then $P_j^2(r) > 0$ if $j \neq 0$. The result follows from Lemma 1. □

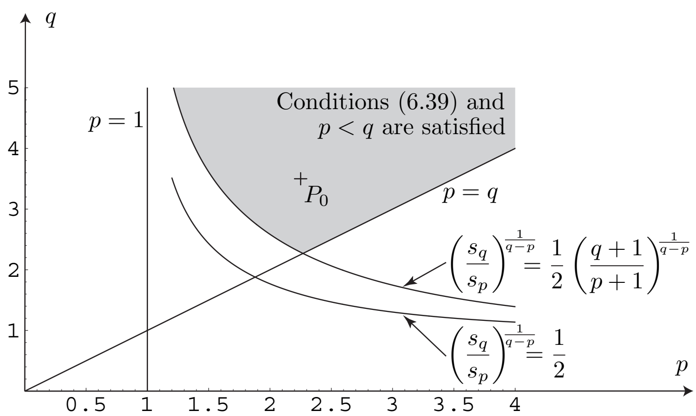

Fig. 2 *Van der Waals forces: regions for which Conditions* (6.1) *and* (6.2) *are satisfied. The point* $P_0 := (2.25, 3.5)$ *corresponding to Fig. 1 is shown. In the gray area, Condition (5.1) is satisfied by* $P^1(r)$ *and* $P^2(r)$.

Conditions (6.1) and (6.2) could easily be improved, for instance by refining the estimates for which $P_j^1 \leq 0$ and $-P_j^2 \leq 0$.

A straightforward consequence of Lemma 2 and Proposition 1 is the following result of stability under compression. This is the main result of this section.

Corollary 3 (Sufficient conditions for Lennard-Jones type potentials to have (A2)). *If (6.2) is satisfied, then Assumption (A2) is satisfied if* $|L^*| \in (r_2/2, \overline{r}_1)$.

Remark 8 In dimension $d \geq 2$, intuitively we expect stability of the chain of atoms when we pull the chain in the range where $W_0'(r) > 0$ and $W_0''(r) > 0$. Nevertheless, we were not able to prove it, because it is more difficult to check Assumption (A2) in such a case.

On the contrary, in the case of compression of a straight chain, i.e., with $W_0'(r) < 0$ and $W_0''(r) > 0$, one atom may decrease the total energy by moving far enough, perpendicularly to the chain. What is stated in Corollary 3 and Theorem 1 shows that the chain of atoms under compression is stable at microscopic level, if the atoms do not move too far perpendicularly to the chain, i.e., if $D_k(X, L^*) \leq \delta_0$ with δ_0 small enough.

Aknowledgments

This work was supported by the ECOS projects C02E06 and C05E02. R.B. was supported by FONDECYT (Chile) project # 106–0651 and CONICYT (Chile) PBCT Proyecto Anillo de Investigación en Ciencia y Tecnologia ACT30/2006.

References

1. S. Bardenhagen and N. Triantafyllidis, *Derivation of higher order gradient continuum theories in* 2, 3*-D nonlinear elasticity from periodic lattice models*, J. Mech. Phys. Solids, 42 (1994), pp. 111–139.
2. X. Blanc, C. Le Bris, and F. Legoll, *Analysis of a prototypical multiscale method coupling atomistic and continuum mechanics: the convex case*, Acta Math. Appl. Sin. Engl. Ser., 23 (2007), pp. 209–216.
3. X. Blanc, C. Le Bris, and P.-L. Lions, *From molecular models to continuum mechanics*, Arch. Ration. Mech. Anal., 164 (2002), pp. 341–381.
4. X. Blanc and R. Monneau, *Screening of an applied electric field inside a metallic layer described by the Thomas-Fermi-von Weizsäcker model*, Adv. Differential Equations, 7 (2002), pp. 847–876.
5. A. Braides and M. S. Gelli, *Limits of discrete systems with long-range interactions*, J. Convex Anal., 9 (2002), pp. 363–399. Special issue on optimization (Montpellier, 2000).
6. A. Braides, M. S. Gelli, and M. Sigalotti, *The passage from nonconvex discrete systems to variational problems in Sobolev spaces: the one-dimensional case*, Tr. Mat. Inst. Steklova, 236 (2002), pp. 408–427.
7. W. E and Z. Huang, *Matching conditions in atomistic-continuum modeling of materials*, Phys. Rev. Lett., 87 (2001), p. 135501.
8. ———, *A dynamic atomistic-continuum method for the simulation of crystalline materials*, J. Comput. Phys., 182 (2002), pp. 234–261.
9. W. E and P. Ming, *Cauchy-Born rule and the stability of crystalline solids: static problems*, Arch. Ration. Mech. Anal., 183 (2007), pp. 241–297.
10. G. Friesecke and R. D. James, *A scheme for the passage from atomic to continuum theory for thin films, nanotubes and nanorods*, J. Mech. Phys. Solids, 48 (2000), pp. 1519–1540. The J. R. Willis 60th anniversary volume.
11. G. Friesecke and F. Theil, *Validity and failure of the Cauchy-Born hypothesis in a two-dimensional mass-spring lattice*, J. Nonlinear Sci., 12 (2002), pp. 445–478.
12. C. S. Gardner and C. Radin, *The infinite-volume ground state of the Lennard-Jones potential*, J. Statist. Phys., 20 (1979), pp. 719–724.

13. R. C. Heitmann and C. Radin, *The ground state for sticky disks*, J. Statist. Phys., 22 (1980), pp. 281–287.
14. R. Monneau, *Uniform elliptic estimate for an infinite plate in linear elasticity*, Comm. Partial Differential Equations, 29 (2004), pp. 989–1016.
15. ———, *A new 3d-2d interior error estimate independent on the geometry of a linear elastic plate*, Asymptot. Anal., 49 (2006), pp. 331–344.
16. C. Radin, *The ground state for soft disks*, J. Statist. Phys., 26 (1981), pp. 365–373.
17. ———, *Classical ground states in one dimension*, J. Statist. Phys., 35 (1984), pp. 109–117.
18. ———, *Low temperature and the origin of crystalline symmetry*, Int. J. Mod. Phys. B, 1 (1987), pp. 1157–1191.
19. C. Radin and L. S. Schulman, *Periodicity of classical ground states*, Phys. Rev. Lett., 51 (1983), pp. 621–622.
20. V. B. Shenoy, R. Miller, E. B. Tadmor, D. Rodney, R. Phillips, and M. Ortiz, *An adaptive finite element approach to atomic-scale mechanics—the quasicontinuum method*, J. Mech. Phys. Solids, 47 (1999), pp. 611–642.
21. E. B. Tadmor, M. Ortiz, and R. Phillips, *Quasicontinuum analysis of defects in solids*, Philosophical Magazine A, 73 (1996), pp. 1529–1563.
22. E. B. Tadmor, R. Phillips, and M. Ortiz, *Mixed atomistic and continuum models of deformation in solids*, Langmuir, 12 (1996), pp. 4529–4534.
23. E. B. Tadmor, G. S. Smith, N. Bernstein, and E. Kaxiras, *Mixed finite element and atomistic formulation for complex crystals*, Phys. Rev. B, 59 (1999), pp. 235–245.
24. N. Triantafyllidis and S. Bardenhagen, *On higher order gradient continuum theories in 1-D nonlinear elasticity. Derivation from and comparison to the corresponding discrete models*, J. Elasticity, 33 (1993), pp. 259–293.
25. W. J. Ventevogel, *On the configuration of a one-dimensional system of interacting particles with minimum potential energy per particle*, Physica A: Statistical and Theoretical Physics, 92 (1978), pp. 343–361.
26. W. J. Ventevogel and B. R. A. Nijboer, *On the configuration of systems of interacting particles with minimum potential energy per particle*, Phys. A, 98 (1979), pp. 274–288.
27. ———, *On the configuration of systems of interacting particles with minimum potential energy per particle*, Phys. A, 99 (1979), pp. 569–580.
28. G. Zanzotto, *On the material symmetry group of elastic crystals and the Born rule*, Arch. Rational Mech. Anal., 121 (1992), pp. 1–36.