Atomic to continuum passage for nanotubes. A discrete Saint-Venant principle and error estimates

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Abstract

We consider general infinite nanotubes of atoms in $\mathbb{R}^3$ where each atom interacts with all the others through a two-body potential. At the equilibrium, the positions of the atoms satisfy an Euler-Lagrange equation. When there are no exterior forces and for a suitable geometry, a particular family of nanotubes is the set of perfect nanotubes at the equilibrium. When exterior forces are applied on the nanotube, we compare the nanotube to nanotubes of the previous family.

In part I of the paper, this quantitative comparison is formulated in our first main result as a discrete Saint-Venant principle. As a corollary, we also give a Liouville classification result. Our Saint-Venant principle can be derived for a large class of potentials (including Lennard-Jones potential), when the perfect nanotubes at the equilibrium are stable. The approach is designed to be applicable to nanotubes that can have general shapes like for instance carbon nanotubes or DNA, under the oversimplified assumption that all the atoms are identical.

In part II of the paper, we derive from our Saint-Venant principle, a macroscopic mechanical model for general nanotubes. We prove that every solution is well approximated by the solution of a continuum model involving stretching and twisting, but no bending. We establish error estimates between the discrete and the continuous solution. More precisely we give two error estimates: one at the microscopic level and one at the macroscopic level.

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1 Introduction

In this paper, we study nanotubes that are collections of atoms in $\mathbb{R}^3$. These atoms are submitted to two-body interactions with all the other atoms and also to exterior forces. Our model can be seen as simplified description of macromolecules like carbon nanotubes or DNA, where all the atoms are assumed to be identical. We distinguish a subclass of nanotubes that are perfect and at the equilibrium with no exterior forces.

In order to give a flavour of our main results (our main results will be stated precisely in Section 2) we first need to introduce a few concepts and notations in Subsection 1.1. We then provide a review of the literature in Subsection 1.2. The organisation of the paper is given in Subsection 1.3.

1.1 Setting of the problem

1.1.1 The macroscopic description

Let us consider three maps

$$\begin{cases} \Phi : \mathbb{R} \longrightarrow \mathbb{R}^3 \\ \alpha : \mathbb{R} \longrightarrow \mathbb{R} \\ \bar{f} : \mathbb{R} \longrightarrow \mathbb{R}^3, \end{cases}$$

that satisfy (as a simplification) the following macroscopic "linear + periodic" conditions

$$(1.1) \qquad \begin{cases} \Phi(x+j) = \Phi(x) + j\,L^0 & \text{for any } j \in \mathbb{Z}\,,\ x \in \mathbb{R} \\ \alpha(x+j) = \alpha(x) + j\,\theta^0 & \text{for any } j \in \mathbb{Z}\,,\ x \in \mathbb{R}\,, \end{cases}$$

$$(1.2) \qquad \bar{f}(x+j) = \bar{f}(x) \quad \text{for any } j \in \mathbb{Z}\,,\ x \in \mathbb{R}\,,$$

for some given vector $L^0 \in \mathbb{R}^3 \backslash \{0\}$ and some given scalar $\theta^0 \in [0, 2\pi)$. Here $\Phi(x)$ describes the position of an arc and $\alpha(x)$ is proportional to the angle of rotation of a microstructure associated to the arc. This is illustrated on Figure 1. Moreover $\bar{f}$ is simply the force acting on the arc.

The periodicity condition provides us some suitable compactness properties, which will simplify the presentation and the proof of the results.
We consider the following macroscopic total energy of a non linear elastic "arc" as

$$(1.3) \qquad \int_{\mathbb{R}/\mathbb{Z}} W(\alpha', \Phi') + \bar{f}\Phi,$$

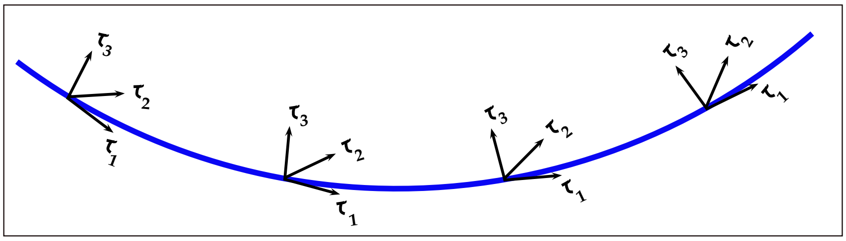

Figure 1: Arc $\Phi(x)$ with rotation of the local basis (τ_1, τ_2, τ_3) under the action of $\alpha(x)$

where W is an (isotropic) energy density that will be defined later (see (2.13)), such that $W(\alpha', \Phi')$ only depends on α' and $|\Phi'|$ (see Lemma 7.3), and the force $\bar{f}$ satisfies the following compatibility condition

$$\int_{\mathbb{R}/\mathbb{Z}} \bar{f}\, dx = 0\,. \tag{1.4}$$

We are interested in macroscopic solutions (α, Φ) of the corresponding Euler-Lagrange equations:

$$\begin{cases} (W'_{\Phi'}(\alpha', \Phi'))' = \bar{f} & \text{on } \mathbb{R} \\ (W'_{\alpha'}(\alpha', \Phi'))' = 0 & \text{on } \mathbb{R}. \end{cases} \tag{1.5}$$

1.1.2 The microscopic description

Given $K \geq 1$ we define

$$\begin{cases} X = (X_j)_{j\in\mathbb{Z}} & \text{with} \quad X_j = (X_{j,l})_{0\leq l\leq K-1} & \text{and} \quad X_{j,l} \in \mathbb{R}^3 \\ f = (f_j)_{j\in\mathbb{Z}} & \text{with} \quad f_j = (f_{j,l})_{0\leq l\leq K-1} & \text{and} \quad f_{j,l} \in \mathbb{R}^3, \end{cases}$$

Here X is a nanotube, X_j is the j^{th} cell (see Figure 2) containing K atoms, and $f_{j,l}$ is the force acting on the atom $X_{j,l}$. We make the following particular choice for the forces $f_{j,l}$

$$f_{j,l} = \frac{1}{K} f_j^0, \tag{1.6}$$

which means that the total force f_j^0 acting on the j^{th} cell is equidistributed on the atoms of the cell.

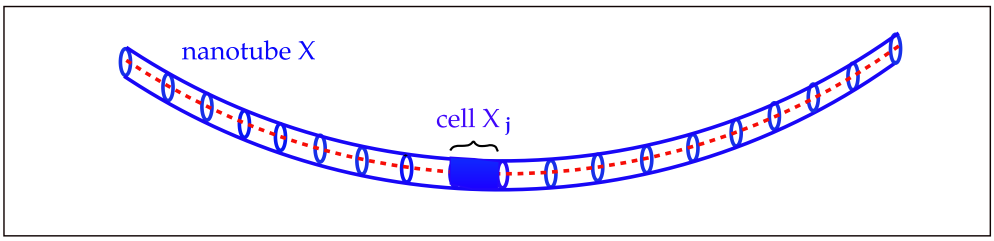

Figure 2: Portion of a nanotube

We consider any integer N_ε large enough, set $\varepsilon = 1/N_\varepsilon$, and when we will compare the microscopic model to the macroscopic one, we will moreover require the following microscopic "linear + periodic" conditions (analogous to (1.1), (1.2))

$$X_{j+N_\varepsilon j'} = N_\varepsilon j' L^0 + X_j \quad \text{for any } j,\ j' \in \mathbb{Z}, \tag{1.7}$$

$$f^0_{j+N_\varepsilon\, j'} = f^0_j \quad \text{for any } j,\ j' \in \mathbb{Z}. \tag{1.8}$$

Given a function $V_0 : (0, \infty) \to \mathbb{R}$, we define the two-body potential as a function of the distance between the atoms:

$$V(L) = V_0(|L|) \quad \text{for every } L \in \mathbb{R}^3 \backslash \{0\}, \tag{1.9}$$

where by convention, we set formally

$$V(0) = 0, \quad \nabla V(0) = 0 \quad \text{and} \quad D^2V(0) = 0. \tag{1.10}$$

For a general nanotube X we consider the following formal microscopic elastic energy as

$$E_0(X) = \frac{1}{2} \sum_{\substack{j,j' \in \mathbb{Z} \\ 0 \le l,l' \le K-1}} V(X_{j,l} - X_{j',l'})$$

and the formal microscopic total energy as

$$E(X) = E_0(X) + \sum_{\substack{j \in \mathbb{Z} \\ 0 \le l \le K-1}} X_{j,l} \cdot f_{j,l}, \tag{1.11}$$

which is analogue to (1.3). When it will be necessary, we will assume the following additional compatibility condition analoguous to (1.4)

$$\sum_{j=1}^{N_\varepsilon} f^0_j = 0. \tag{1.12}$$

Finally we assume that X solves the corresponding Euler-Lagrange equation

$$E'(X) = 0,$$

i.e.

$$f_{j,l} + \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X_{j,l} - X_{j',l'}) = 0 \quad \text{for any } j \in \mathbb{Z},\ 0 \le l \le K-1, \tag{1.13}$$

where we have used convention (1.10) when $(j', l') = (j, l)$.
Similarly $E_0'(X) = 0$ means (1.13) with $f_{j,l} = 0$.

1.1.3 Relationship between macroscopic and microscopic scales

We assume that we have the following relationship on the force of the j^{th} cell and the macroscopic force

$$f_j^0 := \int_{\varepsilon(j-\frac{1}{2})}^{\varepsilon(j+\frac{1}{2})} \bar{f}(x)dx \quad \simeq \quad \varepsilon \bar{f}(j\varepsilon). \tag{1.14}$$

Notice that this relation implies (1.8) and (1.12) from (1.2) and (1.4). The heuristic idea is that for regular enough nanotubes we expect to have roughly the following relation:

$$X_{j+1,l} - \frac{1}{\varepsilon}\Phi((j+1)\varepsilon) \simeq R_{\alpha'(j\varepsilon),\widehat{\Phi'(j\varepsilon)}}(X_{j,l} - \frac{1}{\varepsilon}\Phi(j\varepsilon)) \quad \text{with} \quad \widehat{\Phi'(j\varepsilon)} := \frac{\Phi'(j\varepsilon)}{|\Phi'(j\varepsilon)|}, \tag{1.15}$$

where $R_{\alpha'(j\varepsilon),\widehat{\Phi'(j\varepsilon)}}$ is a rotation of angle $\alpha'(j\varepsilon)$ and of axis $\widehat{\Phi'(j\varepsilon)}$.
The sequence $(\Phi(j\varepsilon))_{j\in\mathbb{Z}}$ gives a good approximation of the mean fiber of the nanotube, and the sequence $(\alpha'(j\varepsilon))_{j\in\mathbb{Z}}$ is also a good approximation of the angle of rotation of X_j into X_{j+1}. Our main motivation is to obtain a quantitative justification of relation (1.15) (see the error estimate of Theorem 2.15 for the details):

Main goal/result: *under certain assumptions we can show a weak version of (1.15).*

In order to obtain such a result, we will first prove a discrete Saint-Venant principle (Theorem 2.13).

1.1.4 Perfect nanotubes

Given an angle $\theta \in [0, 2\pi)$ and a vector $L \in \mathbb{R}^3\backslash\{0\}$, we define the screw displacement $T^{\theta,L}$ by

$$T^{\theta,L}(x) = L + R_{\theta,\widehat{L}}(x) \quad \text{for all}\, x \in \mathbb{R},$$

where $R_{\theta,\widehat{L}}$ is the rotation of angle θ and axis $\widehat{L} = \dfrac{L}{|L|}$.
We define the subclass of **special perfect nanotubes**

$$\mathcal{C}^{\theta,L} = \big\{X = ((X_{j,l})_l)_j \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}, \quad X_{j+1,l} = T^{\theta,L}(X_{j,l})\big\},$$

and the class of **perfect nanotubes**

$$\widehat{\mathcal{C}}^{\theta,L} = \{Y \in ((\mathbb{R}^3)^K)^{\mathbb{Z}},\, \exists a \in \mathbb{R}^3,\, X \in \mathcal{C}^{\theta,L} \quad \text{with} \quad Y_{j,l} = a + X_{j,l}\},$$

which is obtained from $\mathcal{C}^{\theta,L}$ by translations. Finally we see that (1.15), can be interpreted saying that X is well approximated by a perfect nanotube of parameter $(\theta, L) = (\alpha'(j\varepsilon), \Phi'(j\varepsilon))$. Examples of perfect nanotubes are represented on Figures 3 and 4.

1.1.5 Notation

We will constantly use an abuse of notation writing for any rotation $R \in SO(3)$, $a \in \mathbb{R}^3$ and any cell X_j

$$(R(X_j) + a)_l = R(X_{j,l}) + a.$$

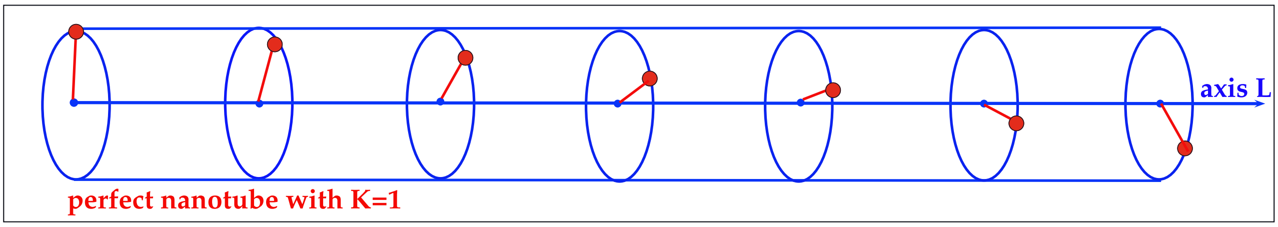

Figure 3: Perfect nanotube with one atom per cell ($K = 1$)

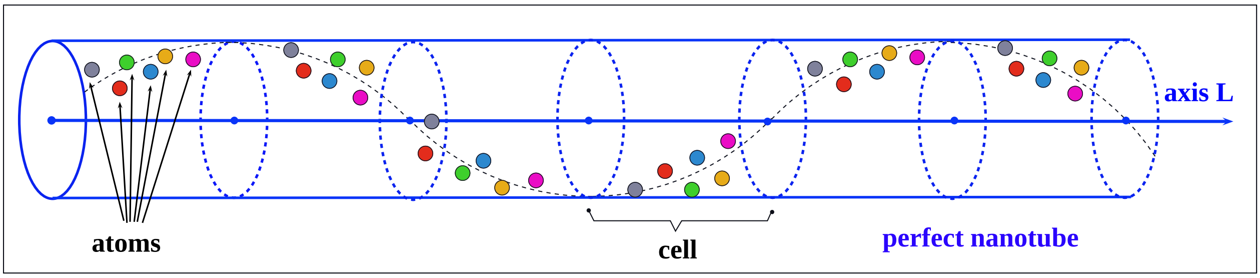

Figure 4: Perfect nanotube with 6 atoms per cell ($K = 6$)

Moreover for a nanotube X we set

$$(R(X) + a)_j = R(X_j) + a.$$

This will also be applied with $\quad R(\cdot) = u \times (\cdot) \quad$ for some $u \in \mathbb{R}^3$.

1.2 Review of the literature

Mathematical approaches

Related to our problem is the question of the structure of minimizers of the microscopic problem. In certain cases, periodic minimizers are expected (see for instance the overview [59] and the recent works [26, 7]). Notice that in our problem, perfect nanotubes are not periodic at all, but are only invariant by a screw displacement $T^{\theta,L}$.

Recall that the Cauchy-Born rule (see [30]), means that the microscopic deformation mimics the macroscopic one. Our Saint-Venant principle (2.15) is a kind of quantitative version of the Cauchy-Born rule, and uses a perturbation argument that shares some similarities with the work [61] on the regularity of solutions of fully non linear elliptic PDEs, or the basic elliptic estimate in [52]. Cases where such Cauchy-Born rule fails (by fracture or melting) have been studied in [11, 18, 68, 33, 23, 31, 17, 16] and a general representation of the macroscopic energy has been given in [2, 19] and in [62, 42, 43] for films. General schemes have been proposed to deduce (assuming the Cauchy-Born rule) macroscopic theories from microscopic ones, see [32, 12, 71, 5]. See also [3, 13] for stochastic lattices. Even if it is different, our approach shares some common points with the Quasi-Continuum Method (see [63]) and some general aspects of multiscale modeling (see the overviews [25, 14]).

A discrete-continuum error estimate has been obtained in [27] (justifying the Cauchy-Born rule) for three-dimensional elasticity starting from microscopic minimizers with two-body interactions of finite range. In [27], the authors use a stability assumption on the Fourier transform of the hessian of the energy, which shares some similarities with our microscopic stability assumption (H2) for nanotubes. Let us mention notable differences: in the present work we do not consider minimizers, but only critical points of the microscopic energy; we do not assume neither a high regularity on the exterior forces. Extension of [27] to the case of the dynamics is presented in [28].

For a general theory of rods, we refer to the book [4] and [67], and for wire ropes, we refer to the book [24]. Let us mention a discrete mechanical approach to rod theory introduced in [38]. For $3D$-$1D$ reduction in the framework of continuum linear and nonlinear elasticity, see [56, 1, 53, 54, 55].

Physical applications

We have in mind that our setting can be an oversimplified framework to modelize mechanical behaviour of macromolecules, like DNA, tropocollagen triple helix (see [20]), micotubules (see [37]), or carbon nanotubes in the regime where bending is neglectable.

For a nice overview of mathematical aspects of DNA, see [65] (where also some references to discrete models for DNA are also indicated). Concerning simplified mechanical models for DNA, involving twist-stretch coupling, we refer to [39, 35, 34] and [36] with the references therein. For a discrete-continuuous comparison of models for DNA, see also [46]. Let us also mention the Elastic Network Model (ENM) method, used for instance to modelize biomolecules (see [64]).

For an overview on the mechanics of carbon nanotubes (including nanoropes with smaller bending stiffness), we refer to [58, 60]. For continuum elastic models of carbon nanotubes, we refer to [41] and the references cited therein. For atomistic derivation of mechanical properties (including torsion) of carbon nanotubes, we refer to [70, 45, 6, 69] mainly with interatomic potentials modeling, and also [22] for a SCC-DFTB atomistic model, and the references therein.

1.3 Organisation of the paper

This paper is divided into two first sections (Section 1 for the introduction and Section 2 for the presentation of the main results), followed by two main parts (parts I and II) and ended by an appendix (Section 13).

On the one hand, part I is devoted to the proof of the discrete Saint-Venant principle (Theorem 2.13) and the Liouville result (Corollary 2.14). On the other hand, part II presents the proof of error estimates: a microscopic error estimate (Theorem 2.15) and a macroscopic error estimate (Corollary 2.16). Part I is independent on part II but uses the first two subsections of the appendix, while part II uses some results in part I and the three first subsections of the appendix.

We now describe the structure of part I. This part is composed of Sections 3 to 6. Section 3 presents certain properties about the equilibrium and the construction (proof of Proposition 2.1) of perfect nanotubes and other properties of the kernel of the hessian of the energy. In Section 4, we prove rough rigidity estimates which are various local and global comparison estimates between nanotubes. In Section 5, we present a fine rigidity estimate (Theorem 5.1) which plays a crucial role in our analysis. This fine estimate compares a general nanotube to a perfect nanotube. In Section 6, we prove the main results of this part, namely Theorem 2.13 and Corollary 2.14.

We now focus on the structure of part II. This part is composed of Sections 7 to 12. In Section 7 we define the line torsion, the line tension and prove their properties, with in particular their relation with the derivatives of the energy for perfect nanotubes (Theorem 7.2 and Theorem 7.9). In Section 8, we define the important discrete notion of mean fiber and prove some of its properties in Theorem 8.2. In Section 9, we mainly prove Theorem 9.1, which is an estimate for a general nanotube on the line tension and the line torsion (i.e. a moment of the forces estimated on the mean fiber). In order to go further, we define in Section 10, the notion of scalar line torsion that we prove to be almost constant (see Theorem 10.2). In Section 11, we mainly prove some estimates between continuum and discrete forces acting on a general nanotube (Theorem 11.1), that is used in Section 12 to prove the main results of part II: namely Theorem 2.15 and Corollary 2.16.

Finally Section 13 is an appendix composed of four subsections. Subsections 13.1 and 13.2 contain respectively properties of rotations and fundamental controls of rotations. Subsection 13.3 gives some technical results on convergent series. We conclude with Subsection 13.4 which is not necessary to establish our main results, but proposes an axiomatic approach to the definition of perfect nanotubes.

2 Main results

In this section we present our main results which are based on the subclass of perfect nanotubes at the equilibrium with no exterior forces.

Our first main result is a quantitative estimate on the distance between a general nanotube and nanotubes of this subclass, namely a Saint-Venant principle (Theorem 2.13), which implies in particular a Liouville classification result (Corollary 2.14).

Those perfect nanotubes at the equilibrium are used to build the macroscopic model for nanotubes deriving from some macroscopic energy W. Our second main result is a set of two error estimates between discrete nanotubes and the solution of the associated macroscopic continuum model (see Theorem 2.15 and Corollary 2.16).

In order to present our main results we need first to present our assumptions in Subsection 2.1. Subsection 2.1 should probably be skipped by the reader in a first reading of this section. Our main results will be given in Subsection 2.2. We finally discuss the main new difficulties of our approach in Subsection 2.3.

2.1 Assumptions

In order to state precisely our main results in Subsection 2.2.1, we need first to introduce several assumptions.

Assumption (H0) (Regularity and decay of the potential)

We assume that $V_0 \in C^2(0,+\infty)$, and for some $p>1$, we assume that

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

Notice that our assumption (H0) allows us to consider Lennard-Jones potential. We define the energy per cell of a special perfect nanotube $X \in \mathcal{C}^{\theta,L}$ by (assuming convention (1.10))

$$\begin{aligned} \mathcal{W}(\theta, L, X_0) &= \frac{1}{2} \sum_{\substack{k \in \mathbb{Z} \\ 0 \le l, m \le K-1}} V(X_{k,l} - X_{0,m}) \\ &= \frac{1}{2} \sum_{\substack{k \in \mathbb{Z} \\ 0 \le l, m \le K-1}} V(kL + R_{k\theta,\widehat{L}}(X_{0,l}) - X_{0,m}), \end{aligned} \tag{2.1}$$

where $X_0 = (X_{0,l})_{0 \le l \le K-1}$ is a cell for the perfect nanotube X. Notice that $\mathcal{W}$, up to its second derivatives, is well defined (when all the atoms of the nanotube are distinct) because of assumption (H0) above.

Assumption (H1) (Stability for a particular perfect nanotube)

i) We assume that there exists $\theta^* \in (0, 2\pi)$, $L^* \in \mathbb{R}^3 \backslash \{0\}$ and $X_0^* = (X_{0,l}^*)_l \in (\mathbb{R}^3)^K$ solution of

$$D_{X_0} \mathcal{W}(\theta^*, L^*, X_0^*) = 0. \tag{2.2}$$

Let the nanotube $X^* = (X_{j,l}^*) \in \mathcal{C}^{\theta^*, L^*}$ with $X_{j,l}^* = jL^* + R_{j\theta^*, \widehat{L}^*}(X_{0,l}^*)$ for $j \in \mathbb{Z}$ and $0 \le l \le K-1$, then we have

$$E_0'(X^*) = 0. \tag{2.3}$$

We also assume that **not all the atoms $X_{j,l}^*$ are aligned** for $j \in \mathbb{Z}$, $l \in \{0, ..., K-1\}$.
ii) We assume that

$$\text{Ker}\, D^2_{X_0 X_0} \mathcal{W}(\theta^*, L^*, X_0^*) = \mathbb{R}(L^* \times X_0^*) + \mathbb{R} \begin{pmatrix} \widehat{L^*} \\ \vdots \\ \vdots \\ \widehat{L^*} \end{pmatrix}. \tag{2.4}$$

where $(L^* \times X_0^*)_l = L^* \times X_{0,l}^*$.

Notice that it is possible to see (see later Proposition 3.3) that (2.2) implies (2.3) in assumption (H1) i).
We will prove later in Proposition 3.4 that under assumption (H1) i) we always have the inclusion

$$\mathbb{R}(L^* \times X_0^*) + \mathbb{R} \begin{pmatrix} \widehat{L^*} \\ \vdots \\ \widehat{L^*} \end{pmatrix} \quad \subset \quad \text{Ker}\, D^2_{X_0 X_0} \mathcal{W}(\theta^*, L^*, X_0^*),$$

and therefore (2.4) is a natural assumption of macroscopic stability of the nanotube X^*. Then we have the following result which will be proven later in Subsection 3.2, which provides a parametrisation by (θ, L) of the unit cell $X_0^* = \mathcal{X}_0^*(\theta, L)$ of special perfect nanotubes at the equilibrium.

Proposition 2.1 (Existence of a suitable map $(\theta, L) \mapsto \mathcal{X}_0^*(\theta, L)$)
i) Existence
Assume (H0) and (H1). Then $\mathcal{W}$ is C^2 (on its domain of definition) and there exists a closed neighborhood $\mathcal{U}_0$ of (θ^*, L^*) in $(0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\})$ and a bounded neighborhood $\mathcal{V}_0^*$ of X_0^* in $(\mathbb{R}^3)^K$, and a C^1 map

$$\begin{array}{cccc} \mathcal{X}_0^* & : & \mathcal{U}_0 & \to & \mathcal{V}_0^* \\ & & (\theta, L) & \mapsto & \mathcal{X}_0^*(\theta, L) \end{array}$$

with $\mathcal{X}_0^*(\theta^*, L^*) = X_0^*$, such that for all $(\theta, L) \in \mathcal{U}_0$, we have

$$D_{X_0}\mathcal{W}(\theta, L, \mathcal{X}_0^*(\theta, L)) = 0 \quad \text{and} \quad \widehat{L} \cdot \left(\sum_{l=0}^{K-1} (\mathcal{X}_0^*)_l(\theta, L) \right) = 0,$$

and every $X_0 \in \mathcal{V}_0^*$ solution of

$$D_{X_0}\mathcal{W}(\theta, L, X_0) = 0 \quad \text{for} \quad (\theta, L) \in \mathcal{U}_0,$$

can be writen

$$X_0 = R_{\beta, \widehat{L}}(\mathcal{X}_0^*(\theta, L)) + \gamma \widehat{L} \quad \text{for some} \quad \beta,\, \gamma \in \mathbb{R}. \tag{2.5}$$

ii) Further technical properties
Up to reduce $\mathcal{U}_0$, we can always show that for any $(\theta, L) \in \mathcal{U}_0$ and

$$\mathcal{X}^*(\theta, L) = (\mathcal{X}_j^*(\theta, L))_{j \in \mathbb{Z}} \quad \text{with} \quad \mathcal{X}_j^*(\theta, L) = R_{j\theta, \widehat{L}}(\mathcal{X}_0^*(\theta, L)) + jL, \tag{2.6}$$

we have

(2.7) *there are at least three atoms of the nanotube $\mathcal{X}^*(\theta, L)$ which are not aligned,*

$$\mathcal{U}_0 = \overline{Int\, \mathcal{U}_0}, \tag{2.8}$$

and there exists $c_0 > 0$ such that

$$\text{for all} \quad (\theta, L),\ (\bar{\theta}, \bar{L}) \in \mathcal{U}_0, \quad \left\{ \begin{array}{l} |\widehat{L} + \widehat{\bar{L}}| \geq c_0 > 0 \\ |L| - |L - \bar{L}| \geq c_0 > 0, \end{array} \right. \tag{2.9}$$

and (for $r \geq 1$ given such that $r\theta^* \neq 0\, (2\pi)$) we have

$$r\theta \neq 0\, (2\pi) \quad \text{for all} \quad (\theta, L) \in \mathcal{U}_0. \tag{2.10}$$

Definition 2.2 (The hessian of the energy)
For a nanotube X^*, the hessian of the energy $E_0''(X^*) : ((\mathbb{R}^3)^K)^{\mathbb{Z}} \to ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ is defined for any $Z \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ by

$$(E_0''(X^*) \cdot Z)_{j,l} = \sum_{\substack{j' \in \mathbb{Z} \\ 0 \leq l' \leq K-1}} D^2V(X_{j,l}^* - X_{j',l'}^*) \cdot (Z_{j,l} - Z_{j',l'}).$$

Assumption (H2) (Microscopic stability by characterisation of the kernel of the hessian)

We assume that there exists a positive constant C such that for any $Z \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ such that

$$\left\{ \begin{array}{l} E_0''(X^*) \cdot Z = 0 \\ |Z_j| \leq C(1+|j|^2), \end{array} \right. \tag{2.11}$$

there exist two vectors $u_1, u_2 \in \mathbb{R}^3$, $(\bar{\theta}, \bar{L}) \in \mathbb{R} \times \mathbb{R}^3$ and $Y \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ such that

$$Z = u_1 + u_2 \times X^* + Y, \tag{2.12}$$

with

$$\left\{ \begin{array}{l} X^* = \mathcal{X}^*(\theta^*, L^*) \\ Y = (\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}^*(\theta^*, L^*) \quad \text{with } \mathcal{X}^*(\theta, L) \text{ defined in (2.6).} \end{array} \right.$$

Notice that all Z as in (2.12) are in the kernel of $E''(X^*)$ by Proposition 3.5. Assumption (H2) claims that the kernel defined by (2.11) does not contain other elements. Therefore assumption (H2) appears as a kind of microscopic stability assumption.

Remark 2.3
We can write

$$\left\{ \begin{array}{l} Y_j = \left(R_{j\theta,\widehat{L}}(Y_0) + \overline{\theta} \cdot (j\widehat{L} \times R_{j\theta,\widehat{L}}(X_0^*)) + \overline{L} \cdot \left(\nabla_L R_{j\theta,\widehat{L}}\right)(X_0^*) + j\overline{L} \right) \Big|_{(\theta,L)=(\theta^*,L^*)} \\ Y_0 = (\overline{\theta}, \overline{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}_0^*(\theta, L) \Big|_{(\theta^*,L^*)}, \end{array} \right.$$

where we recall that $X_0^* = \mathcal{X}_0^*(\theta^*, L^*)$*.*

For later use we introduce the following technical assumption:

Assumption (H3) (Minimal number of cells $2q_0 + 1$ to define the distance D_j)

We introduce conditions on some parameter

$$q_0 = 2r - 1$$

involved later in Definition 2.11, where $2q_0 + 1$ is the minimal number of cells used to define the distance D_j.
If $K \geq 3$ and not all atoms of $\mathcal{X}_0^*(\theta, L)$ are aligned for each $(\theta, L) \in \mathcal{U}_0$, we set

$$r = 1.$$

Otherwise if $K \geq 2$, we set

$$\left\{ \begin{array}{lll} r = 2 & \text{if} & \theta^* \neq \pi \\ r = 3 & \text{if} & \theta^* = \pi. \end{array} \right.$$

If $K = 1$, we set

$$\left\{ \begin{array}{lllll} r = 3 & \text{if} & \theta^* \neq \dfrac{2\pi}{3} & \text{and} & \theta^* \neq \dfrac{4\pi}{3} \\ r = 4 & \text{if} & \theta^* = \dfrac{2\pi}{3} & \text{or} & \theta^* = \dfrac{4\pi}{3}. \end{array} \right.$$

Remark 2.4
Here $q_0 = 2r - 1$ *is such that the atoms of* $X_0(\theta, L)$,..., $X_{r-1}(\theta, L)$ *are always not all aligned when assumption (H1) i) is satisfied. Moreover* $r\theta^* \neq 0\,(2\,\pi)$, *and this condition is used in (2.10).*

Definition 2.5 (Macroscopic energy)
For any $(\theta, L) \in \mathcal{U}_0$, *we define the energy* W *by*

$$W(\theta, L) = \mathcal{W}(\theta, L, \mathcal{X}_0^*(\theta, L)). \tag{2.13}$$

Remark 2.6
For any β, $\gamma \in \mathbb{R}$, *let* $X_0 := R_{\beta,\widehat{L}}(\mathcal{X}_0^*(\theta, L)) + \gamma L$. *Then we have*

$$\mathcal{W}(\theta, L, X_0) = \mathcal{W}(\theta, L, R_{\beta,\widehat{L}}(\mathcal{X}_0^*(\theta, L)) + \gamma L) = \mathcal{W}(\theta, L, \mathcal{X}_0^*(\theta, L)) = W(\theta, L).$$

We have the following regularity:

Proposition 2.7 (Regularity of W)
The energy W *is* C^2 *on* $\mathcal{U}_0$.

We denote by (L_1, L_2, L_3) the coordinates of $L \in \mathbb{R}^3$ and we denote θ by L_0, and we assume that

$$A_{mn} := \frac{\partial^2 W}{\partial L_m \, \partial L_n}(\theta^*, L^*) \quad \text{for any } m,\, n = 0, \cdots, 3$$

satisfies the following non-degeneracy assumption.

Assumption (H4) (Invertibility assumption at the macroscopic level)

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

Remark 2.8
Intuitively, it is expected that assumption (H4) should be related to assumption (H2), but we do not know if (H4) can be deduced from (H2). This question shares some analogies with Lemma 3.1 in [27].

In this paper, when we use the set $\mathcal{U}_0$, we implicitely assume that (H0) and (H1) hold.

2.2 Main results

In order to give our main results in Subsection 2.2.2, we first need some definitions in Subsection 2.2.1.

2.2.1 Perfect nanotubes at the equilibrium, distance and semi-norm

A nanotube $X \in \mathcal{C}^{\theta,L}$ is at the equilibrium if $E_0'(X) = 0$. We introduce the following definitions.

Definition 2.9 (Class $C_*^{\theta,L}$)
For any $(\theta, L) \in \mathcal{U}_0$, we define the subclass of special perfect nanotubes at the equilibrium by

$$\mathcal{C}_*^{\theta,L} = \{Y \in \mathcal{C}^{\theta,L},\ E_0'(Y) = 0,\ \exists(\beta,\gamma) \in \mathbb{R}^2,\ Y_0 = R_{\beta,\widehat{L}}(\mathcal{X}_0^*(\theta, L)) + \gamma\widehat{L}\}.$$

Notice that $\mathcal{X}_0^*(\theta, L)$ is a parametrisation of the unit cell given by Proposition 2.1.

Definition 2.10 (Class $\widehat{C}_*^{\theta,L}$)
For any $(\theta, L) \in \mathcal{U}_0$, we define the class of the perfect nanotubes at the equilibrium by

$$\widehat{\mathcal{C}}_*^{\theta,L} = \{Y \in \widehat{\mathcal{C}}^{\theta,L}, \exists a \in \mathbb{R}^3, X \in \mathcal{C}_*^{\theta,L},\ Y_j = a + X_j\},$$

which is obtained from $\mathcal{C}_*^{\theta,L}$ by translations.

In order to give our main result we need to test the degree of perfection of a nanotube. To this end, we will define a "three cells distance" (when $q = 1$) for a local control of the degree of perfection of a nanotube, and a semi-norm making the local control a global control.

Definition 2.11 (Distance D_j)
For fixed $q \geq q_0 \geq 1$, with q_0 given in (H3), and for any $(\theta, L) \in \mathcal{U}_0$ and a nanotube X we define

$$D_j(X, \theta, L) = \inf_{\widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta,L}} \sup_{|\beta| \leq q} |X_{j+\beta} - \widehat{X}^*_{j+\beta}|,$$

where $|X_j| = \sup_{0 \leq l \leq K-1} |X_{j,l}|$.

Similarly we define for the force $|f_j| = \sup_{0 \leq l \leq K-1} |f_{j,l}|$.

Definition 2.12 (Semi–norm)
We shall say that a subset $J \subset \mathbb{Z}$ of indices is a box, *(i.e. a discrete interval), if and only if it is the intersection of $\mathbb{Z}$ with an interval. For such a box, J, let us define the semi–norm*

$$\mathcal{N}_J(X) := \sup_{j \in J} \inf_{(\theta,L) \in \mathcal{U}_0} D_j(X, \theta, L).$$

Moreover, for a given $\rho > 0$, we set

$$J_\rho := J + Q_\rho,$$

where $Q_\rho := \{e \in \mathbb{Z}, \text{ such that } |e| \leq \rho\}$. We are now ready to state our first main result in the next paragraph, namely our discrete Saint-Venant principle for nanotubes.

2.2.2 Statement of the main results

With the notation of Subsection 2.2.1, we have:

Theorem 2.13 (A Saint-Venant principle for nanotubes)
Assume (H0), (H1), (H2) and (H3), where we recall that $\theta^* \in (0, 2\pi)$ *and* $L^* \in \mathbb{R}^3 \backslash \{0\}$*. Then there exists* $\delta_0 > 0$*,* $\mu \in (0,1)$*,* C_1*,* $C_2 > 0$ *such that, for every nanotube* $X \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ *satisfying the Euler–Lagrange equation (1.13) for some* $f \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ *satisfying (1.6) and*

$$\sup_{j\in\mathbb{Z}} D_j(X, \theta^*, L^*) \leq \delta_0, \tag{2.14}$$

we have for any box $J \subset \mathbb{Z}$

$$\mathcal{N}_J(X) \ \leq \ \mu\, \mathcal{N}_{J_\rho}(X) + C_1 \sup_{j\in J_\rho} |f_j|, \tag{2.15}$$

with

$$\rho^p = \frac{C_2}{\mathcal{N}_J(X)}, \tag{2.16}$$

where we recall that $p > 1$ *is the decay exponent of the two-body potential given in (H0).*

Estimate (2.15) when $f = 0$ on J_ρ is illustrated on Figure 5.

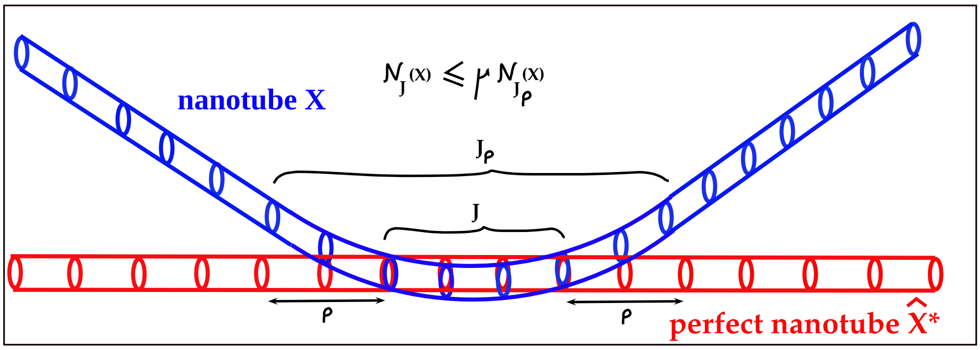

Figure 5: Interpretation of our Saint-Venant principle when $f = 0$ on J_ρ:
X looks more perfect on J than on J_ρ

This Saint-Venant principle (2.15) has been obtained following the general lines of the previous works [8, 15, 50, 51], but with substantial difficulties that are mentionned in Subsection 2.3. Concerning Saint-Venant's principle and exponential decay estimates, we refer the reader to [40, 57, 66] and to [48, 49, 47] for a center manifolds approach.

Corollary 2.14 (Liouville result for nanotubes)
Assume (H0), (H1), (H2) and (H3), where we recall that $\theta^* \in (0, 2\pi)$ *and* $L^* \in \mathbb{R}^3 \backslash \{0\}$*. Then there exists* $\delta_0 > 0$ *such that for every nanotube* $X \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ *satisfying the Euler–Lagrange equation (1.13) with* $f = 0$ *and*

$$\sup_{j\in\mathbb{Z}} D_j(X, \theta^*, L^*) \leq \delta_0, \tag{2.17}$$

then there exists $(\theta_0, L_0) \in \mathcal{U}_0$*, such that*

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta_0,L_0) = 0,$$

and X *is a perfect nanotube.*

Notice that it could also be interesting to try to derive for nanotubes a boundary layer estimate similar Corollary 2 of [8], (this would require some substantial additional work).

Theorem 2.15 (Discrete-continuum error estimate)
Assume that (H0), (H1), (H2), (H3) and (H4) hold with $p > 2$*. Let* $\bar{f} : \mathbb{R} \to \mathbb{R}^3$ *be a function satisfying (1.2), (1.4). There exists* $\varepsilon_0 > 0$*, such that if we have for some constant* $K_0 \geq 0$

$$(2.18) \qquad ||\bar{f}'||_{L^\infty(\mathbb{R})} \leq K_0\,, \quad ||\bar{f}||_{L^\infty(\mathbb{R})} \leq \varepsilon_0\,, \quad \sup_{j\in\mathbb{Z}} D_j(X,\theta^*,L^*) \leq \varepsilon_0,$$

then there exists a constant $C = C(K_0) > 0$ *such that for any discrete solution* X *of (1.13), (1.14), (1.6) and (1.7) with* $\varepsilon \in (0,\varepsilon_0)$*, for* L^0 *defined in (1.7), there exists* $\theta^0 \in \mathbb{R}$ *satisfying*

$$(2.19) \qquad |\theta^0 - \theta^*| \leq C\varepsilon_0\,, \quad |L^0 - L^*| \leq C\varepsilon_0$$

and there exists a solution (α,Φ) *of (1.1) and (1.5) where* W *is defined in (2.13), such that*

$$(2.20) \qquad \sup_{j\in\mathbb{Z}} D_j(X,\alpha'(j\varepsilon),\Phi'(j\varepsilon)) \leq C\varepsilon^\gamma \quad \text{with} \quad \gamma = \min\left(\frac{1}{3}, \frac{p-2}{p}\right).$$

Moreover there exists $\tilde{a}_j \in \mathbb{R}^3$ *for* $j \in \mathbb{Z}$ *such that we have the following error estimate*

$$(2.21) \qquad \left\{\begin{array}{l} |X_j - \tilde{a}_j| \leq C \\ |\tilde{a}_{j+1} - \tilde{a}_j - \Phi'(j\varepsilon)| \leq C\,\varepsilon^\gamma \\ |X_{j+1} - \tilde{a}_{j+1} - R_{\alpha'(j\varepsilon),\widehat{\Phi'(j\varepsilon)}}(X_j - \tilde{a}_j)| \leq C\,\varepsilon^\gamma, \end{array}\right.$$

where we recall the notation $\widehat{z} = \dfrac{z}{|z|}$*.*

The result of Theorem 2.15 is illustrated on Figure 6.

Corollary 2.16 (Macro-micro error estimate)
Under the assumptions and with the notations of Theorem 2.15, we have that there exists $a \in \mathbb{R}^3$ *such that for all* $j \in \mathbb{Z}$ *we have*

$$(2.22) \qquad |\varepsilon X_j - \Phi(j\varepsilon) - a| \leq C\,\varepsilon^\gamma.$$

Result (2.22) of Corollary 2.16 is illustrated on Figure 7.

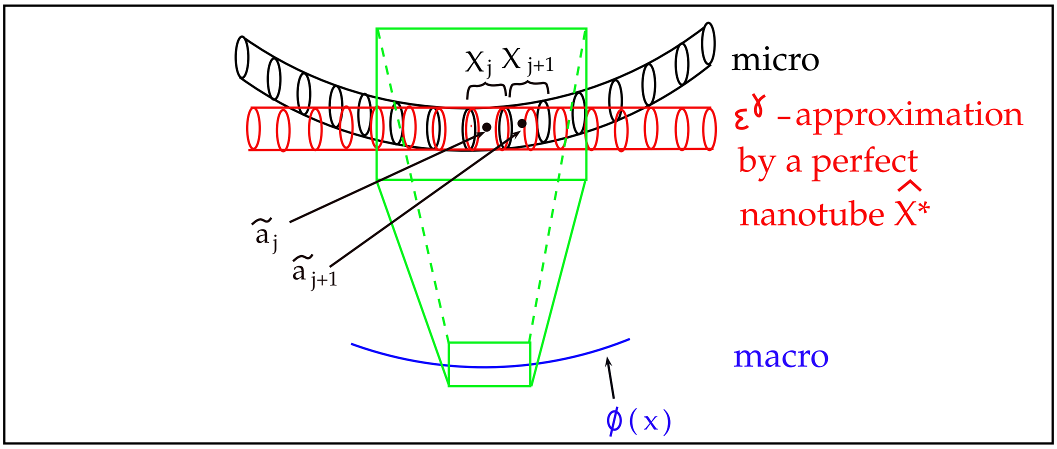

Figure 6: Discrete-continuum error estimates (2.21), (2.20)

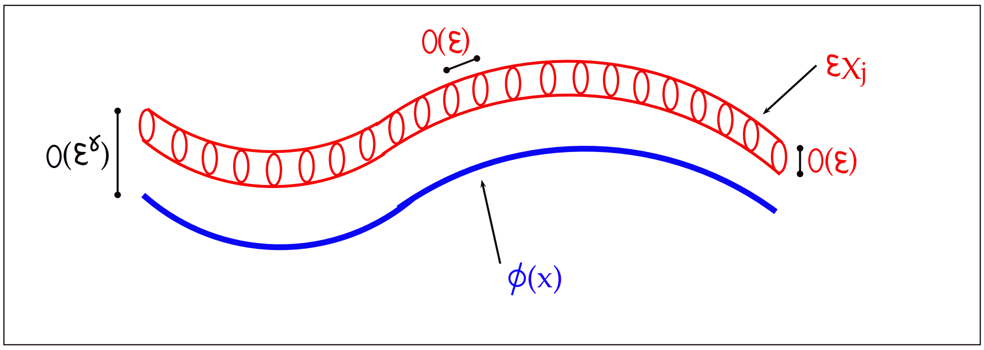

Figure 7: Macro-micro error estimate (2.22) for $a = 0$

2.3 Main difficulties encountered

The starting point of our work was paper [8], where a Saint-Venant principle has been obtained for a linear chain of atoms. This Saint-Venant principle was called a Harnack type inequality in [8]. Our goal was to adapt the method to the case of oversimplified models of nanotubes in $\mathbb{R}^3$, sketching applications for instance to carbon nanotubes and to DNA molecules (in the regime where the bending is neglectable, which is for instance expected when a huge traction is applied). We simplified the analysis, concentrating on the problem with two-body interactions in the case where all the atoms are the same. Nevertheless, we had to face some questions that are several order of magnitude more difficult than in [8]. Even if some proofs may seem elementar from line to line, we had to design from scratch the whole strategy and structure of proof of this paper. For this reason, this paper is fully self-contained.

We list below some of the main difficulties encountered here.

Main difficulties in part I
I.1) the definition of perfect nanotubes:
At a first glance, a perfect nanotube should be a set of atoms that is invariant by a screw displacement $T^{\theta,L}$ (composition of a rotation $R_{\theta,\widehat{L}}$ and a translation in the direction of the

axis L of the rotation). Even if it is very intuitive that we should define a cell repeated by screw displacement, we had to realize that the barycenter of the cell is not necessarily on the axis of the rotation, and then has in general to rotate around this axis. Moreover the parametrisation by $(\theta, L) \in \mathcal{U}_0$ of the family of perfect nanotubes at the equilibrium was not very intuitive, even if it was realised already in [21] that the shape of the microscopic cell of a nanotube can change under homogeneous macroscopic deformations. Moreover, we realised that we had to exclude the case of rotation angle $\theta = 0$ (modulo 2π), which is more singular for at least two reasons: on the one hand several nanotubes families could bifurcate from the case $\theta = 0$ because the dimension of the kernel of $D^2_{X_0X_0}\mathcal{W}$ is higher when $\theta = 0$, and on the other hand, the axis of the identity rotation is not well defined, which makes it impossible to control the axis of perturbed rotations close to the identity. In the same spirit, the suitable stability condition (H2) that we assume on the kernel of the hessian of the microscopic energy was not obvious a priori.

I.2) the notion of curvature to use:

The statement of our Saint-Venant principle (Theorem 2.13) uses a notion of measure of the degree of imperfection of a general nanotube, which we can interprete as a generalised curvature of the nanotube. When each cell X_k reduces to a single atom and $\theta = 0$ (as in [8]), we can simply consider $D_j(X) := |(X_{k+1} - X_k) - (X_k - X_{k-1})|$ which measures the curvature of the chain of atoms. At the beginning of our work, it was not clear what should be the right corresponding notion $D_j(X, \theta, L)$ for nanotubes and how to use it.

I.3) rigidity estimates on nanotubes:

Contrarily to the chain of atoms, we have to consider the action of rotations of the nanotube around its axis. This creates a lot of difficulties to estimate the long range position of a general nanotube, from its local generalised curvature $\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X, \theta, L)$.

Main difficulties in part II

II.1) the macroscopic model:

The macroscopic model is now built on the family of perfect nanotubes at the equilibrium, parametrized by $(\theta, L) \in \mathcal{U}_0$, and creates an isotropic energy $W(\theta, L)$ such that $W(\theta, L) = \widetilde{W}(\theta, |L|)$. This was absolutely not clear at the beginning of our work, even if a posteriori this is related to the energetic regime that we consider, which allows "large" deformations (with respect to the solution of minimum energy). We also realised that those parameters can be interpreted as

$$(\theta, L) = (\alpha', \Phi')$$

where $\Phi(x)$ is the macroscopic arc of a continuous mechanical model, and α can be interpreted as the angle of rotation of an orthonormal basis (whose first vector is tangent to the arc, see Figure 1) associated to each point of the arc with respect to the natural Bishop frame corresponding to zero torsion of the macroscopic arc (see [9, 44, 10]).

II.2) the line torsion and the mean fiber:

In comparison to [8] where line tension was introduced, we had additionnaly to introduce the notion of line torsion at the microscopic level, which is a moment of the internal forces, evaluated at some point. But this notion was difficult to use, and we had to define the right point where to evaluate this moment. We discovered that this moment has to be evaluated on the mean fiber $\tilde{a}_k$, a suitable notion that we also had to introduce (and which corresponds to the projection of the barycenter of the cell on the axis of the nanotube, when this nanotube is perfect). We introduced this notion of mean fiber for general nanotubes.

II.3) microscopic scalar torsion at large scale:
For simplicity, we assumed (as in [8]) some large scale (of order $1/\varepsilon$) periodicity conditions on the microscopic nanotube. To this end, we imposed the large scale translation L^0/ε of atoms, but it was impossible to prescribe the large scale torsion of the nanotube. This is of course natural, because even if the nanotube is anisotropic at the microscopic level, it turns out that it is isotropic at the macroscopic level (in the regime that we consider). This also creates a lot of difficulties to evaluate the microscopic line torsion and to relate it to the macroscopic one. In order to do that, we had to introduce the notion of scalar microscopic line torsion m_i (instead of the vectorial line torsion), that we have shown in Theorem 10.2 to be almost constant, i.e. (for $p \geq 3$)

$$m_i - m_0 = O\left(\frac{1}{N} + N^2\varepsilon\right) = O(\varepsilon^{\frac{1}{3}}).$$

This has been obtained by averaging rotations of the cells of the nanotube on a window of size $N << N_\varepsilon = \varepsilon^{-1}$ and optimizing the error with $N = \varepsilon^{-\frac{1}{3}}$. Here the averaging was possible because $\theta \neq 0\,(2\pi)$. Notice also that this is the only part of the proof where we use the Lipschitz regularity of the forces $\bar{f}$.

Part I
A discrete Saint-Venant principle

3 Properties of perfect nanotubes

This section is divided into three subsections. In Subsection 3.1 we mainly prove Proposition 3.3 for the equilibrium of perfect nanotubes. In Subsection 3.2 we show Proposition 2.1 and Proposition 3.4 for the construction of a family of perfect nanotubes at the equilibrium. Finaly in Subsection 3.3 we get Proposition 3.5 on the properties of the kernel of the hessian of the energy.

3.1 The equilibrium of perfect nanotubes

In this subsection, we grasp a few results that will be used later in the paper. We first notice that using (H0) we can estimate the rest of the series defining $\mathcal{W}$, $D\mathcal{W}$ and $D^2\mathcal{W}$, and then show that $\mathcal{W} \in C^2$, while there are no pairs of atoms in X that touch each other.

Lemma 3.1 (Computation of $D_{X_{0,l}}\mathcal{W}(\theta, L, X_0)$)
Let us consider a nanotube $X \in \mathcal{C}^{\theta,L}$, then for the energy per cell defined in (2.1) we have

$$D_{X_{0,l}}\mathcal{W}(\theta, L, X_0) = \sum_{\substack{j' \in \mathbb{Z} \\ 0 \leq l' \leq K-1}} \nabla V(X_{0,l} - X_{j',l'}).$$

Proof of Lemma 3.1
We have $\quad \mathcal{W}(\theta, L, X_0) = \dfrac{1}{2} \displaystyle\sum_{\substack{j' \in \mathbb{Z} \\ 0 \leq l,l' \leq K-1}} V(X_{0,l} - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'})).$

Then

$$\begin{aligned}
D_{X_{0,p}}\mathcal{W}(\theta,L,X_0) &= \frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l,l'\le K-1}} \delta_{lp}\nabla V(X_{0,l}-j'L-R_{j'\theta,\widehat{L}}(X_{0,l'}))\\
&- \frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l,l'\le K-1}} \delta_{l'p}R_{-j'\theta,\widehat{L}}\nabla V(X_{0,l}-j'L-R_{j'\theta,\widehat{L}}(X_{0,l'}))\\
&= \frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V(X_{0,p}-j'L-R_{j'\theta,\widehat{L}}(X_{0,l'}))\\
&- \frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l\le K-1}} R_{-j'\theta,\widehat{L}}\nabla V(X_{0,l}-j'L-R_{j'\theta,\widehat{L}}(X_{0,p})).
\end{aligned}$$

Using Lemma 13.4 in the appendix, we compute

$$\begin{aligned}
&-\frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l\le K-1}} R_{-j'\theta,\widehat{L}}\nabla V(X_{0,l}-j'L-R_{j'\theta,\widehat{L}}(X_{0,p}))\\
&= -\frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l\le K-1}} \nabla V\Big(R_{-j'\theta,\widehat{L}}\big(X_{0,l}-j'L-R_{j'\theta,\widehat{L}}(X_{0,p})\big)\Big)\\
&= -\frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V\big(R_{-j'\theta,\widehat{L}}(X_{0,l'})-j'L-X_{0,p}\big)\\
&= \frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V\big(X_{0,p}-(-j'L)-R_{-j'\theta,\widehat{L}}(X_{0,l'})\big)\\
&= \frac{1}{2}\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V\big(X_{0,p}-j'L-R_{j'\theta,\widehat{L}}(X_{0,l'})\big),
\end{aligned}$$

then we have

$$D_{X_{0,p}}\mathcal{W}(\theta,L,X_0) = \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V\big(X_{0,p}-j'L-R_{j'\theta,\widehat{L}}(X_{0,l'})\big),$$

and finally

$$D_{X_{0,l}}\mathcal{W}(\theta,L,X_0) = \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V(X_{0,l}-X_{j',l'}).$$

□

Lemma 3.2 (Rotation of the external forces)
If $X\in\mathcal{C}^{\theta,L}$ solves (1.13), then we have

$$f_{j+1} = R_{\theta,\widehat{L}}(f_j),$$

and

$$\widehat{L}\cdot\sum_{l=0}^{K-1} f_{j,l}=0 \quad \textit{for all} \quad j\in\mathbb{Z}. \tag{3.1}$$

Proof of Lemma 3.2
Step 1: Proof of $f_{j+1}=R_{\theta,\widehat{L}}(f_j)$
We recall (1.13) for any $j\in\mathbb{Z}$ and $0\le l\le K-1$

$$f_{j,l}+A_{j,l}=0 \quad \text{with} \quad A_{j,l}=\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V(X_{j,l}-X_{j',l'}). \tag{3.2}$$

Now we compute

$$\begin{aligned}
A_{j+1,l} &= \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V(X_{j+1,l}-X_{j'+1,l'})\\
&= \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V(L+R_{\theta,\widehat{L}}(X_{j,l})-L-R_{\theta,\widehat{L}}(X_{j',l'})))\\
&= \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V(R_{\theta,\widehat{L}}(X_{j,l}-X_{j',l'}))\\
&= R_{\theta,\widehat{L}}\Bigg(\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}} \nabla V(X_{j,l}-X_{j',l'})\Bigg)\\
&= R_{\theta,\widehat{L}}(A_{j,l}),
\end{aligned}$$

where we have used Lemma 13.4 in the fourth line. From (3.2), we deduce that

$$f_{j+1,l}=R_{\theta,\widehat{L}}(f_{j,l}).$$

Step 2: Proof of $\widehat{L}\cdot\sum_{l=0}^{K-1} f_{j,l}=0$
Using (3.2), we get

$$\widehat{L}\cdot\sum_{l=0}^{K-1} f_{j,l}+\widehat{L}\cdot\sum_{l=0}^{K-1} A_{j,l}=0. \tag{3.3}$$

We compute

$$\begin{aligned}
\widehat{L}\cdot\sum_{l=0}^{K-1} A_{j,l} &= \widehat{L}\cdot \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l,l'\le K-1}} \nabla V((j-j')L+R_{j\theta,\widehat{L}}(X_{0,l})-R_{j'\theta,\widehat{L}}(X_{0,l'}))\\
&= \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l,l'\le K-1}} \widehat{L}\cdot\nabla V\big(R_{j\theta,\widehat{L}}\big((j-j')L+X_{0,l}-R_{(j'-j)\theta,\widehat{L}}(X_{0,l'})\big)\big)\\
&= \sum_{\substack{j'\in\mathbb{Z}\\ 0\le l,l'\le K-1}} R_{-j\theta,\widehat{L}}(\widehat{L})\cdot\nabla V((j-j')L+X_{0,l}-R_{(j'-j)\theta,\widehat{L}}(X_{0,l'})),
\end{aligned}$$

where we have used Lemma 13.4 in the last line. This shows that

$$\widehat{L}\cdot\sum_{l=0}^{K-1}A_{j,l}=\sum_{\substack{k\in\mathbb{Z}\\ 0\le l,l'\le K-1}}\widehat{L}\cdot\nabla V(kL+X_{0,l}-R_{-k\theta,\widehat{L}}(X_{0,l'})),$$

Using similar arguments, we get

$$\begin{aligned}
\widehat{L}\cdot\sum_{l=0}^{K-1}A_{j,l} &= \sum_{\substack{k\in\mathbb{Z}\\ 0\le l,l'\le K-1}}\widehat{L}\cdot\nabla V(-kL+X_{0,l}-R_{k\theta,\widehat{L}}(X_{0,l'}))\\
&= \sum_{\substack{k\in\mathbb{Z}\\ 0\le l,l'\le K-1}}\widehat{L}\cdot\nabla V(R_{k\theta,\widehat{L}}(-kL+R_{-k\theta,\widehat{L}}(X_{0,l})-X_{0,l'}))\\
&= \sum_{\substack{k\in\mathbb{Z}\\ 0\le l,l'\le K-1}}R_{-k\theta,\widehat{L}}(\widehat{L})\cdot\nabla V(-kL+R_{-k\theta,\widehat{L}}(X_{0,l'})-X_{0,l})\\
&= \sum_{\substack{k\in\mathbb{Z}\\ 0\le l,l'\le K-1}}\widehat{L}\cdot\nabla V(kL+R_{k\theta,\widehat{L}}(X_{0,l'})-X_{0,l})\\
&= -\widehat{L}\cdot\sum_{l=0}^{K-1}A_{j,l}.
\end{aligned}$$

This implies that $\widehat{L}\cdot\sum_{l=0}^{K-1}A_{j,l}=0$, which with (3.3) implies (3.1).

□

Finally we have

Proposition 3.3 (Euler-Lagrange equations deriving from $\mathcal{W}$ and E) *Given a solution $X\in\mathcal{C}^{\theta,L}$ of Euler-Lagrange equation (1.13), we have*

$$-D_{X_{0,p}}\mathcal{W}(\theta,L,X)=f_{0,p}, \tag{3.4}$$

and

$$D_{X_{0,p}}\mathcal{W}(\theta,L,X)=0\quad\Longleftrightarrow\quad E_0'(X)=0.$$

Proof of Proposition 3.3

By Lemma 3.1, we have

$$D_{X_{0,l}}\mathcal{W}(\theta,L,X_0)=\sum_{\substack{j'\in\mathbb{Z}\\ 0\le l'\le K-1}}\nabla V(X_{0,l}-X_{j',l'}).$$

Using (1.13), we obtain

$$-D_{X_{0,p}}\mathcal{W}(\theta,L,X_0)=f_{0,p}.$$

If $E_0'(X)=0$, then $f_0=0$ and finally

$$D_{X_{0,p}}\mathcal{W}(\theta,L,X_0)=0.$$

Reciprocically, let us assume that $f_0=0$. Then by Lemma 3.2 we have $f_{j+1}=R_{\theta,\widehat{L}}(f_j)$, and then $f_j=0$ for all $j\in\mathbb{Z}$, which implies

$$E_0'(X)=0.$$

□

3.2 Stability of perfect nanotubes at the equilibrium

Proposition 3.4 (On assumption (H1) ii))
Under assumption (H1) i), we have

$$\mathbb{R}(L^* \times X_0^*) + \mathbb{R}\begin{pmatrix} \widehat{L^*} \\ \vdots \\ \widehat{L^*} \end{pmatrix} \quad \subset \quad Ker\, D^2_{X_0X_0}\mathcal{W}(\theta^*, L^*, X_0^*).$$

Proof of Proposition 3.4
To simplify the presentation, we set $\lambda = (\theta, L)$, $X = X_0$ and $\lambda^* = (\theta^*, L^*)$, $X^* = X_0^*$.
Step 1: Invariance by translation along L
From the explicit expression of $D_X\mathcal{W}(\lambda, X)$ given by Lemma 3.1, we see that

$$D_X\mathcal{W}(\lambda, X + \gamma\widehat{L}) = D_X\mathcal{W}(\lambda, X) \quad \text{for all } \gamma \in \mathbb{R}.$$

By derivation with respect to γ, we deduce in particular that

$$\begin{pmatrix} \widehat{L} \\ \vdots \\ \widehat{L} \end{pmatrix} \cdot D^2_{XX}\mathcal{W}(\lambda, X) = 0,$$

which shows that $\mathbb{R}\begin{pmatrix} \widehat{L} \\ \vdots \\ \widehat{L} \end{pmatrix} \quad \subset \quad \text{Ker}\, D^2_{XX}\mathcal{W}(\lambda, X).$
Step 2: Invariance by rotation
We have

$$\mathcal{W}(\lambda, R_{\alpha,\widehat{L}}(X)) = \mathcal{W}(\lambda, X) \quad \text{for all } \alpha \in \mathbb{R}.$$

Taking the derivative with respect to α, we obtain

$$D_X\mathcal{W}(\lambda, R_{\alpha,\widehat{L}}(X)) \cdot (\widehat{L} \times R_{\alpha,\widehat{L}}(X)) = 0 \quad \text{for all } \alpha \in \mathbb{R}. \tag{3.5}$$

Taking again the derivative with respect to α at $\alpha = 0$, we obtain

$$D^2_{XX}\mathcal{W}(\lambda, X) \cdot (\widehat{L} \times X, \widehat{L} \times X) + D_X\mathcal{W}(\lambda, X) \cdot (\widehat{L} \times (\widehat{L} \times X)) = 0.$$

Using $D_X\mathcal{W}(\lambda^*, X^*) = 0$, we deduce that

$$\widehat{L^*} \times X^* \in \text{Ker}\, D^2_{XX}\mathcal{W}(\lambda^*, X^*),$$

and then

$$\mathbb{R}(L^* \times X^*) \quad \subset \quad \text{Ker}\, D^2_{XX}\mathcal{W}(\lambda^*, X^*).$$

□

Proof of Proposition 2.1
Step 1: Definition and properties of ψ
We keep the notations $\lambda, X, \lambda^*, X^*$ of the proof of Proposition 3.4.
We introduce the following map

$$\psi(\lambda, X) := D_X\mathcal{W}(\lambda, X). \tag{3.6}$$

We know that $\psi(\lambda^*, X^*) = 0$, and we want to find a solution $X(\lambda)$ of $\psi(\lambda, X(\lambda)) = 0$, using an inverse function theorem. We notice that we have $D_X\psi(\lambda, X) = D^2_{XX}\mathcal{W}(\lambda, X)$, with $\ker D^2_{XX}\mathcal{W}(\lambda^*, X^*) \neq \{0\}$ by Proposition 3.4.
On the other hand we know by (3.4) and (3.1) that

$$\widehat{\mathcal{L}} \cdot \psi(\lambda, X) = 0 \quad \text{with} \quad \widehat{\mathcal{L}} := \begin{pmatrix} \widehat{L} \\ \vdots \\ \widehat{L} \end{pmatrix},$$

i.e.

$$\psi(\lambda, X) \in \widehat{\mathcal{L}}^{\perp}. \tag{3.7}$$

Moreover computation (3.5) shows that

$$\psi(\lambda, X) \in (AX)^{\perp} \quad \text{with} \quad AX := L \times X. \tag{3.8}$$

From Lemma 3.1 and Lemma 13.4, we have for all $\alpha, \gamma \in \mathbb{R}$

$$\psi(\lambda, R_{\alpha,\widehat{L}}(X) + \gamma\widehat{L}) = R_{\alpha,\widehat{L}}(\psi(\lambda, X)). \tag{3.9}$$

Step 2: Setting for invertibility
We set

$$V_1 = (A^*X^*)^{\perp} \cap \widehat{\mathcal{L}^*}^{\perp} \quad \text{with} \quad \widehat{\mathcal{L}}^* := \begin{pmatrix} \widehat{L}^* \\ \vdots \\ \widehat{L}^* \end{pmatrix} \quad \text{and} \quad A^*X^* := L^* \times A^*,$$

and notice that $A^*X^* \neq 0$ because not all the atoms are aligned (as a consequence of assumption (H1) i)). We consider (with the orthogonal projection on V_1)

$$\tilde{\psi}(\lambda, \cdot) := Proj\Big|_{V_1}\left(\psi(\lambda, \cdot)\Big|_{X^*+V_1}\right). \tag{3.10}$$

We now want to apply the inverse function theorem to $\tilde{\psi}$. To this end, we compute

$$D_X\tilde{\psi}(\lambda^*, X^*) = Proj\Big|_{V_1}\left(D^2_{XX}\mathcal{W}(\lambda^*, X^*)\Big|_{V_1}\right).$$

But $D^2_{XX}\mathcal{W}(\lambda^*, X^*)$ is a symmetric matrix whose kernel is $V_1^{\perp}$ by assumption (H1) ii). Therefore $D^2_{XX}\mathcal{W}(\lambda^*, X^*)$ is invertible from V_1 to V_1, which shows the invertibility of $D_X\tilde{\psi}(\lambda^*, X^*)$. From the inverse function theorem, there exist a bounded neighborhood $\mathcal{U}_0$ of λ^* and a bounded neighborhood $\tilde{\mathcal{V}}_0^*$ of X^* in $X^* + V_1$ and a C^1-map (because the map $(\lambda, X) \mapsto \mathcal{W}(\lambda, X)$ is C^2 by assumption (H0))

$$\begin{array}{rcccl} \mathcal{X}_0^* & : & \mathcal{U}_0 & \to & \tilde{\mathcal{V}}_0^* \\ & & \lambda & \mapsto & \mathcal{X}_0^*(\lambda), \end{array}$$

such that the equation

$$\tilde{\psi}(\lambda, X) = 0 \quad \text{for} \quad X \in \tilde{\mathcal{V}}_0^*$$

has a unique solution which is $\mathcal{X}_0^*(\lambda)$.

Step 3: Consequences

Notice that $\tilde{\psi}(\lambda, X) = 0$ means

$$\psi(\lambda, X) - \alpha A^* X^* - \beta \widehat{\mathcal{L}}^* = 0 \quad \text{with} \quad \left\{ \begin{array}{l} \alpha = \dfrac{(A^* X^*) \cdot \psi(\lambda, X)}{|A^* X^*|^2} \\ \beta = \dfrac{\widehat{\mathcal{L}}^* \cdot \psi(\lambda, X)}{|\widehat{\mathcal{L}}^*|^2}, \end{array} \right. \tag{3.11}$$

where we have substracted to ψ its orthogonal projection on $V_1^\perp$, namely

$$V_1^\perp = \mathbb{R}(A^* X^*) \overset{\perp}{\oplus} \mathbb{R}\widehat{\mathcal{L}}^*.$$

Taking respectively the scalar product with AX and $\widehat{\mathcal{L}}$ in (3.11), and using respectively (3.8) and (3.7), we get

$$\left\{ \begin{array}{l} 0 - \alpha\,(A^* X^* \cdot AX) - \beta\,(\widehat{\mathcal{L}}^* \cdot AX) = 0 \\ 0 - \alpha\,(A^* X^* \cdot \widehat{\mathcal{L}}) - \beta\,(\widehat{\mathcal{L}}^* \cdot \widehat{\mathcal{L}}) = 0. \end{array} \right.$$

For

$$\Delta(L, X) := \det \begin{pmatrix} (A^* X^* \cdot AX) & (\widehat{\mathcal{L}}^* \cdot AX) \\ (A^* X^* \cdot \widehat{\mathcal{L}}) & (\widehat{\mathcal{L}}^* \cdot \widehat{\mathcal{L}}) \end{pmatrix},$$

we have

$$\Delta(L^*, X^*) = |A^* X^*|^2 |\widehat{\mathcal{L}}^*|^2 \neq 0,$$

and $\Delta(L, X) \neq 0$ for (L, X) close enough to (L^*, X^*) (which is true for $X = \mathcal{X}_0^*(\lambda)$ and $\lambda = (\theta, L) \in \mathcal{U}_0$, up to reduce $\mathcal{U}_0$). Therefore $\alpha = \beta = 0$ which implies that

$$\psi(\lambda, X) = 0 \quad \text{for all } X = \mathcal{X}_0^*(\lambda) \quad \text{and} \quad \lambda \in \mathcal{U}_0.$$

Step 4: Further properties

With notation (2.6), recall that not all the atoms in the nanotube $\mathcal{X}^*(\lambda^*)$ are aligned. Because $\mathcal{X}_0^*$ is a continuous map, we deduce that not all the atoms in $\mathcal{X}^*(\lambda)$ are aligned, for $\lambda \in \mathcal{U}_0$ with $\mathcal{U}_0$ small enough, which shows (2.6). Moreover up to reduce $\mathcal{U}_0$, we can assume (2.8), (2.9) and (2.10).

Step 5: Conclusion for the existence of $\mathcal{V}_0^*$

We define

$$\begin{array}{rcccc} \mathcal{F} & : & (0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\}) \times (X^* + V_1) \times \mathbb{R} \times \mathbb{R} & \longrightarrow & (0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\}) \times (\mathbb{R}^3)^K \\ & & (\theta, L, X, \alpha, \gamma) & \longmapsto & (\theta, L, R_{\alpha, \widehat{L}}(X) + \gamma \widehat{L}). \end{array}$$

We have $\mathcal{F}(\theta^*, L^*, X^*, 0, 0) = (\theta^*, L^*, X^*)$, and we compute

$$D\mathcal{F}(\theta^*, L^*, X^*, 0, 0) \cdot (\bar{\theta}, \bar{L}, \bar{X}, \bar{\alpha}, \bar{\gamma}) = (\bar{\theta}, \bar{L}, \bar{X} + \bar{\alpha} \widehat{L}^* \times X^* + \bar{\gamma} \widehat{L}^*).$$

This shows that $D\mathcal{F}$ is invertible at this point. Because $\mathcal{F}$ is C^1, we deduce from the inverse function theorem that there exists a bounded neighborhood $\mathcal{V}_0^*$ of X^* in $(\mathbb{R}^3)^K$ such that (up to reduce $\mathcal{U}_0$ and choose $\mathcal{V}_0^*$ small enough) for all $(\theta, L, X) \in \mathcal{U}_0 \times \mathcal{V}_0^*$, there exists a unique $(\theta, L, \tilde{X}, \alpha, \gamma) \in \mathcal{U}_0 \times \tilde{\mathcal{V}}_0^* \times B_r(0)$, with $B_{r_0}(0) \subset \mathbb{R}^2$ for some small $r_0 > 0$, such that

$$\mathcal{F}(\theta, L, \tilde{X}, \alpha, \gamma) = (\theta, L, X).$$

As a consequence if $(\theta, L, X) \in \mathcal{U}_0 \times \mathcal{V}_0^*$ and $\psi(\theta, L, X) = 0$, then

$$X = R_{\alpha,\widehat{L}}(\tilde{X}) + \gamma\widehat{L} \quad \text{with} \quad \tilde{X} \in X^* + V_1.$$

Therefore from (3.9), we deduce

$$\psi(\theta, L, \tilde{X}) = 0 \quad \text{with} \quad \tilde{X} \in X^* + V_1.$$

From Step 2, we deduce that

$$\tilde{X} = \mathcal{X}_0^*(\theta, L),$$

and then

$$X = R_{\alpha,\widehat{L}}(\tilde{\mathcal{X}}_0^*(\theta, L)) + \gamma\widehat{L},$$

which shows (2.5).

□

3.3 The kernel of the hessian

Proposition 3.5 (The kernel of the hessian)
We set

$$Z_j = u_1 + u_2 \times X_j^* + Y_j,$$

with u_1, $u_2 \in \mathbb{R}^3$, $X^* \in \mathcal{C}_*^{\theta^*,L^*}$, *with* $X^* = \mathcal{X}^*(\theta^*, L^*)$ *and for* $(\overline{\theta}, \overline{L}) \in \mathbb{R} \times \mathbb{R}^3$

$$Y := (\overline{\theta}, \overline{L}).\nabla_{(\theta,L)}\mathcal{X}^*(\theta^*, L^*), \tag{3.12}$$

where $\mathcal{X}^*$ *is defined in Proposition 2.1. Then*
i) for $Z = (Z_j)_{j\in\mathbb{Z}}$, *we have* $Z \in Ker\, E_0''(X^*)$,
ii) there exists a constant $C > 0$ *such that* $|Z_j| \le C(1 + |j|)$.

Proof of Proposition 3.5
Proof of i)
Action of translations
For $\mathcal{Y} = X^* + tu_1$, we have $\mathcal{Y}_{j,l} - \mathcal{Y}_{j',l'} = X_{j,l}^* - X_{j',l'}^*$ and then $E_0'(X^* + tu_1) = E_0'(X^*)$. Therefore

$$0 = \frac{d}{dt}(E_0'(X^* + tu_1))\big|_{t=0} = E_0''(X^*) \cdot u_1$$

and finally

$$u_1 \in \text{Ker}\, E_0''(X^*). \tag{3.13}$$

Action of rotations
For $\alpha \in \mathbb{R}$ and $\mathcal{Y} = R_{\alpha,\widehat{u}_2}(X^*)$, we have $\mathcal{Y}_{j,l} - \mathcal{Y}_{j',l'} = R_{\alpha,\widehat{u}_2}(X_{j,l}^* - X_{j',l'}^*)$, then we write

$$E_0'(R_{\alpha,\widehat{u}_2}(X^*)) = R_{\alpha,\widehat{u}_2}(E_0'(X^*)) = 0,$$

where we have used Lemma 13.4 and the fact that $E_0'(X^*) = 0$.
Therefore for $\alpha = t|u_2|$, we get

$$0 = \frac{d}{dt} E_0'(R_{t|u_2|,\widehat{u}_2}(X^*))\big|_{\alpha=0} = E_0''(X^*) \cdot (u_2 \times X^*),$$

and finally

$$u_2 \times X^* \in \operatorname{Ker} E_0''(X^*). \tag{3.14}$$

Perturbation of $\mathcal{X}^*(\theta, L)$
We have

$$E_0'(\mathcal{X}^*(\theta, L)) = 0.$$

Therefore for $(\theta, L) = (\theta^*, L^*) + t(\bar{\theta}, \bar{L})$, we have

$$0 = \frac{d}{dt} E_0'(\mathcal{X}^*(\theta^* + t\bar{\theta}, L^* + t\bar{L})) = E_0''(\mathcal{X}^*(\theta^*, L^*)) \cdot Y,$$

with $Y = (\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}^*(\theta^*, L^*)$. And finally

$$Y \in \operatorname{Ker} E_0''(X^*). \tag{3.15}$$

Conclusion
From (3.13), (3.14) and (3.15), we deduce that $Z \in \operatorname{Ker} E_0''(X^*)$.
Proof of ii)
On the one hand, there exists a constant $C_1 > 0$ such that

$$|X_j^*| \le C_1(1 + |j|), \tag{3.16}$$

which can be deduced, for instance, from the independent Lemma 4.4.
On the other hand, we have

$$\mathcal{X}_j^*(\theta, L) = jL + R_{j\theta,\widehat{L}}(\mathcal{X}_0^*(\theta, L)).$$

This gives

$$\begin{aligned} Y_j &= (\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}_j^*(\theta^*, L^*) \\ &= j\bar{L} + j\bar{\theta} R_{j\theta^* + \frac{\pi}{2}, \widehat{L}^*}(\mathcal{X}_0^*(\theta^*, L^*)) + \left(\bar{L} \cdot \nabla_L R_{j\theta^*,\widehat{L}}\right)\Big|_{L=L^*} (\mathcal{X}_0^*(\theta^*, L^*)) \\ &\quad + R_{j\theta^*,\widehat{L}^*}\left((\bar{\theta}, \bar{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}_0^*(\theta^*, L^*)\right), \end{aligned}$$

and then (using Lemma 13.7) there exists a constant C_2 such that

$$|Y_j| \le C_2(1 + |j|). \tag{3.17}$$

From (3.16) and (3.17) we deduce that there exists a constant C such that

$$|Z_j| \le C(1 + |j|).$$

□

4 Rough rigidity estimates

The goal of this section is to prove Propositions 4.5 and 4.6 about finite differences of a single nanotube. This is done in Subsection 4.2. In Subsection 4.1, we present preliminary results about comparaison between two nanotubes, that are used in Subsection 4.2 and also later in Section 6.

4.1 Comparison between two nanotubes

Lemma 4.1 (Long distance error estimate for perfect nanotubes)
Let us consider two perfect nanotubes $X \in \widehat{\mathcal{C}}^{\theta,L}$ and $\bar{X} \in \widehat{\mathcal{C}}^{\bar{\theta},\bar{L}}$ for (θ, L), $(\bar{\theta}, \bar{L}) \in \mathcal{U}_0$ such that

$$\begin{cases} \sup_{\alpha=0,-1} |X_\alpha - \bar{X}_\alpha| \leq \varepsilon \\ |\theta - \bar{\theta}| \leq \varepsilon_0 \leq \varepsilon \\ |L - \bar{L}| \leq \varepsilon_0 \leq \varepsilon. \end{cases}$$

Assume moreover that we can write

$$X = a + Y \quad \text{with} \quad Y \in \mathcal{C}^{\theta,L} \quad \text{and} \quad \inf_{\gamma\in\mathbb{R}} \sup_{0\leq l\leq K-1} |Y_{0,l} - \gamma L| \leq c_1. \tag{4.1}$$

Then there exists a constant $C_0 = C_0(c_1) > 0$ such that

$$|X_j - \bar{X}_j| \leq C_0(\varepsilon + \varepsilon_0|j|), \tag{4.2}$$

and there exists a constant $C_1 = C_1(j, c_1)$ such that we have

$$|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)| \leq C_1(\varepsilon_0 + \varepsilon|j' - j| + \varepsilon_0|j' - j|^2). \tag{4.3}$$

Error estimate (4.2) is illustrated on Figure 8.

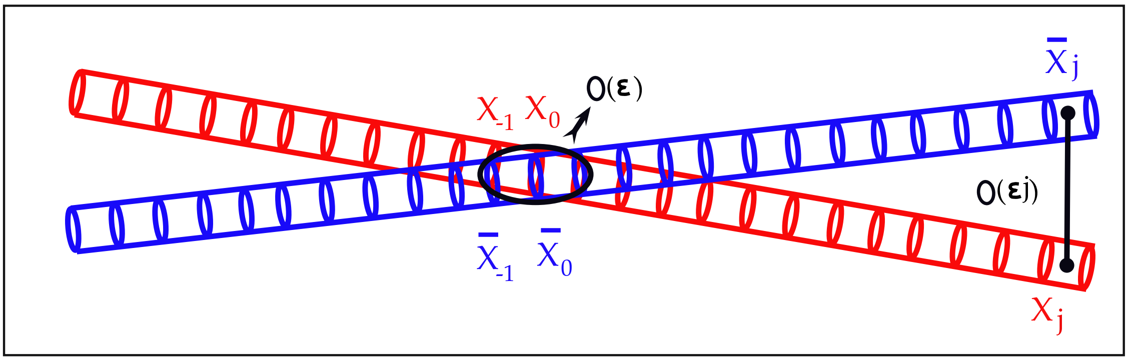

Figure 8: Illustration of error estimate (4.2)

Remark 4.2
In statement of Lemma 4.1, we assumed for simplicity that (θ, L), $(\bar{\theta}, \bar{L}) \in \mathcal{U}_0$. Indeed the result is still true if $|R_{\bar{\theta},\widehat{\bar{L}}} - I|$ is bounded from bellow by a positive constant.

Proof of Lemma 4.1
Step 1: Estimate on rotations
We have $|L-\bar{L}| \le \varepsilon_0$, then by Lemma 13.9 there exists a constant $c>0$ such that

$$|\widehat{L}-\widehat{\bar{L}}| \le c\varepsilon_0.$$

By Lemma 13.8, we have

$$\begin{aligned} |R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}}| &\le |j\theta - j\bar{\theta}| + 5|\widehat{L}-\widehat{\bar{L}}| \\ &\le (|j|+5c)\varepsilon_0, \end{aligned}$$

where we have used the fact that $|\theta-\bar{\theta}| \le \varepsilon_0$.
Then there exists $c_0>0$ such that (with the difference of identity matrices for $j=0$)

$$|R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}}| \le c_0|j|\varepsilon_0.$$

Step 2: First estimate on $|X_j-\bar{X}_j|$
We recall that

$$\begin{cases} X_j = a + R_{j\theta,\widehat{L}}(X_0-a) + jL & \text{with} \quad a \in \mathbb{R}^3 \\ \bar{X}_j = \bar{a} + R_{j\bar{\theta},\widehat{\bar{L}}}(\bar{X}_0-\bar{a}) + j\bar{L} & \text{with} \quad \bar{a} \in \mathbb{R}^3, \end{cases}$$

where up to change a in $a+\gamma L$, we can assume that we can take $\gamma=0$ in (4.1). We have

$$|X_j-\bar{X}_j| = |(a + R_{j\theta,\widehat{L}}(X_0-a) + jL) - (\bar{a} + R_{j\bar{\theta},\widehat{\bar{L}}}(\bar{X}_0-\bar{a}) + j\bar{L})|,$$

and then

$$|X_j-\bar{X}_j| = |a-\bar{a}-R_{j\bar{\theta},\widehat{\bar{L}}}(a-\bar{a}) + (R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}})(X_0-a) + R_{j\bar{\theta},\widehat{\bar{L}}}(X_0-\bar{X}_0) + j(L-\bar{L})|. \tag{4.4}$$

This implies

$$\begin{aligned} |X_j-\bar{X}_j| &\le |a-\bar{a}-R_{j\bar{\theta},\widehat{\bar{L}}}(a-\bar{a})| + |R_{j\theta,\widehat{L}} - R_{j\bar{\theta},\widehat{\bar{L}}}||X_0-a| + |X_0-\bar{X}_0| + |j||L-\bar{L}| \\ &\le A_j + c_1c_0|j|\varepsilon_0 + \varepsilon + |j|\varepsilon_0, \end{aligned}$$

with

$$A_j = |a-\bar{a}-R_{j\bar{\theta},\widehat{\bar{L}}}(a-\bar{a})|.$$

This gives

$$|X_j-\bar{X}_j| \le A_j + c_4(\varepsilon + \varepsilon_0|j|), \tag{4.5}$$

with $c_4 = \max(1, c_1c_0+1)$.
Step 3: Control of A_1
Again from (4.4), we get (using $\varepsilon_0 \le \varepsilon$)

$$A_j \le |X_j-\bar{X}_j| + c_4(1+|j|)\varepsilon.$$

For $j=1$, this gives

$$A_1 \le \varepsilon + 2c_4\varepsilon \le c_5\varepsilon,$$

with $c_5 = 1 + 2c_4$.

Step 4: Control of A_j

We get with $u = a - \bar{a}$

$$A_1 = |u - R_{\bar{\theta},\widehat{\bar{L}}}(u)| \leq c_5\varepsilon. \tag{4.6}$$

Let $u^\perp = u - (u \cdot \widehat{\bar{L}})\widehat{\bar{L}}$. Then using (4.6) and $(\bar{\theta}, \bar{L}) \in \mathcal{U}_0$ which implies that $|R_{\bar{\theta},\widehat{\bar{L}}} - I|$ is bounded from below by some positive constant, there exists $c_6 > 0$ such that

$$|u^\perp| \leq c_6\varepsilon,$$

and for all $j \in \mathbb{Z}$

$$A_j = |u - R_{j\bar{\theta},\widehat{\bar{L}}}(u)| = |u^\perp - R_{j\bar{\theta},\widehat{\bar{L}}}(u^\perp)| \leq 2c_6\varepsilon.$$

Step 5: Conclusion

Similarly we get

$$|X_j - \bar{X}_j| \leq A_j + c_4(\varepsilon + \varepsilon_0|j|) \leq 2c_6\varepsilon + c_4(\varepsilon + \varepsilon_0|j|) \leq C(\varepsilon + \varepsilon_0|j|),$$

with $C = 2c_6 + c_4$, which shows (4.2).

Step 6: Bound on $|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)|$

We compute (using (4.2)),

$$\begin{aligned} |(X_{k+1} - \bar{X}_{k+1}) - (X_k - \bar{X}_k)| &\leq C(\varepsilon + \varepsilon_0|k+1|) + C(\varepsilon + \varepsilon_0|k|) \\ &\leq C_1(\varepsilon + \varepsilon_0|k|). \end{aligned} \tag{4.7}$$

Up to change (j, j') in $(-j, -j')$ we can assume that $j' > j$. Then by iteration of (4.7), we have

$$|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)| \leq C_1\left(\varepsilon|j' - j| + \varepsilon_0\sum_{k=j}^{j'-1}|k|\right) \quad \text{for } j' > j. \tag{4.8}$$

We distinguish the cases

$$\sum_{k=j}^{j'-1}|k| = \begin{cases} \displaystyle\sum_{k=j}^{j'-1} k & \text{if } \quad j \geq 0 \\ \displaystyle -\sum_{k=1-j'}^{j} k & \text{if } \quad j' - 1 \leq 0 \\ \displaystyle -\sum_{k=j}^{0} k + \sum_{k=0}^{j'-1} k & \text{if } \quad j < 0 < j' - 1. \end{cases}$$

In each case, we deduce that there exists a constant $c_7 = c_7(j)$ such that we have

$$\sum_{k=j}^{j'-1}|k| \leq c_7(1 + |j' - j|^2),$$

Joint to (4.8), we deduce that there exists a constant $C_2 = C_2(j)$ such that we have

$$|(X_{j'} - X_j) - (\bar{X}_{j'} - \bar{X}_j)| \leq C_2(\varepsilon_0 + \varepsilon|j' - j| + \varepsilon_0|j' - j|^2).$$

□

Lemma 4.3 (Estimate between a general and a perfect nanotube)
Let us consider a nanotube X *and* $(\theta_0, L_0) \in \mathcal{U}_0$. *Let us assume that we have*

$$\sup_{|\alpha|\le 1} |X_\alpha - \widehat{X}^*_\alpha| \le \varepsilon \quad \textit{with} \quad \widehat{X}^* \in \widehat{\mathcal{C}}^{\theta_0, L_0}_*.$$

Let us assume the existence of sequences $(\theta_j, L_j) \in \mathcal{U}_0$ *such that for some* $\varepsilon > 0$, *we have*

$$D_j(X, \theta_j, L_j) \le \varepsilon \quad \textit{for } M \le j \le N \quad \textit{with } M \le 0 \le N, \tag{4.9}$$

and for some $\varepsilon_0 \ge 0$

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j| \le \varepsilon_0 \le \varepsilon \\ |L_{j+1} - L_j| \le \varepsilon_0 \le \varepsilon \end{array} \right| \qquad \textit{for } M \le j \le N-1.$$

Then there exists a constant $c > 0$ *such that*

$$|X_j - \widehat{X}^*_j| \le c\big(\varepsilon(1+|j|) + \varepsilon_0 j^2\big) \quad \textit{for} \quad M \le j \le N. \tag{4.10}$$

Error estimate (4.10) is illustrated on Figure 9.

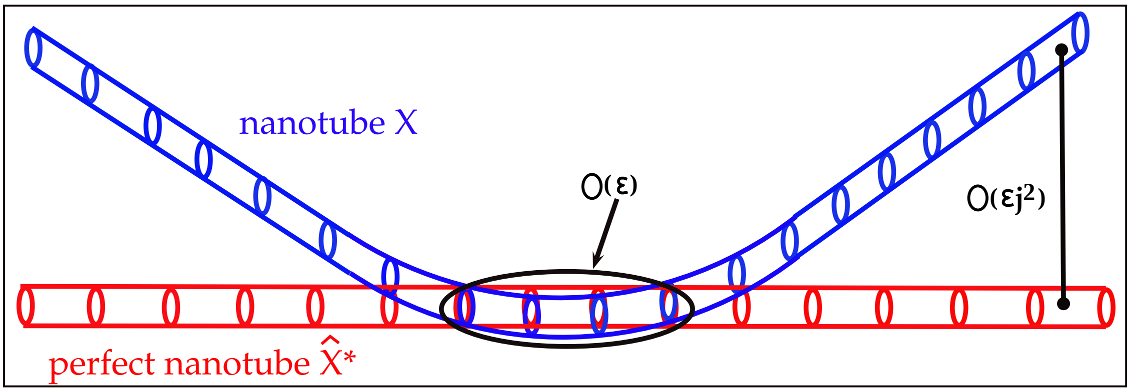

Figure 9: Illustration of error estimate (4.10) between a general and a perfect nanotube

Proof of Lemma 4.3
Let us consider a perfect nanotube $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta_j, L_j}$ that achieves the infimum in $D_j(X, \theta_j, L_j)$, which satisfies in particular

$$\sup_{|\alpha|\le 1} |X_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \le \varepsilon,$$

with the choice $\widehat{X}^{*,0} := \widehat{X}^*$.
We see that (4.9) implies for $M \le j \le N$

$$\left\{ \begin{array}{l} |X_j - \widehat{X}^{*,j}_j| \le \varepsilon \\ |X_{j+1} - \widehat{X}^{*,j}_{j+1}| \le \varepsilon \\ |X_{j-1} - \widehat{X}^{*,j}_{j-1}| \le \varepsilon. \end{array} \right. \tag{4.11}$$

Similarly for j replaced by $j-1$ with $M \le j-1 \le N$, we have

$$\left\{ \begin{array}{l} |X_{j-1} - \widehat{X}^{*,j-1}_{j-1}| \le \varepsilon \\ |X_j - \widehat{X}^{*,j-1}_j| \le \varepsilon \\ |X_{j-2} - \widehat{X}^{*,j-1}_{j-2}| \le \varepsilon. \end{array} \right. \tag{4.12}$$

Using the first line in (4.11) and the second line in (4.12) , we get

$$|\widehat{X}_j^{*,j} - \widehat{X}_j^{*,j-1}| \leq 2\varepsilon. \tag{4.13}$$

Using the last line in (4.11) and the first line in (4.12) , we get

$$|\widehat{X}_{j-1}^{*,j} - \widehat{X}_{j-1}^{*,j-1}| \leq 2\varepsilon. \tag{4.14}$$

We summarize (4.13) and (4.14) as

$$\sup_{\alpha=0,-1} |\widehat{X}_{j+\alpha}^{*,j} - \widehat{X}_{j+\alpha}^{*,j-1}| \leq 2\varepsilon \quad \text{for } M+1 \leq j \leq N.$$

Because we have $|\theta_j - \theta_{j-1}| \leq \varepsilon_0$ and $|L_j - L_{j-1}| \leq \varepsilon_0$, using (4.2) in Lemma 4.1 then there exists $c_0 = 2C_0 > 0$ such that we have

$$|\widehat{X}_k^{*,j} - \widehat{X}_k^{*,j-1}| \leq c_0(\varepsilon + \varepsilon_0|j-k|). \tag{4.15}$$

Therefore, we can write for $0 \leq j \leq N$

$$\begin{array}{rcl} |\widehat{X}_j^{*,j} - \widehat{X}_j^{*,0}| & = & |(\widehat{X}_j^{*,j} - \widehat{X}_j^{*,j-1}) + (\widehat{X}_j^{*,j-1} - \widehat{X}_j^{*,j-2}) + ... + (\widehat{X}_j^{*,1} - \widehat{X}_j^{*,0})| \\ & \leq & |\widehat{X}_j^{*,j} - \widehat{X}_j^{*,j-1}| + |\widehat{X}_j^{*,j-1} - \widehat{X}_j^{*,j-2}| + ... + |\widehat{X}_j^{*,1} - \widehat{X}_j^{*,0}| \\ & \leq & c_0\big((\varepsilon + 0\varepsilon_0) + (\varepsilon + 1\varepsilon_0) + ... + (\varepsilon + |j-1|\varepsilon_0)\big) \\ & \leq & c_0(\varepsilon|j| + \varepsilon_0 j^2), \end{array} \tag{4.16}$$

where in the third line we have used (4.15). Similarly we get the same result for $M \leq j \leq 0$ and then for $M \leq j \leq N$. Finally, we have for $M \leq j \leq N$

$$\begin{array}{rcl} |X_j - \widehat{X}_j^*| & \leq & |X_j - \widehat{X}_j^{*,j}| + |\widehat{X}_j^{*,j} - \widehat{X}_j^*| \\ & = & |X_j - \widehat{X}_j^{*,j}| + |\widehat{X}_j^{*,j} - \widehat{X}_j^{*,0}| \\ & \leq & \varepsilon + c_0(\varepsilon|j| + \varepsilon_0 j^2) \\ & \leq & c(\varepsilon(1+|j|) + \varepsilon_0 j^2), \end{array}$$

with $c = \max\{1, c_0\}$ and where in the third line we have used (4.16) and the first line of (4.11).

□

4.2 Finite differences for a single nanotube

In order to prove Propositions 4.5 and 4.6 we need first the following result:

Lemma 4.4 (Estimate on perfect nanotubes)
For $(\theta, L) \in \mathcal{U}_0$, let us consider $X \in \mathcal{C}^{\theta,L}$. Then we have

$$|X_{j',l'} - X_{j,l} - (j'-j)L| \leq 4C_0, \tag{4.17}$$

with $C_0 = \inf_{\gamma\in\mathbb{R}} \sup_{0\leq l\leq K-1} |X_{0,l} - \gamma L|$.

Proof of Lemma 4.4
We have

$$\begin{array}{rcl} X_{j,l} - X_{j',l'} & = & jL + R_{j\theta,\widehat{L}}(X_{0,l}) - j'L - R_{j'\theta,\widehat{L}}(X_{0,l'}) \\ & = & (j-j')L + (R_{j\theta,\widehat{L}} - R_{j'\theta,\widehat{L}})(X_{0,l}) + R_{j'\theta,\widehat{L}}(X_{0,l} - X_{0,l'}), \\ & = & (j-j')L + (R_{j\theta,\widehat{L}} - R_{j'\theta,\widehat{L}})(X_{0,l} - V) + R_{j'\theta,\widehat{L}}((X_{0,l} - V) - (X_{0,l'} - V)), \end{array}$$

for any vector $V = \gamma L$ for $\gamma \in \mathbb{R}$. We deduce that (4.17) holds.

□

Proposition 4.5 (Estimate on a general nanotube)
There exists a constant C such that the following holds.
For any general nanotube X, $(\theta, L) \in \mathcal{U}_0$ and $\delta \in (0,1)$, satisfying

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta,L) \le \delta,$$

we have

$$|X_{j',l'} - X_{j,l} - (j'-j)L| \le C(1 + \delta|j'-j|). \tag{4.18}$$

Moreover there exists $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta,L}$ such that

$$|X_{j',l'} - X_{j,l} - (\widehat{X}^{*,j}_{j',l'} - \widehat{X}^{*,j}_{j,l})| \le C\delta(1 + |j'-j|). \tag{4.19}$$

Proof of Proposition 4.5
We recall that there exists $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta,L}_*$ such that

$$D_j(X,\theta,L) = \sup_{|\alpha|\le q} |X_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \le \delta. \tag{4.20}$$

Writing $\widehat{X}^{*,j} = X^{*,j} + a_j$ with $X^{*,j} \in \mathcal{C}^{\theta,L}_*$ and $a_j \in L^\perp$, we deduce from Lemma 4.4 that there exists a constant C_1 such that

$$|X^{*,j}_{j,l} - X^{*,j}_{j',l'} - (j-j')L| \le C_1. \tag{4.21}$$

Because of (4.20), we can apply (4.10) in Lemma 4.3 with $\varepsilon_0 = 0$, and get the existence of a constant C_2 such that we have

$$|X_{j',l'} - X^{*,j}_{j',l'}| \le C_2\delta(1 + |j-j'|) \quad \text{for all } j \in \mathbb{Z}.$$

In particular for $(j',l') = (j,l)$, we get

$$|X_{j,l} - X^{*,j}_{j,l}| \le C_2\delta,$$

Subtracting the two last lines, we get that there exists a constant C_3 such that

$$|X_{j,l} - X_{j',l'} - (X^{*,j}_{j,l} - X^{*,j}_{j',l'})| \le C_3\delta(1 + |j-j'|),$$

which shows (4.19).
Using (4.21), we see that there exists a constant C_4 such that we have

$$|X_{j,l} - X_{j',l'} - (j-j')L| \le C_4(1 + \delta|j-j'|). \tag{4.22}$$

□

Proposition 4.6 (Another estimate on a general nanotube)
There exist $\eta \in (0,1)$ *and* $C_0 > 0$ *such that the following holds. Let us consider* $(\theta, L) \in \mathcal{U}_0$, $\delta \in (0,\eta)$ *and a nanotube* X, *satisfying*

$$\sup_{j\in\mathbb{Z}} D_j(X,\theta,L) \le \delta,$$

such that for some $(\theta^0, L^0) \in \mathcal{U}_0$, *there exists* $\widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta^0,L^0}$ *satisfying*

$$\sup_{|\alpha|\le q} |X_\alpha - \widehat{X}^*_\alpha| \le \delta.$$

Then for $t \in [0,1]$

$$Z_{j,l}(t) = tX_{j,l} + (1-t)\widehat{X}^*_{j,l},$$

we have

$$|Z_{j,l}(t) - Z_{j',l'}(t)| \ge C_0|j'-j| \quad \textit{if} \quad |j-j'| \ge \frac{1}{C_0}. \tag{4.23}$$

Proof of Proposition 4.6
From Lemma 4.4 and Proposition 4.5, we get respectively

$$|\widehat{X}^*_{j,l} - \widehat{X}^*_{j',l'} - (j-j')L^0| \le C_1, \tag{4.24}$$

and

$$|X_{j,l} - X_{j',l'} - (j-j')L| \le C_2(1+\delta|j-j'|). \tag{4.25}$$

with C_1, $C_2 > 0$. If we multiply (4.24) by $1-t$ and (4.25) by t, we can deduce that

$$\begin{aligned} |Z_{j,l}(t) - Z_{j',l'}(t) - (tL+(1-t)L^0)(j-j')| &\le tC_2(1+\delta|j-j'|) + (1-t)C_1 \\ &\le C_3\delta|j-j'| + C_3, \end{aligned}$$

with $C_3 > 0$. We can write

$$tL + (1-t)L^0 = L + (1-t)(L^0 - L).$$

We compute

$$|Z_{j,l}(t) - Z_{j',l'}(t) - (j-j')L)| \le C_3\delta|j-j'| + C_3 + |j-j'||L^0-L|.$$

This implies

$$\begin{aligned} |Z_{j,l}(t) - Z_{j',l'}(t)| &\ge |j-j'||L| - C_3 - |j-j'||L^0-L| - C_3\delta|j-j'| \\ &= |j-j'|(|L| - |L^0-L| - C_3\delta) - C_3. \end{aligned}$$

Recall that we have from (2.9)

$$|L| - |L^0 - L| \ge c_0 > 0.$$

Therefore

$$|L| - |L^0-L| - C_3\delta \ge \frac{c_0}{2} \quad \text{for} \quad \delta \le \eta := \frac{c_0}{2C_3},$$

and we deduce that there exist constants C_4 and C_5 such that we have

$$|Z_{j,l}(t) - Z_{j',l'}(t)| \ge C_4|j-j'| - C_5.$$

Then there exists a constant $C_0 > 0$ such that if $|j-j'| \ge \dfrac{1}{C_0}$, we have

$$|Z_{j,l}(t) - Z_{j',l'}(t)| \ge C_0|j-j'|. \tag{4.26}$$

□

5 Fine rigidity results for nanotubes

The main result of this section is the following:

Theorem 5.1 (Main rigidity estimate)
There exists a constant $C > 0$, such that for every nanotube X, and any $\varepsilon \in (0,1)$, if

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X,\theta,L) \le \varepsilon \qquad \text{for } M \le j \le N \quad \text{with } M < 0 < N,$$

then the following holds.
If for some $(\theta^0, L^0) \in \mathcal{U}_0$, we have $\widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta^0,L^0}$ and $\sup_{|\alpha|\le q} |X_\alpha - \widehat{X}^*_\alpha| \le \varepsilon$.
Then $\bar{X} := X - \widehat{X}^*$ satisfies

$$|\bar{X}_j| \le C\varepsilon(1+|j|^2) \qquad \text{for} \quad M \le j \le N, \tag{5.1}$$

and for all $M+1 \le j \le N-1$, there exists a constant $C' = C'(j)$ such that we have

$$|\bar{X}_{j'} - \bar{X}_j| \le C'\varepsilon(1+|j'-j|^2) \qquad \text{for all} \quad M \le j' \le N. \tag{5.2}$$

In order to prove this result, we need Lemma 5.2 and Proposition 5.4 below.

Lemma 5.2 (A quantitative estimate for perfect nanotubes)
Assume that $X \in \widehat{\mathcal{C}}^{\theta,L}$, $\bar{X} \in \widehat{\mathcal{C}}^{\bar{\theta},\bar{L}}$, with (θ,L), $(\bar{\theta},\bar{L}) \in [0,2\pi) \times (\mathbb{R}^3\backslash\{0\})$, with

$$\left\{\begin{array}{l} \sup_{\alpha=0,1} |\bar{X}_\alpha - X_\alpha| \le \varepsilon \\ |\widehat{\bar{L}} - \widehat{L}| \le \varepsilon. \end{array}\right. \tag{5.3}$$

If moreover

$$X = a + Y \quad \text{with} \quad Y \in \mathcal{C}^{\theta,L},$$

and

$$\left\{\begin{array}{l} \inf_{\gamma\in\mathbb{R}} \sup_{0\le l\le K-1} |Y_{0,l} - \gamma L| \le c_1 \\ |L| \le c_1, \end{array}\right. \tag{5.4}$$

then there exists $C = C(c_1) > 0$, such that

$$\big||L| - |\bar{L}|\big| \le C\,\varepsilon. \tag{5.5}$$

Proof of Lemma 5.2
We recall that

$$X_1 - a = R_{\theta,\widehat{L}}(X_0 - a) + L,$$

and then

$$\widehat{L} \cdot (X_1 - X_0) = |L|, \tag{5.6}$$

and similarly

$$\widehat{\bar{L}} \cdot (\bar{X}_1 - \bar{X}_0) = |\bar{L}|. \tag{5.7}$$

From (5.3), we deduce
$$|(\bar{X}_1 - \bar{X}_0) - (X_1 - X_0)| \leq 2\varepsilon.$$
Taking the scalar product with $\widehat{\bar{L}}$, we get
$$|\widehat{\bar{L}} \cdot (\bar{X}_1 - \bar{X}_0) - \widehat{\bar{L}} \cdot (X_1 - X_0)| \leq 2\varepsilon.$$
i.e. (using (5.7))
$$||\bar{L}| - \widehat{\bar{L}} \cdot (X_1 - X_0)| \leq 2\varepsilon.$$
Using moreover (5.6), we deduce
$$||\bar{L}| - |L|| \leq 2\varepsilon + |(X_1 - X_0) \cdot (\widehat{\bar{L}} - \widehat{L})|.$$
We also have for any $\gamma \in \mathbb{R}$
$$X_1 - X_0 = L + (R_{\theta,\widehat{L}} - I)(Y_0 - \gamma L),$$
and (5.4) implies
$$||\bar{L}| - |L|| \leq 2\varepsilon + 3c_1\varepsilon,$$
which implies (5.5).

□

In order to prove Proposition 5.4 below, we need to introduce the following:

Definition 5.3 (Barycenter and centered cell)
We define the barycenter b_j of the cell X_j of a nanotube $X = ((X_{j,l})_{0\leq l\leq K-1})_{j\in\mathbb{Z}}$ by
$$b_j = \frac{1}{K} \sum_{l=0}^{K-1} X_{j,l}.$$
And we define the centered cell X'_j by
$$X'_{j,l} = X_{j,l} - b_j \quad \textit{and} \quad X'_j = (X'_{j,l})_{0\leq l\leq K-1}.$$

Proposition 5.4 (Error estimate on the angles and the axes)
There exists a constant $C > 0$ and $\varepsilon_1 > 0$ such that if a nanotube X satisfies for some $\varepsilon \in [0, \varepsilon_1)$
$$D_k(X, \theta_k, L_k) \leq \varepsilon \quad \textit{for } k = j,\ j+1,$$
then we have
$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j| \leq C\varepsilon \\ |L_{j+1} - L_j| \leq C\varepsilon. \end{array} \right. \tag{5.8}$$

Proof of Proposition 5.4
We have
$$D_k(X, \theta_k, L_k) \leq \varepsilon \quad \text{for } k = j,\ j+1,$$
which implies that there exists $\widehat{X}^{*,k} \in \widehat{\mathcal{C}}_*^{\theta_k, L_k}$ such that
$$\sup_{|\alpha|\leq q} |X_{k+\alpha} - \widehat{X}^{*,k}_{k+\alpha}| \leq \varepsilon. \tag{5.9}$$

Taking the difference for $k = j$ and $\alpha = 0, 1$ (respectively $k = j+1$ and $\alpha = -1, 0$), we get

$$\sup_{\beta=0,1} |\widehat{X}^{*,j+1}_{j+\beta} - \widehat{X}^{*,j}_{j+\beta}| \le 2\varepsilon. \tag{5.10}$$

Step 1: Preliminary estimate

Writing

$$\widehat{X}^{*,k} = a_k + X^{*,k} \quad \text{with} \quad X^{*,k} \in \mathcal{C}_*^{\theta_k, L_k} \quad \text{and} \quad \left\{ \begin{array}{l} \inf\limits_{\gamma\in\mathbb{R}} \sup\limits_{0\le l\le K-1} |X^{*,k}_{k,l} - \gamma L_k| \le c_1 \\ |L_k| \le c_1, \end{array} \right. \tag{5.11}$$

with $c_1 > 0$, we deduce (by convexity) for the centered cell (see Definition 5.3)

$$\sup_{\beta=0,1} |(X^{*,j+1}_{j+\beta})' - (X^{*,j}_{j+\beta})'| \le 2\varepsilon. \tag{5.12}$$

Applying the rotation $R_{\theta_{j+1},\widehat{L}_{j+1}}$ to (5.12) for $\beta = 0$, we get

$$|R_{\theta_{j+1},\widehat{L}_{j+1}}(X^{*,j+1}_j)' - R_{\theta_{j+1},\widehat{L}_{j+1}}(X^{*,j}_j)'| \le 2\varepsilon. \tag{5.13}$$

Recall that

$$(X^{*,k}_{j+1})' = R_{\theta_k,\widehat{L}_k}(X^{*,k}_j)'.$$

Then (5.12) for $\beta = 1$ can be rewritten as

$$|R_{\theta_{j+1},\widehat{L}_{j+1}}(X^{*,j+1}_j)' - R_{\theta_j,\widehat{L}_j}(X^{*,j}_j)'| \le 2\varepsilon. \tag{5.14}$$

Substracting (5.13) and (5.14), we get

$$|(R_{\theta_{j+1},\widehat{L}_{j+1}} - R_{\theta_j,\widehat{L}_j})(X^{*,j}_j)'| \le 4\varepsilon. \tag{5.15}$$

Step 2: Estimate on $|(\theta_{j+1}, \widehat{L}_{j+1}) - (\theta_j, \widehat{L}_j)|$

Case 1: $q \ge 1$ and three atoms of $\mathcal{X}_0^*(\theta, L)$ are not aligned for each $(\theta, L) \in \mathcal{U}_0$

Because we can find at least three atoms not aligned in $X^{*,j}_j$, this implies that there exist two vectors v_i, $i = 1, 2$ in the centered cell $(X^{*,j}_j)'$ such that

$$|v_1|, |v_2| \le \frac{1}{c_0} \quad \text{and} \quad |v_1 \times v_2| \ge c_0 > 0, \tag{5.16}$$

for some constant c_0 uniform in $(\theta_j, L_j) \in \mathcal{U}_0$.

If $\theta_j \in [0, \pi]$, using the fact that

$$\overline{\mathcal{U}_0} \subset (0, 2\pi) \times \mathbb{R}^3 \backslash \{0\}, \tag{5.17}$$

then we can apply Lemma 13.10 to (5.15) and deduce that there exists a constant $C_1 > 0$ and $m \in \mathbb{Z}$ such that

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j - 2m\pi| \le C_1\varepsilon \\ |\widehat{L}_{j+1} - \widehat{L}_j| \le C_1\varepsilon. \end{array} \right. \tag{5.18}$$

or (using $R_{2\pi-\theta_{j+1},-\widehat{L}_{j+1}} = R_{\theta_{j+1},\widehat{L}_{j+1}}$)

$$\left\{ \begin{array}{l} |2\pi - \theta_{j+1} - \theta_j - 2m\pi| \le C_1\varepsilon \\ |-\widehat{L}_{j+1} - \widehat{L}_j| \le C_1\varepsilon. \end{array} \right. \tag{5.19}$$

The last line of (5.19) is impossible for $(\theta_k, L_k) \in \mathcal{U}_0$, $k = j, j+1$ and ε small enough, because of (2.9). Notice that (5.17) implies $m = 0$ for ε in (5.18) small enough. Similarly if $\theta_j \in [\pi, 2\pi]$, we set $\bar{\theta}_k = 2\pi - \theta_k$, $\bar{L}_k = -L_k$ for $k = j, j+1$ and apply the previous reasoning to $\bar{\theta}_j \in [0, \pi]$. Then in all cases this shows

$$\text{(5.20)} \qquad \begin{cases} |\theta_{j+1} - \theta_j| \le C_1 \varepsilon \\ |\widehat{L}_{j+1} - \widehat{L}_j| \le C_1 \varepsilon. \end{cases}$$

Case 2: The general case

Let us consider the new supercell $\tilde{X}_0^{*,k}$ (see Figure 10) for $k = j, j+1$ built from the r cells $X_j^{*,k}, X_{j+1}^{*,k}, ..., X_{j+r-1}^{*,k}$ for $r \ge 2$, with

$$\begin{cases} \tilde{X}_m^{*,k} = (\tilde{X}_{m,\tilde{l}}^{*,k})_{0 \le \tilde{l} \le \tilde{K}-1} \quad \text{with} \quad \tilde{K} = rK, \\ \tilde{X}_{m,pK+l}^{*,k} = X_{j+mr+p,l}^{*,k} \quad \text{for} \quad p = 0, ..., r-1 \quad \text{and} \quad l = 0, ..., K-1. \end{cases}$$

Because $X^{*,k} \in \mathcal{C}^{\theta_k, L_k}$, we get $\tilde{X}^{*,k} \in \mathcal{C}^{\tilde{\theta}_k, \tilde{L}_k}$ with $\tilde{\theta}_k = r\theta_k$ and $\tilde{L}_k = rL_k$, and $\tilde{X}^{*,k}$ satisfies

$$\tilde{X}_{m+1}^{*,k} = R_{\tilde{\theta}_k, \widehat{\tilde{L}}_k}(\tilde{X}_m^{*,k}) + \tilde{L}_k.$$

Now if all the atoms of $\tilde{X}_0^{*,k}$ are aligned, applying T^{θ_k, L_k} to the cells $X_j^{*,k}, X_{j+1}^{*,k}, ..., X_{j+r-1}^{*,k}$, we get that all the atoms of $X_{j+1}^{*,k}, X_{j+2}^{*,k}, ..., X_{j+r}^{*,k}$ are also aligned.
If $r \ge 3$, whatever is the value $K \ge 1$, we conclude that all the atoms of $X_j^{*,k}, X_{j+1}^{*,k}, ..., X_{j+r}^{*,k}$ are aligned.

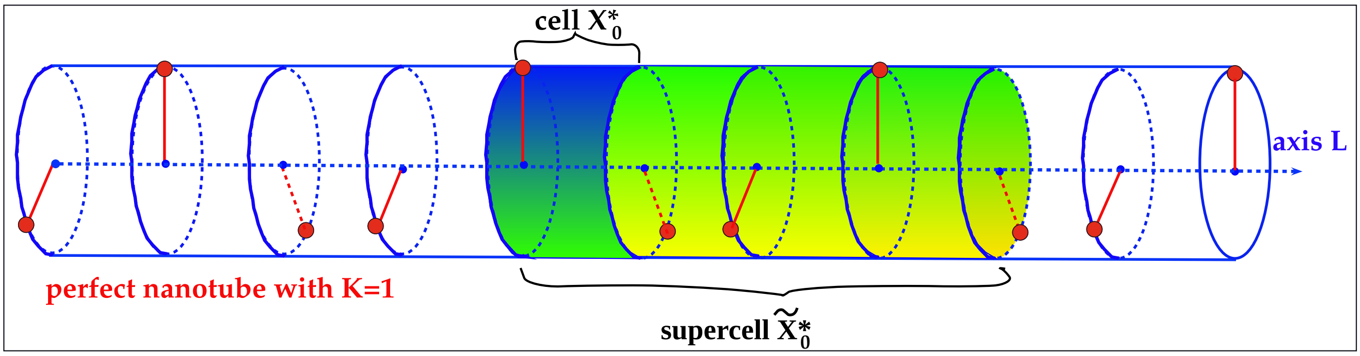

Figure 10: The supercell $\tilde{X}_0^*$ constructed using $X_0^*, ..., X_{r-1}^*$ for $r = 4$, $\theta = \dfrac{2\pi}{3}$, and $K = 1$

If $K \ge 2$ and $r \ge 2$, we also conclude that all the atoms of $X_j^{*,k}, ..., X_{j+r}^{*,k}$ are aligned.
By iteration, this implies that all atoms of $X^{*,k}$ are aligned, which is excluded by assumption (2.7). We conclude that we can find three atoms not aligned in $\tilde{X}_0^{*,k}$.
Recalling the definition of a_k in (5.11), we define

$$\widehat{\tilde{X}}_m^{*,k} := a_k + \tilde{X}_m^{*,k}.$$

Following assumption (H3), and using (2.10), we get that $r\theta \ne 0\,(2\pi)$ for all $(\theta, L) \in \mathcal{U}_0$.
Recall that (5.9) implies (by difference) for $k = j$ and $k = j+1$ and $q \ge q_0 \ge 2r-1 \ge r \ge 1$

$$|\widehat{X}_{j+\beta}^{*,j+1} - \widehat{X}_{j+\beta}^{*,j}| \le 2\varepsilon \quad \text{for} \quad 0 \le \beta \le 2r-1.$$

This implies

$$|\widehat{\tilde{X}}^{*,j+1}_{\tilde{\beta}} - \widehat{\tilde{X}}^{*,j}_{\tilde{\beta}}| \leq 2\varepsilon \quad \text{for} \quad \tilde{\beta} = 0, 1, \tag{5.21}$$

which is exactly similar to (5.10).
This shows that we can apply Step 1 and Step 2 (case 1) using (5.21) in place of (5.10). Because by construction there are at least three atoms not aligned in the centered cell $(\tilde{X}^{*,j}_j)'$ with $\tilde{\theta}_j = r\theta_j \neq 0\,(2\,\pi)$ and $\tilde{L}_j = rL_j$, we conclude that

$$\left\{ \begin{array}{l} |\tilde{\theta}_{j+1} - \tilde{\theta}_j| \leq C_1\varepsilon \\ |\widehat{\tilde{L}}_{j+1} - \widehat{\tilde{L}}_j| \leq C_1\varepsilon, \end{array} \right.$$

which implies (5.20).
Step 3: Proof of $|L_{j+1} - L_j| \leq C\varepsilon$.
Because

$$|\widehat{L}_{j+1} - \widehat{L}_j| \leq C_1\varepsilon, \tag{5.22}$$

we can apply Lemma 5.2, using (5.10) and (5.11) and checking that (5.4) is satisfied because $(\theta_j, L_j) \in \mathcal{U}_0$. We deduce that there exists a constant C_2 such that

$$\big||L_{j+1}| - |L_j|\big| \leq C_2\varepsilon. \tag{5.23}$$

We can compute

$$\begin{array}{rcl} |L_{j+1} - L_j| & = & \big||L_{j+1}|\widehat{L}_{j+1} - |L_j|\widehat{L}_j\big| \\ & = & \big||L_{j+1}|\widehat{L}_{j+1} - |L_{j+1}|\widehat{L}_j + |L_{j+1}|\widehat{L}_j - |L_j|\widehat{L}_j\big| \\ & \leq & |L_{j+1}||\widehat{L}_{j+1} - \widehat{L}_j| + \big||L_{j+1}| - |L_j|\big||\widehat{L}_j|. \end{array}$$

Using (5.23) and (5.22), we deduce that there exists a constant C_3 such that

$$|L_{j+1} - L_j| \leq C_3\varepsilon,$$

This last inequality and (5.20) imply (5.8).

□

Proof of Theorem 5.1
Step 1: Proof of (5.1)
We have

$$\left\{ \begin{array}{ll} \displaystyle\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X,\theta,L) \leq \varepsilon & \quad \text{for } M \leq j \leq N \\ \displaystyle\sup_{|\alpha|\leq q} |X_\alpha - \widehat{X}^*_\alpha| \leq \varepsilon, & \end{array} \right.$$

then for $M \leq j \leq N$, there exists $(\theta_j, L_j) \in \mathcal{U}_0$ such that

$$\left\{ \begin{array}{l} D_j(X, \theta_j, L_j) \leq \varepsilon \\ \text{with } \theta_0 = \theta^0 \text{ and } L_0 = L^0. \end{array} \right. \tag{5.24}$$

Then by Proposition 5.4 we deduce that there exists a constant $c > 0$ such that we have

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j| \leq c\varepsilon \\ |L_{j+1} - L_j| \leq c\varepsilon \end{array} \right| \text{for } M \leq j \leq N-1. \tag{5.25}$$

Moreover because $D_j(X,\theta_j,L_j) \le \varepsilon$ for $M \le j \le N$ and $\sup_{|\alpha|\le q} |X_\alpha - \widehat{X}^*_\alpha| \le \varepsilon$, we can apply Lemma 4.3 and we deduce that there exists a constant C such that we have

$$|\bar{X}_j| \le C\varepsilon(1+|j|^2) \qquad \text{for } M \le j \le N.$$

Step 2: Proof of (5.2)
Step 2-1: Preliminary result: proof of (5.27)
By (5.1), we have for $M+1 \le j \le N$

$$|X_{j+\alpha} - \widehat{X}^*_{j+\alpha}| \le C\varepsilon(1+|j+\alpha|^2) \quad \text{for } \alpha = -1, 0.$$

Because of (5.24), we get

$$|X_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \le \varepsilon \quad \text{for } \alpha = -1, 0 \quad \text{and } M \le j \le N.$$

Substracting these two lines, we get that there exists a constant C_1 such that

$$(5.26) \qquad |\widehat{X}^*_{j+\alpha} - \widehat{X}^{*,j}_{j+\alpha}| \le C_1\varepsilon(1+|j+\alpha|^2) \quad \text{for } \alpha = -1, 0 \quad \text{and } M+1 \le j \le N.$$

On the other hand, by an iteration of (5.25) we have for $M \le j \le N-1$

$$\begin{cases} |\theta_0 - \theta_j| \le c\varepsilon|j| \\ |L_0 - L_j| \le c\varepsilon|j|. \end{cases}$$

Moreover using (5.26), we can apply (4.3) in Lemma 4.1, and we deduce that there exists a constant $C_2 = C_2(j)$ such that we have for $M+1 \le j \le N-1$ and any $j' \in \mathbb{Z}$,

$$(5.27) \qquad |(\widehat{X}^*_{j'} - \widehat{X}^*_j) - (\widehat{X}^{*,j}_{j'} - \widehat{X}^{*,j}_j)| \le C_2\varepsilon(1+|j'-j|^2).$$

Step 2-2: Proof of (5.29)
We have

$$D_j(X,\theta_j,L_j) \le \varepsilon \quad \text{for } M \le j \le N,$$

then for $M \le j', j \le N$, there exist $\widehat{X}^{*,j'} \in \widehat{\mathcal{C}}^{\theta_{j'},L_{j'}}_*$ and $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta_j,L_j}_*$ such that we have

$$\begin{cases} |X_{j'} - \widehat{X}^{*,j'}_{j'}| \le \varepsilon \\ |X_j - \widehat{X}^{*,j}_j| \le \varepsilon. \end{cases}$$

Substracting the two lines we deduce that

$$|X_{j'} - X_j - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_j)| \le 2\varepsilon.$$

Using

$$\bar{X}_{j'} - \bar{X}_j = X_{j'} - X_j - (\widehat{X}^*_{j'} - \widehat{X}^*_j),$$

we deduce

$$|\bar{X}_{j'} - \bar{X}_j + (\widehat{X}^*_{j'} - \widehat{X}^*_j) - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_j)| \le 2\varepsilon,$$

and then for $M \le j', j \le N$, we get

$$(5.28) \qquad |\bar{X}_{j'} - \bar{X}_j + (\widehat{X}^*_{j'} - \widehat{X}^*_j) - (\widehat{X}^{*,j}_{j'} - \widehat{X}^{*,j}_j) - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_{j'})| \le 2\varepsilon.$$

Using moreover (5.27), we deduce that there exists a constant $C_3 = C_3(j)$ such that for $M+1 \le j \le N-1$ we have

$$|\bar{X}_{j'} - \bar{X}_j - (\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_{j'})| \le C_3\varepsilon(1+|j'-j|^2) \quad \text{for all } M \le j' \le N. \tag{5.29}$$

Step 2-3: Conclusion
By a generalization of (5.1) (replace $\widehat{X}^* = \widehat{X}^{*,0}$ by $\widehat{X}^{*,j}$ for $M+1 \le j \le N-1$) we deduce that there exists a constant C_4 such that we have for $M \le j' \le N$

$$|X_{j'} - \widehat{X}^{*,j}_{j'}| \le C_4\varepsilon(1+|j'-j|^2).$$

But because $D_{j'}(X, \theta'_j, L'_j) \le \varepsilon$ for $M \le j' \le N$, we deduce $|X_{j'} - \widehat{X}^{*,j'}_{j'}| \le \varepsilon$ for $M \le j' \le N$, and then

$$|\widehat{X}^{*,j'}_{j'} - \widehat{X}^{*,j}_{j'}| \le C_4\varepsilon(1+|j'-j|^2) + \varepsilon \quad \text{for} \quad M \le j' \le N \quad \text{and} \quad M+1 \le j \le N-1.$$

Using moreover (5.29), we deduce for $M+1 \le j \le N-1$ and $M \le j' \le N$ that

$$|\bar{X}_{j'} - \bar{X}_j| \le C_4\varepsilon(1+|j'-j|^2) + \varepsilon + C_3\varepsilon(1+|j'-j|^2),$$

which implies (5.2).

□

6 Proof of a discrete Saint-Venant principle: Theorem 2.13 and Corollary 2.14

Proof of Theorem 2.13
We do the proof by contradiction in several steps.
Step 1: Construction of sequences
Assume by contradiction that the statement of Theorem 2.13 is false. This means that for every $\delta_0 > 0$, $\mu \in (0,1)$, $C_1, C_2 > 0$, there exists X satisfying (1.13) with forces $(f_j)_{j\in Z}$ and (11.1), and there exists a box J such that (2.15) is false with the definition (11.2) of ρ. We can choose 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 $(X^n)_{n\in\mathbb{N}}$, $(J^n)_{n\in\mathbb{N}}$, $(\rho^n)_{n\in\mathbb{N}}$, $(f^n)_{n\in\mathbb{N}}$ such that

$$\begin{cases} \sup_{j\in\mathbb{Z}} D_j(X^n, \theta^*, L^*) \le \delta_0^n \to 0, \\ (\rho^n)^p = \dfrac{C_2^n}{\mathcal{N}_{J^n}(X^n)} \to +\infty, \\ \mathcal{N}_{J^n}(X^n) \ > \ \mu^n\, \mathcal{N}_{J^n_{\rho^n}}(X^n) + C_1^n \sup_{j\in J^n_{\rho^n}} |f_j^n|, \\ X^n \text{ satisfies (1.13) with forces } f^n. \end{cases} \tag{6.1}$$

Then we set

$$\varepsilon^n := \mathcal{N}_{J^n}(X^n).$$

We have

$$\mathcal{N}_{J^n}(X^n) = \sup_{j\in J^n} \inf_{(\theta,L)\in\mathcal{U}_0} D_j(X^n,\theta,L) \le \sup_{j\in\mathbb{Z}} D_j(X^n,\theta^*,L^*) \le \delta_0^n \to 0. \tag{6.2}$$

which implies

$$\varepsilon^n \to 0. \tag{6.3}$$

When J^n is bounded, we can define $j^n \in J^n$ and $(\theta^n, L^n) \in \mathcal{U}_0$ such that

$$\varepsilon^n = \mathcal{N}_{J^n}(X^n) = \sup_{j\in J^n} \inf_{(\theta,L)\in\mathcal{U}_0} D_j(X^n,\theta,L) = \inf_{(\theta,L)\in\mathcal{U}_0} D_{j^n}(X^n,\theta,L) = D_{j^n}(X^n,\theta^n,L^n). \tag{6.4}$$

When J^n is not bounded, we can use an approximation argument and for instance assume that there exists $j^n \in J^n$ such that

$$\varepsilon^n \ge \frac{n}{n+1}\left(\inf_{(\theta,L)\in\mathcal{U}_0} D_{j^n}(X^n,\theta,L)\right) = \frac{n}{n+1} D_{j^n}(X^n,\theta^n,L^n).$$

In order to simplify the presentation, we restrict the proof to the case of J^n bounded, but the adaptation to the general case is straightforward.

Step 2: Proof that $(\theta^n, L^n, X^n_{j^n+\cdot}) \to (\theta^*, L^*, \widehat{X}^{**,\infty})$ for $\widehat{X}^{**,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$

Step 2-1: Proof that $X^n_{j^n+\cdot} \to \widehat{X}^{**,\infty}$ for $\widehat{X}^{**,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$

By (6.2) and by definition of $D_{j^n}(X^n,\theta^*,L^*)$, there exists $\widehat{X}^{**,j^n} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$ such that

$$\sup_{|\alpha|\le q} |X^n_{j^n+\alpha} - \widehat{X}^{**,j^n}_{j^n+\alpha}| \le \delta_0^n. \tag{6.5}$$

Up to substract a suitable constant, we can assume that $\widehat{X}^{**,j^n}_{j^n}$ is bounded.
Using (6.2) and (6.5), we can apply (5.1) of Theorem 5.1 and we deduce that there exists a constant C_1 such that

$$|X^n_{j^n+j} - \widehat{X}^{**,j^n}_{j^n+j}| \le C_1\delta_0^n(1+|j|^2).$$

Because $\delta_0^n \to 0$, we deduce that

$$\lim_n X^n_{j^n+j} = \lim_n \widehat{X}^{**,j^n}_{j^n+j} = \widehat{X}^{**,\infty}_j \quad \text{with } \widehat{X}^{**,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}. \tag{6.6}$$

Step 2-2: Proof of $(\theta^n, L^n) \to (\theta^*, L^*)$

From (6.2), we have

$$D_j(X^n,\theta^*,L^*) \le \delta_0^n \quad \text{for all } j\in\mathbb{Z},$$

and then in particular

$$D_{j^n+1}(X^n,\theta^*,L^*) \le \delta_0^n.$$

Recall that from (6.2) and (6.4), we also have

$$D_{j^n}(X^n,\theta^n,L^n) \le \delta_0^n, \tag{6.7}$$

We can apply Proposition 5.4, and deduce that there exists a constant C_2 such that we have

$$\left\{ \begin{array}{l} |\theta^n - \theta^*| \leq C_2 \delta_0^n \\ |L^n - L^*| \leq C_2 \delta_0^n, \end{array} \right.$$

which implies in the limit $\delta_0^n \to 0$ that

$$(\theta^n, L^n) \to (\theta^*, L^*). \tag{6.8}$$

Step 3: A priori estimates for renormalized quantities
Let us define

$$\bar{X}_j^n = \frac{X_{j+j^n}^n - \widehat{X}_{j+j^n}^{*,j^n}}{\varepsilon^n},$$

with $(\widehat{X}_j^{*,j^n})_{j\in\mathbb{Z}} = \widehat{X}^{*,j^n} \in \widehat{\mathcal{C}}_*^{\theta^n, L^n}$, where we recall that

$$D_{j^n}(X^n, \theta^n, L^n) = \sup_{|\alpha|\leq q} |X_{j^n+\alpha}^n - \widehat{X}_{j^n+\alpha}^{*,j^n}|.$$

Let us define

$$\bar{D}_j^n(\bar{X}^n, \theta, L) := \frac{1}{\varepsilon^n} D_{j+j^n}(X^n, \theta, L), \tag{6.9}$$

we have

$$\inf_{(\theta,L)\in\mathcal{U}_0} \bar{D}_0^n(\bar{X}^n, \theta, L) = \inf_{(\theta,L)\in\mathcal{U}_0} \frac{1}{\varepsilon^n} D_{j^n}(X^n, \theta, L) = 1. \tag{6.10}$$

On the other hand we have from (6.1)

$$\begin{array}{rcll} \varepsilon^n = \mathcal{N}_{J^n}(X^n) & > & \mu^n \mathcal{N}_{J_{\rho^n}^n}(X^n) + C_1^n \sup_{j\in J_{\rho^n}^n} |f_j^n| & \\ & \geq & \mu^n \mathcal{N}_{J_{\rho^n}^n}(X^n) & \\ & = & \mu^n \sup_{j+j^n\in J_{\rho^n}^n} \inf_{(\theta,L)\in\mathcal{U}_0} D_{j+j^n}^n(X^n, \theta, L) & \\ & = & \mu^n \sup_{j+j^n\in J_{\rho^n}^n} \inf_{(\theta,L)\in\mathcal{U}_0} \varepsilon^n \bar{D}_j^n(\bar{X}^n, \theta, L) & \\ & \geq & \varepsilon^n \mu^n \inf_{(\theta,L)\in\mathcal{U}_0} \bar{D}_j^n(\bar{X}^n, \theta, L) & \text{for all } j + j^n \in J_{\rho^n}^n, \end{array}$$

hence we obtain

$$\inf_{(\theta,L)\in\mathcal{U}_0} \bar{D}_j^n(\bar{X}^n, \theta, L) < \frac{1}{\mu^n} \quad \text{for all} \quad j \in J_{\rho^n}^n - j^n \supset Q_{\rho^n} = \{-\rho^n, \cdots, \rho^n\}. \tag{6.11}$$

On the other hand by (6.4) we have $D_{j^n}(X^n, \theta^n, L^n) \leq \varepsilon^n$, then we deduce

$$\sup_{|\alpha|\leq q} |X_{j^n+\alpha}^n - X_{j^n+\alpha}^{*,j^n}| \leq \varepsilon^n.$$

Using moreover (6.11), and taking into account the definition (6.9) of $\bar{D}_j^n$, we can apply Theorem 5.1 and we deduce that there exists a constant C_3 such that we have

$$|\bar{X}_j^n| \leq \frac{C_3}{\mu^n}(1 + j^2) \quad \text{for } j \in Q_{\rho^n}. \tag{6.12}$$

and a constant $C_4 = C_4(j)$ such that

$$|\bar{X}^n_{j'} - \bar{X}^n_j| < \frac{C_4}{\mu^n}(1 + |j - j'|^2) \quad \text{for } j', j \in Q_{\rho^n - 1}. \tag{6.13}$$

Step 4: Definition and equation verified by g^n_j

Let us define

$$g^n_j := \frac{f^n_{j+j^n}}{\varepsilon^n} \quad \text{for all} \quad j \in J^n_{\rho^n} - j^n,$$

we have

$$\varepsilon^n > C^n_1 \sup_{j \in J^n_{\rho^n} - j^n} |f^n_{j+j^n}| = \varepsilon^n C^n_1 \sup_{j \in J^n_{\rho^n} - j^n} |g^n_j|,$$

then g^n_j satisfies

$$|g^n_j| < \frac{1}{C^n_1} \to 0 \quad \text{as} \quad n \to +\infty, \quad \text{for each } j \in \mathbb{Z}. \tag{6.14}$$

From (1.13) we deduce that

$$f^n_{j+j^n,l} + \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(X^n_{j+j^n,l} - X^n_{j'+j^n,l'}) = 0 \qquad \text{for all } j \in \mathbb{Z},\ 0 \le l \le K - 1.$$

i.e.

$$\varepsilon^n g^n_{j,l} + \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(\varepsilon^n(\bar{X}^n_{j,l} - \bar{X}^n_{j',l'}) + \widehat{X}^{*,j^n}_{j+j^n,l} - \widehat{X}^{*,j^n}_{j'+j^n,l'}) = 0 \qquad \text{for all } j \in \mathbb{Z},\ 0 \le l \le K-1.$$

On the other hand, we have

$$\sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} \nabla V(\widehat{X}^{*,j^n}_{j+j^n,l} - \widehat{X}^{*,j^n}_{j'+j^n,l'}) = 0.$$

Taking the difference, we get with

$$Z^n_{j,l}(t) = tX^n_{j+j^n,l} + (1-t)\widehat{X}^{*,j^n}_{j+j^n,l},$$

that

$$g^n_{j,l} + \int_0^1 dt \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} D^2V\big(Z^n_{j,l}(t) - Z^n_{j',l'}(t)\big) \cdot (\bar{X}^n_{j,l} - \bar{X}^n_{j',l'}) = 0, \tag{6.15}$$

In order to pass to the limit in (6.15), we nead some further estimates. To this end, we will estimate for any fixed $j \in Q_{\rho^n/2}$ separately a short distance contribution

$$S^n_j := \sum_{\substack{j' \in (j + Q_{\rho^n/2}) \\ 0 \le l' \le K-1}} D^2V\big(Z^n_{j,l}(t) - Z^n_{j',l'}(t)\big) \cdot (\bar{X}^n_{j,l} - \bar{X}^n_{j',l'}),$$

and for a far away contribution

$$F_j^n := \sum_{\substack{j' \in \mathbb{Z}\backslash(j+Q_{\rho^n/2}) \\ 0 \le l' \le K-1}} D^2V\big(Z_{j,l}^n(t) - Z_{j',l'}^n(t)\big) \cdot (\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n).$$

Step 5: useful controls
Step 5-1: A long distance control of $|\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n|$
By the definition of $\bar{X}_j^n$, we have

$$|\bar{X}_j^n - \bar{X}_{j'}^n| = \frac{1}{\varepsilon^n}|X_{j+j^n}^n - X_{j'+j^n}^n - (\widehat{X}_{j+j^n}^{*,j^n} - \widehat{X}_{j'+j^n}^{*,j^n})|.$$

By Proposition 4.5 applied both to $X_{j^n+\cdot}^n$ and $\widehat{X}_{j^n+\cdot}^{*,j^n}$, we get that there exists a constant C_4 such that

$$\text{(6.16)} \qquad \begin{cases} |X_{j+j^n,l}^n - X_{j'+j^n,l'}^n| \le C_4(1+|j-j'|) \\ |\widehat{X}_{j+j^n,l}^{*,j^n} - \widehat{X}_{j'+j^n,l'}^{*,j^n}| \le C_4(1+|j-j'|). \end{cases}$$

This implies

$$\text{(6.17)} \qquad |\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n| \le \frac{2C_4}{\varepsilon^n}(1+|j-j'|),$$

Step 5-2: Control on $|Z_{j,l}^n(t) - Z_{j',l'}^n(t)|$
Recall that

$$\sup_{|\alpha|\le q} |X_{j+j^n+\alpha,l}^n - \widehat{X}_{j+j^n+\alpha,l}^{*,j^n}| \le \delta_0^n,$$

and

$$\sup_{j\in\mathbb{Z}} D_j(X^n, \theta^*, L^*) \le \delta_0^n.$$

Therefore by definition of $Z_{j,l}^n(t)$ and by Proposition 4.6, there exists a constant C_5 such that we have

$$\text{(6.18)} \qquad |Z_{j,l}^n(t) - Z_{j',l'}^n(t)| \ge C_5|j-j'| \quad \text{for } |j-j'| \ge \frac{1}{C_5} > 0.$$

As a consequence, by assumption (H0), there exists a constant C_6 such that we have

$$\text{(6.19)} \qquad |D^2V\big(Z_{j,l}^n(t) - Z_{j',l'}^n(t)\big)| \le \frac{C_6}{|j-j'|^{p+2}} \quad \text{for } |j-j'| \ge \frac{1}{C_5}$$

Step 6: Passing to the limit
Up to extraction of convergent subsequences, by (6.12) , (6.14), (6.8) and (6.6) we can assume that

$$\text{(6.20)} \qquad \begin{cases} \bar{X}_j^n \to \bar{X}_j^\infty \\ g_j^n \to 0 \\ L^n \to L^* \\ \theta^n \to \theta^* \\ \widehat{X}_{j^n+\cdot}^{*,j^n} \to \widehat{X}^{*,\infty} := \widehat{X}^{**,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}. \end{cases}$$

Passing to the limit in (6.12) we get

$$(6.21) \qquad |\bar{X}_j^\infty| \le C_3(1+|j|^2).$$

We now want to pass to the limit in (6.15).
On the one hand from (6.17) and (6.19), there exist a constant C_7 and a constant C_8 such that we have

$$|F_j^n| \le \sum_{\substack{j' \in \mathbb{Z}\backslash(j+Q_{\rho^n/2}) \\ 0 \le l' \le K-1}} \frac{C_6}{|j-j'|^{p+2}} \frac{2C_4}{\varepsilon^n}(1+|j-j'|) \le \frac{2C_4C_6C_7}{\varepsilon^n(\rho^n)^p} = \frac{C_8}{C_2^n} \to 0,$$

where we have used the definition of ρ^n in (6.1) and the fact that $C_2^n \to +\infty$.
On the other hand from (6.13), (6.19) and the dominated convergence theorem, we deduce that for $p > 1$ we have

$$S_j^n \to S_j^\infty := \sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} D^2V(\widehat{X}_{j,l}^{*,\infty} - \widehat{X}_{j',l'}^{*,\infty}) \cdot (\bar{X}_{j,l}^\infty - \bar{X}_{j',l'}^\infty).$$

Then we have (uniformly in $t \in [0,1]$)

$$\sum_{\substack{j' \in \mathbb{Z} \\ 0 \le l' \le K-1}} D^2V\big(t\varepsilon^n(\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n) + (\widehat{X}_{j,l}^{*,n} - \widehat{X}_{j',l'}^{*,n})\big) \cdot (\bar{X}_{j,l}^n - \bar{X}_{j',l'}^n) \quad = \quad S_j^n + F_j^n \quad \to \quad S_j^\infty.$$

Therefore we can pass to the limit in (6.15) and get that

$$0 = 0 + \int_0^1 dt\, S_j^\infty = S_j^\infty,$$

and by Definition 2.2 of the hessian of the energy, we have

$$(E_0''(\widehat{X}^{*,\infty}) \cdot \bar{X}^\infty)_{j,l} = 0,$$

i.e.

$$(6.22) \qquad E_0''(\widehat{X}^{*,\infty}) \cdot \bar{X}^\infty = 0.$$

Step 7: Getting a contradiction
Because $\widehat{X}^{*,\infty} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$, there exists $(\alpha^*, a^*) \in \mathbb{R} \times \mathbb{R}^3$ such that

$$(6.23) \qquad \widehat{X}_j^{*,\infty} - a^* = (T^{\theta^*,L^*})^j (R_{\alpha^*,\widehat{L}^*} \mathcal{X}_0^*(\theta^*, L^*)).$$

Using Lemma 13.5 and (6.22) we get

$$0 = E_0''(\widehat{X}^{*,\infty}) \cdot \bar{X}^\infty = R_{\alpha^*,\widehat{L}}\big\{E_0''(X^*) \cdot (R_{-\alpha^*,\widehat{L}}(\bar{X}^\infty))\big\} \quad \text{with} \quad X^* := \mathcal{X}^*(\theta^*, L^*).$$

Then using (6.21) and assumption (H2), we deduce that there exist two vectors $u_1, u_2 \in \mathbb{R}^3$, $(\bar{\theta}, \bar{L}) \in \mathbb{R} \times \mathbb{R}^3$ and $Y \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ such that

$$(6.24) \qquad \begin{cases} R_{-\alpha^*,\widehat{L}^*}(\bar{X}^\infty) = u_1 + u_2 \times X^* + Y \\ Y = (\overline{\theta}, \overline{L}) \cdot \nabla_{(\theta,L)} \mathcal{X}^*(\theta^*, L^*). \end{cases}$$

We recall (6.10), i.e.

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_{j^n}(X^n,\theta,L)=\varepsilon^n.$$

Then we have

$$\inf_{\substack{(\theta,L)\,\in\,\mathcal{U}_0\\ \widehat{X}^*\,\in\,\widehat{\mathcal{C}}_*^{\theta,L}}} \sup_{|\beta|\le q} |\varepsilon^n \bar{X}^n_\beta + \widehat{X}^{*,j^n}_{j^n+\beta} - \widehat{X}^*_{j^n+\beta}| = \varepsilon^n,$$

which implies

$$\sup_{|\beta|\le q}\left|\bar{X}^n_\beta + \frac{1}{\varepsilon^n}(\widehat{X}^{*,j^n}_{j^n+\beta} - \widehat{X}^*_{j^n+\beta})\right| \ge 1 \quad \text{for} \quad \widehat{X}^*\in\widehat{\mathcal{C}}_*^{\theta,L} \quad \text{with} \quad (\theta,L)\in\mathcal{U}_0. \tag{6.25}$$

Because $\widehat{X}^{*,j^n}_{j^n+\cdot}\in\widehat{\mathcal{C}}_*^{\theta^n,L^n}$, there exists $(\alpha^n,a^n)\in\mathbb{R}\times\mathbb{R}^3$ such that

$$\widehat{X}^{*,j^n}_{j^n+\beta} = (T^{\theta^n,L^n})^\beta(R_{\alpha^n,\widehat{L}^n}(\mathcal{X}^*_0(\theta^n,L^n))) + a^n, \tag{6.26}$$

where (6.20) and $(\theta^n,L^n)\to(\theta^*,L^*)$ imply that $(\alpha^n,a^n)\to(\alpha^*,a^*)$, where $(\alpha^*,a^*)\in\mathbb{R}\times\mathbb{R}^3$ is given in (6.23). We deduce

$$R_{-\alpha^n,\widehat{L}^n}\widehat{X}^{*,j^n}_{j^n+\beta} = \mathcal{X}^*_\beta(\theta^n,L^n) + R_{-\alpha^n,\widehat{L}^n}a^n.$$

From Lemma 13.6 i), recall that

$$R_{-\alpha^n,\widehat{L}^n}\widehat{X}^*_{j^n+\cdot}\in\widehat{\mathcal{C}}_*^{\theta,\tilde{L}} \quad \text{with} \quad \tilde{L}=R_{-\alpha^n,\widehat{L}^n}(L),$$

and

$$R_{-\alpha^n,\widehat{L}^n}\widehat{X}^{*,j^n}_{j^n+\cdot}\in\widehat{\mathcal{C}}_*^{\theta^n,L^n} \quad \text{with} \quad L^n=R_{-\alpha^n,\widehat{L}^n}(L^n).$$

We set

$$\tilde{X}^* = -R_{-\alpha^n,\widehat{L}^n}(a^n) + R_{-\alpha^n,\widehat{L}^n}\widehat{X}^*_{j^n+\cdot}\in\widehat{\mathcal{C}}_*^{\theta,\tilde{L}},$$

with $(\theta,\tilde{L})\in\mathcal{U}_0$ (which is true for (θ,L) close to (θ^n,L^n)). We deduce from (6.25)

$$1\le\sup_{|\beta|\le q}\left|R_{-\alpha^n,\widehat{L}^n}(\bar{X}^n_\beta) + \frac{1}{\varepsilon^n}(\mathcal{X}^*_\beta(\theta^n,L^n) - \tilde{X}^*_\beta)\right|. \tag{6.27}$$

Choice of $\tilde{X}^*$
We choose

$$\tilde{X}^*_\beta = \varepsilon^n u_1 + R_{\varepsilon^n|u_2|,\widehat{u}_2}(\mathcal{X}^*_\beta(\theta,\tilde{L})) \quad \text{with} \;\; (\theta,\tilde{L}) = (\theta^n+\varepsilon^n\bar{\theta}, L^n+\varepsilon^n\bar{L}).$$

Passing to the limit in (6.27), we get

$$1\le\sup_{|\beta|\le q}\left|R_{-\alpha^*,\widehat{L}^*}(\bar{X}^\infty_\beta) - (u_1 + u_2\times\mathcal{X}^*_\beta(\theta^*,L^*) + (\bar{\theta},\bar{L})\cdot\nabla_{(\theta,L)}\mathcal{X}^*_\beta(\theta^*,L^*)\right| = 0 \quad \text{by (6.24)}.$$

Contradiction. This ends the proof of Theorem 2.13.

□

Proof of Corollary 2.14
We can apply Theorem 2.13 for $J=\mathbb{Z}$, we deduce for $\mu\in(0,1)$ that

$$\mathcal{N}_\mathbb{Z}(X)\le\mu\mathcal{N}_\mathbb{Z}(X),$$

and then

$$\mathcal{N}_{\mathbb{Z}}(X) = 0.$$

Given $j \in \mathbb{Z}$, we consider $(\theta_j, L_j) \in \mathcal{U}_0$, such that

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X,\theta,L) = D_j(X,\theta_j,L_j),$$

we deduce that

$$D_j(X,\theta_j,L_j) = 0.$$

Moreover we can apply Proposition 5.4 for $\varepsilon = 0$ and deduce that

$$\begin{cases} \theta_{j+1} = \theta_j \\ L_{j+1} = L_j, \end{cases}$$

and then X is a perfect nanotube.

□

Part II
Error estimates

7 Line tension and line torsion

In this section we introduce the notion of line tension (Definition 7.1) and line torsion (Definition 7.7) for a general nanotube X. Those notions are formal but can be seen as rigorous definitions if we assume for instance assumption (H0) and (1.7) with $L^0 \neq 0$ and that

$$X_{j,l} \neq X_{k,m} \quad \text{if} \quad (j,l) \neq (k,m). \tag{7.1}$$

When we will apply these notions in the next sections, we will assume (H1) i) and X locally close to an $X^* \in \mathcal{C}_*^{\theta^*,L^*}$ which will imply (7.1).

We start to prove the regularity of W.
Proof of Proposition 2.7
With the notation $\lambda = (\theta, L)$, we write

$$W(\lambda) = \mathcal{W}(\lambda, \mathcal{X}_0^*(\lambda)).$$

We compute

$$W'(\lambda) = \mathcal{W}'_\lambda(\lambda, \mathcal{X}_0^*(\lambda)) + \mathcal{W}'_{X_0}(\lambda, \mathcal{X}_0^*(\lambda)) \cdot (\mathcal{X}_0^*)'_\lambda(\lambda).$$

By definition of $\mathcal{X}_0^*$, we have $\mathcal{W}'_{X_0}(\lambda, \mathcal{X}_0^*(\lambda)) = 0$, and then

$$W'(\lambda) = \mathcal{W}'_\lambda(\lambda, \mathcal{X}_0^*(\lambda)).$$

Because $\mathcal{W}$ is C^2 and $\mathcal{X}_0^*(\lambda)$ is C^1 (see Proposition 2.1) we deduce that W' is C^1, and then W is C^2 on $\mathcal{U}_0$.

□

7.1 Line tension

In this section, we define the line tension of a nanotube as follows

Definition 7.1 (Line tension)
We define the line tension T_i of the nanotube X by

$$T_i = \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} \nabla V(X_{\alpha,l} - X_{\beta,m}).$$

The main result of this subsection is the following theorem that proves a relationship between line tension and a partial derivative of the energy.

Theorem 7.2 (Line tension as a gradient of the energy)
Let $(\theta, L) \in \mathcal{U}_0$ and $X \in \mathcal{C}_*^{\theta,L}$. Then we have the following relationship between the line tension and the derivative of the energy

$$T_i = W'_L(\theta, L). \tag{7.2}$$

In order to prove Theorem 7.2, we will need several lemmata.

Lemma 7.3 (Invariance of the energy by rotation)
Let $(\theta, L) \in \mathcal{U}_0$ and $R \in SO(3)$ such that $(\theta, RL) \in \mathcal{U}_0$. We have $W(\theta, RL) = W(\theta, L)$.

Proof of Lemma 7.3
We first compute (using convention (1.10))

$$\begin{aligned} \mathcal{W}(\theta, RL, RX_0) &= \frac{1}{2} \sum_{k \in \mathbb{Z}} \sum_{0 \leq l,m \leq K-1} V(kRL + R_{k\theta, R\widehat{L}}(R(X_{0,l})) - RX_{0,m}) \\ &= \frac{1}{2} \sum_{k \in \mathbb{Z}} \sum_{0 \leq l,m \leq K-1} V(R\{kL + (R^{-1} R_{k\theta, R\widehat{L}} R)(X_{0,l}) - X_{0,m}\}) \\ &= \mathcal{W}(\theta, L, X_0), \end{aligned}$$

where in the third line we have used Lemma 13.6 ii) in the appendix and the fact that $V(p)$ only depends on $|p|$. From (2.13), we deduce using Lemma 13.6 i) that

$$W(\theta, RL) = \mathcal{W}(\theta, RL, RX_0) = \mathcal{W}(\theta, L, X_0) = W(\theta, L).$$

□

Corollary 7.4 (The direction of $W'_L(\theta, L)$)
Let $(\theta, L) \in \mathcal{U}_0$, if $X \in \mathcal{C}_*^{\theta,L}$, then $W'_L(\theta, L)$ is parallel to L.

Proof of Corollary 7.4
Let us consider a vector ξ perpendicular to $\widehat{L}$ with $|\xi| = 1$. We set $n = \widehat{L} \times \xi$.
We consider the rotation $R_{\alpha,n} \in SO(3)$ of angle $\alpha \in \mathbb{R}$ and axis $n \in \mathbb{S}^2$.
In particular we have

$$R_{\alpha,n} L = |L| \big((\cos \alpha) \widehat{L} + (\sin \alpha) \xi \big). \tag{7.3}$$

By Lemma 7.3, for $(\theta, L) \in \operatorname{Int}\mathcal{U}_0$, we also have $W(\theta, R_{\alpha,n}L) = W(\theta, L)$ for any $\alpha \in \mathbb{R}$ small enough, from which we deduce

$$\begin{aligned} 0 &= \frac{d}{d\alpha}\big(W(\theta, R_{\alpha,n}L)\big)_{|\alpha=0} \\ &= W_L'(\theta, L) \cdot \left(\frac{d}{d\alpha}(R_{\alpha,n}L)_{|\alpha=0}\right) \\ &= W_L'(\theta, L) \cdot (|L|\xi), \end{aligned}$$

where in the third line we have used (7.3) to compute $\frac{d}{d\alpha}(R_{\alpha,n}L)$.
Because $W_L'(\theta, L) \cdot \xi = 0$ for any $\xi \perp \widehat{L}$, we deduce that $W_L'(\theta, L)$ is parallel to L for any $(\theta, L) \in \operatorname{Int}\mathcal{U}_0$. By continuity of W_L' (using Proposition 2.7), this is also true for all $(\theta, L) \in \mathcal{U}_0$ (using (2.8)).

□

Lemma 7.5 (The rotation of the line tension)
If $X \in \mathcal{C}^{\theta,L}$, then we have $T_i = R_{\theta,\widehat{L}}(T_{i-1})$.

Proof of Lemma 7.5
We have

$$T_i = \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} \nabla V(X_{\alpha,l} - X_{\beta,m}).$$

Using the fact that our nanotube is a special perfect nanotube, we compute

$$X_{\alpha,l} = \alpha L + R_{\alpha\theta,\widehat{L}}(X_{0,l}),$$

then

$$\begin{aligned} T_i &= \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} \nabla V\big((\alpha-\beta)L + R_{\alpha\theta,\widehat{L}}(X_{0,l}) - R_{\beta\theta,\widehat{L}}(X_{0,m})\big) \\ &= R_{\theta,\widehat{L}}\Bigg(\sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} \nabla V\big((\alpha-\beta)L + R_{(\alpha-1)\theta,\widehat{L}}(X_{0,l}) - R_{(\beta-1)\theta,\widehat{L}}(X_{0,m})\big)\Bigg) \\ &= R_{\theta,\widehat{L}}\Bigg(\sum_{\substack{\alpha \geq i \\ \beta \leq i-1}} \sum_{0 \leq l,m \leq K-1} \nabla V\big((\alpha-\beta)L + R_{\alpha\theta,\widehat{L}}(X_{0,l}) - R_{\beta\theta,\widehat{L}}(X_{0,m})\big)\Bigg) \\ &= R_{\theta,\widehat{L}}(T_{i-1}), \end{aligned}$$

where in the second line we use Lemma 13.4 in the appendix.

□

Lemma 7.6 (Line tension and the external force)
If X is a solution of equation (1.13) with our definition (1.6) of $f_{j,l}$, then we have the following relationship between the line tension and the external force

$$T_i - T_{i-1} = f_i^0.$$

This result holds true if equation (1.13) and the T_i are well defined.
This is for instance the case under assumption (H0) assuming (1.7) with $L^0 \neq 0$ and (7.1).

Proof of Lemma 7.6
We have

$$\begin{aligned} T_i &= \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{\beta,m}) \\ &= \sum_{\substack{\alpha \geq i \\ \beta \leq i}} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{\beta,m}) - \sum_{\substack{\alpha = i \\ \beta \leq i}} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{\beta,m}). \end{aligned}$$

Similarly we have

$$T_{i-1} = \sum_{\substack{\alpha \geq i \\ \beta \leq i}} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{\beta,m}) - \sum_{\substack{\alpha \geq i \\ \beta = i}} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{\beta,m}).$$

We deduce

$$\begin{aligned} T_i - T_{i-1} &= \sum_{\alpha\geq i} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) - \sum_{\alpha\leq i} \sum_{0\leq l,m\leq K-1} \nabla V(X_{i,l} - X_{\alpha,m}) \\ &= \sum_{\alpha\geq i} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) + \sum_{\alpha\leq i} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) \\ &= \sum_{\alpha\in\mathbb{Z}} \sum_{0\leq l,m\leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) + A \\ &= \sum_{0\leq m\leq K-1} \sum_{\substack{\alpha \in \mathbb{Z} \\ 0 \leq l \leq K-1}} \nabla V(X_{\alpha,l} - X_{i,m}) + 0 \\ &= \sum_{0\leq m\leq K-1} f_{i,m} = f_i^0, \end{aligned} \tag{7.4}$$

where in the second term of the first line we have changed β in α, in the second line we have used the antisymmetry of ∇V and exchanged l and m, in the third line we have set

$$A := \sum_{0\leq l,m\leq K-1} \nabla V(X_{i,l} - X_{i,m}).$$

In the fourth line of (7.4), we have used the fact that $A = 0$. This follows from the antisymmetry of ∇V and from the fact that l and m play a symmetric role. In the last line of (7.4) we have used the equation of equilibrium (1.13), the definition of the forces (1.6) and the antisymmetry of ∇V.

□

Proof of Theorem 7.2
From the definition of $\mathcal{C}_*^{\theta,L}$, X solves (1.13) with $f_i = 0$, and satisfies $X_{\alpha,l} = \alpha L + R_{\alpha\theta,\widehat{L}}(X_{0,l})$. Then from Lemma 7.6 we have $T_i = T_{i-1}$, and from Lemma 7.5, $T_i = R_{\theta,\widehat{L}}(T_i)$, and because $\theta \neq 0 \bmod(2\pi)$, we deduce that T_i is parallel to L.
From Corollary 7.4, we see that it suffices to show that $\widehat{L} \cdot T_i = \widehat{L} \cdot W_L'(\theta, L)$.

Therefore we compute

$$\begin{aligned}
\widehat{L}\cdot T_i &= \widehat{L}\cdot \sum_{\substack{\alpha\ge i+1\\ \beta\le i}}\ \sum_{0\le l,m\le K-1} \nabla V((\alpha-\beta)L + R_{\alpha\theta,\widehat{L}}(X_{0,l}) - R_{\beta\theta,\widehat{L}}(X_{0,m}))\\
&= \sum_{\substack{\alpha\ge i+1\\ \beta\le i}}\ \sum_{0\le l,m\le K-1} \widehat{L}\cdot R_{\beta\theta,\widehat{L}}\big(\nabla V((\alpha-\beta)L + R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big)\\
&= \sum_{\substack{\alpha\ge i+1\\ \beta\le i}}\ \sum_{0\le l,m\le K-1} \widehat{L}\cdot \nabla V((\alpha-\beta)L + R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m}),
\end{aligned}$$

where in the second line we get out the rotation $R_{\beta\theta,\widehat{L}}$ using Lemma 13.4.
We now call $q=\alpha-\beta$ and get

$$\widehat{L}\cdot T_i = \sum_{q\ge 1}\ \sum_{0\le l,m\le K-1} q\widehat{L}\cdot \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}). \tag{7.5}$$

From this expression we deduce

$$\begin{aligned}
\widehat{L}\cdot T_i &= \sum_{q\ge 1}\ \sum_{0\le l,m\le K-1} q\widehat{L}\cdot R_{q\theta,\widehat{L}}\big(\nabla V(qL - R_{-q\theta,\widehat{L}}(X_{0,m}) + X_{0,l})\big)\\
&= \sum_{-q\ge 1}\ \sum_{0\le l,m\le K-1} -q\widehat{L}\cdot \nabla V(-qL - R_{q\theta,\widehat{L}}(X_{0,m}) + X_{0,l}),
\end{aligned}$$

where in the first line we get out the rotation $R_{q\theta,\widehat{L}}$ using again Lemma 13.4, and in the second line we have changed $-q$ in q.
Now using the antisymmetry of ∇V and exchanging the position of l and m, we get

$$\widehat{L}\cdot T_i = \sum_{q\le -1}\ \sum_{0\le l,m\le K-1} q\widehat{L}\cdot \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}), \tag{7.6}$$

which is an expression similar to (7.5) but with $q\le -1$.
Summing (7.5) and (7.6) we get

$$\widehat{L}\cdot T_i = \widehat{L}\cdot\left\{\frac{1}{2}\sum_{q\in\mathbb{Z}}\ \sum_{0\le l,m\le K-1} q\nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\right\},$$

where for $q=0$ and $l=m$ we use convention (1.10), for which we have $\nabla V(0)=0$. Then, using Lemma 13.7 which shows that $\widehat{L}\cdot\nabla_L(R_{q\theta,\widehat{L}})=0$, we get

$$\widehat{L}\cdot T_i = \widehat{L}\cdot \mathcal{W}'_L(\theta,L,X_0). \tag{7.7}$$

On the one hand, we have $W(\theta,L)=\mathcal{W}(\theta,L,X_0)$ with $X_0=\mathcal{X}_0^*(\theta,L)$. Then we have

$$W'_L(\theta,L) = \nabla_L\{\mathcal{W}(\theta,L,\mathcal{X}_0^*(\theta,L))\} = \mathcal{W}'_L(\theta,L,X_0) + \mathcal{W}'_{X_0}(\theta,L,X_0)\cdot(\mathcal{X}_0^*)'_L(\theta,L). \tag{7.8}$$

On the other hand by Proposition 3.3 we have

$$\mathcal{W}'_{X_0}(\theta,L,X_0)=0.$$

This shows with (7.7), (7.8) that

$$\widehat{L}\cdot T_i = \widehat{L}\cdot W'_L(\theta,L),$$

from which we conclude that

$$T_i = W'_L(\theta,L).$$

□

7.2 Line torsion

In this section, we define the line torsion (as a moment) for a nanotube as follows

Definition 7.7 (Line torsion of a nanotube)
We define the line torsion M_i of a nanotube $X \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$ at a point $A \in \mathbb{R}^3$ by

$$M_i(A) = \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} (X_{\alpha,l} - A) \times \nabla V(X_{\alpha,l} - X_{\beta,m}).$$

In the sequel we set $M_i = M_i(0)$.

Then we have the following straightforward property (whose we skip the proof):

Proposition 7.8 (Torsor)
The couple (T_i, M_i) defines a torsor, i.e. for any $A, B \in \mathbb{R}^3$, we have

$$M_i(B) = M_i(A) + \overrightarrow{BA} \times T_i.$$

The main result of this subsection is the following theorem that proves a relationship between line torsion and a partial derivative of the energy.

Theorem 7.9 (Line torsion and the gradient of the energy)
Let $(\theta, L) \in \mathcal{U}_0$ and $X \in \mathcal{C}_*^{\theta,L}$. Then we have the following relationship between the line torsion and the derivative of the energy

$$M_i = W'_\theta(\theta, L)\widehat{L}. \tag{7.9}$$

In order to prove Theorem 7.9, we will need several Lemmata. We first start to prove a subcase of Theorem 7.9, namely:

Lemma 7.10 (Projected line torsion as a gradient of the energy)
Let $(\theta, L) \in \mathcal{U}_0$ and $X \in \mathcal{C}_*^{\theta,L}$. Then we have the following relationship between the line torsion and the derivative of the energy

$$\widehat{L} \cdot M_i = W'_\theta(\theta, L). \tag{7.10}$$

Proof of Lemma 7.10
We compute

$$\begin{aligned}
\widehat{L} \cdot M_i &= \widehat{L} \cdot \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} X_{\alpha,l} \times \nabla V(X_{\alpha,l} - X_{\beta,m}) \\
&= \widehat{L} \cdot \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} (\alpha L + R_{\alpha\theta,\widehat{L}}(X_{0,l})) \times \nabla V((\alpha-\beta)L + R_{\alpha\theta,\widehat{L}}(X_{0,l}) - R_{\beta\theta,\widehat{L}}(X_{0,m})) \\
&= \widehat{L} \cdot \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} (R_{\alpha\theta,\widehat{L}}(X_{0,l})) \times R_{\beta\theta,\widehat{L}}\big(\nabla V((\alpha-\beta)L + R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big) \\
&= \widehat{L} \cdot \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} (R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l})) \times \nabla V((\alpha-\beta)L + R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m}),
\end{aligned}$$

where in the second line we have used the fact that X is a special perfect nanotube, in the third line we have used Lemma 13.4 to get the rotation, and in the fourth line we have used Lemma 13.2.
Therefore we get with $q = \alpha - \beta$

$$\widehat{L} \cdot M_i = \widehat{L} \cdot \sum_{q \geq 1} \sum_{0 \leq l,m \leq K-1} q(R_{q\theta,\widehat{L}}(X_{0,l})) \times \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}). \tag{7.11}$$

From this expresion we get

$$\begin{aligned}
& \widehat{L} \cdot M_i \\
= & \widehat{L} \cdot \sum_{q \geq 1} \sum_{0 \leq l,m \leq K-1} -q(R_{q\theta,\widehat{L}}(X_{0,l})) \times \nabla V(-qL + X_{0,m} - R_{q\theta,\widehat{L}}(X_{0,l})) \\
= & \widehat{L} \cdot \sum_{q \geq 1} \sum_{0 \leq l,m \leq K-1} -qX_{0,l} \times \nabla V(-qL + R_{-q\theta,\widehat{L}}(X_{0,m}) - X_{0,l}) \\
= & \widehat{L} \cdot \sum_{q \leq -1} \sum_{0 \leq l,m \leq K-1} qX_{0,m} \times \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}) \\
= & \widehat{L} \cdot \sum_{q \leq -1} \sum_{0 \leq l,m \leq K-1} q(X_{0,m} - qL - R_{q\theta,\widehat{L}}(X_{0,l}) + R_{q\theta,\widehat{L}}(X_{0,l})) \times \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}),
\end{aligned}$$

where in the first equality we have used the antisymmetry of ∇V, in the second equality we have used Lemma 13.4 and Lemma 13.2 to eliminate the rotation $R_{q\theta,\widehat{L}}$, in the third equality we have changed q in $-q$ and exchanged the position of m and l.
Using the fact that $\nabla V(p)$ is parallel to p we obtain

$$\widehat{L} \cdot M_i = \widehat{L} \cdot \sum_{q \leq -1} \sum_{0 \leq l,m \leq K-1} qR_{q\theta,\widehat{L}}(X_{0,l}) \times \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}). \tag{7.12}$$

which is an expression similar to (7.11) but with $q \leq -1$.
Summing (7.11) and (7.12) we obtain

$$\widehat{L} \cdot M_i = \frac{1}{2} \sum_{q \in \mathbb{Z}} \sum_{0 \leq l,m \leq K-1} q\, \widehat{L} \cdot \big(R_{q\theta,\widehat{L}}(X_{0,l}) \times \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big). \tag{7.13}$$

Using Lemma 13.3 we obtain

$$\widehat{L} \cdot M_i = \frac{1}{2} \sum_{q \in \mathbb{Z}} \sum_{0 \leq l,m \leq K-1} q \left(\big(R_{q\theta + \frac{\pi}{2},\widehat{L}}(X_{0,l})\big)^{\perp_{\widehat{L}}} \cdot \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}) \right).$$

Notice that

$$\frac{d}{d\theta} R_{q\theta,\widehat{L}}(X_{0,l}) = q\big(R_{\frac{\pi}{2}+q\theta,\widehat{L}}(X_{0,l})\big)^{\perp_{\widehat{L}}}.$$

Therefore

$$\widehat{L} \cdot M_i = \mathcal{W}'_\theta(\theta, L, X_0). \tag{7.14}$$

On the one hand, we have $W(\theta, L) = \mathcal{W}(\theta, L, X_0)$ with $X_0 = \mathcal{X}_0^*(\theta, L)$. Then we have

$$W'_\theta(\theta, L) = \nabla_\theta\{\mathcal{W}(\theta, L, \mathcal{X}_0^*(\theta, L))\} = \mathcal{W}'_\theta(\theta, L, X_0) + \mathcal{W}'_{X_0}(\theta, L, X_0) \cdot (\mathcal{X}_0^*)'_\theta(\theta, L). \tag{7.15}$$

On the other hand by Proposition 3.3 we have

$$\mathcal{W}'_{X_0}(\theta, L, X_0) = 0.$$

This shows with (7.14) and (7.15) that

$$\widehat{L} \cdot M_i = W'_\theta(\theta, L).$$

$\square$

Lemma 7.11 **(M_i in terms of M_{i-1} and T_{i-1} for a special perfect nanotube)**
If $X \in \mathcal{C}^{\theta,L}$, then we have

$$M_i = R_{\theta,\widehat{L}}(M_{i-1} + L \times T_{i-1}).$$

Proof of Lemma 7.11
We have

$$\begin{aligned}
M_i &= \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} X_{\alpha,l} \times \nabla V(X_{\alpha,l} - X_{\beta,m}) \\
&= \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} (\alpha L + R_{\alpha\theta,\widehat{L}}(X_{0,l})) \times \nabla V\big((\alpha-\beta)L + R_{\alpha\theta,\widehat{L}}(X_{0,l}) - R_{\beta\theta,\widehat{L}}(X_{0,m})\big) \\
&= \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} (\alpha L + R_{\alpha\theta,\widehat{L}}(X_{0,l})) \times R_{\beta\theta,\widehat{L}}\big(\nabla V((\alpha-\beta)L + R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big) \\
&= \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0 \leq l,m \leq K-1} R_{\beta\theta,\widehat{L}}\big\{(\alpha L + R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l})) \times \nabla V((\alpha-\beta)L + R_{(\alpha-\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big\},
\end{aligned}$$

where in the third line we have used Lemma 13.4 and in the fourth line we have used Lemma 13.1. Let us define

$$\begin{cases} \bar{\alpha} := \alpha - 1 \\ \bar{\beta} := \beta - 1, \end{cases}$$

then we compute

$$\begin{aligned}
& M_i \\
&= \sum_{\substack{\bar{\alpha} \geq i \\ \bar{\beta} \leq i-1}} \sum_{0 \leq l,m \leq K-1} R_{(\bar{\beta}+1)\theta,\widehat{L}}\big\{(\bar{\alpha} L + R_{(\bar{\alpha}-\bar{\beta})\theta,\widehat{L}}(X_{0,l})) \times \nabla V((\bar{\alpha}-\bar{\beta})L + R_{(\bar{\alpha}-\bar{\beta})\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big\} \\
&+ \sum_{\substack{\bar{\alpha} \geq i \\ \bar{\beta} \leq i-1}} \sum_{0 \leq l,m \leq K-1} R_{(\bar{\beta}+1)\theta,\widehat{L}}\big\{L \times \nabla V((\bar{\alpha}-\bar{\beta})L + R_{(\bar{\alpha}-\bar{\beta})\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big\} \\
&= R_{\theta,\widehat{L}} \left\{ \begin{array}{l} \displaystyle\sum_{\substack{\bar{\alpha} \geq i \\ \bar{\beta} \leq i-1}} \sum_{0 \leq l,m \leq K-1} R_{\bar{\beta}\theta,\widehat{L}}\{\ldots\} \\ \displaystyle + \sum_{\substack{\bar{\alpha} \geq i \\ \bar{\beta} \leq i-1}} \sum_{0 \leq l,m \leq K-1} R_{\bar{\beta}\theta,\widehat{L}}\{\ldots\} \end{array} \right\}.
\end{aligned}$$

Then we have

$$
\begin{aligned}
&M_i\\
&= R_{\theta,\widehat{L}} \left\{ \begin{array}{l} \displaystyle\sum_{\substack{\bar\alpha \geq i \\ \bar\beta \leq i-1}} \sum_{0\leq l,m\leq K-1} (\bar\alpha L + R_{\bar\alpha\theta,\widehat{L}}(X_{0,l})) \times R_{\bar\beta\theta,\widehat{L}}\big(\nabla V((\bar\alpha-\bar\beta)L + R_{(\bar\alpha-\bar\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big) \\ \displaystyle + \sum_{\substack{\bar\alpha \geq i \\ \bar\beta \leq i-1}} \sum_{0\leq l,m\leq K-1} L \times R_{\bar\beta\theta,\widehat{L}}\big(\nabla V((\bar\alpha-\bar\beta)L + R_{(\bar\alpha-\bar\beta)\theta,\widehat{L}}(X_{0,l}) - X_{0,m})\big) \end{array} \right\}\\
&= R_{\theta,\widehat{L}} \left\{ \begin{array}{l} \displaystyle\sum_{\substack{\bar\alpha \geq i \\ \bar\beta \leq i-1}} \sum_{0\leq l,m\leq K-1} (\bar\alpha L + R_{\bar\alpha\theta,\widehat{L}}(X_{0,l})) \times \nabla V((\bar\alpha-\bar\beta)L + R_{\bar\alpha\theta,\widehat{L}}(X_{0,l}) - R_{\bar\beta\theta,\widehat{L}}(X_{0,m})) \\ \displaystyle +L \times \sum_{\substack{\bar\alpha \geq i \\ \bar\beta \leq i-1}} \sum_{0\leq l,m\leq K-1} \nabla V((\bar\alpha-\bar\beta)L + R_{\bar\alpha\theta,\widehat{L}}(X_{0,l}) - R_{\bar\beta\theta,\widehat{L}}(X_{0,m})) \end{array} \right\}\\
&= R_{\theta,\widehat{L}}\big(M_{i-1} + L \times T_{i-1}\big),
\end{aligned}
$$

where in the first equality we have used Lemma 13.1 and in the second equality we have used Lemma 13.4.

□

Lemma 7.12 (Line torsion and external force for a general nanotube)
Let X be a solution of equation (1.13) and with our definition (1.6) of $f_{j,l}$. Then we have the following relationship between the line torsion, the barycenter b_i of the cell X_i (see Definition 5.3) and the external force

$$M_i - M_{i-1} = b_i \times f_i^0.$$

This result holds true if equation (1.13) and the M_i are well defined.
This is for instance the case under assumption (H0) assuming (1.7) with $L^0 \neq 0$ and (7.1).

Proof of Lemma 7.12
Step 1 : Main computation.
We have

$$M_i = \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i}} \sum_{0\leq l,m\leq K-1} X_{\alpha,l} \times \nabla V(X_{\alpha,l} - X_{\beta,m}).$$

Then

$$M_i = \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i-1}} \sum_{0\leq l,m\leq K-1} X_{\alpha,l}\times\nabla V(X_{\alpha,l}-X_{\beta,m}) \quad + \sum_{\substack{\alpha \geq i+1 \\ \beta = i}} \sum_{0\leq l,m\leq K-1} X_{\alpha,l}\times\nabla V(X_{\alpha,l}-X_{\beta,m}).$$

Similarly we have

$$M_{i-1} = \sum_{\substack{\alpha \geq i+1 \\ \beta \leq i-1}} \sum_{0\leq l,m\leq K-1} X_{\alpha,l}\times\nabla V(X_{\alpha,l}-X_{\beta,m}) \quad + \sum_{\substack{\alpha = i \\ \beta \leq i-1}} \sum_{0\leq l,m\leq K-1} X_{\alpha,l}\times\nabla V(X_{\alpha,l}-X_{\beta,m}).$$

Then we have

$$
\begin{aligned}
& M_i - M_{i-1} \\
= & \sum_{\substack{\alpha \geq i+1 \\ \beta = i}} \sum_{0\leq l,m\leq K-1} X_{\alpha,l} \times \nabla V(X_{\alpha,l} - X_{\beta,m}) - \sum_{\substack{\alpha = i \\ \beta \leq i-1}} \sum_{0\leq l,m\leq K-1} X_{\alpha,l} \times \nabla V(X_{\alpha,l} - X_{\beta,m}) \\
= & \sum_{\alpha\geq i+1} \sum_{0\leq l,m\leq K-1} X_{\alpha,l} \times \nabla V(X_{\alpha,l} - X_{i,m}) + \sum_{\alpha\leq i-1} \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{\alpha,l} - X_{i,m}) \\
= & \sum_{\alpha\geq i+1} \sum_{0\leq l,m\leq K-1} (X_{\alpha,l} - X_{i,m} + X_{i,m}) \times \nabla V(X_{\alpha,l} - X_{i,m}) + \sum_{\alpha\leq i-1} \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{\alpha,l} - X_{i,m}) \\
= & \sum_{\alpha\geq i+1} \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{\alpha,l} - X_{i,m}) + \sum_{\alpha\leq i-1} \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{\alpha,l} - X_{i,m}) \\
= & \sum_{\alpha\neq i} \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{\alpha,l} - X_{i,m}),
\end{aligned}
$$

where in the second term of the second equality we have replaced β by α, used the anti-symmetry of ∇V and exchanged l and m. In the fourth equality we have used the fact that $\nabla V(p)$ is parallel to p.

We have the following result which will be proven later:

Claim : $\displaystyle\sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{i,l} - X_{i,m}) = 0.$

Using this claim we obtain

$$
\begin{aligned}
M_i - M_{i-1} &= \sum_{\alpha\in\mathbb{Z}} \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{\alpha,l} - X_{i,m}) \\
&= \sum_{0\leq m\leq K-1} \left(X_{i,m} \times \sum_{\alpha\in\mathbb{Z}} \sum_{0\leq l\leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) \right) \\
&= \sum_{0\leq m\leq K-1} X_{i,m} \times f_{i,m} \\
&= \left(\sum_{0\leq m\leq K-1} X_{i,m} \right) \times \frac{1}{K} f_i^0 \\
&= b_i \times f_i^0.
\end{aligned}
$$

where in the third line we have used (1.13), in the fourth line we have used (1.6), and in the fifth line we have used the definition of the barycenter b_i of the cell X_i.

Step 2 : Proof of the claim

We compute

$$
\begin{aligned}
A &:= \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{i,l} - X_{i,m}) \\
&= \sum_{0\leq l,m\leq K-1} (X_{i,m} - X_{i,l} + X_{i,l}) \times \nabla V(X_{i,l} - X_{i,m}) \\
&= \sum_{0\leq l,m\leq K-1} X_{i,l} \times \nabla V(X_{i,l} - X_{i,m}) \\
&= \sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{i,m} - X_{i,l}) \\
&= -\sum_{0\leq l,m\leq K-1} X_{i,m} \times \nabla V(X_{i,l} - X_{i,m}) \\
&= -A,
\end{aligned}
$$

where in the third line we have used the fact that $\nabla V(p)$ is parallel to p, in the fourth line we have exchanged l and m, and in the fifth line we have used the antisymmetry of ∇V. Therfore we get A=0.

$\square$

Proof of Theorem 7.9
Step 1: $M_i = R_{\theta,\widehat{L}}(M_{i-1})$
By Corollary 7.4 and by Theorem 7.2, we deduce that $L \times T_{i-1} = 0$.
Then by Lemma 7.11 we get

$$M_i = R_{\theta,\widehat{L}}(M_{i-1}). \tag{7.16}$$

Step 2: Conclusion
By Lemma 7.12 and the fact that $X \in \mathcal{C}_*^{\theta,L}$, we have $f_i^0 = 0$ and

$$M_i = M_{i-1},$$

and by Step 1, we deduce that

$$M_i = R_{\theta,\widehat{L}}(M_i).$$

Because $\theta \neq 0\,(2\pi)$ for any $(\theta, L) \in \mathcal{U}_0$, we deduce that M_i is parallel to $\widehat{L}$, and finally by Lemma 7.10, we get

$$M_i = (\widehat{L} \cdot M_i)\widehat{L} = W'_\theta(\theta, L)\widehat{L}.$$

$\square$

8 The mean fiber

The goal of this section is to define the mean fiber $\tilde{a}_i$ of a general nanotube and to prove geometric estimates (see Theorem 8.2).

Definition 8.1 (Mean fiber $\tilde{a}_i$)
Let X be a nanotube. Let $(\theta_i, L_i) \in \mathcal{U}_0$ and $\widehat{X}^{*,i} \in \widehat{\mathcal{C}}_*^{\theta_i,L_i}$ such that

$$D_i(X, \theta_i, L_i) = \sup_{|\alpha| \leq q} |X_{i+\alpha} - \widehat{X}^{*,i}_{i+\alpha}|.$$

Then there exists a unique $a_i \in L_i^\perp$ and $X^{*,i} \in \mathcal{C}_*^{\theta_i,L_i}$ such that $\widehat{X}^{*,i} = a_i + X^{*,i}$. We define the mean fiber $\tilde{a}_i$ by

$$\tilde{a}_i = a_i + (b_i^{*,i} \cdot \widehat{L}_i)\widehat{L}_i, \tag{8.1}$$

where $b_i^{*,i} = \dfrac{1}{K}\displaystyle\sum_{l=0}^{K} X^{*,i}_{i,l}$ is the barycenter of the cell $X_i^{*,i}$.

For an illustration of the mean fiber, see Figure 11.
Notice that for a special perfect nanotube, the mean fiber is simply the projection of the barycenter of the cell on the axis of the nanotube. Notice also that for a general nanotube the mean fiber may be not unique.

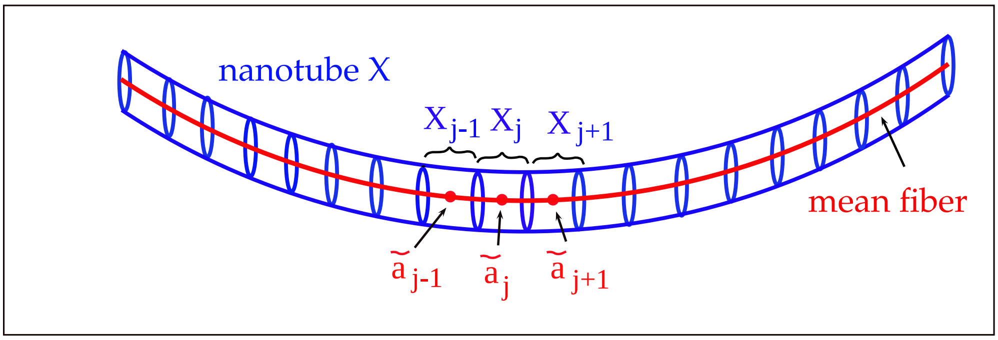

Figure 11: Mean fiber $\tilde{a}_j$ of a nanotube

Theorem 8.2 (An estimate on $\tilde{a}_i$)
There exists a constant $C > 0$ such that if a nanotube X satisfies for some $\varepsilon \in (0,1)$ and for fixed $i_0 \in \mathbb{Z}$

(8.2) $$D_i(X, \theta_i, L_i) \leq \varepsilon \qquad \text{for } i \in \{i_0, i_0+1\},$$

then for any mean fiber $\tilde{a}_{i_0}$, $\tilde{a}_{i_0+1}$ given by Definition 8.1, we have

(8.3) $$|b_{i_0} - \tilde{a}_{i_0}| \leq C,$$

(8.4) $$|X'_{i_0}| \leq C,$$

(8.5) $$|(\tilde{a}_{i_0+1} - \tilde{a}_{i_0})^{\perp_{\widehat{L}_{i_0+1}}}| \leq C\,\varepsilon,$$

(8.6) $$|\tilde{a}_{i_0+1} - \tilde{a}_{i_0} - L_{i_0}| \leq C\,\varepsilon,$$

(8.7) $$|b_{i_0+1} - \tilde{a}_{i_0+1} - R_{\theta_{i_0}, \widehat{L}_{i_0}}(b_{i_0} - \tilde{a}_{i_0})| \leq C\,\varepsilon,$$

(8.8) $$|X'_{i_0+1} - R_{\theta_{i_0}, \widehat{L}_{i_0}}(X'_{i_0})| \leq C\varepsilon,$$

with the centrered cell $X'_i = X_i - b_i$ and the barycenter $b_i = \dfrac{1}{N} \displaystyle\sum_{0 \leq l \leq K-1} X_{i,l}$.

Proof of Theorem 8.2
As a preliminary, we use the fact that $\mathcal{U}_0$ is closed (in Proposition 2.1) to recall (for later use) that

(8.9) $$\overline{\mathcal{U}_0} = \mathcal{U}_0 \subset (0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\}).$$

On the other hand, because of (8.2), we can apply Proposition 5.4 and deduce that there exists a constant $C_0 > 0$ such that we have

(8.10) $$|\theta_{i_0+1} - \theta_{i_0}| \leq C_0 \varepsilon,$$

and

$$|L_{i_0+1} - L_{i_0}| \leq C_0\varepsilon. \tag{8.11}$$

Step 1: Proof that $b_{i_0} - \tilde{a}_{i_0}$ and X'_{i_0} are bounded
Let $X^{*,i_0} \in \mathcal{C}_*^{\theta_{i_0},L_{i_0}}$ and $a_{i_0} \in L_{i_0}^{\perp}$ such that $\widehat{X}^{*,i_0} = a_{i_0} + X^{*,i_0}$ minimizes the infimum defining the distance $D_{i_0}(X, \theta_{i_0}, L_{i_0})$ as in Definition 8.1. We know that there exists a constant $C_1 > 0$ such that

$$|(X_j^{*,i_0})^{\perp_{\widehat{L}_{i_0}}}| \leq C_1,$$

and by (8.2), we have

$$|X_{i_0} - a_{i_0} - X_{i_0}^{*,i_0}| \leq \varepsilon. \tag{8.12}$$

Then

$$|(X_{i_0} - a_{i_0})^{\perp_{\widehat{L}_{i_0}}}| \leq C_1 + \varepsilon.$$

In particular we deduce that

$$|(b_{i_0} - a_{i_0})^{\perp_{\widehat{L}_{i_0}}}| \leq C_1 + \varepsilon,$$

i.e.

$$|b_{i_0} - (b_{i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0} - a_{i_0}| \leq C_1 + \varepsilon. \tag{8.13}$$

We deduce from (8.12) that

$$|(b_{i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0} - (b_{i_0}^{*,i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0}| \leq \varepsilon. \tag{8.14}$$

Using moreover (8.13), we get

$$|b_{i_0} - \tilde{a}_{i_0}| \leq C_1 + 2\varepsilon \leq C_2,$$

which proves (8.3). On the other hand, (8.12) implies for the centered cells

$$|X'_{i_0} - (X_{i_0}^{*,i_0})'| \leq \varepsilon,$$

and we deduce (8.4) from the fact that $(X_{i_0}^{*,i_0})'$ is bounded.
Step 2: Proof of $|\tilde{a}_{i_0+1} - \tilde{a}_{i_0} - L_{i_0}| \leq C_7\varepsilon$
Step 2-1: Proof of $|(\tilde{a}_{i_0+1} - \tilde{a}_{i_0})^{\perp_{L_{i_0+1}}}| \leq C_4\varepsilon$
We compute

$$\begin{aligned} & |b_{i_0+1} - a_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(b_{i_0} - a_{i_0}) - L_{i_0}| \\ = \ & |b_{i_0+1} - a_{i_0} - (b_{i_0}^{*,i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(b_{i_0} - a_{i_0} - (b_{i_0}^{*,i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0}) - L_{i_0}| \\ = \ & |b_{i_0+1} - \tilde{a}_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(b_{i_0} - \tilde{a}_{i_0}) - L_{i_0}| \end{aligned}$$

Using (8.2) in case $i = i_0$, we get

$$\left\{ \begin{array}{l} |X_{i_0+1} - a_{i_0} - X_{i_0+1}^{*,i_0}| \leq \varepsilon \\ |X_{i_0} - a_{i_0} - X_{i_0}^{*,i_0}| \leq \varepsilon, \end{array} \right.$$

i.e.

$$\begin{cases} |X_{i_0+1} - a_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(X^{*,i_0}_{i_0}) - L_{i_0}| \le \varepsilon \\ |R_{\theta_{i_0},\widehat{L}_{i_0}}(X_{i_0} - a_{i_0}) - R_{\theta_{i_0},\widehat{L}_{i_0}}(X^{*,i_0}_{i_0})| \le \varepsilon. \end{cases}$$

Substracting the two last lines, we get

$$|X_{i_0+1} - a_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(X_{i_0} - a_{i_0}) - L_{i_0}| \le 2\varepsilon, \tag{8.15}$$

which implies

$$|b_{i_0+1} - \tilde{a}_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(b_{i_0} - \tilde{a}_{i_0}) - L_{i_0}| \le 2\varepsilon. \tag{8.16}$$

Similarly using (8.2) in case $i = i_0 + 1$, we get

$$|X_{i_0+1} - a_{i_0+1} - R_{\theta_{i_0+1},\widehat{L}_{i_0+1}}(X_{i_0} - a_{i_0+1}) - L_{i_0+1}| \le 2\varepsilon,$$

which implies

$$|b_{i_0+1} - \tilde{a}_{i_0+1} - R_{\theta_{i_0+1},\widehat{L}_{i_0+1}}(b_{i_0} - \tilde{a}_{i_0+1}) - L_{i_0+1}| \le 2\varepsilon. \tag{8.17}$$

Substracting (8.16) and (8.17), we get (using (8.11))

$$|\tilde{a}_{i_0+1} - \tilde{a}_{i_0} + (R_{\theta_{i_0+1},\widehat{L}_{i_0+1}} - R_{\theta_{i_0},\widehat{L}_{i_0}})(b_{i_0} - \tilde{a}_{i_0}) - R_{\theta_{i_0+1},\widehat{L}_{i_0+1}}(\tilde{a}_{i_0+1} - \tilde{a}_{i_0})| \le (4 + C_0)\varepsilon.$$

Using (8.3) to bound $b_{i_0} - \tilde{a}_{i_0}$ and Lemma 13.8 to bound $R_{\theta_{i_0+1},\widehat{L}_{i_0+1}} - R_{\theta_{i_0},\widehat{L}_{i_0}}$ (with (8.10) and (8.11)), we deduce that there exists a constant C_3 such that we have

$$|(I - R_{\theta_{i_0+1},\widehat{L}_{i_0+1}})(\tilde{a}_{i_0+1} - \tilde{a}_{i_0})| \le C_3\varepsilon.$$

Using (8.9), we get that there exists a constant $C_4 > 0$ such that

$$|(\tilde{a}_{i_0+1} - \tilde{a}_{i_0})^{\perp_{\widehat{L}_{i_0+1}}}| \le C_4\varepsilon$$

Step 2-2: $|((\tilde{a}_{i_0+1} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0+1})\widehat{L}_{i_0+1} - L_{i_0}| \le C_6\varepsilon$
We compute

$$\begin{aligned} & (b_{i_0+1} - \tilde{a}_{i_0+1} - R_{\theta_{i_0+1},\widehat{L}_{i_0+1}}(b_{i_0} - \tilde{a}_{i_0+1}) - L_{i_0+1}) \cdot \widehat{L}_{i_0+1} \\ = \ & (b_{i_0+1} - \tilde{a}_{i_0+1}) \cdot \widehat{L}_{i_0+1} - (b_{i_0} - \tilde{a}_{i_0+1}) \cdot \widehat{L}_{i_0+1} - |L_{i_0+1}| \\ = \ & (b_{i_0+1} - \tilde{a}_{i_0+1}) \cdot \widehat{L}_{i_0+1} - (b_{i_0} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0+1} + (\tilde{a}_{i_0+1} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0+1} - |L_{i_0+1}| \\ = \ & (b_{i_0+1} - \tilde{a}_{i_0+1}) \cdot \widehat{L}_{i_0+1} - (b_{i_0} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0} - (b_{i_0} - \tilde{a}_{i_0}) \cdot (\widehat{L}_{i_0+1} - \widehat{L}_{i_0}) \\ & + (\tilde{a}_{i_0+1} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0+1} - |L_{i_0+1}|. \end{aligned}$$

Using (8.14), notice that $(b_{i_0} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0} = O(\varepsilon)$ and similarly $(b_{i_0+1} - \tilde{a}_{i_0+1}) \cdot \widehat{L}_{i_0+1} = O(\varepsilon)$. Using moreover the fact that $b_{i_0} - \tilde{a}_{i_0}$ is bounded (see (8.3)) joint to Lemma 13.9 ii), and (8.17), we deduce that there exists a constant C_5 such that

$$|(\tilde{a}_{i_0+1} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0+1} - |L_{i_0+1}|| \le C_5\varepsilon,$$

and then

$$|((\tilde{a}_{i_0+1} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0+1})\widehat{L}_{i_0+1} - L_{i_0+1}| \le C_5\varepsilon.$$

Because $|L_{i_0+1} - L_{i_0}| \leq C_0\varepsilon$, we deduce that there exists a constant C_6 such that

$$|((\tilde{a}_{i_0+1} - \tilde{a}_{i_0}) \cdot \widehat{L}_{i_0+1})\widehat{L}_{i_0+1} - L_{i_0}| \leq C_6\varepsilon. \tag{8.18}$$

Step 2-3: Conclusion
By (8.5) and (8.18), we see that we control both parallel and orthogonal parts of $\tilde{a}_{i_0+1} - \tilde{a}_{i_0}$ and then there exists a constant $C_7 > 0$ such that we have

$$|\tilde{a}_{i_0+1} - \tilde{a}_{i_0} - L_{i_0}| \leq C_7\varepsilon.$$

Step 3: Proof of (8.7) and (8.8)
Inequality (8.7) is a consequence of (8.16) and (8.6). Moreover (8.8) is implied by (8.15).

□

9 An estimate about the line tension, the line torsion and the partial derivatives of the energy

The goal of this section is to prove the following theorem which indicates an accurate estimate for the difference between line tension and a partial derivative of the energy and the difference between line torsion and a another partial derivative of the energy.

Theorem 9.1 (An estimate about the line tension and the line torsion)
Let us consider a nanotube X under the assumptions of Theorem 2.15. Then there exists a constant $C > 0$ (independent on X) such that for all $i \in \mathbb{Z}$ there exist $(\theta_i, L_i) \in \mathcal{U}_0$, and a mean fiber $\tilde{a}_i \in \mathbb{R}^3$ given by Definition 8.1 such that we have with the notation of Definitions 7.1 and 7.7, for all $i \in \mathbb{Z}$

$$D_i(X, \theta_i, L_i) \leq C\varepsilon, \tag{9.1}$$

and

$$|T_i - W'_L(\theta_i, L_i)| \leq C\varepsilon^{\frac{p-1}{p+1}}, \tag{9.2}$$

and

$$|M_i(\tilde{a}_i) - W'_\theta(\theta_i, L_i)\widehat{L}_i| \leq C\varepsilon^{\frac{p-2}{p}}, \tag{9.3}$$

where $p > 2$ appears in assumption (H0).

Remark 9.2
Notice that $\varepsilon^{\frac{p-2}{p}} = \varepsilon^{\frac{q-1}{q+1}}$ with $q = p - 1$. This difference between the error estimate (9.2) and (9.3) comes from the fact the line torsion M_i has the following homogeneity

$$M_i \simeq \textit{length} \times T_i.$$

This explains the difference of exponent $q = p - 1$ (in order to estimate the rest of the series defining M_i and T_i).

In a first subsection, we state and prove two results on two-body interactions, that are used in a second subsection to prove Theorem 9.1.

9.1 Preliminary estimates on two-body interactions

In this subsection we present two estimates on two-body interactions: Proposition 9.3 and Proposition 9.5.

Proposition 9.3 (A uniform estimate on two-body interactions)
Assume (H0). Then there exists $\varepsilon_0 > 0$ *small enough and a constant* $C > 0$*, such that for every nanotube* X *and* $(\theta^*, L^*) \in \mathcal{U}_0$*, such that*

$$\sup_{j\in\mathbb{Z}} D_j(X, \theta^*, L^*) \le \varepsilon_0,$$

we have

$$|\nabla V(X_{j,l} - X_{j',l'})| \le \frac{C}{|j-j'|^{p+1}} \quad \textit{for } |j-j'| \ge 1, \tag{9.4}$$

and

$$|X_j - X_{j'}| \le C(1 + |j - j'|) \quad \textit{for all} \quad j,\, j' \in \mathbb{Z}. \tag{9.5}$$

Remark 9.4
Notice that under assumption (H1), we automatically have $(\theta^*, L^*) \in \mathcal{U}_0$ *by Proposition 2.1.*

Proof of Proposition 9.3
Step 1: Preliminary
From Proposition 4.5, we deduce estimate (9.5) and that there exists a constant $C_1 > 0$ such that

$$|X_{j',l'} - X_{j,l}| \ge (|L| - C_1\varepsilon_0)|j' - j| - C_1, \tag{9.6}$$

and moreover that there exists $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}_*^{\theta^*,L^*}$ such that

$$|X_{j',l'} - X_{j,l} - (\widehat{X}^{*,j}_{j',l'} - \widehat{X}^{*,j}_{j,l})| \le C_1\varepsilon_0(1 + |j' - j|). \tag{9.7}$$

Step 2: Proof of (9.4)
Case 1: $|j - j'| \ge C_3$
Using (9.6) there exists a constant $C_2 > 0$ and a constant C_3 (large enough) such that we have

$$|X_{j,l} - X_{j',l'}| \ge C_2|j - j'| \quad \text{for } |j - j'| \ge C_3.$$

Case 2: $1 \le |j - j'| \le C_3$
Notice that there exists a constant δ such that

$$|\widehat{X}^{*,j}_{j,l} - \widehat{X}^{*,j}_{j',l'}| \ge \delta > 0 \quad \text{if } j \ne j'.$$

From (9.7), we get

$$|X_{j,l} - X_{j',l'}| \ge \delta - C_1\varepsilon_0(1 + |j - j'|).$$

For $\varepsilon_0 < \dfrac{\delta}{4C_1C_3}$, we get

$$|X_{j,l} - X_{j',l'}| \ge \frac{\delta}{2} \quad \text{for } 1 \le |j - j'| \le C_3.$$

Using the conclusions of case 1 and case 2 and assumption (H0), we see that there exists a constant $C > 0$ such that (9.4) holds.

□

Proposition 9.5 (A short distance estimate on the two-body interactions)
Assume (H0). Then there exist constants $C > 0$ and $\varepsilon_1 > 0$ such that for every nanotube X and any $\varepsilon \in (0, 1)$, if

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_j(X, \theta, L) \le \varepsilon \qquad \text{for } j \in \mathbb{Z},$$

then the following holds.
If for some $(\theta_0, L_0) \in \mathcal{U}_0$, we have $\widehat{X}^* \in \widehat{\mathcal{C}}_*^{\theta_0,L_0}$ and $\sup_{|\alpha|\le q} |X_\alpha - \widehat{X}^*_\alpha| \le \varepsilon$,
then for $j, j' \in Q_\rho$ where $\rho > 1$ is such that $\varepsilon\rho^2 \le \varepsilon_1$, we have

$$|\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\hat{X}^*_{j,l} - \hat{X}^*_{j',l'})| \le \frac{C\varepsilon\rho^2}{|j - j'|^{p+2}}. \tag{9.8}$$

Proof of Proposition 9.5
Step 1: Definition of $\bar{X}$ and Taylor expansion
We define

$$\bar{X} := \frac{X - \widehat{X}^*}{\varepsilon}.$$

Then we can apply Theorem 5.1 and deduce that there exists a constant C_1 such that we have

$$|\bar{X}_j| \le C_1(1 + |j|^2) \quad \text{for } j \in \mathbb{Z}.$$

Therefore for $j \in Q_\rho$ with $\rho > 1$, there exists a constant $C_2 > 0$ such that we have

$$|\bar{X}_j| \le C_2\rho^2. \tag{9.9}$$

By the definition of $\bar{X}_j$, we have

$$X_{j,l} - X_{j',l'} = \widehat{X}^*_{j,l} - \widehat{X}^*_{j',l'} + \varepsilon(\bar{X}_{j,l} - \bar{X}_{j',l'}).$$

Using the Taylor expansion with integral rest, we get

$$\nabla V(X_{j,l} - X_{j',l'}) = \nabla V(\widehat{X}^*_{j,l} - \widehat{X}^*_{j',l'}) + \varepsilon(\bar{X}_{j,l} - \bar{X}_{j',l'}) \int_0^1 D^2V(A(t))\, dt, \tag{9.10}$$

with

$$A(t) = Z_{j,l}(t) - Z_{j',l'}(t) \quad \text{and} \quad Z_{j,l}(t) = \widehat{X}^*_{j,l} + t\varepsilon\bar{X}_{j,l}.$$

Step 2: Conclusion
From Proposition 4.6, we deduce that there exist constants C_3, C_4 such that

$$|A(t)| \ge C_4|j - j'| \quad \text{if} \quad |j - j'| \ge C_3. \tag{9.11}$$

Case 1: $|j - j'| > C_3$
Then by assumption (H0), there exists a constant $C_5 > 0$ such that

$$|D^2V(A(t))| \le \frac{C_5}{|j - j'|^{p+2}}.$$

Case 2: $1 \le |j - j'| \le C_3$
Assume that $1 \le |j - j'| \le C_3$. Because of (9.9), we deduce

$$|\bar{X}_{j,l} - \bar{X}_{j',l'}| \le 2C_2\rho^2.$$

Then we compute

$$\begin{array}{rcl} |A(t) - (\widehat{X}^*_{j,l} - \widehat{X}^*_{j',l'})| & = & |t\varepsilon(\bar{X}_{j,l} - \bar{X}_{j',l'})| \\ & \le & 2C_2\varepsilon\rho^2, \end{array}$$

and because $|\widehat{X}^*_{j,l} - \widehat{X}^*_{j',l'}| \ge \delta > 0$ if $(j,l) \neq (j',l')$, we deduce for the choice $\varepsilon\rho^2 \le \varepsilon_1$ (for ε_1 small enough) that there exists a constant C_6 such that

$$|A(t)| \ge C_6.$$

Using moreover assumption (H0), there exists a constant $C_7 > 0$ such that

$$|D^2V(A(t))| \le C_7 \le \frac{C_7}{|j-j'|^{p+2}}.$$

Using the conclusions of case 1 and case 2, we deduce that there exists a constant $C_8 > 0$ such that

$$\left|\int_0^1 D^2V(A(t))dt\right| \le \frac{C_8}{|j-j'|^{p+2}}.$$

Moreover because of (9.9) and (9.10), we deduce that there exists a constant $C > 0$ such that we have (9.8).

□

9.2 Proof of Theorem 9.1

Proof of Theorem 9.1

Step 1: Control of $\mathcal{N}_{\mathbb{Z}}(X)$ and $D_i(X,\theta_i,L_i)$

We apply our Saint-Venant principle (2.15) of Theorem 2.13 with $J = \mathbb{Z}$ and we get

$$\mathcal{N}_{\mathbb{Z}}(X) \le \frac{C_1}{1-\mu}\sup_{j\in\mathbb{Z}}|f_j|.$$

We compute

$$\begin{array}{rcl} \sup_{j\in\mathbb{Z}}|f_j| & = & \sup_{j\in\mathbb{Z}}\sup_{0\le l\le K-1}|f_{j,l}| \\ & = & \sup_{j\in\mathbb{Z}}|\frac{1}{K}f^0_j| \\ & = & \frac{1}{K}\sup_{j\in\mathbb{Z}}|\int_{\varepsilon(j-\frac{1}{2})}^{\varepsilon(j+\frac{1}{2})}\bar{f}(x)dx| \\ & \le & \frac{\varepsilon}{K}\sup_x|\bar{f}(x)|, \end{array}$$

where in the second line we have used (1.6) and in the third line we have used (1.14). Using (2.18) to bound $\bar{f}$, we deduce that for some constant $C_0 > 0$, we have

$$\mathcal{N}_{\mathbb{Z}}(X) \le \bar{\varepsilon} \quad \text{with} \quad \bar{\varepsilon} := C_0\varepsilon. \tag{9.12}$$

Given $i \in \mathbb{Z}$, we consider $(\theta_i, L_i) \in \mathcal{U}_0$, such that

$$\inf_{(\theta,L)\in\mathcal{U}_0} D_i(X,\theta,L) = D_i(X,\theta_i,L_i),$$

and $\widehat{X}^{*,i} \in \widehat{\mathcal{C}}_*^{\theta_i,L_i}$ such that

$$D_i(X,\theta_i,L_i) = \sup_{|\alpha|\le q} |X_{i+\alpha} - \widehat{X}^{*,i}_{i+\alpha}|.$$

Using (9.12), we have

$$D_i(X,\theta_i,L_i) \le \bar{\varepsilon}. \tag{9.13}$$

For later use, we write (uniquely) $\widehat{X}^{*,i} = a_i + X^{*,i}$ with $a_i \in L_i^\perp$ and $X^{*,i} \in \mathcal{C}_*^{\theta_i,L_i}$.

Step 2: Error estimate on the line tension

We recall the definition of the line tension

$$T_i[X] := T_i = \sum_{\substack{j\ge i+1\\ j'\le i}} \sum_{0\le l,l'\le K-1} \nabla V(X_{j,l} - X_{j',l'}),$$

where we show the dependence of T_i on X. We write

$$T_i[X] = S_i(X) + F_i(X),$$

with the short distance contribution for $\rho \ge 1$:

$$S_i(X) = \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} \nabla V(X_{j,l} - X_{j',l'}),$$

and the far away contribution

$$F_i(X) = \sum_{\substack{j> i+\rho\\ j'\le i}} \sum_{0\le l,l'\le K-1} \nabla V(X_{j,l} - X_{j',l'}) + \sum_{\substack{i+1\le j\le i+\rho\\ j'< i-\rho}} \sum_{0\le l,l'\le K-1} \nabla V(X_{j,l} - X_{j',l'}).$$

Step 2-1: Error estimate on $S_i(X)$

Assuming that $\bar{\varepsilon}\rho^2 < 1$ (see later on our choice (9.18)), we can apply (9.8) in Proposition 9.5 and deduce that there exists a constant C_2 such that for $|j-i|, |j'-i| \le \rho$:

$$|\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\widehat{X}^{*,i}_{j,l} - \widehat{X}^{*,i}_{j',l'})| \le \frac{C_2\bar{\varepsilon}\rho^2}{|j-j'|^{p+2}}. \tag{9.14}$$

Then we compute

$$\begin{aligned}
|S_i(X) - S_i(\widehat{X}^{*,i})| &\le \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} |\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\widehat{X}^{*,i}_{j,l} - \widehat{X}^{*,i}_{j',l'})| \\
&\le \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} \frac{C_2\bar{\varepsilon}\rho^2}{|j-j'|^{p+2}} \\
&\le \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \frac{K^2C_2\bar{\varepsilon}\rho^2}{|j-j'|^{p+2}} \\
&\le K^2C_2\bar{\varepsilon}\rho^2 \sum_{\substack{1\le \bar{j}\le \rho\\ 0\le \bar{j}'\le \rho}} \frac{1}{|\bar{j}+\bar{j}'|^{p+2}} \\
&\le K^2C_2\bar{\varepsilon}\rho^2 \sum_{\substack{\bar{j}\ge 1\\ \bar{j}'\ge 0}} \frac{1}{|\bar{j}+\bar{j}'|^{p+2}},
\end{aligned}$$

where $\bar{j} := j - i$ and $\bar{j}' := i - j'$.
By Lemma 13.12 (with $\rho = 1$) with $p > 0$, there exists a constant C_3 such that we have

$$|S_i(X) - S_i(\widehat{X}^{*,i})| \leq C_3 \bar{\varepsilon} \rho^2. \tag{9.15}$$

Step 2-2: Error estimate on $F_i(X)$
By (2.18) we have

$$\sup_{j \in \mathbb{Z}} D_j(X, \theta^*, L^*) \leq \varepsilon_0.$$

Using (9.4) in Proposition 9.3, we deduce that there exists a constant $C_4 > 0$ such that

$$|\nabla V(X_{j,l} - X_{j',l'})| \leq \frac{C_4}{|j - j'|^{p+1}} \qquad \text{for } |j - j'| \geq \rho \geq 1. \tag{9.16}$$

Then
(9.17)

$$\begin{aligned}
|F_i(X)| &\leq C_4 \Bigg(\sum_{\substack{j > i + \rho \\ j' \leq i}} \sum_{0 \leq l, l' \leq K-1} \frac{1}{|j - j'|^{p+1}} + \sum_{\substack{i+1 \leq j \leq i + \rho \\ j' < i - \rho}} \sum_{0 \leq l, l' \leq K-1} \frac{1}{|j - j'|^{p+1}} \Bigg) \\
&\leq K^2 C_4 \Bigg(\sum_{\substack{\bar{j} > \rho \\ \bar{j}' \geq 0}} \frac{1}{(\bar{j} + \bar{j}')^{p+1}} + \sum_{\substack{1 \leq \bar{j} \leq \rho \\ \bar{j}' > \rho}} \frac{1}{(\bar{j} + \bar{j}')^{p+1}} \Bigg) \\
&\leq 2K^2 C_4 \sum_{\substack{\bar{j} > \rho \\ \bar{j}' \geq 0}} \frac{1}{(\bar{j} + \bar{j}')^{p+1}}.
\end{aligned}$$

where $\bar{j} := j - i$ and $\bar{j}' := i - j'$. By Lemma 13.12 with $p > 1$, there exists a constant C_5 such that

$$|F_i(X)| \leq \frac{C_5}{\rho^{p-1}}.$$

Similarly we have

$$|F_i(\widehat{X}^{*,i})| \leq \frac{C_5}{\rho^{p-1}}.$$

Step 2-3: Conclusion
We compute

$$\begin{aligned}
\left| T_i[X] - T_i[\widehat{X}^{*,i}] \right| &\leq |S_i(X) - S_i(\widehat{X}^{*,i})| + |F_i(X)| + |F_i(\widehat{X}^{*,i}))| \\
&\leq C_3 \bar{\varepsilon} \rho^2 + \frac{C_5 + C_5}{\rho^{p-1}} \\
&\leq C_6 (\bar{\varepsilon} \rho^2 + \frac{1}{\rho^{p-1}}),
\end{aligned}$$

with $C_6 = \max(C_3, 2C_5)$. With the choice

$$\bar{\varepsilon} \rho^{p+1} = 1, \tag{9.18}$$

which is optimal up to a numerical constant, the right hand side becomes $2C_6 \bar{\varepsilon}^{\frac{p-1}{p+1}}$ and we get

$$\left| T_i[X] - T_i[\widehat{X}^{*,i}] \right| \leq C_7 \bar{\varepsilon}^{\frac{p-1}{p+1}},$$

with $C_7 = 2C_6$. Finally by Theorem 7.2 we have $T_i[\widehat{X}^{*,i}] = T_i[X^{*,i}] = W_L'(\theta_i, L_i)$. Therefore

$$|T_i - W_L'(\theta_i, L_i)| \leq C\varepsilon^{\frac{p-1}{p+1}},$$

with $C \geq C_7 C_0^{\frac{p-1}{p+1}}$.

Step 3: Error estimate on the line torsion

We recall the definition of the line torsion

$$M_i[X] := M_i = \sum_{\substack{j \geq i+1 \\ j' \leq i}} \sum_{0 \leq l,l' \leq K-1} X_{j,l} \times \nabla V(X_{j,l} - X_{j',l'}).$$

where we show the dependence of M_i on X. The goal of this step is to prove (9.3) with the mean fiber (see Definition 8.1)

$$\tilde{a}_i = a_i + (b_i^{*,i} \cdot \widehat{L}_i)\widehat{L}_i.$$

We write (from Definition 7.7 and Proposition 7.8)

$$M_i[X] = M_i[X](0) = M_i[X](\tilde{a}_i) + \tilde{a}_i \times T_i[X] = \mathbb{S}_i(X - \tilde{a}_i) + \mathbb{F}_i(X - \tilde{a}_i) + \tilde{a}_i \times T_i[X], \tag{9.19}$$

with the short distance contribution for $\rho \geq 1$

$$\mathbb{S}_i(X - \tilde{a}_i) = \sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} (X_{j,l} - \tilde{a}_i) \times \nabla V(X_{j,l} - X_{j',l'}),$$

and the far away contribution

$$\begin{aligned} \mathbb{F}_i(X - \tilde{a}_i) \quad = \quad & \sum_{\substack{j > i+\rho \\ j' \leq i}} \sum_{0 \leq l,l' \leq K-1} (X_{j,l} - \tilde{a}_i) \times \nabla V(X_{j,l} - X_{j',l'}) \\ & + \sum_{\substack{i+1 \leq j \leq i+\rho \\ j' < i-\rho}} \sum_{0 \leq l,l' \leq K-1} (X_{j,l} - \tilde{a}_i) \times \nabla V(X_{j,l} - X_{j',l'}). \end{aligned}$$

Step 3-0: Definition and properties of $\tilde{X}^{*,i}$

We define for $j \in \mathbb{Z}$

$$\tilde{X}_j^{*,i} := X_j^{*,i} - (b_i^{*,i} \cdot \widehat{L}_i)\widehat{L}_i.$$

Then we have

$$\tilde{X}^{*,i} \in \mathcal{C}_*^{\theta_i, L_i}. \tag{9.20}$$

We compute

$$X_i - \widehat{X}_i^{*,i} = X_i - a_i - X_i^{*,i} = X_i - (a_i + (b_i^{*,i} \cdot \widehat{L}_i)\widehat{L}_i) - (X_i^{*,i} - (b_i^{*,i} \cdot \widehat{L}_i)\widehat{L}_i) = X_i - \tilde{a}_i - \tilde{X}_i^{*,i}.$$

By (9.13) we deduce

$$|X_i - \tilde{a}_i - \tilde{X}_i^{*,i}| \leq \bar{\varepsilon}, \tag{9.21}$$

and then (with $\tilde{b}_i^{*,i}$ the barycenter of $\tilde{X}_i^{*,i}$)

$$|b_i - \tilde{a}_i - \tilde{b}_i^{*,i}| \leq \bar{\varepsilon}. \tag{9.22}$$

Using (8.3) we deduce that $\tilde{b}_i^{*,i}$ is bounded. Moreover because the centered cell $(\tilde{X}_{i,l}^{*,i})'_l = (\tilde{X}_{i,l}^{*,i} - \tilde{b}_i^{*,i})_l$ is bounded, we deduce that there exists a constant $C_8 > 0$ such that

$$|\tilde{X}_i^{*,i}| \leq C_8. \tag{9.23}$$

Step 3-1: Error estimate on $\mathbb{S}_i(X - \tilde{a}_i)$
We compute (using the fact that $\tilde{X}_{j,l}^{*,i} - \tilde{X}_{j',l'}^{*,i} = \widehat{X}_{j,l}^{*,i} - \widehat{X}_{j',l'}^{*,i}$)

$$\begin{aligned}
&\mathbb{S}_i(X - \tilde{a}_i) - \mathbb{S}_i(\tilde{X}^{*,i}) \\
= &\sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} \left((X_{j,l} - \tilde{a}_i) \times \nabla V(X_{j,l} - X_{j',l'}) - \tilde{X}_{j,l}^{*,i} \times \nabla V(\tilde{X}_{j,l}^{*,i} - \tilde{X}_{j',l'}^{*,i})\right) \\
= &\sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} \left((X_{j,l} - \tilde{a}_i) \times \nabla V(X_{j,l} - X_{j',l'}) - \tilde{X}_{j,l}^{*,i} \times \nabla V(\widehat{X}_{j,l}^{*,i} - \widehat{X}_{j',l'}^{*,i})\right) \\
= &\ \mathbb{S}_i^1 + \mathbb{S}_i^2 + \mathbb{S}_i^3,
\end{aligned}$$

with

$$\begin{cases}
\mathbb{S}_i^1 = \displaystyle\sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} (X_{j,l} - \tilde{a}_i - \tilde{X}_{j,l}^{*,i}) \times \nabla V(X_{j,l} - X_{j',l'}) \\
\mathbb{S}_i^2 = \displaystyle\sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} \left(R_{(j-i)\theta_i, \widehat{L}_i}(\tilde{X}_{i,l}^{*,i})\right) \times \left(\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\widehat{X}_{j,l}^{*,i} - \widehat{X}_{j',l'}^{*,i})\right) \\
\mathbb{S}_i^3 = \displaystyle\sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} (j-i)L_i \times \left(\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\widehat{X}_{j,l}^{*,i} - \widehat{X}_{j',l'}^{*,i})\right),
\end{cases}$$

where we have used (9.20).
Using (9.16) and (9.21), we deduce that there exists a constant C_9 such that we have

$$|\mathbb{S}_i^1| \leq \sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} \frac{C_4 \bar{\varepsilon}}{|j-j'|^{p+1}} \leq \sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} C_4 K^2 \bar{\varepsilon} \leq C_9 \bar{\varepsilon} \rho^2.$$

Using (9.14) and (9.23), we deduce that

$$\begin{aligned}
|\mathbb{S}_i^2| &\leq \sum_{\substack{i+1 \leq j \leq i+\rho \\ i-\rho \leq j' \leq i}} \sum_{0 \leq l,l' \leq K-1} \frac{C_8 C_2 \bar{\varepsilon} \rho^2}{|j-j'|^{p+1}} \leq C_8 C_2 K^2 \bar{\varepsilon} \rho^2 \sum_{\substack{1 \leq \bar{j} \leq \rho \\ 0 \leq \bar{j}' \leq \rho}} \frac{1}{|\bar{j} + \bar{j}'|^{p+1}} \\
&\leq C_8 C_2 K^2 \bar{\varepsilon} \rho^2 \sum_{\substack{\bar{j} \geq 1 \\ \bar{j}' \geq 0}} \frac{1}{|\bar{j} + \bar{j}'|^{p+1}},
\end{aligned}$$

where $\bar{j} = j - i$ and $\bar{j}' = i - j'$. By Lemma 13.12 (with $\rho = 1$) with $p > 1$, we deduce that there exists a constant C_{10} such that

$$|\mathbb{S}_i^2| \leq C_{10} \bar{\varepsilon} \rho^2.$$

Using (9.14), we deduce that there exists a constant C_{11} such that we have

$$|\mathbb{S}_i^3| \leq C_{11}\bar{\varepsilon}\rho^2 \sum_{\substack{i+1\leq j\leq i+\rho \\ i-\rho\leq j'\leq i}} \frac{|j-i|}{|j-j'|^{p+2}} = C_{11}\bar{\varepsilon}\rho^2 \sum_{\substack{1\leq \bar{j}\leq \rho \\ 0\leq \bar{j}'\leq \rho}} \frac{\bar{j}}{(\bar{j}+\bar{j}')^{p+2}} \leq C_{11}\bar{\varepsilon}\rho^2 \sum_{\substack{\bar{j}\geq 1 \\ \bar{j}'\geq 0}} \frac{\bar{j}}{(\bar{j}+\bar{j}')^{p+2}},$$

where $\bar{j} := j-i$ and $\bar{j}' := i-j'$.
By Lemma 13.12 (with $\rho = 1$) with $p > 1$, then there exists a constant C_{12} such that we have

$$|\mathbb{S}_i^3| \leq C_{12}\bar{\varepsilon}\rho^2.$$

Finally we get

$$|\mathbb{S}_i(X-\tilde{a}_i) - \mathbb{S}_i(\tilde{X}^{*,i})| \leq C_{13}\bar{\varepsilon}\rho^2, \tag{9.24}$$

with $C_{13} = C_9 + C_{10} + C_{12}$.
Step 3-2: Error estimate on $\mathbb{F}_i(X-\tilde{a}_i)$
Using (9.5), (9.21) and (9.23), we deduce that

$$\begin{aligned} |X_j - \tilde{a}_i| &\leq |X_j - X_i| + |X_i - \tilde{a}_i - \tilde{X}_i^{*,i}| + |\tilde{X}_i^{*,i}| \\ &\leq C_{14}(1+|j-i|), \end{aligned}$$

with $C_{14} > 0$. Using moreover (9.16), we get

$$\begin{aligned} |\mathbb{F}_i(X-\tilde{a}_i)| &= \left| \begin{array}{l} \displaystyle\sum_{\substack{j>i+\rho \\ j'\leq i}} \sum_{0\leq l,l'\leq K-1} (X_{j,l}-\tilde{a}_i)\times \nabla V(X_{j,l}-X_{j',l'}) \\ \displaystyle+ \sum_{\substack{i+1\leq j\leq i+\rho \\ j'<i-\rho}} \sum_{0\leq l,l'\leq K-1} (X_{j,l}-\tilde{a}_i)\times \nabla V(X_{j,l}-X_{j',l'}) \end{array} \right| \\ &\leq K^2 C_4 \left(\sum_{\substack{j>i+\rho \\ j'\leq i}} \frac{C_{14}(1+|j-i|)}{|j-j'|^{p+1}} + \sum_{\substack{i+1\leq j\leq i+\rho \\ j'<i-\rho}} \frac{C_{14}(1+|j-i|)}{|j-j'|^{p+1}} \right) \\ &\leq K^2 C_4 C_{14} \Bigg(\sum_{\substack{\bar{j}>\rho \\ \bar{j}'\geq 0}} \frac{1+\bar{j}}{(\bar{j}+\bar{j}')^{p+1}} + \sum_{\substack{1\leq\bar{j}\leq\rho \\ \bar{j}'>\rho}} \frac{1+\bar{j}}{(\bar{j}+\bar{j}')^{p+1}} \Bigg), \end{aligned}$$

with $\bar{j} = j-i$ and $\bar{j}' = i-j'$. Using Lemmata 13.11 and 13.12 with $p > 2$, we deduce that there exists a constant C_{15} such that we have

$$|\mathbb{F}_i(X-\tilde{a}_i)| \leq \frac{C_{15}}{\rho^{p-2}}.$$

Similarly, we have

$$|\mathbb{F}_i(\tilde{X}^{*,i})| \leq \frac{C_{15}}{\rho^{p-2}}. \tag{9.25}$$

Step 3-3: Conclusion
We compute

$$\begin{aligned}\left|M_i[X] - \tilde{a}_i \times T_i[X] - M_i[\tilde{X}^{*,i}]\right| &\leq |\mathbb{S}(X-\tilde{a}_i) - \mathbb{S}(\tilde{X}^{*,i})| + |\mathbb{F}_i(X-\tilde{a}_i)| + |\mathbb{F}_i(\tilde{X}^{*,i})| \\ &\leq C_{16}\left(\bar{\varepsilon}\rho^2 + \frac{1}{\rho^{p-2}}\right),\end{aligned}$$

with $C_{16} = \max\{C_{13}, 2C_{15}\}$. With the choice of ρ such that

$$\bar{\varepsilon}\rho^p = 1,$$

which is optimal up to numerical constant, we have $\bar{\varepsilon}\rho^2 \leq \varepsilon_1$ (using $p > 2$) and the right hand side becomes $C_{17}\bar{\varepsilon}^{\frac{p-2}{p}}$, which gives

$$\left|M_i[X] - \tilde{a}_i \times T_i[X] - M_i[\tilde{X}^{*,i}]\right| \leq C_{17}\bar{\varepsilon}^{\frac{p-2}{p}}.$$

Finally using Lemma 7.9, we get $M_i[\tilde{X}^{*,i}] = W'_\theta(\theta_i, L_i)\widehat{L}_i$ and then

$$\left|M_i[X] - \tilde{a}_i \times T_i[X] - W'_\theta(\theta_i, L_i)\widehat{L}_i\right| \leq C_{17}\bar{\varepsilon}^{\frac{p-2}{p}},$$

that we can write (using (9.19))

$$\left|M_i[X](\tilde{a}_i) - W'_\theta(\theta_i, L_i)\widehat{L}_i\right| \leq C\varepsilon^{\frac{p-2}{p}},$$

with $C \geq C_{17}C_0^{\frac{p-2}{p}}$, which means exactly (9.3).

□

10 An estimate about the scalar line torsion

In order to use later (in Section 11) the estimates of Theorem 9.1 about T_i and $M_i(\tilde{a}_i)$, we need first to compute these quantities. Recall that we have $T_i - T_{i-1} = f_i^0$, and a simple iteration is sufficient to get $T_i = T_0 + \sum_{j=1}^{i} f_i^0$. But a simple similar raisoning for the line torsion $M_i(\tilde{a}_i)$ is not possible. The goal of this section is to solve this problem and to this end we introduce the following scalar line torsion.

Definition 10.1 (Scalar line torsion)
Given a nanotube $X \in ((\mathbb{R}^3)^K)^{\mathbb{Z}}$, we define a scalar line torsion as

$$m_i := M_i(\tilde{a}_i) \cdot \widehat{L}_i,$$

where L_i and $\tilde{a}_i$ are introduced in Definition 8.1.

The main result of this section is the following estimate about the scalar line torsion

Theorem 10.2 (Almost constant scalar line torsion)
Let us consider a nanotube X under the assumptions of Theorem 2.15. Then there exist constants $\bar{m}_0 \in \mathbb{R}$ and $C > 0$ such that we have for all $i \in \mathbb{Z}$

$$|m_i - \bar{m}_0| \le C\varepsilon^\gamma \quad \textit{with} \quad \gamma = \min\left(\frac{1}{3}, \frac{p-2}{p}\right). \tag{10.1}$$

Notice that (10.1) means that the scalar line torsion m_i is almost constant which is the discrete analogue of the second equation of (1.5).
In order to prove Theorem 10.2 we first need the following lemma:

Lemma 10.3 (Estimate on $m_i - m_{i-1}$)
Let us consider a nanotube X under the assumptions of Theorem 2.15. Then we have for all $i \in \mathbb{Z}$

$$m_i - m_{i-1} = -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times f_i^0) + O(\varepsilon^{1+\bar{\bar{\gamma}}}), \tag{10.2}$$

with $\bar{\bar{\gamma}} = \dfrac{p-2}{p}$.

Proof of Lemma 10.3
By Theorem 9.1, we have (9.1), i.e.

$$D_i(X, \theta_i, L_i) \le C\varepsilon. \tag{10.3}$$

We also have the general relations

$$\begin{cases} M_i - M_{i-1} = b_i \times f_i^0 \\ M_i(\tilde{a}_i) = M_i - \tilde{a}_i \times T_i \\ T_i - T_{i-1} = f_i^0. \end{cases}$$

Then we compute

$$\begin{aligned} M_i(\tilde{a}_i) - M_{i-1}(\tilde{a}_{i-1}) &= b_i \times f_i^0 - \tilde{a}_i \times T_i + \tilde{a}_{i-1} \times T_{i-1} \\ &= b_i \times (T_i - T_{i-1}) - \tilde{a}_i \times T_i + \tilde{a}_{i-1} \times T_{i-1} \\ &= (b_i - \tilde{a}_i) \times T_i - (b_i - \tilde{a}_{i-1}) \times T_{i-1}, \end{aligned}$$

which implies

$$\widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_i \cdot M_{i-1}(\tilde{a}_{i-1}) = \widehat{L}_i \cdot \big((b_i - \tilde{a}_i) \times T_i\big) - \widehat{L}_i \cdot \big((b_i - \tilde{a}_{i-1}) \times T_{i-1}\big),$$

and then

$$\widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_i \cdot M_{i-1}(\tilde{a}_{i-1}) = -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_i) + (b_i - \tilde{a}_{i-1}) \cdot (\widehat{L}_i \times T_{i-1}). \tag{10.4}$$

We compute with $\bar{\gamma} = \dfrac{p-1}{p+1}$

$$\begin{aligned} (b_i - \tilde{a}_{i-1}) \cdot (\widehat{L}_i \times T_{i-1}) &= (b_i - \tilde{a}_{i-1}^{\perp_{\widehat{L}_i}}) \cdot (\widehat{L}_i \times T_{i-1}) \\ &= (b_i - \tilde{a}_i^{\perp_{\widehat{L}_i}} + O(\varepsilon)) \cdot (\widehat{L}_i \times T_{i-1}) \\ &= (b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_{i-1}) + O(\varepsilon) \cdot ((\widehat{L}_{i-1} + O(\varepsilon)) \times T_{i-1}) \\ &= (b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_{i-1}) + O(\varepsilon^2) + O(\varepsilon) \cdot (\widehat{L}_{i-1} \times T_{i-1}) \\ &= (b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_{i-1}) + O(\varepsilon^2) + O(\varepsilon) \cdot O(\varepsilon^{\bar{\gamma}}) \\ &= (b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_{i-1}) + O(\varepsilon^{1+\bar{\gamma}}), \end{aligned}$$

where in the second line we have used (8.5), in the third line we have used (10.3), Lemma 5.4 and Lemma 13.9 ii), and in the fifth line we have used (9.2) and the fact that $W'_L(\theta_{i-1}, L_{i-1})$ is parallel to L_{i-1} (see Corollary 7.4). Therefore from (10.4), we get

$$\begin{array}{rcl} \widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_i \cdot M_{i-1}(\tilde{a}_{i-1}) & = & -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_i) + (b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_{i-1}) + O(\varepsilon^{1+\bar{\gamma}}) \\ & = & -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times (T_i - T_{i-1})) + O(\varepsilon^{1+\bar{\gamma}}) \\ & = & -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times f_i^0) + O(\varepsilon^{1+\bar{\gamma}}). \end{array}$$

On the other hand we compute

$$\begin{array}{rcl} (\widehat{L}_i - \widehat{L}_{i-1}) \cdot M_{i-1}(\tilde{a}_{i-1}) & = & (\widehat{L}_i - \widehat{L}_{i-1}) \cdot (W'_\theta(\theta_{i-1}, L_{i-1})\widehat{L}_{i-1} + O(\varepsilon^{\bar{\bar{\gamma}}})) \\ & = & W'_\theta(\theta_{i-1}, L_{i-1})(\widehat{L}_i \cdot \widehat{L}_{i-1} - 1) + O(\varepsilon^{1+\bar{\bar{\gamma}}}) \\ & = & O(\varepsilon^2) + O(\varepsilon^{1+\bar{\bar{\gamma}}}) = O(\varepsilon^{1+\bar{\bar{\gamma}}}), \end{array}$$

where in the first line we have used (9.3) and in the last line we have used the square of the relation $\widehat{L}_i - \widehat{L}_{i-1} = O(\varepsilon)$. We compute

$$\begin{array}{rcl} m_i - m_{i-1} & = & \widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_{i-1} \cdot M_{i-1}(\tilde{a}_{i-1}) \\ & = & \widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_i \cdot M_{i-1}(\tilde{a}_{i-1}) + (\widehat{L}_i - \widehat{L}_{i-1}) \cdot M_{i-1}(\tilde{a}_{i-1}) \\ & = & -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times f_i^0) + O(\varepsilon^{1+\bar{\gamma}}) + O(\varepsilon^{1+\bar{\bar{\gamma}}}), \end{array}$$

and finally, because $\bar{\bar{\gamma}} < \bar{\gamma}$, we deduce (10.2).

□

Proof of Theorem 10.2

We recall that by Lemma 5.4, there exists a constant $C_1 > 0$ such that we have

$$\left\{ \begin{array}{l} |\theta_{i+1} - \theta_i| \le C_1 \varepsilon \\ |L_{i+1} - L_i| \le C_1 \varepsilon. \end{array} \right. \tag{10.5}$$

Step 1: Proof of $m_i - m_{i-1} = -(b_i - \tilde{a}_i) \cdot (\widehat{L}_0 \times f_0^0) + O(i\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}})$

We recall (10.2) in Lemma 10.3, i.e.

$$m_i - m_{i-1} = -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times f_i^0) + O(\varepsilon^{1+\bar{\bar{\gamma}}}).$$

By (1.14) and the fact that $\bar{f}$ is Lipschitz, we have

$$f_i^0 = f_0^0 + O(i\varepsilon^2),$$

and because $\bar{f}$ is bounded in L^∞, we get

$$f_0^0 = O(\varepsilon).$$

From (10.5) and Lemma 13.9 ii) we have $\widehat{L}_i = \widehat{L}_{i-1} + O(\varepsilon)$, and we get by iteration $\widehat{L}_i = \widehat{L}_0 + O(i\varepsilon)$. We compute for $0 \le i \le \dfrac{1}{\varepsilon}$

$$\begin{array}{rcl} m_i - m_{i-1} & = & -(b_i - \tilde{a}_i) \cdot \big((\widehat{L}_0 + O(i\varepsilon)) \times (f_0^0 + O(i\varepsilon^2))\big) + O(\varepsilon^{1+\bar{\bar{\gamma}}}) \\ & = & -(b_i - \tilde{a}_i) \cdot (\widehat{L}_0 \times f_0^0) + O(i\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}). \end{array}$$

Step 2: A refined estimate on $b_i - \tilde{a}_i$
We already know from (8.3) that $b_i - \tilde{a}_i$ is bounded, but for later use it is crucial to get a refined algebraic expression for $b_i - \tilde{a}_i$. From (8.7), we have

$$\begin{aligned} b_i - \tilde{a}_i &= R_{\theta_{i-1},\widehat{L}_{i-1}}(b_{i-1} - \tilde{a}_{i-1}) + O(\varepsilon) \\ &= R_{\theta_0,\widehat{L}_0}(b_{i-1} - \tilde{a}_{i-1}) + (R_{\theta_{i-1},\widehat{L}_{i-1}} - R_{\theta_0,\widehat{L}_0})(b_{i-1} - \tilde{a}_{i-1}) + O(\varepsilon). \end{aligned}$$

Because $b_{i-1} - \tilde{a}_{i-1}$ is bounded (see (8.3)) , $\theta_{i-1} = \theta_0 + O((i-1)\varepsilon)$, $L_{i-1} = L_0 + O((i-1)\varepsilon)$, using Lemma 13.8 and Lemma 13.9 ii), we deduce for $i \geq 1$

$$b_i - \tilde{a}_i = R_{\theta_0,\widehat{L}_0}(b_{i-1} - \tilde{a}_{i-1}) + O(i\varepsilon).$$

We compute for $i \geq 1$

$$\begin{aligned} b_i - \tilde{a}_i &= R_{\theta_0,\widehat{L}_0}(b_{i-1} - \tilde{a}_{i-1}) + O(i\varepsilon) \\ &= R_{\theta_0,\widehat{L}_0}\big(R_{\theta_0,\widehat{L}_0}(b_{i-2} - \tilde{a}_{i-2}) + O((i-1)\varepsilon)\big) + O(i\varepsilon) \\ &= R_{2\theta_0,\widehat{L}_0}(b_{i-2} - \tilde{a}_{i-2})) + O((i-1)\varepsilon) + O(i\varepsilon) \\ &= R_{i\theta_0,\widehat{L}_0}(b_0 - \tilde{a}_0) + O\left(\frac{i(i+1)}{2}\varepsilon\right) \end{aligned}$$

and then we have for $i \geq 0$

$$b_i - \tilde{a}_i = R_{i\theta_0,\widehat{L}_0}(b_0 - \tilde{a}_0) + O(i^2\varepsilon). \tag{10.6}$$

Step 3: An estimate on $m_i - m_{i-1}$
By Step 1 and (10.6), using $f_0^0 = O(\varepsilon)$, $b_0 - \tilde{a}_0 = O(1)$ and $\bar{\gamma} \leq 1$, for $i \geq 0$ we compute

$$\begin{aligned} m_i - m_{i-1} &= -\big(R_{i\theta_0,\widehat{L}_0}(b_0 - \tilde{a}_0) + O(i^2\varepsilon)\big) \cdot \big(\widehat{L}_0 \times f_0^0\big) + O(i\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}) \\ &= -R_{i\theta_0,\widehat{L}_0}(b_0 - \tilde{a}_0) \cdot (\widehat{L}_0 \times f_0^0) + O(i\varepsilon^2 + i^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}) \\ &= -(b_0 - \tilde{a}_0) \cdot R_{-i\theta_0,\widehat{L}_0}(\widehat{L}_0 \times f_0^0) + O(i^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}) \\ &= -(b_0 - \tilde{a}_0) \cdot (\widehat{L}_0 \times R_{-i\theta_0,\widehat{L}_0}(f_0^0)) + O(i^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}), \end{aligned}$$

then we have for $i \geq 0$

$$m_i - m_{i-1} = -\big((b_0 - \tilde{a}_0) \times \widehat{L}_0\big) \cdot (R_{-i\theta_0,\widehat{L}_0}(f_0^0))^{\perp_{\widehat{L}_0}} + O(i^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}),$$

More generally, we have for $i \geq 0$ and $j \in \mathbb{Z}$

$$m_{j+i} - m_{j+i-1} = -\big((b_j - \tilde{a}_j) \times \widehat{L}_j\big) \cdot (R_{-i\theta_j,\widehat{L}_j}(f_j^0))^{\perp_{\widehat{L}_j}} + O(i^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}). \tag{10.7}$$

Step 4: An estimate on $\bar{m}_i$
We define for some N to choose later

$$\bar{m}_j = \frac{1}{N}\sum_{k=1}^{N} m_{j+k},$$

which is an average of the scalar line torsion on a window of length N. We rewrite (10.7) as

$$m_{j+k} - m_{j+k-1} = -\big((b_j - \tilde{a}_j) \times \widehat{L}_j\big) \cdot (R_{-k\theta_j,\widehat{L}_j}(f_j^0))^{\perp_{\widehat{L}_j}} + O(k^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}),$$

and we compute

$$\begin{aligned}
& \bar{m}_j - \bar{m}_{j-1} \\
= \; & \frac{1}{N}\sum_{k=1}^{N}\big(m_{j+k} - m_{j+k-1}\big) \\
= \; & -\big((b_j - \tilde{a}_j)\times \widehat{L}_j\big)\cdot\left(\frac{1}{N}\sum_{k=1}^{N} R_{-k\theta_j,\widehat{L}_j}(f_j^0)\right)^{\perp_{\widehat{L}_j}} + \frac{1}{N}\sum_{k=1}^{N} O(k^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}) \\
= \; & A + B,
\end{aligned}$$

with

$$\begin{cases} A = -\big((b_j - \tilde{a}_j)\times \widehat{L}_j\big)\cdot (Q\, f_j^0)^{\perp_{\widehat{L}_j}} \quad \textit{with} \quad Q = \dfrac{1}{N}\displaystyle\sum_{k=1}^{N} R_{-k\theta_j,\widehat{L}_j}, \\ B = \dfrac{1}{N}\displaystyle\sum_{k=1}^{N} O(k^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}). \end{cases}$$

Step 4-1: An estimate on the matrix Q

We consider a direct orthonormal basis (g_1, g_2, g_3) with $g_3 = \widehat{L}_j$, and we write $x = \sum_{k=1}^{3} x_k\, g_k$ and $Q\,x = \sum_{k=1}^{3} y_k\, g_k$. Then we get with $i \in \mathbb{C}$ such that $i^2 = -1$:

$$\begin{cases} y_3 = x_3 \\ y_1 + iy_2 = q\,(x_1 + ix_2) \quad \text{with} \quad q = \dfrac{1}{N}\displaystyle\sum_{k=1}^{N} e^{-ik\theta_j}. \end{cases}$$

We compute

$$q = \frac{1}{N}\sum_{k=1}^{N} e^{-ik\theta_j} = \frac{1}{N}\left(\frac{1 - e^{-iN\theta_j}}{1 - e^{-i\theta_j}}\right) e^{-ik\theta_j}.$$

Because $\overline{\mathcal{U}_0} = \mathcal{U}_0 \subset (0, 2\,\pi)\times(\mathbb{R}^3\backslash\{0\})$, we have $\inf_{k\in\mathbb{Z}} |\theta_j - 2k\pi| \geq \delta > 0$ and there exists a constant $C > 0$ such that

$$|q| \leq \frac{C}{N},$$

and then

$$|(Q\,x)^{\perp_{\widehat{L}_j}}| \leq \frac{C}{N}|x|.$$

Step 4-2: An estimate on B

We compute

$$\begin{aligned}
B \; & = \; \frac{1}{N}\sum_{k=1}^{N} O(k^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}) \\
& = \; \frac{1}{N} O\left(\frac{N(N+1)(2N+1)}{6}\varepsilon^2 + N\varepsilon^{1+\bar{\bar{\gamma}}}\right) \\
& = \; O\left(\frac{(N+1)(2N+1)}{6}\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}\right) \\
& = \; O\big(N^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}\big).
\end{aligned}$$

Step 4-3: An estimate on $\bar{m}_j$
From Step 4-1 and 4-2, we deduce

$$\bar{m}_j - \bar{m}_{j-1} = O\left(\frac{\varepsilon}{N} + N^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}\right).$$

With the choice

$$1 << N = \frac{1}{\varepsilon^{\frac{1}{3}}} << \frac{1}{\varepsilon},$$

we get

$$\bar{m}_j - \bar{m}_{j-1} = O\big(\varepsilon^{\frac{4}{3}} + \varepsilon^{1+\bar{\bar{\gamma}}}\big).$$

This implies

$$\bar{m}_j - \bar{m}_{j-1} = O(\varepsilon^{1+\gamma}),$$

with

$$\gamma = \min\left(\frac{1}{3}, \bar{\bar{\gamma}}\right) = \begin{cases} \frac{1}{3} & \text{if} \quad p \geq 3 \\ \bar{\bar{\gamma}} & \text{if} \quad p \in (2,3). \end{cases}$$

By iteration, we get for $0 \leq j \leq \frac{1}{\varepsilon}$

$$\bar{m}_j = \bar{m}_0 + O(\varepsilon^{\gamma}). \tag{10.8}$$

Step 5: An estimate on m_i
Using (9.3) in Theorem 9.1, we get that

$$m_i = W'_\theta(\theta_i, L_i) + O(\varepsilon^{\bar{\bar{\gamma}}}). \tag{10.9}$$

We compute

$$\begin{aligned} |\bar{m}_i - m_i| &= \left|\frac{1}{N}\sum_{k=1}^{N}(m_{i+k} - m_i)\right| \\ &= \left|\frac{1}{N}\sum_{k=1}^{N}(W'_\theta(\theta_{i+k}, L_{i+k}) - W'_\theta(\theta_i, L_i) + O(\varepsilon^{\bar{\bar{\gamma}}}))\right| \\ &\leq O(\varepsilon^{\bar{\bar{\gamma}}}) + \frac{1}{N}\sum_{k=1}^{N}|W'_\theta(\theta_{i+k}, L_{i+k}) - W'_\theta(\theta_i, L_i)| \\ &\leq O(\varepsilon^{\bar{\bar{\gamma}}}) + \frac{C}{N}\sum_{k=1}^{N}O(k\varepsilon) \qquad \text{with} \quad C = |W''|_\infty \\ &\leq O(\varepsilon^{\bar{\bar{\gamma}}}) + C\frac{N+1}{2}\varepsilon \\ &= O(\varepsilon^{\bar{\bar{\gamma}}}) + O(\varepsilon^{\frac{2}{3}}), \end{aligned}$$

where in the second line we have used (10.9) and in the fourth line we have used Proposition 2.1 which implies that W is C^2 using its definition (2.13) (i.e. W'' is C^0) in the closed set $\mathcal{U}_0$, i.e. W'' is bounded. Using (10.8) and the $\frac{1}{\varepsilon}$-periodicity, we get

$$m_i = \bar{m}_0 + O(\varepsilon^{\gamma}) \qquad \text{for all } i \in \mathbb{Z}.$$

□

11 Estimate between discrete and continuous forces

The goal of this section is to prove the following Theorem 11.1, giving an error estimate between the discrete and the continuous forces.

Theorem 11.1 (Error estimate between discrete and continuous forces)
There exists a constant $C > 0$ such that the following holds. Let us consider a nanotube X under the assumptions of Theorem 2.15 with $p > 2$ and $(\theta_i, L_i) \in \mathcal{U}_0$ as in Theorem 9.1. There exists $\varepsilon_1 > 0$, such that if

$$|\theta^0 - \theta^*| \leq \varepsilon_1 \quad \text{and} \quad |L^0 - L^*| \leq \varepsilon_1,$$

then there exists (α, Φ) solution of (1.1) and (1.5) and constants $\Sigma_0 \in \mathbb{R}^3$, $\sigma_0 \in \mathbb{R}$ such that we have for any $x \in [(i - \frac{1}{2})\varepsilon, (i + \frac{1}{2})\varepsilon]$

$$(11.1) \qquad |\Sigma_0 + W'_L(\alpha'(x), \Phi'(x)) - W'_L(\theta_i, L_i)| \leq C\varepsilon^{\bar{\gamma}}$$

and

$$(11.2) \qquad |\sigma_0 + W'_\theta(\alpha'(x), \Phi'(x)) - W'_\theta(\theta_i, L_i)| \leq C\varepsilon^{\gamma}.$$

where $\bar{\gamma} = \dfrac{p-1}{p+1}$ and $\gamma = \min\left(\dfrac{1}{3}, \dfrac{p-2}{p}\right)$.

In order to prove Theorem 11.1 we need the following Proposition 11.2 giving the existence of a solution of the Euler-Lagrange system (1.5).

Proposition 11.2 (Existence of a solution of the Euler-Lagrange system)
Assume (H4) and let $\bar{f} : \mathbb{R} \to \mathbb{R}^3$ satisfying (1.2) and (1.4). Then there exists $\varepsilon_1 > 0$ such that if $|(\theta^0, L^0) - (\theta^*, L^*)| \leq \varepsilon_1$ and $|\bar{f}|_{L^\infty(\mathbb{R})} \leq \varepsilon_1$ then there exists $(\alpha, \Phi) : \mathbb{R} \to \mathbb{R} \times \mathbb{R}^3$ with $(\alpha, \Phi) \in W^{2,\infty}(\mathbb{R}, \mathbb{R} \times \mathbb{R}^3)$, such that $(\alpha', \Phi') : \mathbb{R} \to \mathcal{U}_0$, solution of the Euler-Lagrange system (1.5), namely

$$\begin{cases} (W'_{\Phi'}(\alpha', \Phi'))' = \bar{f} & \text{on } \mathbb{R} \\ (W'_{\alpha'}(\alpha', \Phi'))' = 0 & \text{on } \mathbb{R}, \end{cases}$$

satisfying the periodic conditions (1.1).
Moreover there exists a constant $C > 0$ such that

$$(11.3) \qquad |(\alpha', \Phi') - (\theta^0, L^0)|_{L^\infty(\mathbb{R})} \leq C|\bar{f}|_{L^\infty(\mathbb{R})}.$$

Proof of Proposition 11.2
We look for $\Lambda = (\alpha, \phi) \in W^{1,\infty}(\mathbb{R}, \mathbb{R}^4)$ solution of (1.1) and (1.5) and we will show later that $\Lambda = (\alpha, \phi) \in W^{2,\infty}(\mathbb{R}, \mathbb{R}^4)$.
Step 1: Preliminaries
Without loss of generality, we can assume that

$$(11.4) \qquad \Lambda(0) = 0.$$

Then let us define

$$\lambda^0 = (\theta^0, L^0),$$

and

$$\mathcal{V}_1 = \{\Lambda \in W^{1,\infty}(\mathbb{R},\mathbb{R}^4);\ \Lambda(x+1) = \Lambda(x) + \lambda^0 \quad \text{with (11.4)}\,\}$$
$$\mathcal{V}_2 = \{g = h' \text{ with } h \in L^\infty(\mathbb{R},\mathbb{R}^4);\ h(x+1) = h(x)\}\,.$$

We embed the space $\mathcal{V}_2$ with the norm

$$|g|_{\mathcal{V}_2} = \inf_{c\in\mathbb{R}} |h-c|_{L^\infty(\mathbb{R})} \quad \text{with} \quad g = h' \quad \text{and} \quad h(x+1) = h(x),$$

and notice that $(\mathcal{V}_2, |\cdot|_{\mathcal{V}_2})$ is a Banach space. Let us define

$$\mathcal{U}_1 = \{\Lambda \in \mathcal{V}_1;\ \exists\delta > 0,\ B_\delta(0) + \Lambda'(x) \subset \mathcal{U}_0,\ \text{for almost every } x \in \mathbb{R}\},$$

where we easily check that $\mathcal{U}_1$ is an open set in $\mathcal{V}_1$. We call $\lambda = (\theta, L) \in \mathcal{U}_0$ and let us consider the map

$$\begin{array}{rcccc} \Psi & : & \mathcal{U}_1 & \longrightarrow & \mathcal{V}_2 \\ & & \Lambda & \mapsto & (W'_\lambda(\Lambda'))'. \end{array}$$

Step 2: Ψ is C^1

We compute

$$\begin{array}{rcl} |\Psi(\Lambda_2) - \Psi(\Lambda_1)|_{\mathcal{V}_2} & \le & |W'_\lambda(\Lambda'_2) - W'_\lambda(\Lambda'_1)|_{L^\infty(\mathbb{R})} \\ & \le & |D^2W|_{L^\infty(\mathcal{U}_0)} |\Lambda'_2 - \Lambda'_1|_{L^\infty(\mathbb{R})} \\ & \le & |D^2W|_{L^\infty(\mathcal{U}_0)} |\Lambda_2 - \Lambda_1|_{W^{1,\infty}(\mathbb{R})}. \end{array}$$

We compute

$$D_\Lambda\Psi(\Lambda)\cdot\bar\Lambda = (D^2W(\Lambda')\cdot\bar\Lambda')'.$$

Therefore

$$\begin{array}{rl} & |D_\Lambda\Psi(\Lambda_2)\cdot\bar\Lambda_2 - D_\Lambda\Psi(\Lambda_1)\cdot\bar\Lambda_1|_{\mathcal{V}_2} \\ \le & |D^2W(\Lambda'_2)\cdot\bar\Lambda'_2 - D^2W(\Lambda'_1)\cdot\bar\Lambda'_1|_{L^\infty(\mathbb{R})} \\ \le & |D^2W(\Lambda'_2) - D^2W(\Lambda'_1)|_{L^\infty(\mathcal{U}_0)}|\bar\Lambda'_2|_{L^\infty(\mathbb{R})} + |D^2W|_{L^\infty(\mathcal{U}_0)}|\bar\Lambda'_2 - \bar\Lambda'_1|_{L^\infty(\mathbb{R})} \\ & \longrightarrow 0 \quad \text{as} \quad |(\Lambda_2,\bar\Lambda_2) - (\Lambda_1,\bar\Lambda_1)|_{\mathcal{V}_1\times\mathcal{V}_1} \longrightarrow 0, \end{array}$$

where we have used the fact that W is C^2 by Proposition 2.7. This shows the continuity of $D\Psi$. Therefore Ψ is C^1.

Step 3: Inverse function theorem

Let $\Lambda_0(x) = x\lambda^0$ for $x \in \mathbb{R}$. We have

$$D_\Lambda\Psi(\Lambda_0)\cdot\bar\Lambda = (D^2W(\lambda^0)\cdot\bar\Lambda')'.$$

Let $g \in \mathcal{V}_2$, then there exists $h \in L^\infty(\mathbb{R},\mathbb{R}^4)$ with $h(x+1) = h(x)$ such that $g = h'$ and $|g|_{\mathcal{V}_2} = \inf_{c\in\mathbb{R}} |h-c|_{L^\infty} = |h|_{L^\infty}$.

This shows that

$$D_\Lambda\Psi(\Lambda_0)\cdot\bar\Lambda = g, \tag{11.5}$$

means

$$D^2W(\lambda^0)\cdot\bar\Lambda' = h + k \quad \text{for some constant} \quad k \in \mathbb{R}.$$

Integrating on $(0,1)$, this implies $k = -\int_0^1 h(x)\,dx$.
Recall that by assumption (H4)

$$A = D^2W(\lambda^*) \quad \text{is invertible with} \quad \lambda^* = (\theta^*, L^*).$$

Therefore there exists $\varepsilon_0 > 0$, such that for $|\lambda^0 - \lambda^*| < \varepsilon_0$, $A^0 = D^2W(\lambda^0)$ is still invertible and

$$\bar\Lambda' = (A^0)^{-1}(h + k).$$

This shows that

$$\bar\Lambda(x) = \int_0^x (A^0)^{-1}(h(y) + k)\,dy$$

satisfies $\bar\Lambda \in \mathcal{V}_1$ and is the unique solution of (11.5) satisfying (11.4). Moreover there exists a constant $C > 0$ such that

$$\begin{aligned} |\bar\Lambda|_{W^{1,\infty}(\mathbb{R})} &\leq C|(A^0)^{-1}|_{L^\infty}|h+k|_{L^\infty(\mathbb{R})} \\ &\leq 2C|(A^0)^{-1}|_{L^\infty}|h|_{L^\infty(\mathbb{R})} \\ &\leq 2C|(A^0)^{-1}|_{L^\infty}|g|_{\mathcal{V}_2}. \end{aligned}$$

This shows that $(D_\Lambda\Psi(\Lambda_0))^{-1}$ exists and is continous from $\mathcal{V}_2$ to $W^{1,\infty}(\mathbb{R})$. We have

$$\Psi(\Lambda_0) = 0. \tag{11.6}$$

Therefore we can apply the inverse function theorem in Banach spaces. This shows that (up to reduce $\varepsilon_1 > 0$) for every $\bar f$ such that $|\bar f|_{L^\infty} < \varepsilon_1$ with $\bar f(x+1) = \bar f(x)$ and $\int_{\mathbb{R}/\mathbb{Z}} \bar f = 0$, there exists $\Lambda \in \mathcal{U}_1$ such that

$$\Psi(\Lambda) = (0, \bar f). \tag{11.7}$$

Step 4: Conclusion
Therefore

$$(W'_\lambda(\Lambda'))' = (0, \bar f),$$

and then for some constant $\bar k \in \mathbb{R}^4$

$$W'_\lambda(\Lambda') = (0, \int_0^x \bar f(y)\,dy) + \bar k.$$

Again $D^2W(\lambda^0)$ is inversible and the inverse function theorem applies to W'_λ and gives (again up to reduce $\varepsilon_1 > 0$)

$$\Lambda' = (W'_\lambda)^{-1}\left((0, \int_0^x \bar f(y)\,dy) + \bar k\right),$$

which shows that $\Lambda'' \in L^\infty(\mathbb{R})$ and $\Lambda \in W^{2,\infty}(\mathbb{R})$.
Step 5: Proof of (11.3)
Because of (11.6) and (11.7) and the fact that Ψ is invertible, we deduce

$$\Lambda = \Psi^{-1}((0,\bar f)) \quad \text{and} \quad \Lambda_0 = \Psi^{-1}((0,0)).$$

Using moreover the fact that Ψ^{-1} is C^1, we deduce that there exists a constant C such that

$$|\Lambda - \Lambda_0|_{W^{1,\infty}(\mathbb{R})} \leq C|(0,\bar f) - (0,0)|_{\mathcal{V}_2} \leq C|\bar f|_{L^\infty(\mathbb{R})},$$

which implies (11.3).

□

Proof of Theorem 11.1

By Proposition 11.2, given $\bar{f}$ satisfying (1.2) and (1.4), and given any (θ^0, L^0) satisfying $|(\theta^0, L^0) - (\theta^*, L^*)| \leq \varepsilon_1$, there exists a solution (α, Φ) of the Euler-Lagrange system (1.5) namely

$$\begin{cases} (W'_{\Phi'}(\alpha', \Phi'))' = \bar{f} & \text{on } \mathbb{R} \\ (W'_{\alpha'}(\alpha', \Phi'))' = 0 & \text{on } \mathbb{R}, \end{cases}$$

satisfying the periodic conditions (1.1).

Step 1: Proof of (11.1)

We have $(W'_{\Phi'}(\alpha', \Phi'))' = \bar{f}$, then there exists a constant $\tilde{\Sigma}_0 \in \mathbb{R}^3$ such that

$$W'_{\Phi'}(\alpha'(x), \Phi'(x)) = \tilde{\Sigma}_0 + \int_0^x \bar{f}(y)\, dy. \tag{11.8}$$

On the other hand, we have $T_i = T_0 + \sum_{j=1}^{i} f_j^0$ which shows using (1.14)

$$T_i = T_0 + \sum_{j=1}^{i} \int_{\varepsilon(j-\frac{1}{2})}^{\varepsilon(j+\frac{1}{2})} \bar{f}(y)\, dy = T_0 + \int_{\frac{\varepsilon}{2}}^{\varepsilon(i+\frac{1}{2})} \bar{f}(y)\, dy.$$

From (9.2), we get

$$|T_0 + \int_{\frac{\varepsilon}{2}}^{\varepsilon(i+\frac{1}{2})} \bar{f}(y)\, dy - W'_L(\theta_i, L_i)| \leq C_1 \varepsilon^{\frac{p-1}{p+1}}.$$

Using (11.8), we get for $x \in [(i-\frac{1}{2})\varepsilon, (i+\frac{1}{2})\varepsilon]$ (using the fact that $\bar{f}$ is bounded in L^∞)

$$|T_0 - \tilde{\Sigma}_0 + W'_{\Phi'}(\alpha'(x), \Phi'(x)) - W'_L(\theta_i, L_i)| \leq C_2 \varepsilon^{\frac{p-1}{p+1}}. \tag{11.9}$$

This implies (11.1) with $\Sigma_0 = T_0 - \tilde{\Sigma}_0$.

Step 2: Proof of (11.2)

We have $(W'_{\alpha'}(\alpha', \Phi'))' = 0$, then there exists a constant $\tilde{\sigma}_0 \in \mathbb{R}$ such that

$$W'_{\alpha'}(\alpha', \Phi') = \tilde{\sigma}_0. \tag{11.10}$$

From (9.3), there exists a constant $C_3 > 0$ such that we have for $m_i = M_i(\tilde{a}_i) \cdot \hat{L}_i$

$$|m_i - W'_\theta(\theta_i, L_i)| \leq C_3 \varepsilon^{\bar{\bar{\gamma}}}.$$

Using (10.1), we get

$$|\bar{m}_0 - W'_\theta(\theta_i, L_i)| \leq C_4 \varepsilon^{\gamma}.$$

Using (11.10), we get for $x \in [(i-\frac{1}{2})\varepsilon, (i+\frac{1}{2})\varepsilon]$

$$|\bar{m}_0 - \tilde{\sigma}_0 + W'_{\alpha'}(\alpha'(x), \Phi'(x)) - W'_\theta(\theta_i, L_i)| \leq C_4 \varepsilon^{\gamma}. \tag{11.11}$$

which implies (11.2) with $\sigma_0 = \bar{m}_0 - \tilde{\sigma}_0$.

□

12 Proof of error estimates: Theorem 2.15 and Corollary 2.16

The goal of this section is to prove Theorem 2.15 and Corollary 2.16.

Proof of Theorem 2.15
Step 1: Definition of $(\tilde{\alpha},\tilde{\Phi})$ **and** (α,Φ)
Step 1-1: Definition of $(\tilde{\alpha},\tilde{\Phi})$
Let us define an approximation $(\tilde{\alpha},\tilde{\Phi})$ (that we think to be close to (α,Φ) to define later) by setting

$$\tag{12.1} \left\{\begin{array}{l} \tilde{\alpha}'(x) = (1-t)\theta_i + t\theta_{i+1} \\ \tilde{\Phi}'(x) = (1-t)L_i + tL_{i+1} \end{array}\right. \Bigg| \quad \text{with } t = \frac{x-i\varepsilon}{\varepsilon} \quad \text{for} \quad i\varepsilon \le x \le (i+1)\varepsilon.$$

where (θ_i, L_i) are given in Theorem 11.1. Notice that because of (1.7), we can choose (θ_i, L_i) and $\tilde{a}_i$ given in Theorem 8.2 such that we have

$$\left\{\begin{array}{rcl} (\theta_{i+N_\varepsilon}, L_{i+N_\varepsilon}) & = & (\theta_i, L_i) \\ \tilde{a}_{i+N_\varepsilon} & = & \tilde{a}_i + N_\varepsilon L^0. \end{array}\right.$$

From (8.6) we have $\tilde{a}_{i+1} - \tilde{a}_i - L_i = O(\varepsilon)$. With L^0 defined in (1.7), we get

$$N_\varepsilon L^0 = \sum_{i=0}^{N_\varepsilon - 1} \tilde{a}_{i+1} - \tilde{a}_i = O(N_\varepsilon \varepsilon) + \sum_{i=0}^{N_\varepsilon - 1} L_i,$$

which implies

$$L^0 = O(\varepsilon) + \varepsilon \sum_{i=0}^{N_\varepsilon - 1} L_i.$$

We compute

$$\begin{aligned} \int_0^1 \tilde{\Phi}'(x)\,dx &= \sum_{i=0}^{N_\varepsilon-1} \int_{i\varepsilon}^{i\varepsilon+\varepsilon} \tilde{\Phi}'(x)\,dx = \sum_{i=0}^{N_\varepsilon-1} \int_0^1 \big((1-t)L_i + tL_{i+1}\big)\varepsilon\,dt \\ &= \varepsilon \sum_{i=0}^{N_\varepsilon-1} \Big[(t-\frac{t^2}{2})L_i + \frac{t^2}{2}L_{i+1}\Big]_0^1 = \varepsilon \sum_{i=0}^{N_\varepsilon-1} \frac{1}{2}(L_i + L_{i+1}). \end{aligned}$$

Using the N_ε-periodicity of L_i and the fact that $N_\varepsilon = \dfrac{1}{\varepsilon}$, we get

$$\tag{12.2} \int_0^1 \tilde{\Phi}'(x)\,dx = O(\varepsilon) + \varepsilon \sum_{i=0}^{N_\varepsilon-1} L_i = L^0 + O(\varepsilon).$$

Similarly we have

$$\tag{12.3} \int_0^1 \tilde{\alpha}'(x)\,dx = O(\varepsilon) + \varepsilon \sum_{i=0}^{N_\varepsilon-1} \theta_i := \theta^0.$$

Step 1-2: Properties of (θ^0, L^0)
By (9.1) and (2.18) we deduce that there exists a constant $C > 0$ such that we have respectively

$$D_i(X, \theta_i, L_i) \le C\varepsilon_0,$$

and

$$D_{i+1}(X, \theta^*, L^*) \le C\varepsilon_0.$$

Therefore we can apply Proposition 5.4 and deduce for $\varepsilon \le \varepsilon_0$ with ε_0 small enough that

$$\left\{ \begin{array}{l} |\theta_i - \theta^*| \le C\varepsilon_0 \\ |L_i - L^*| \le C\varepsilon_0. \end{array} \right. \tag{12.4}$$

Using (12.2) and (12.3), this implies (2.19), i.e.

$$\left\{ \begin{array}{l} |\theta^0 - \theta^*| \le C\varepsilon_0 \\ |L^0 - L^*| \le C\varepsilon_0. \end{array} \right. \tag{12.5}$$

Step 1-3: Definition of (α, Φ)
For ε_0 small enough, we deduce from (12.5) that $|\theta^0 - \theta^*| \le \varepsilon_1$ and $|L^0 - L^*| \le \varepsilon_1$ and then we can apply Theorem 11.1 which shows the existence of a solution (α, Φ) of (1.1), (1.5). We get in particular

$$\left\{ \begin{array}{l} \displaystyle\int_0^1 \tilde{\Phi}'(x)\,dx = \int_0^1 \Phi'(x)\,dx + O(\varepsilon) \\ \displaystyle\int_0^1 \tilde{\alpha}'(x)\,dx = \int_0^1 \alpha'(x)\,dx. \end{array} \right. \tag{12.6}$$

Step 2: Estimate on the differences of W'
By (12.1) we have

$$\left\{ \begin{array}{l} \tilde{\alpha}' = \theta_i + t(\theta_{i+1} - \theta_i) \\ \tilde{\Phi}' = L_i + t(L_{i+1} - L_i). \end{array} \right.$$

By (9.1) and (5.8), we have $\theta_{i+1} - \theta_i = O(\varepsilon)$ and $L_{i+1} - L_i = O(\varepsilon)$, and then

$$\left\{ \begin{array}{l} |\tilde{\alpha}' - \theta_i| = O(\varepsilon) \\ |\tilde{\Phi}' - L_i| = O(\varepsilon). \end{array} \right.$$

Using the regularity of W, we deduce from (11.1) and (11.2) that there exists a constant C_1 such that we have

$$\left\{ \begin{array}{l} |\Sigma_0 + W'_L(\alpha'(x), \Phi'(x)) - W'_L(\tilde{\alpha}'(x), \tilde{\Phi}'(x))| \le C_1\varepsilon^{\bar{\gamma}} \\ |\sigma_0 + W'_\theta(\alpha'(x), \Phi'(x)) - W'_\theta(\tilde{\alpha}'(x), \tilde{\Phi}'(x))| \le C_1\varepsilon^{\gamma}. \end{array} \right. \tag{12.7}$$

For simplicity, we denote

$$\left\{ \begin{array}{l} u^0 = (\theta^0, L^0) \\ c_0 = (\sigma_0, \Sigma_0) \\ \tilde{u}(x) = (\tilde{\alpha}'(x), \tilde{\Phi}'(x)) \\ u(x) = (\alpha'(x), \Phi'(x)). \end{array} \right.$$

Because $\bar{\gamma} > \gamma$, we see that there exists a constant C_2 such that for $\lambda = (\theta, L)$

$$|c_0 + W'_\lambda(u(x)) - W'_\lambda(\tilde{u}(x))| \le C_2\varepsilon^{\gamma}. \tag{12.8}$$

Step 3: Estimate on $u - \tilde{u}$
We consider the Taylor expansion

$$W'_\lambda(\tilde{u}(x)) = W'_\lambda(u(x)) + D^2W(u(x)) \cdot (\tilde{u}(x) - u(x)) + O\big(|\tilde{u}(x) - u(x)|\omega(|\tilde{u} - u|_{L^\infty})\big),$$

where ω is the modulus of continuity of D^2W on $\mathcal{U}_0$.
Taking into account the invertibility of $D^2W(u(x))$, which follows from assumption (H4) (for u close to u^0 and u^0 close to (θ^*, L^*)), we deduce

$$|\tilde{u}(x) - u(x) - \big(D^2W(u(x))\big)^{-1}(c_0)| \le O\big(\varepsilon^\gamma + |\tilde{u}(x) - u(x)|\omega(|\tilde{u} - u|_{L^\infty})\big), \tag{12.9}$$

and then we deduce that there exists a constant C_3 such that we have
(12.10)

$$|\tilde{u}(x) - u(x) - \big(D^2W(u^0)\big)^{-1}(c_0)| \le C_3\Big(\varepsilon^\gamma + |\tilde{u} - u|_{L^\infty}\omega(|\tilde{u} - u|_{L^\infty}) + |c_0|\,\omega(|u - u^0|_{L^\infty})\Big).$$

Using (12.6), we deduce

$$\int_0^1 \tilde{u}(x)\,dx = \int_0^1 (\tilde{\alpha}'(x), \tilde{\Phi}'(x))\,dx = \int_0^1 (\alpha'(x), \Phi'(x))\,dx + O(\varepsilon) = \int_0^1 u(x)\,dx + O(\varepsilon).$$

Then integrating (12.10) on the interval $(0,1)$, we get

$$|\big(D^2W(u^0)\big)^{-1}(c_0)| \le C_3(\varepsilon^\gamma + |\tilde{u} - u|_{L^\infty}\omega(|\tilde{u} - u|_{L^\infty}) + |c_0|\,\omega(|u - u^0|_{L^\infty}) + O(\varepsilon).$$

Up to reduce ε_0, we can choose $|u - u^0|_{L^\infty}$ small enough using (11.3), and then there exists a constant C_4 such that

$$|c_0| \le C_4(\varepsilon^\gamma + |\tilde{u} - u|_{L^\infty}\omega(|\tilde{u} - u|_{L^\infty})).$$

Hence (12.9) implies that there exists a constant C_5 such that we have

$$|\tilde{u} - u|_{L^\infty} \le C_5\varepsilon^\gamma,$$

where we have used the fact that $|\tilde{u} - u|_{L^\infty}$ is small because $u(x)$ and $\tilde{u}(x)$ are both close to u^0, respectively by (11.3) and (12.4), for ε_0 small enough.
Step 4: Conclusion
Then we have

$$\begin{cases} |\tilde{\alpha}' - \alpha'|_{L^\infty} \le C_5\varepsilon^\gamma \\ |\tilde{\Phi}' - \Phi'|_{L^\infty} \le C_5\varepsilon^\gamma. \end{cases}$$

For the choice $x = j\varepsilon$, we get that there exists a constant C_6 such that

$$\begin{cases} |\theta_j - \alpha'(j\varepsilon)| \le C_6\varepsilon^\gamma \\ |L_j - \Phi'(j\varepsilon)| \le C_6\varepsilon^\gamma. \end{cases} \tag{12.11}$$

Using (8.3) and (8.4), we deduce that there exists a constant C_7 such that we have

$$|X_j - \tilde{a}_j| \le C_7. \tag{12.12}$$

Using (8.7) and (8.8), we deduce that there exists a constant C_8 such that

$$|X_{j+1} - \tilde{a}_{j+1} - R_{\theta_j, \widehat{L}_j}(X_j - \tilde{a}_j)| \le C_8\varepsilon.$$

Using (12.11), (12.12), Lemma 13.8 and Lemma 13.9 ii), we deduce that there exists a constant C_9 such that we have

$$|X_{j+1} - \tilde{a}_{j+1} - R_{\alpha'(j\varepsilon),\widehat{\Phi'(j\varepsilon)}}(X_j - \tilde{a}_j)| \leq C_9\varepsilon^\gamma. \tag{12.13}$$

Using (8.6) and (12.11), we deduce that there exists a constant C_{10} such that we have

$$|\tilde{a}_{j+1} - \tilde{a}_j - \Phi'(j\varepsilon)| \leq C_{10}\varepsilon^\gamma. \tag{12.14}$$

Finally (12.13), (12.14),(12.12) and the choice $C = \max(C_7, C_9, C_{10})$ prove (2.21).

Step 5: Proof of (2.20)

By Theorem 9.1 we have (9.1), i.e. there exists a constant C_{11} such that

$$D_j(X, \theta_j, L_j) \leq C_{11}\varepsilon.$$

Therefore there exists $\widehat{X}^{*,j} \in \widehat{\mathcal{C}}^{\theta_j,L_j}$ such that

$$\sup_{|\beta|\leq q} |X_{j+\beta} - \widehat{X}^{*,j}_{j+\beta}| \leq C_{11}\varepsilon. \tag{12.15}$$

We can write $\widehat{X}^{*,j} = a_j + X^{*,j}$ with $a_j \in L_j^\perp$ and $X^{*,j} \in \mathcal{C}^{\theta_j,L_j}$. Moreover there exists $(\delta,\eta) \in \mathbb{R}\times\mathbb{R}$ such that $X^{*,j}_j = R_{\delta,\widehat{L}_j}(\mathcal{X}^*_0(\theta_j, L_j)) + \eta\widehat{L}_j$. Then we can write

$$\widehat{X}^{*,j}_j = Y^{*,j}_j + c_j \quad \text{with} \quad Y^{*,j}_j := R_{\delta,\widehat{L}_j}(\mathcal{X}^*_0(\theta_j, L_j)) \quad \text{and} \quad c_j = \eta\widehat{L}_j + a_j.$$

We define

$$\widehat{\bar{X}}^{*,j}_j = \bar{Y}^{*,j}_j + c_j \quad \text{with} \quad \bar{Y}^{*,j}_j := R_{\delta,\widehat{\bar{L}}_j}(\mathcal{X}^*_0(\bar{\theta}_j, \bar{L}_j)) \quad \text{and} \quad \begin{cases} \bar{\theta}_j := \alpha'(j\varepsilon) \\ \bar{L}_j := \Phi'(j\varepsilon), \end{cases}$$

with

$$\widehat{\bar{X}}^{*,j} \in \widehat{\mathcal{C}}^{\bar{\theta}_j,\bar{L}_j}. \tag{12.16}$$

For $|\beta| \leq q$, we compute

$$\begin{aligned}
& \widehat{\bar{X}}^{*,j}_{j+\beta} - \widehat{X}^{*,j}_{j+\beta} \\
= \; & \bar{Y}^{*,j}_{j+\beta} - Y^{*,j}_{j+\beta} \\
= \; & R_{\beta\bar{\theta}_j,\widehat{\bar{L}}_j}\left(R_{\delta,\widehat{\bar{L}}_j}(\mathcal{X}^*_0(\bar{\theta}_j, \bar{L}_j))\right) + \beta\bar{L}_j - R_{\beta\theta_j,\widehat{L}_j}\left(R_{\delta,\widehat{L}_j}(\mathcal{X}^*_0(\theta_j, L_j))\right) + \beta L_j \\
= \; & R_{\beta\bar{\theta}_j+\delta,\widehat{\bar{L}}_j}\left(\mathcal{X}^*_0(\bar{\theta}_j, \bar{L}_j) - \mathcal{X}^*_0(\theta_j, L_j)\right) + \left(R_{\beta\bar{\theta}_j+\delta,\widehat{\bar{L}}_j} - R_{\beta\theta_j+\delta,\widehat{L}_j}\right)(\mathcal{X}^*_0(\theta_j, L_j)) + \beta(\bar{L}_j - L_j).
\end{aligned}$$

We deduce

$$|\widehat{\bar{X}}^{*,j}_{j+\beta} - \widehat{X}^{*,j}_{j+\beta}| \leq |\mathcal{X}^*_0(\bar{\theta}_j, \bar{L}_j) - \mathcal{X}^*_0(\theta_j, L_j)| + |R_{\beta\bar{\theta}_j+\delta,\widehat{\bar{L}}_j} - R_{\beta\theta_j+\delta,\widehat{L}_j}||\mathcal{X}^*_0(\theta_j, L_j)| + |\beta||\bar{L}_j - L_j|.$$

Using the Lipschitz regularity of the map $\mathcal{X}^*_0$, Lemma 13.8 and (12.11), we deduce that there exists a constant $C_{12} > 0$ such that

$$|\widehat{\bar{X}}^{*,j}_{j+\beta} - \widehat{X}^{*,j}_{j+\beta}| \leq C_{12}(|\bar{\theta}_j - \theta_j| + |\bar{L}_j - L_j|) \leq C_{12}\varepsilon^\gamma.$$

From (12.15), we deduce that there exists a constant $C > 0$ such that

$$\sup_{|\beta|\leq q} |X_{j+\beta} - \widehat{\widehat{X}}^{*,j}_{j+\beta}| \leq C\varepsilon^\gamma,$$

which proves (2.20). This ends the proof of Theorem 2.15.

□

Proof of Corollary 2.16
Step 1: Proof of (12.17)
We recall the second line in (2.21)

$$|\tilde{a}_{j+1} - \tilde{a}_j - \Phi'(j\varepsilon)| \leq C\varepsilon^\gamma.$$

Then we get

$$|\varepsilon\tilde{a}_{j+1} - \varepsilon\tilde{a}_j - \varepsilon\Phi'(j\varepsilon)| \leq C\varepsilon^{1+\gamma}.$$

On the other hand we deduce by Proposition 11.2 that $\Phi \in W^{2,\infty}$, and then

$$|\Phi((j+1)\varepsilon) - \Phi(j\varepsilon) - \varepsilon\Phi'(j\varepsilon)| \leq C\varepsilon^2.$$

Using the two last inequalities, we get

$$|e_{j+1} - e_j| \leq C\varepsilon^{1+\gamma} \quad \text{with} \quad e_j := \varepsilon\tilde{a}_j - \Phi(j\varepsilon),$$

and then by iteration for $0 \leq j \leq \frac{1}{\varepsilon} - 1$, we get

$$|e_j - e_0| \leq C\varepsilon^\gamma,$$

i.e.

$$|\varepsilon\tilde{a}_j - \Phi(j\varepsilon) - a| \leq C\varepsilon^\gamma, \tag{12.17}$$

with $a = e_0$.
Step 2: Conclusion
Using the first line of (2.21) and (12.17), we obtain (2.22).

□

13 Appendix

This appendix is composed of four independent subsections. In Subsection 13.1, we present miscellaneous results about the action of rotations. In Subsection 13.2, we give some estimates on rotations. In the Subsection 13.3, we give a few estimates on some series. Finally in Subsection 13.4, we propose an axiomatic approach to the introduction of perfect nanotubes, which is not necessary for the proof of the results in this paper, but which should shed some light on the notion of perfect nanotubes.

13.1 Action of rotations

Lemma 13.1 (Rotation and cross product)
Let us consider a rotation $R \in SO(3)$. Then for every $x, y \in \mathbb{R}^3$, we have

$$R(x) \times R(y) = R(x \times y).$$

Proof of Lemma 13.1
Let $z \in \mathbb{R}^3$, then we have

$$Rz \cdot (Rx \times Ry) = \det(Rz, Rx, Ry) = \det(R)\det(z, x, y) = z \cdot (x \times y) = Rz \cdot R(x \times y).$$

This is true for all $Rz \in \mathbb{R}^3$, and then $R(x) \times R(y) = R(x \times y)$.

□

Lemma 13.2 (Elimination of the rotation)
Let us set $R = R_{\theta,\widehat{L}}$. Then for every $x, y \in \mathbb{R}^3$ we have

$$L \cdot (R(x) \times R(y)) = L \cdot (x \times y).$$

Proof of Lemma 13.2
This is a straightforward consequence of Lemma 13.1.

□

Lemma 13.3 (Rewriting the mixed product)
Let $L \neq 0$ and $x, y \in \mathbb{R}^3$. Then we have

$$\widehat{L} \cdot (x \times y) = (R_{\frac{\pi}{2},\widehat{L}}(x))^{\perp_{\widehat{L}}} \cdot y,$$

where $(R_{\frac{\pi}{2},\widehat{L}}(x))^{\perp_{\widehat{L}}}$ is the component of $(R_{\frac{\pi}{2},\widehat{L}}(x))$ orthogonal to $\widehat{L}$.

Proof of Lemma 13.3
We compute

$$\widehat{L} \cdot (x \times y) = (\widehat{L} \times x) \cdot y = (R_{\frac{\pi}{2},\widehat{L}}(x))^{\perp_{\widehat{L}}} \cdot y.$$

□

Lemma 13.4 (Composition of a rotation with the gradient of the potential)
For every $x \in \mathbb{R}^3$ and any rotation R, and with our definition (1.9) of V we have

$$\nabla V(R(x)) = R(\nabla V(x)).$$

Proof of Lemma 13.4
We have $V(x) = V_0(|x|)$, then $\nabla V(x) = V_0'(|x|).\dfrac{x}{|x|}$, and we have:

$$\nabla V(R(x)) = V_0'(|R(x)|).\frac{R(x)}{|R(x)|} = R\left(V_0'(|x|) \cdot \frac{x}{|x|}\right) = R(\nabla V(x)).$$

□

Lemma 13.5 (Composition of a rotation with the hessian of the potential)
For every $x \in \mathbb{R}^3$ and any rotation R, and with our definition (1.9) of V we have

$$RD^2V(R^{-1}x) = D^2V(x)R.$$

Proof of Lemma 13.5
By Lemma 13.4 and for every $y \in \mathbb{R}^3$, we have $\nabla V(Ry) = R(\nabla V(y))$, which can be written in coordinates (with the Einstein convention of summation on repeated indices)

$$R_{ij}(\nabla_j V(y)) = \nabla_i V(Ry)),$$

and by derivation we have

$$R_{ij}D^2_{jk}V(y) = D^2_{ij'}V(Ry)R_{j'k},$$

i.e.

$$RD^2V(y) = D^2V(Ry)R.$$

Finally setting $x = Ry$, we deduce

$$RD^2V(R^{-1}x) = D^2V(x)R.$$

□

Lemma 13.6 (Rotation of a special perfect nanotube)
Let $\theta \in \mathbb{R}$, $L \in \mathbb{R}^3\backslash\{0\}$. Then for any rotation $R \in SO(3)$ we have
i) $X \in \mathcal{C}^{\theta,RL}$ if and only if $X = RY$ with $Y \in \mathcal{C}^{\theta,L}$.
ii) we have

$$R^{-1}R_{\theta,R\widehat{L}}R = R_{\theta,\widehat{L}}. \tag{13.1}$$

Proof of Lemma 13.6
Proof of ii)
Let us consider a direct orthonormal basis (e_1, e_2, e_3) of $\mathbb{R}^3$ with $e_3 = \widehat{L}$.
Then we know that $(Re_1, Re_2, Re_3 = R\widehat{L})$ is also a direct orthonormal basis.
To show (13.1), it suffices to show that

$$\big(R^{-1}R_{\theta,R\widehat{L}}R\big)(e_i) = R_{\theta,\widehat{L}}(e_i) \quad \text{for} \quad i \in \{1,2,3\}. \tag{13.2}$$

For $e_3 = \widehat{L}$, we have

$$\big(R^{-1}R_{\theta,R\widehat{L}}R\big)(\widehat{L}) = R^{-1}\big(R_{\theta,R\widehat{L}}(R\widehat{L})\big) = R^{-1}(R\widehat{L}) = \widehat{L} = R_{\theta,\widehat{L}}(\widehat{L}).$$

We do the computation for e_1

$$\begin{aligned}\big(R^{-1}R_{\theta,R\widehat{L}}R\big)(e_1) &= R^{-1}\big(R_{\theta,R\widehat{L}}(Re_1)\big)\\ &= R^{-1}\big((\cos\theta)Re_1 + (\sin\theta)Re_2\big)\\ &= (\cos\theta)R^{-1}(Re_1) + (\sin\theta)R^{-1}(Re_2)\\ &= (\cos\theta)e_1 + (\sin\theta)e_2\\ &= R_{\theta,\widehat{L}}(e_1),\end{aligned}$$

where in the second line we have used the fact that $(Re_1, Re_2, Re_3 = R\widehat{L})$ is a direct orthonormal basis, joint to the definition of $R_{\theta,R\widehat{L}}$.
For e_2, a similar computation shows (13.2) for $i = 2$.
Proof of i)
Let us consider $X = RY$.

$$\begin{array}{lll} X \in \mathcal{C}^{\theta,RL} & \text{iff} & X_{j+1} = RL + R_{\theta,\widehat{RL}}(X_j) \\ & \text{iff} & RY_{j+1} = RL + R_{\theta,\widehat{RL}}(RY_j) \\ & \text{iff} & Y_{j+1} = L + R^{-1}R_{\theta,\widehat{RL}}RY_j \\ & \text{iff} & Y_{j+1} = L + R_{\theta,\widehat{L}}(Y_j) \\ & \text{iff} & Y \in \mathcal{C}^{\theta,L}, \end{array}$$

where we have used (13.1) in the fourth line.

□

We have the following result whose proof is straightforward.

Lemma 13.7 (Derivative of rotations)
For $u \in \mathbb{R}^3$, we have

$$R_{\theta,\widehat{L}}(u) = (u.\widehat{L})\widehat{L} + (\cos\theta)(u - (u.\widehat{L})\widehat{L}) + (\sin\theta)(\widehat{L} \times u). \tag{13.3}$$

We also have

$$\bar{L}.\nabla_L(R_{\theta,\widehat{L}}(u)) = \big((u.\bar{\bar{L}})\widehat{L} + (u.\widehat{L})\bar{\bar{L}}\big)(1 - \cos\theta) + (\sin\theta)(\bar{\bar{L}} \times u), \tag{13.4}$$

with

$$\bar{\bar{L}} := \bar{L}.\nabla_L(\widehat{L}) = \frac{\bar{L}}{|L|} - \frac{L}{|L|^3}(L.\bar{L}). \tag{13.5}$$

13.2 Estimates on rotations

Lemma 13.8 (Control of rotations by angles and axes)
Let us consider two angles $\theta_2, \theta_1 \in \mathbb{R}$ and two axes $\widehat{L}_2, \widehat{L}_1 \in \mathbb{R}^3$, then we have

$$|R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_1}| \le 5|\widehat{L}_2 - \widehat{L}_1| + |\theta_2 - \theta_1|.$$

Proof of Lemma 13.8
Step 1: Control by axes
For $x \in \mathbb{R}^3$, we recall that

$$R_{\theta_2,\widehat{L}_i}(x) = (x \cdot \widehat{L}_i)\widehat{L}_i + (x - (x \cdot \widehat{L}_i)\widehat{L}_i)\cos\theta_2 + (\widehat{L}_i \times x)\sin\theta_2 \quad \text{for} \quad i = 1, 2.$$

Then we have for $x \in \mathbb{R}^3$

$$(R_{\theta_2,\widehat{L}_2} - R_{\theta_2,\widehat{L}_1})(x) = ((x \cdot \widehat{L}_2)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_1)(1 - \cos\theta_2) + ((\widehat{L}_2 - \widehat{L}_1) \times x)\sin\theta_2. \tag{13.6}$$

But we have

$$\begin{array}{rcl} (x \cdot \widehat{L}_2)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_1 & = & (x \cdot \widehat{L}_2)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_2 + (x \cdot \widehat{L}_1)\widehat{L}_2 - (x \cdot \widehat{L}_1)\widehat{L}_1 \\ & = & (x \cdot (\widehat{L}_2 - \widehat{L}_1))\widehat{L}_2 + (x \cdot \widehat{L}_1)(\widehat{L}_2 - \widehat{L}_1), \end{array}$$

and then

$$|(x\cdot\widehat{L}_2)\widehat{L}_2-(x\cdot\widehat{L}_1)\widehat{L}_1|\le 2|x||\widehat{L}_2-\widehat{L}_1|.$$

Using (13.6), we deduce

$$\begin{aligned}|(R_{\theta_2,\widehat{L}_2}-R_{\theta_2,\widehat{L}_1})(x)| &\le 2|x||\widehat{L}_2-\widehat{L}_1||1-\cos\theta_2|+|x||\widehat{L}_2-\widehat{L}_1||\sin\theta_2|\\ &\le 5|x||\widehat{L}_2-\widehat{L}_1|,\end{aligned}$$

and finally we deduce

$$|R_{\theta_2,\widehat{L}_2}-R_{\theta_2,\widehat{L}_1}|\le 5|\widehat{L}_2-\widehat{L}_1|.$$

Step 2: Control by angles
We have

$$\begin{aligned}&(R_{\theta_2,\widehat{L}_2}-R_{\theta_1,\widehat{L}_2})(x)\\ =\;&(\cos\theta_2-\cos\theta_1)(x-(x\cdot\widehat{L}_2)\widehat{L}_2)+(\sin\theta_2-\sin\theta_1)(\widehat{L}_2\times x)\\ =\;&-2\sin\left(\frac{\theta_2+\theta_1}{2}\right)\sin\left(\frac{\theta_2-\theta_1}{2}\right)(x-(x\cdot\widehat{L}_2)\widehat{L}_2)+2\cos\left(\frac{\theta_2+\theta_1}{2}\right)\sin\left(\frac{\theta_2-\theta_1}{2}\right)(\widehat{L}_2\times x)\\ =\;&2\sin\left(\frac{\theta_2-\theta_1}{2}\right)\left(-\sin\left(\frac{\theta_2+\theta_1}{2}\right)(x-(x\cdot\widehat{L}_2)\widehat{L}_2)+\cos\left(\frac{\theta_2+\theta_1}{2}\right)(\widehat{L}_2\times x)\right).\end{aligned}$$

But we have

$$\begin{cases}|x-(x\cdot\widehat{L}_2)\widehat{L}_2|\le|x|\\ |\widehat{L}_2\times x|\le|x|.\end{cases}$$

Using the fact that $x-(x\cdot\widehat{L}_2)\widehat{L}_2$ and $\widehat{L}_2\times x$ are orthogonal with the same length, we get

$$\begin{aligned}|(R_{\theta_2,\widehat{L}_2}-R_{\theta_1,\widehat{L}_2})(x)| &\le 2|\sin(\frac{\theta_2-\theta_1}{2})||x|\\ &\le |\theta_2-\theta_1||x|.\end{aligned}$$

And finally we have

$$|R_{\theta_2,\widehat{L}_2}-R_{\theta_1,\widehat{L}_2}|\le|\theta_2-\theta_1|.$$

Step 3: General control
We deduce

$$\begin{aligned}|R_{\theta_2,\widehat{L}_2}-R_{\theta_1,\widehat{L}_1}| &\le |R_{\theta_2,\widehat{L}_2}-R_{\theta_1,\widehat{L}_2}|+|R_{\theta_1,\widehat{L}_2}-R_{\theta_1,\widehat{L}_1}|\\ &\le |\theta_2-\theta_1|+5|\widehat{L}_2-\widehat{L}_1|,\end{aligned}$$

where in the last line we have used Step 1 and Step 2.

□

Lemma 13.9 (A control of the axes)
Let us consider two axes L and L' such that

$$(13.7)\qquad |L|\ge\delta>0\qquad \textit{for some}\quad \delta>0.$$

If

$$|L-L'|\le\varepsilon,$$

then there exists a constant $C=C(\delta)$ such that we have
i) $\big||L|-|L'|\big|\le\varepsilon$,
ii) $|\widehat{L}-\widehat{L'}|\le C\varepsilon$.

Proof of Lemma 13.9
Proof of i)
We notice that the map $L \mapsto |L|$ is 1−Lipschitz.
Proof of ii)

$$\begin{array}{rcl} |L - L'| & = & \big||L|\widehat{L} - |L'|\widehat{L}'\big| \\ & = & \big||L|\widehat{L} - |L|\widehat{L}' + |L|\widehat{L}' - |L'|\widehat{L}'\big| \\ & = & \big||L|(\widehat{L} - \widehat{L}') + (|L| - |L'|)\widehat{L}'\big| \\ & \geq & |L||\widehat{L} - \widehat{L}'| - \big||L| - |L'|\big|. \end{array}$$

Then we deduce

$$|L||\widehat{L} - \widehat{L}'| \leq \big||L| - |L'|\big| + |L - L'| \leq 2\varepsilon.$$

Using (13.7), we deduce

$$|\widehat{L} - \widehat{L}'| \leq C\varepsilon \qquad \text{with} \quad C = \frac{2}{\delta}.$$

□

Lemma 13.10 (Error estimate on rotations)
Let $v_i \in \mathbb{R}^3$, $i = 1, 2$ two vectors satisfying:

$$|v_1|,\, |v_2| \leq \frac{1}{c_0}, \quad |v_1 \times v_2| \geq c_0 > 0, \tag{13.8}$$

for some constant $c_0 > 0$. Then there exists $c = c(c_0) > 0$, such that the following holds. Let R, $R^* \in SO(3)$, then

$$|(R - R^*)(v_i)| \leq \varepsilon \quad \textit{for} \quad i = 1, 2 \quad \textit{implies} \quad |R - R^*| \leq c\,\varepsilon.$$

If $R^* = R_{\theta^*, \widehat{L}^*}$ with $\pi \geq \theta^* \geq \delta > 0$, then there exists $c_\delta = c_\delta(c_0)$ such that we can write $R = R_{\tilde{\theta}, \widehat{\tilde{L}}}$ with $(\tilde{\theta}, \tilde{L}) \in \mathbb{R} \times (\mathbb{R}^3 \backslash \{0\})$, and

$$\left\{ \begin{array}{l} |\widehat{\tilde{L}} - \widehat{L}^*| \leq c_\delta \varepsilon \\ |\tilde{\theta} - \theta^*| \leq c_\delta \varepsilon. \end{array} \right. \tag{13.9}$$

Proof of Lemma 13.10
Step 1: Proof of $|R - R^*| \leq c_1\,\varepsilon$
If $R = R^*$, we have nothing to prove. So we assume now that $R \neq R^*$.
Then (up to change $\widehat{l}$ in $-\widehat{l}$) there exists an angle $\alpha \in (0, \pi]$ such that

$$R_{\alpha, \widehat{l}} = R^{-1} R^*.$$

Let us consider an orthonormal basis (e_1, e_2, e_3) of $\mathbb{R}^3$ with $e_3 = \widehat{l}$, and a vector $x = x_1 e_1 + x_2 e_2 + x_3 e_3 \in \mathbb{R}^3$.
We have

$$\begin{array}{rcl} |(R - R^*)(x)| & = & |(I - R_{\alpha, \widehat{l}})(x)| \\ & = & \left| \left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} - \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \right| \\ & = & \left| \begin{pmatrix} (1 - \cos\alpha)x_1 + (\sin\alpha)x_2 \\ (-\sin\alpha)x_1 + (1 - \cos\alpha)x_2 \\ 0 \end{pmatrix} \right| \\ & = & 2\left(\sin\dfrac{\alpha}{2}\right)\sqrt{x_1^2 + x_2^2}. \end{array} \tag{13.10}$$

Then we have

$$|(R - R^*)(x)| \leq 2\left(\sin\frac{\alpha}{2}\right)|x|. \tag{13.11}$$

Because of (13.8), we know that v_1 and v_2 generate a plane which contains at least a vector perpendicular to $\widehat{l}$, that we can call e_2 without loss of generality.
Therefore, we can write

$$e_2 = a_1 v_1 + a_2 v_2.$$

We have for $i = 1, 2$, $e_2 \times v_i = a_j v_j \times v_i$ for $j \in \{1, 2\}\backslash\{i\}$.
Therefore

$$|a_j| \leq \frac{|v_i|}{|v_1 \times v_2|} \leq \frac{1}{(c_0)^2}.$$

From (13.10), we deduce

$$2\sin\frac{\alpha}{2} = |(R - R^*)(e_2)| \leq (|a_1| + |a_2|)\varepsilon \leq \frac{2}{(c_0)^2}\,\varepsilon,$$

i.e.

$$2\sin\frac{\alpha}{2} \leq c_1\,\varepsilon. \tag{13.12}$$

with $c_1 = \dfrac{2}{(c_0)^2}$.
Then by (13.11), we deduce

$$|(R - R^*)(x)| \leq c_1\,\varepsilon|x|,$$

and finally we have

$$|R - R^*| \leq c_1\,\varepsilon. \tag{13.13}$$

Step 2: Control of the axis of rotation
Let $\beta \in [0, \pi]$ be the angle between $\widehat{L}$ and $\widehat{L}^*$. From (13.13), we have

$$|(R_{\theta,\widehat{L}} - R_{\theta^*,\widehat{L}^*})(\widehat{L})| \leq c_1\varepsilon|\widehat{L}|,$$

i.e.

$$|\widehat{L} - R_{\theta^*,\widehat{L}^*}(\widehat{L})| \leq c_1\varepsilon.$$

We define u as the orthogonal projection of $\widehat{L}$ on $\mathbb{R}L^*$ by $u = (\widehat{L}\cdot\widehat{L}^*)\widehat{L}^*$ and set $u' = \widehat{L} - u$.
Then we have

$$|u'| = \sin\beta \leq 1.$$

Case 1: $\beta \in \left[0, \dfrac{\pi}{2}\right]$
We compute

$$c_1\varepsilon \geq |\widehat{L} - R_{\theta^*,\widehat{L}^*}(\widehat{L})| = |u' - R_{\theta^*,\widehat{L}^*}(u')| = 2\left|\sin\frac{\theta^*}{2}\right||u'|.$$

Using the fact that $\theta^* \in [0, \pi]$ and $|\theta^*| \geq \delta > 0$, we get

$$\left|\sin\frac{\theta^*}{2}\right| \geq \frac{\theta^*}{\pi} \geq \frac{\delta}{\pi}.$$

We deduce that

$$\sin\beta = |u'| \leq \frac{\pi c_1}{2\delta}\varepsilon.$$

Because $\beta \in \left[0, \frac{\pi}{2}\right]$, we have

$$|\widehat{L} - \widehat{L}^*| = 2\sin\frac{\beta}{2} \leq \beta \leq \frac{\pi}{2}\sin\beta \leq c_3\varepsilon,$$

with $c_3 = \left(\frac{\pi}{2}\right)^2 \frac{c_1}{\delta}$.

Case 2: $\beta \in \left[\frac{\pi}{2}, \pi\right]$

Let $\bar{\theta} = 2\pi - \theta \in [\pi, 2\pi]$, $\bar{\beta} = \pi - \beta \in \left[0, \frac{\pi}{2}\right]$ and $\bar{L} = -L$.

Notice that $\bar{\beta}$ is the angle between $\widehat{L}^*$ and $\widehat{\bar{L}}$ and $R_{\theta,\widehat{L}} = R_{\bar{\theta},\widehat{\bar{L}}}$.

Applying case 1, we get

$$|\widehat{L}^* - \widehat{\bar{L}}| = 2\sin\frac{\bar{\beta}}{2} \leq \bar{\beta} \leq c_3\varepsilon.$$

Finally we set

$$(\tilde{\theta}, \tilde{L}) = \begin{cases} (\theta, L) & \text{if} \quad \beta \in \left[0, \frac{\pi}{2}\right] \\ (\bar{\theta}, \bar{L}) & \text{if} \quad \beta \in \left(\frac{\pi}{2}, \pi\right], \end{cases}$$

and we have proved that there exists a constant $c_3 > 0$ such that

$$|\widehat{\tilde{L}} - \widehat{L}^*| \leq c_3\varepsilon. \tag{13.14}$$

Step 3: Control on the angle of rotation

Then we can compute

$$\begin{aligned} \left|2\sin\left(\frac{\tilde{\theta} - \theta^*}{2}\right)\right| &= |R_{\tilde{\theta},\widehat{L}^*} - R_{\theta^*,\widehat{L}^*}| \\ &\leq |R_{\tilde{\theta},\widehat{L}^*} - R_{\tilde{\theta},\widehat{\tilde{L}}}| + |R_{\tilde{\theta},\widehat{\tilde{L}}} - R_{\theta^*,\widehat{L}^*}| \\ &\leq 5|\widehat{L}^* - \widehat{\tilde{L}}| + |R_{\theta,\widehat{L}} - R_{\theta^*,\widehat{L}^*}| \\ &\leq 5c_3\varepsilon + c_1\varepsilon \\ &\leq c_4\varepsilon, \end{aligned}$$

where in the third line we have used Lemma 13.8 , in the fourth line we have used (13.13) and (13.14) and in the last line we set $c_4 = 5c_3 + c_1$.

Let $\gamma \in \left[0, \frac{\pi}{2}\right]$ such that $\sin\gamma = \left|\sin\left(\frac{\tilde{\theta} - \theta^*}{2}\right)\right|$.

We have

$$0 \leq \gamma \leq \frac{\pi}{2}\sin\gamma \leq \frac{1}{2}c_5\varepsilon,$$

with $c_5 = \frac{\pi}{2}c_4$. Then we have

$$\frac{\tilde{\theta} - \theta^*}{2} = \pm\gamma \mod(\pi).$$

This implies that there exists $k \in \mathbb{Z}$ such that

$$|\tilde{\theta} - \theta^* - 2k\pi| \leq c_5 \varepsilon.$$

Up to change $\tilde{\theta}$ in $\tilde{\theta} - 2k\pi$ we deduce (13.9).

□

13.3 Convergent series

Lemma 13.11 (Convergent series)
Let $n \in \{0, 1, 2\}$, $q > 1$ and $\rho \geq 1$. Then there exists a constant $C = C(q, n)$ such that

$$\sum_{\substack{1 \leq j \leq \rho \\ j' \geq \rho}} \frac{1 + j^n}{(j + j')^{q+n}} \leq \frac{C}{\rho^{q-2}}.$$

The proof of Lemma 13.11 is easy and is left to the reader.

Lemma 13.12 (Convergent series)
Let $n \in \{0, 1, 2\}$, $q > 2$ and $\rho \geq 1$. Then there exists a constant $C = C(q, n)$ such that

$$\sum_{\substack{j \geq \rho \\ j' \geq 0}} \frac{1 + j^n}{(j + j')^{q+n}} \leq \frac{C}{\rho^{q-2}}.$$

Proof of Lemma 13.12
Case $\rho \geq 3$:
For $j \geq \rho$ and $j' \geq 0$, for $x \in [j, j+1]$ and $y \in [j', j'+1]$ we have $3 \leq \rho \leq x + y \leq j + j' + 2$ and

$$\frac{1 + j^n}{(j + j')^{q+n}} \leq \frac{1 + x^n}{(x + y - 2)^{q+n}}.$$

Therefore

$$\begin{aligned}
\sum_{\substack{j \geq \rho \\ j' \geq 0}} \frac{1 + j^n}{(j + j')^{q+n}} &\leq \sum_{\substack{j \geq \rho \\ j' \geq 0}} \int_{(j,j')+[0,1]^2} \frac{1 + x^n}{(x + y - 2)^{q+n}} dx dy \\
&= \int_{x \geq \rho, y \geq 0} \frac{1 + x^n}{(x + y - 2)^{q+n}} dx dy \\
&= \int_{x \geq \rho} \frac{1 + x^n}{(q + n - 1)(x - 2)^{q+n-1}} dx \\
&\leq C_1 \int_{\bar{x} \geq \rho - 2} \frac{1}{(q + n - 1)\bar{x}^{q-1}} d\bar{x} \\
&\leq \frac{C_2}{(\rho - 2)^{q-2}} \\
&\leq \frac{C}{\rho^{q-2}},
\end{aligned}$$

where in the fourth line we have set $x - 2 = \bar{x}$ and expanded the polynomial $x^n = (\bar{x} + 2)^n$, and where C_1 is a constant which depends on n and C_2 is a constant which depends on n and q.
Case $\rho \geq 1$:

We split the series as $\sum_{\substack{j \geq \rho \\ j' \geq 0}} = \sum_{\substack{j \geq 3 \\ j' \geq 0}} + \sum_{\substack{j = 1,2 \\ j' \geq 0}}$, where we bounded the last series directly.

□

13.4 Axiomatic approach to perfect nanotubes

Definition 13.13 (Axioms for a perfect nanotube)
A perfect nanotube Y of axis $L_0 \in \mathbb{R}^3 \backslash \{0\}$ is a collection of atoms i.e. $Y = \{y_j \in \mathbb{R}^3,\, j \in \mathbb{Z}\}$ satisfying the following axioms

i) **(Tube shape)**
there exists a constant C such that $d(y_j, \mathbb{R}L_0) \leq C$ for all $j \in \mathbb{Z}$

ii) **(Maximum density)**
there exists a constant $c > 0$ such that $\inf_{j \neq k} |y_j - y_k| \geq c > 0$

iii) **(Minimum density)**
there exists $\rho > 0$, such that for all $b \in \mathbb{R}L_0$, we have $B(b, \rho) \cap Y \neq \emptyset$ where $B(b, \rho)$ is the closed ball of center b and radius ρ,

and such that there exists an even isometry $T : \mathbb{R}^3 \to \mathbb{R}^3$ which leaves Y invariant, i.e.

$$T(Y) = Y, \tag{13.15}$$

and which has no fixed point, i.e.

$$T(x) \neq x \quad \text{for all } x \in \mathbb{R}^3. \tag{13.16}$$

We recall that an even isometry T is a map such that $|T(x) - T(0)| = |x - 0|$, and which transforms a direct orthonormal basis $(e_i)_{1 \leq i \leq 3}$ into a direct orthonormal basis $(T(e_i) - T(0))_{1 \leq i \leq 3}$. Then it is possible to show the following result (whose proof is left to the reader, see [29] for a proof).

Proposition 13.14 (Perfect nanotubes)
Given a perfect nanotube Y of axis $L_0 \in \mathbb{R}^3 \backslash \{0\}$ (in the sense of Definition 13.13), there exists an angle $\theta \in [0, 2\pi)$, a vector $L \in \mathbb{R}L_0 \backslash \{0\}$ and a vector $a \in \mathbb{R}^3$ such that we have

$$T(Y) = a + T^{\theta,L}(Y - a),$$

where $T(Y) = \{T(y_j),\, j \in \mathbb{Z}\}$ and $Y - a = \{y_j - a,\, j \in \mathbb{Z}\}$.
Then $X := Y - a$ is perfect nanotube of axis L_0 that satisfies

$$T^{\theta,L}(X) = X.$$

Moreover, there exists $K \in \mathbb{N} \backslash \{0\}$ and a set of K distinct atoms $\{X_{0,0}, \cdots, X_{0,K-1}\} \subset X$ such that

$$X_{0,l} \neq (T^{\theta,L})^j (X_{0,m}) \quad \text{for all} \quad j \in \mathbb{Z} \backslash \{0\} \quad \text{and} \quad m \in \{0, \cdots, K-1\},$$

and

$$X_{j,l} = (T^{\theta,L})^j (X_{0,l}) \quad \text{for all} \quad j \in \mathbb{Z} \quad \text{and} \quad l \in \{0, \cdots, K-1\},$$

such that

$$X = \bigcup_{\substack{j \in \mathbb{Z} \\ 0 \leq l \leq K-1}} \{X_{j,l}\}.$$

Notice that we can replace the set X by our standard notation for a nanotube (as it is given in the introduction of this paper)

$$X = (X_j)_{j\in\mathbb{Z}} = ((X_{j,l})_{0\le l\le K-1})_{j\in\mathbb{Z}},$$

where each $X_j = (X_{j,l})_{0\le l\le K-1}$ in $(\mathbb{R}^3)^K$ is a cell of K atoms $X_{j,l}$ in $\mathbb{R}^3$.
Notice also that the choice of the cell X_0 is not unique.

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