Atomic to continuum passage for nanotubes. Part II: error estimates

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Abstract

We consider deformations in $\mathbb{R}^3$ of an infinite general nanotube of atoms where each atom interacts with all the other through a two-body potential. We compute the effect of an external force applied to the nanotube. At the equilibrium, the positions of the atoms satisfy an Euler-Lagrange equation. For large classes of potentials (including Lennard-Jones potential) and under suitable stability assumptions, we prove that every solution is well approximated by the solution of a continuum model involving stretching and twisting, but no bending. We establish an error estimate between the discrete and the continuous solution based on a Saint-Venant principle that the reader can find in the companion paper [25] (part I).

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1 Introduction

In this paper, we study nanotubes that are collections of atoms in $\mathbb{R}^3$. Those atoms are submitted to two-body interactions with all the other atoms and also to exterior forces. Our model can be seen as a simplified description of macromolecules like carbon nanotubes or DNA. We distinguish a subclass of nanotubes that are perfect and at the equilibrium with no exterior forces. Those perfect nanotubes at the equilibrium are used to built the macroscopic model for nanotubes deriving from some macroscopic energy W. Our main result is an error estimate between discrete nanotubes and the solution of the associated macroscopic continuum model (see Theorem 1.12 and Corollary 1.13). In order to present our main result we need first to introduce a few concepts and notations in Subsection 1.1. Our assumptions are presented in Subsection 1.2, and should probably be skipped by the reader in a first reading of the introduction. Our main results will be given in Subsection 1.3. We discuss the main new difficulties of our approach in Subsection 1.4, and give a brief review of the literature in Subsection 1.5. The organisation of the paper is given in Subsection 1.6.

1.1 Setting of the problem

1.1.1 The macroscopic description

Let us consider three maps

$$\left\{\begin{array}{l}\Phi : \mathbb{R} \longmapsto \mathbb{R}^3\\ \alpha : \mathbb{R} \longmapsto \mathbb{R}\\ \bar{f} : \mathbb{R} \longmapsto \mathbb{R}^3\end{array}\right.$$

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

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

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

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.

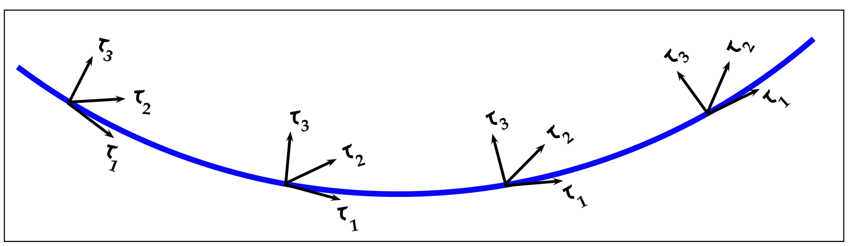

Figure 1: Arc $\Phi(x)$ with rotation of the local basis (τ_1, τ_2, τ_3) under the action of $\alpha(x)$

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

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

where W is an (isotropic) energy density that will be defined later (see (1.26)), such that $W(\alpha', \Phi')$ only depends on α' and $|\Phi'|$ (see Lemma 2.4), and the force $\bar{f}$ satisfies the following compatibility condition

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

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

$$(1.5) \qquad \left\{\begin{array}{ll}(W'_{\Phi'}(\alpha', \Phi'))' = \bar{f} & \text{on } \mathbb{R}\\ (W'_{\alpha'}(\alpha', \Phi'))' = 0 & \text{on } \mathbb{R}.\end{array}\right.$$

1.1.2 The microscopic description

For the microscopic description, we follow [25]. Given $K \geq 1$ we define

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

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 $X_{j,l}$. Our particular expression of $f_{j,l}$ i.e.

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

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

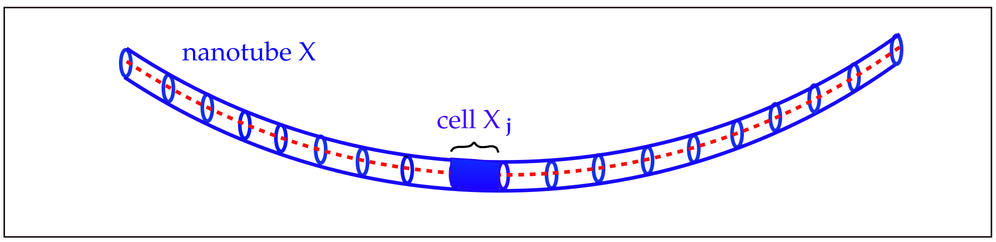

Figure 2: Portion of a nanotube

We consider any integer N_ε large enough, assume that $\varepsilon = 1/N_\varepsilon$, and we require the following microscopic "linear + periodic" conditions

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

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

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

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

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

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

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), with the compatibility condition analogue to (1.4)

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

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 relationships on the force of the j^{th} cell and the macroscopic force

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

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:

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

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 result is the quantitative justification of relation (1.15) (see Theorem 1.12 for the details):

Main result: *under certain assumptions we have a weak version of (1.15).*

1.1.4 Perfect nanotubes

As in [25], 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**

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

and the class of **perfect nanotubes** (see Figure 3)

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

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 $(\theta, L) = (\alpha'(j\varepsilon), \Phi'(j\varepsilon))$.

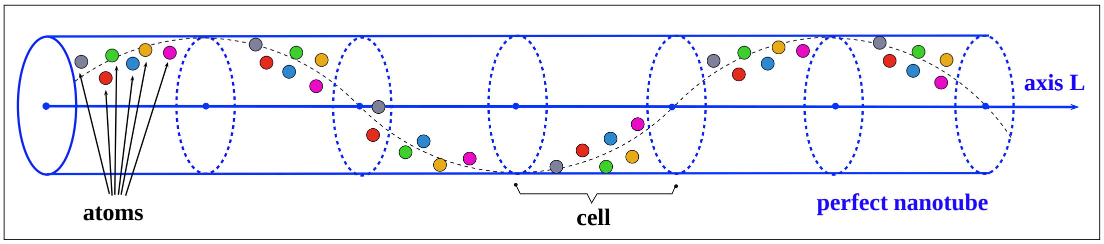

Figure 3: Microscopic perfect nanotube for $K = 6$

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

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

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 $u \in \mathbb{R}^3$.

Definition 1.1 (Barycenter b_j of a cell X_j)
For a general nanotube X, we define the barycenter b_j of the cell $X_j = (X_{j,l})_{0 \le l \le K-1}$ by

$$b_j = \frac{1}{K} \sum_{0 \le l \le K-1} X_{j,l}.$$

1.2 Assumptions

In order to state precisely our main results in Subsection 1.3.1, we need first to introduce several assumptions. We consider assumptions (H0), (H1), (H2) and (H3) listed in [25], that we recall below.

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))

$$\mathcal{W}(\theta,L,X_0) = \frac{1}{2} \sum_{\substack{k\in\mathbb{Z} \\ 0\leq l,m\leq K-1}} V(kL + R_{k\theta,\widehat{L}}(X_{0,l}) - X_{0,m}), \tag{1.16}$$

where $X_0 = (X_{0,l})_{0\leq l\leq K-1}$ is a cell for the perfect nanotube.

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

$$D_{X_0}\mathcal{W}(\theta^*,L^*,X_0^*) = 0. \tag{1.17}$$

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 $0\leq l\leq K-1$, then we have

$$E_0'(X^*) = 0. \tag{1.18}$$

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

$$\mathrm{Ker}\, D^2_{X_0X_0}\mathcal{W}(\theta^*,L^*,X_0^*) = \mathbb{R}(L^*\times X_0^*) + \mathbb{R}\begin{pmatrix}\widehat{L^*}\\ \vdots \\ \vdots \\ \widehat{L^*}\end{pmatrix}. \tag{1.19}$$

where $(L^*\times X_0^*)_l = L^*\times X_{0,l}^*$.
We have the following result which is Proposition 1.1 in the companion [25], and 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 1.2 (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 $X_0 = R_{\beta,\widehat{L}}(\mathcal{X}_0^*(\theta, L)) + \gamma\widehat{L}$ *for some* β, $\gamma \in \mathbb{R}$.

ii) Further technical properties

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

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

we have

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

$$\mathcal{U}_0 = \overline{\mathit{Int}\,\mathcal{U}_0} \tag{1.21}$$

and there exists $c_0 > 0$ *such that*

$$\text{for all} \quad (\theta, L),\ (\bar\theta, \bar L) \in \mathcal{U}_0, \qquad \left\{ \begin{array}{l} |\widehat{L} + \widehat{\bar L}| \geq c_0 > 0 \\ |L| - |L - \bar L| \geq c_0 > 0. \end{array} \right. \tag{1.22}$$

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

$$r\theta \neq 0\,(2\pi) \quad \text{for all} \quad (\theta, L) \in \mathcal{U}_0. \tag{1.23}$$

Definition 1.3 (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

$$\left\{ \begin{array}{l} E_0''(X^*) \cdot Z = 0 \\ |Z_j| \leq C(1 + |j|^2) \end{array} \right. \tag{1.24}$$

then 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

$$Z = u_1 + u_2 \times X^* + Y, \tag{1.25}$$

with

$$\left\{ \begin{array}{l} X^* = \mathcal{X}^*(\theta^*, L^*) = (\mathcal{X}_j^*(\theta^*, L^*))_{j\in\mathbb{Z}} \quad \text{with} \quad \mathcal{X}_j^*(\theta, L) = R_{j\theta,\widehat{L}}(\mathcal{X}_0^*(\theta, L)) + jL \\ Y = (\bar\theta, \bar L) \cdot \nabla_{(\theta,L)}\mathcal{X}^*(\theta, L). \end{array} \right.$$

We will need 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 1.11, 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

$$\begin{cases} r = 2 & \text{if} \quad \theta^* \neq \pi \\ r = 3 & \text{if} \quad \theta^* = \pi. \end{cases}$$

If $K = 1$, we set

$$\begin{cases} r = 3 & \text{if} \quad \theta^* \neq \dfrac{2\pi}{3} \quad \text{and} \quad \theta^* \neq \dfrac{4\pi}{3} \\ r = 4 & \text{if} \quad \theta^* = \dfrac{2\pi}{3} \quad \text{or} \quad \theta^* = \dfrac{4\pi}{3}. \end{cases}$$

Remark 1.4
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 (1.23).

Definition 1.5 (Macroscopic energy)
For any $(\theta, L) \in \mathcal{U}_0$, we define the energy W by

$$W(\theta, L) = \mathcal{W}(\theta, L, \mathcal{X}_0^*(\theta, L)). \tag{1.26}$$

Remark 1.6
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 1.7 (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 1.8
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 [23].

1.3 Main results

In order to give our main results in Subsection 1.3.2, we first need some definitions in Subsection 1.3.1.

1.3.1 Perfect nanotubes at the equilibrium

A nanotube $X \in \mathcal{C}^{\theta,L}$ is at the equilibrium if $E_0'(X) = 0$. We recall from [25] the following definitions.

Definition 1.9 (Class $C_*^{\theta,L}$)
For any $(\theta, L) \in \mathcal{U}_0$, we define the subclass of 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 1.2.

Definition 1.10 (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.

Definition 1.11 (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 the force $|f_j| = \sup_{0 \leq l \leq K-1} |f_{j,l}|$

1.3.2 Statement of the main results

Theorem 1.12 (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 $K_0 \geq 0$

$$(1.27) \qquad ||\bar{f}'||_{L^\infty(\mathbb{R})} \leq K_0\,, \quad ||\bar{f}||_{L^\infty(\mathbb{R})} \leq \varepsilon_0\,, \quad \sup_{j \in \mathbb{Z}} D_j(X, \theta^*, L^*) \leq \varepsilon_0,$$

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

$$(1.28) \qquad |\theta^0 - \theta^*| \leq C\varepsilon_0\,, \quad |L^0 - L^*| \leq C\varepsilon_0$$

and there exists a solution (α, Φ) of (1.1) and (1.5) where W is defined in (1.26), such that

$$(1.29) \qquad \sup_{j \in \mathbb{Z}} D_j(X, \alpha'(j\varepsilon), \Phi'(j\varepsilon)) \leq C\varepsilon^\gamma \quad \textit{with} \quad \gamma = \min\left(\frac{1}{3}, \frac{p-2}{p}\right).$$

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

$$\left\{ \begin{array}{l} |X_j - \tilde a_j| \le C \\ |\tilde a_{j+1} - \tilde a_j - \Phi'(j\varepsilon)| \le C\,\varepsilon^\gamma \\ |X_{j+1} - \tilde a_{j+1} - R_{\alpha'(j\varepsilon),\widehat{\Phi'(j\varepsilon)}}(X_j - \tilde a_j)| \le C\,\varepsilon^\gamma, \end{array} \right. \tag{1.30}$$

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

The result of Theorem 1.12 is illustrated on Figure 4.

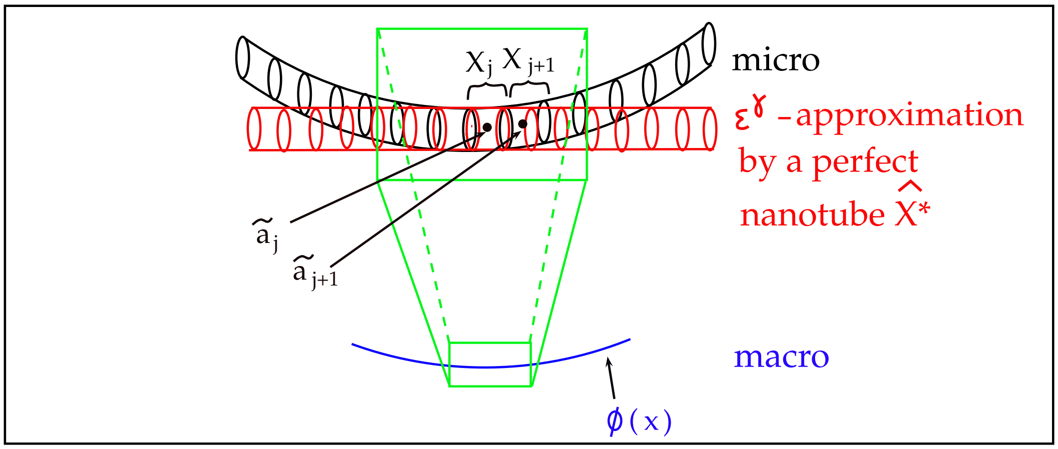

Figure 4: Discrete-continuum error estimates (1.30), (1.29)

Corollary 1.13 (Macro-micro error estimate)
Under the assumptions and with the notations of Theorem 1.12, we have that there exists $a \in \mathbb{R}^3$ such that for all $j \in \mathbb{Z}$ we have

$$|\varepsilon X_j - \Phi(j\varepsilon) - a| \le C\,\varepsilon^\gamma. \tag{1.31}$$

Result (1.31) of Corollary 1.13 is illustrated on Figure 5.

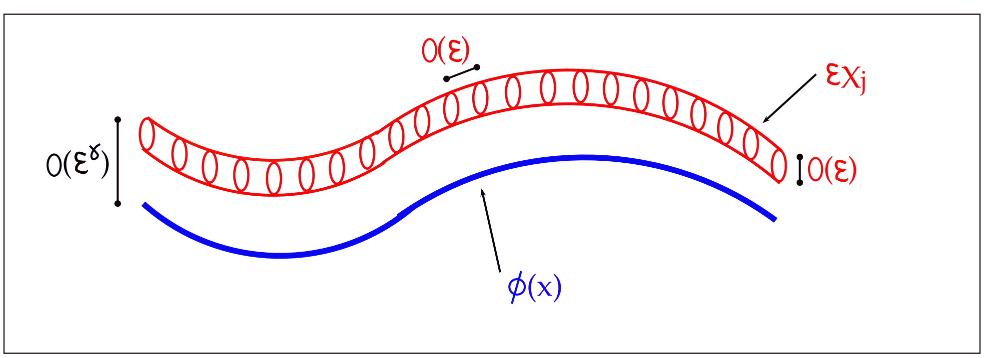

Figure 5: Macro-micro error estimate (1.31) for $a = 0$

1.4 Main difficulties encountered

Our goal was to adapt the method of [25] to the case of nanotubes in $\mathbb{R}^3$, covering 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 large 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 [7]. We list below some of the main difficulties encountered here:

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 $W(\theta, L) = \tilde{W}(\theta, |L|)$. 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 [8, 38, 9]).

2) the line torsion and the mean fiber:

In comparison to [7] 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.

3) microscopic scalar torsion at large scale:

For simplicity, we assumed (as in [7]) 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, indeed even if θ would be equal to zero). 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 5.2 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 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 $\bar{f}$.

1.5 Brief review of the literature

Mathematical approaches

For a general theory of rods, we refer to the book [4] and [51], and for wire ropes, we refer to the book [21]. Let us mention a discrete mechanical approach to rod theory introduced in [33]. For $3D$-$1D$ reduction in the framework of continuum linear and nonlinear elasticity, see [44, 1, 41, 42, 43].

Recall that the Cauchy-Born rule (see [26]), means that the microscopic deformation mimics the macroscopic one. Cases where such Cauchy-Born rule fails (by fracture or melting) have been studied in [10, 16, 52, 28, 20, 27, 15, 14] and a general representation of the macroscopic energy has been given in [2, 17] and in [47, 36, 37] for films. General schemes have been proposed to deduce (assuming the Cauchy-Born rule) macroscopic theories from microscopic ones, see [11, 55, 5]. See also [3, 12] for stochastic lattices. Even if it is different, our approach shares some common points with the Quasi-Continuum Method (see [48]) and some general aspect of multiscale modeling (see the overviews [22, 13]).

A discrete-continuum error estimate has been obtained in [23] (justifying the Cauchy-Born rule) for three-dimensional elasticity starting from microscopic minimizers with two-body interactions of finite range. In [23], 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 [23] to the case of the dynamics is presented in [24].

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 [18]), micotubules (see [32]), or carbon nanotubes in the regime where bending is neglectable.

For a nice overview of mathematical aspects of DNA, see [50] (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 [34, 30, 29], [31] and the references therein. For a discrete-continuuous comparison of models for DNA, see also [40]. Let us also mention the Elastic Network Model (ENM) method, used for instance to modelize biomolecules (see [49]).

For an overview on the mechanics of carbon nanotubes (including nanoropes with smaller bending stiffness), we refer to [45] and also [46] and the references therein. For continuum elastic models of carbon nanotubes, we refer to [35] and the references cited therein. For atomistic derivation of mechanical properties (including torsion) of carbon nanotubes, we refer to [54, 39, 6, 53] mainly with interatomic potentials modeling, and also [19] for a SCC-DFTB atomistic model, and the references therein.

1.6 Organisation of the paper

This paper is divided into eight sections. In Section 2 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 2.2 and Theorem 2.11). In Section 3, we recall crucial known results (including a discrete Saint-Venant principle (Theorem 3.2)) proved in the companion paper [25] to the present work. We also define the important discrete notion of mean fiber and prove some of its properties in Theorem 3.8. In Section 4, we mainly prove Theorem 4.1, 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 5, the notion of scalar line torsion that we prove to be almost constant (see Theorem 5.2). In Section 6, we mainly prove some estimates between continuum and discrete forces acting on a general nanotube (Theorem 6.1), that is used in Section 7 to prove the main results of this paper, namely Theorem 1.12 and Corollary 1.13. Finally Section 8 is an appendix, which contains some results about rotations and on convergent series.

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

2 Line tension and line torsion

In this section we introduce the notion of line tension (Definition 2.1) and line torsion (Definition 2.9) 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

$$X_{j,l} \neq X_{k,m} \quad \text{if} \quad (j,l) \neq (k,m). \tag{2.1}$$

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 (2.1).

We start to prove the regularity of W.
Proof of Proposition 1.7
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 1.2) we deduce that W' is C^1, and then W is C^2 on $\mathcal{U}_0$.

□

2.1 Line tension

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

Definition 2.1 (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 2.2 (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

$$T_i = W'_L(\theta, L). \tag{2.2}$$

In order to prove Theorem 2.2, we will need several lemmata.
We recall the following result (which is Lemma 6.3 in [25]):

Lemma 2.3 (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

$$R^{-1} R_{\theta,R\widehat{L}} R = R_{\theta,\widehat{L}}. \tag{2.3}$$

Lemma 2.4 (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 2.4
We first compute (using convention (1.10))

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

where in the third line we have used Lemma 2.3 ii) and the fact that $V(p)$ only depends on $|p|$. From (1.26), we deduce using Lemma 2.3 i) that

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

$\square$

Corollary 2.5 (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 2.5
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

$$R_{\alpha,n} L = |L| \big((\cos\alpha)\widehat{L} + (\sin\alpha)\xi \big). \tag{2.4}$$

By Lemma 2.4, 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 (2.4) to compute $\dfrac{d}{d\alpha}(R_{\alpha,n}L)$.
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 1.7), this is also true for all $(\theta, L) \in \mathcal{U}_0$ (using (1.21)).

□

Lemma 2.6 (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 2.6
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

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

in the second line we use Lemma 8.6 in the appendix.

□

Lemma 2.7 (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 (2.1).

Proof of Lemma 2.7
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

$$\begin{aligned} T_i - T_{i-1} &= \sum_{\alpha \geq i} \sum_{0 \leq l,m \leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) - \sum_{\alpha \leq i} \sum_{0 \leq l,m \leq K-1} \nabla V(X_{i,l} - X_{\alpha,m}) \\ &= \sum_{\alpha \geq i} \sum_{0 \leq l,m \leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) + \sum_{\alpha \leq i} \sum_{0 \leq l,m \leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) \\ &= \sum_{\alpha \in \mathbb{Z}} \sum_{0 \leq l,m \leq K-1} \nabla V(X_{\alpha,l} - X_{i,m}) + A \\ &= \sum_{0 \leq m \leq K-1} \sum_{\substack{\alpha \in \mathbb{Z} \\ 0 \leq l \leq K-1}} \nabla V(X_{\alpha,l} - X_{i,m}) + 0 \\ &= \sum_{0 \leq m \leq K-1} f_{i,m} = f_i^0, \end{aligned} \tag{2.5}$$

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 (2.5), 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 (2.5) we have used the equation of equilibrium (1.13), the definition of the forces (1.6) and the antisymmetry of ∇V.

□

We recall the following result (which is Proposition 2.3 in [25])

Lemma 2.8 (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

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

and

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

Proof of Theorem 2.2
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 2.7 we have $T_i = T_{i-1}$, and from Lemma 2.6, $T_i = R_{\theta,\widehat{L}}(T_i)$, and because $\theta \neq 0 \bmod(2\pi)$, we deduce that T_i is parallel to L.
From Corollary 2.5, we see that it suffices to show that $\widehat{L} \cdot T_i = \widehat{L} \cdot W'_L(\theta, L)$.
Therefore we compute

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

where in the second line we get out the rotation $R_{\beta\theta,\widehat{L}}$ using Lemma 8.6.
We now call $q = \alpha - \beta$ and get

$$\widehat{L} \cdot T_i = \sum_{q \geq 1} \sum_{0 \leq l,m \leq K-1} q\widehat{L} \cdot \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}). \tag{2.6}$$

From this expression we deduce

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

where in the first line we get out the rotation $R_{q\theta,\widehat{L}}$ using again Lemma 8.6, 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

$$\widehat{L} \cdot T_i = \sum_{q \leq -1} \sum_{0 \leq l,m \leq K-1} q\widehat{L} \cdot \nabla V(qL + R_{q\theta,\widehat{L}}(X_{0,l}) - X_{0,m}) \tag{2.7}$$

which is an expression similar to (2.6) but with $q \leq -1$.
Summing (2.6) and (2.7) we get

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

where for $q = 0$ and $l = m$ we use convention (1.10), for which we have $\nabla V(0) = 0$. Then, using Lemma 8.7 which shows that $\widehat{L} \cdot \nabla_L(R_{q\theta,\widehat{L}}) = 0$, we get

$$\widehat{L} \cdot T_i = \widehat{L} \cdot \mathcal{W}'_L(\theta, L, X_0). \tag{2.8}$$

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

$$W'_L(\theta, L) = \nabla_L\{\mathcal{W}(\theta, L, \mathcal{X}_0^*(\theta, L))\} = \mathcal{W}'_L(\theta, L, X_0) + \mathcal{W}'_{X_0}(\theta, L, X_0) \cdot (\mathcal{X}_0^*)'_L(\theta, L). \tag{2.9}$$

On the other hand by Lemma 2.8 we have

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

This shows with (2.8), (2.9) that

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

from which we conclude that

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

□

2.2 Line torsion

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

Definition 2.9 (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 2.10 (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 2.11 (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

$$M_i = W'_\theta(\theta, L)\widehat{L}. \tag{2.10}$$

In order to prove Theorem 2.11, we will need several Lemmata. We first start to prove a subcase of Theorem 2.11, namely:

Lemma 2.12 (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

$$\widehat{L} \cdot M_i = W'_\theta(\theta, L). \tag{2.11}$$

Proof of Lemma 2.12

We compute

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

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 8.6 to get the rotation, and in the fourth line we have used Lemma 8.2.

Therefore we get with $q=\alpha-\beta$

$$\widehat{L}\cdot M_i=\widehat{L}\cdot\sum_{q\geq 1}\sum_{0\leq l,m\leq K-1} q(R_{q\theta,\widehat{L}}(X_{0,l}))\times\nabla V(qL+R_{q\theta,\widehat{L}}(X_{0,l})-X_{0,m}). \tag{2.12}$$

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 8.6 and Lemma 8.2 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

$$\widehat{L}\cdot M_i=\widehat{L}\cdot\sum_{q\leq -1}\sum_{0\leq l,m\leq K-1} qR_{q\theta,\widehat{L}}(X_{0,l})\times\nabla V(qL+R_{q\theta,\widehat{L}}(X_{0,l})-X_{0,m}). \tag{2.13}$$

which is an expression similar to (2.12) but with $q\leq -1$.

Summing (2.12) and (2.13) we obtain

$$\widehat{L}\cdot M_i=\frac{1}{2}\sum_{q\in\mathbb{Z}}\sum_{0\leq l,m\leq K-1} q\,\widehat{L}\cdot\big(R_{q\theta,\widehat{L}}(X_{0,l})\times\nabla V(qL+R_{q\theta,\widehat{L}}(X_{0,l})-X_{0,m})\big). \tag{2.14}$$

Using Lemma 8.3 we obtain

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

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

$$\widehat{L}\cdot M_i = \mathcal{W}'_\theta(\theta,L,X_0). \tag{2.15}$$

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

$$W'_\theta(\theta,L)=\nabla_\theta\{\mathcal{W}(\theta,L,\mathcal{X}_0^*(\theta,L))\}=\mathcal{W}'_\theta(\theta,L,X_0)+\mathcal{W}'_{X_0}(\theta,L,X_0)\cdot(\mathcal{X}_0^*)'_\theta(\theta,L). \tag{2.16}$$

On the other hand by Lemma 2.8 we have

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

This shows with (2.15) and (2.16) that

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

$\square$

Lemma 2.13 (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 2.13
We have

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

where in the third line we have used Lemma 8.6 and in the fourth line we have used Lemma 8.1. Let us define

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

then we compute

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

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 8.1 and in the second equality we have used Lemma 8.6.

□

Lemma 2.14 (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 (1.1)) 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 (2.1).

Proof of Lemma 2.14
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

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

Similarly we have

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

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

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

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

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.

□

Proof of Theorem 2.11

Step 1: $M_i = R_{\theta,\widehat{L}}(M_{i-1})$

By Corollary 2.5 and by Theorem 2.2, we deduce that $L \times T_{i-1} = 0$.

Then by Lemma 2.13 we get

$$M_i = R_{\theta,\widehat{L}}(M_{i-1}). \tag{2.17}$$

Step 2: Conclusion

By Lemma 2.14 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 2.12, we get

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

□

3 Known results and the mean fiber $\tilde{a}_i$

3.1 Known results

The goal of this subsection is to recall some useful results proven in the companion paper [25].

Definition 3.1 (Semi-norm)
We 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*

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

For a given $\rho > 0$, let us set

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

where $Q_\rho := \{e \in \mathbb{Z}, \text{ such that } |e| \leq \rho\}$. Then we have the following generalization of Saint-Venant's principle for discrete nanotubes.

Theorem 3.2 (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

$$\sup_{j \in \mathbb{Z}} D_j(X,\theta^*,L^*) \leq \delta_0, \tag{3.1}$$

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

$$\mathcal{N}_J(X) \ \leq \ \mu \, \mathcal{N}_{J_\rho}(X) + C_1 \sup_{j \in J_\rho} |f_j|, \tag{3.2}$$

with

$$\rho^p = \frac{C_2}{\mathcal{N}_J(X)}. \tag{3.3}$$

Theorem 3.3 (Main rigidity estimate)
There exists a constant $C > 0$, such that for every nanotube X, and any $\varepsilon \in (0,1)$, if

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

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 $\sup_{|\alpha| \leq q} |X_\alpha - \widehat{X}^*_\alpha| \leq \varepsilon$,
then

$$|X_j - \widehat{X}^*_j| \leq C\varepsilon(1 + |j|^2) \qquad \text{for } M \leq j \leq N. \tag{3.4}$$

Proposition 3.4 (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 $\varepsilon \in (0, \varepsilon_1)$

$$D_k(X,\theta_k,L_k) \leq \varepsilon \quad \text{for } k = j,\ j+1,$$

then we have

$$\left\{ \begin{array}{l} |\theta_{j+1} - \theta_j| \leq C\varepsilon \\ |L_{j+1} - L_j| \leq C\varepsilon. \end{array} \right. \tag{3.5}$$

Proposition 3.5 (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

$$|X_{j',l'} - X_{j,l} - (j'-j)L| \le C(1+\delta|j'-j|). \tag{3.6}$$

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

$$|X_{j',l'} - X_{j,l} - (\widehat{X}^{*,j}_{j',l'} - \widehat{X}^{*,j}_{j,l})| \le C\delta(1+|j'-j|). \tag{3.7}$$

Proposition 3.6 (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

$$|Z_{j,l}(t) - Z_{j',l'}(t)| \ge C_0|j'-j| \quad \text{if} \quad |j-j'| \ge \frac{1}{C_0}. \tag{3.8}$$

Theorem 3.2, Theorem 3.3, Proposition 3.4, Proposition 3.5 and Proposition 3.6 correspond respectively to Theorem 1.9, Theorem 4.1, Proposition 4.4 ,Proposition 3.5 and Proposition 3.6 in [25].

3.2 Mean fiber $\tilde{a}_i$

The goal of this subsection is to define the mean fiber $\tilde{a}_i$ of a general nanotube and to prove geometric estimates (see Theorem 3.8).

Definition 3.7 (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

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

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

$$\tilde{a}_i = a_i + (b^{*,i}_i \cdot \widehat{L}_i)\widehat{L}_i, \tag{3.9}$$

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 6.
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.

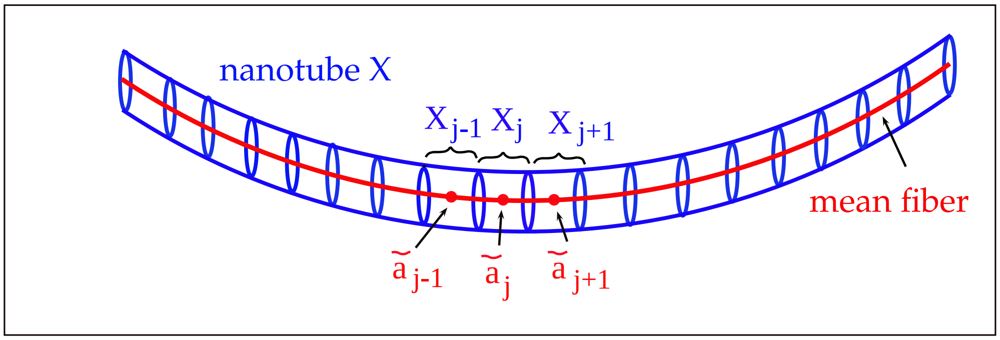

Figure 6: Mean fiber $\tilde{a}_j$ of a nanotube

Theorem 3.8 (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 $i_0 \in \mathbb{Z}$

$$D_i(X, \theta_i, L_i) \leq \varepsilon \qquad \text{for } i \in \{i_0, i_0+1\} \tag{3.10}$$

then for any mean fiber $\tilde{a}_{i_0}$, $\tilde{a}_{i_0+1}$ given by Definition 3.7, we have

$$|b_{i_0} - \tilde{a}_{i_0}| \leq C, \tag{3.11}$$

$$|X'_{i_0}| \leq C, \tag{3.12}$$

$$|(\tilde{a}_{i_0+1} - \tilde{a}_{i_0})^{\perp \widehat{L}_{i_0+1}}| \leq C\,\varepsilon, \tag{3.13}$$

$$|\tilde{a}_{i_0+1} - \tilde{a}_{i_0} - L_{i_0}| \leq C\,\varepsilon, \tag{3.14}$$

$$|b_{i_0+1} - \tilde{a}_{i_0+1} - R_{\theta_{i_0}, \widehat{L}_{i_0}}(b_{i_0} - \tilde{a}_{i_0})| \leq C\,\varepsilon, \tag{3.15}$$

$$|X'_{i_0+1} - R_{\theta_{i_0}, \widehat{L}_{i_0}}(X'_{i_0})| \leq C\varepsilon, \tag{3.16}$$

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 3.8
As a preliminary, we use the fact that $\mathcal{U}_0$ is closed (in Proposition 1.2) to recall (for later use) that

$$\overline{\mathcal{U}_0} = \mathcal{U}_0 \subset (0, 2\pi) \times (\mathbb{R}^3 \backslash \{0\}). \tag{3.17}$$

On the other hand, because of (3.10), we can apply Proposition 3.4 and deduce that there exists a constant $C_0 > 0$ such that we have

$$|\theta_{i_0+1} - \theta_{i_0}| \le C_0\varepsilon, \tag{3.18}$$

and

$$|L_{i_0+1} - L_{i_0}| \le C_0\varepsilon. \tag{3.19}$$

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 3.7. We know that there exists a constant $C_1 > 0$ such that

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

and by (3.10), we have

$$|X_{i_0} - a_{i_0} - X_{i_0}^{*,i_0}| \le \varepsilon. \tag{3.20}$$

Then

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

In particular we deduce that

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

i.e.

$$|b_{i_0} - (b_{i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0} - a_{i_0}| \le C_1 + \varepsilon. \tag{3.21}$$

We deduce from (3.20) that

$$|(b_{i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0} - (b_{i_0}^{*,i_0} \cdot \widehat{L}_{i_0})\widehat{L}_{i_0}| \le \varepsilon. \tag{3.22}$$

Using moreover (3.21), we get

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

which proves (3.11). On the other hand, (3.20) implies for the centered cells

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

and we deduce (3.12) from the fact that $(X_{i_0}^{*,i_0})'$ is bounded.
Step 2: Proof of $|\tilde{a}_{i_0+1} - \tilde{a}_{i_0} - L_{i_0}| \le C_7\varepsilon$
Step 2-1: Proof of $|(\tilde{a}_{i_0+1} - \tilde{a}_{i_0})^{\perp_{L_{i_0+1}}}| \le C_4\varepsilon$
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 (3.10) in case $i = i_0$, we get

$$\begin{cases} |X_{i_0+1} - a_{i_0} - X^{*,i_0}_{i_0+1}| \le \varepsilon \\ |X_{i_0} - a_{i_0} - X^{*,i_0}_{i_0}| \le \varepsilon, \end{cases}$$

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

$$|X_{i_0+1} - a_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(X_{i_0} - a_{i_0}) - L_{i_0}| \le 2\varepsilon, \tag{3.23}$$

which implies

$$|b_{i_0+1} - \tilde{a}_{i_0} - R_{\theta_{i_0},\widehat{L}_{i_0}}(b_{i_0} - \tilde{a}_{i_0}) - L_{i_0}| \le 2\varepsilon. \tag{3.24}$$

Similarly using (3.10) 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

$$|b_{i_0+1} - \tilde{a}_{i_0+1} - R_{\theta_{i_0+1},\widehat{L}_{i_0+1}}(b_{i_0} - \tilde{a}_{i_0+1}) - L_{i_0+1}| \le 2\varepsilon. \tag{3.25}$$

Substracting (3.24) and (3.25), we get (using (3.19))

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

Using (3.11) to bound $b_{i_0} - \tilde{a}_{i_0}$ and Lemma 8.4 to bound $R_{\theta_{i_0+1},\widehat{L}_{i_0+1}} - R_{\theta_{i_0},\widehat{L}_{i_0}}$ (with (3.18) and (3.19)), 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 (3.17), 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 (3.22), 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 (3.11)) joint to Lemma 8.5 ii), and (3.25), 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 $|L_{i_0+1}-L_{i_0}|\le C_0\varepsilon$, we deduce that there exists a constant C_6 such that

$$|((\tilde{a}_{i_0+1}-\tilde{a}_{i_0})\cdot\widehat{L}_{i_0+1})\widehat{L}_{i_0+1}-L_{i_0}|\le C_6\varepsilon \tag{3.26}$$

Step 2-3: Conclusion

By (3.13) and (3.26), 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

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

Step 3: Proof of (3.15) and (3.16)

Inequality (3.15) is a consequence of (3.24) and (3.14). Moreover (3.16) is implied by (3.23).

□

4 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 4.1 (An estimate about the line tension and the line torsion)

Let us consider a nanotube X under the assumptions of Theorem 1.12. 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 3.7 such that we have with the notation of Definitions 2.1 and 2.9, for all $i\in\mathbb{Z}$

$$D_i(X,\theta_i,L_i)\le C\varepsilon, \tag{4.1}$$

and

$$|T_i-W'_L(\theta_i,L_i)|\le C\varepsilon^{\frac{p-1}{p+1}}, \tag{4.2}$$

and

$$|M_i(\tilde{a}_i)-W'_\theta(\theta_i,L_i)\widehat{L}_i|\le C\varepsilon^{\frac{p-2}{p}}, \tag{4.3}$$

where $p>2$ appears in assumption (H0).

Remark 4.2

Notice that $\varepsilon^{\frac{p-2}{p}}=\varepsilon^{\frac{q-1}{q+1}}$ with $q=p-1$. This difference between the error estimate (4.2) and (4.3) 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 4.1.

4.1 Preliminary estimates on two-body interactions

In this subsection we present two estimates on two-body interactions: Proposition 4.3 and Proposition 4.5.

Proposition 4.3 (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

$$\sup_{j\in\mathbb{Z}} D_j(X, \theta^*, L^*) \leq \varepsilon_0,$$

we have

$$|\nabla V(X_{j,l} - X_{j',l'})| \leq \frac{C}{|j-j'|^{p+1}} \quad \text{for } |j-j'| \geq 1, \tag{4.4}$$

and

$$|X_j - X_{j'}| \leq C(1 + |j-j'|) \quad \text{for all} \quad j,\, j' \in \mathbb{Z}. \tag{4.5}$$

Remark 4.4
Notice that under assumption (H1), we automatically have $(\theta^*, L^*) \in \mathcal{U}_0$ by Proposition 1.2.

Proof of Proposition 4.3
Step 1: Preliminary
From Proposition 3.5, we deduce estimate (4.5) and that there exists a constant $C_1 > 0$ such that

$$|X_{j',l'} - X_{j,l}| \geq (|L| - C_1\varepsilon_0)|j'-j| - C_1, \tag{4.6}$$

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

$$|X_{j',l'} - X_{j,l} - (\widehat{X}^{*,j}_{j',l'} - \widehat{X}^{*,j}_{j,l})| \leq C_1\varepsilon_0(1 + |j'-j|). \tag{4.7}$$

Step 2: Proof of (4.4)
Case 1: $|j-j'| \geq C_3$
Using (4.6) there exists a constant $C_2 > 0$ and a constant C_3 (large enough) such that we have

$$|X_{j,l} - X_{j',l'}| \geq C_2|j-j'| \quad \text{for } |j-j'| \geq C_3.$$

Case 2: $1 \leq |j-j'| \leq C_3$
Notice that there exists a constant δ such that

$$|\widehat{X}^{*,j}_{j,l} - \widehat{X}^{*,j}_{j',l'}| \geq \delta > 0 \quad \text{if } j \neq j'.$$

From (4.7), we get

$$|X_{j,l} - X_{j',l'}| \geq \delta - C_1\varepsilon_0(1 + |j-j'|).$$

For $\varepsilon_0 < \dfrac{\delta}{4C_1C_3}$, we get

$$|X_{j,l} - X_{j',l'}| \geq \frac{\delta}{2} \quad \text{for } 1 \leq |j-j'| \leq C_3.$$

Using the conclusions of case 1 and case 2 and assumption (H0), we see that there exists a constant $C > 0$ such that (4.4) holds.

□

Proposition 4.5 (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

$$|\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\hat{X}^*_{j,l} - \hat{X}^*_{j',l'})| \le \frac{C\varepsilon\rho^2}{|j-j'|^{p+2}}. \tag{4.8}$$

Proof of Proposition 4.5
Step 1: Definition of $\bar{X}$ and Taylor expansion
We define

$$\bar{X} := \frac{X - \widehat{X}^*}{\varepsilon}.$$

Then we can apply Theorem 3.3 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

$$|\bar{X}_j| \le C_2\rho^2. \tag{4.9}$$

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

$$\nabla V(X_{j,l} - X_{j',l'}) = \nabla V(\widehat{X}^*_{j,l} - \widehat{X}^*_{j',l'}) + \varepsilon(\bar{X}_{j,l} - \bar{X}_{j',l'}) \int_0^1 D^2V(A(t))\,dt, \tag{4.10}$$

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 3.6, we deduce that there exist constants C_3, C_4 such that

$$|A(t)| \ge C_4|j-j'| \quad \text{if} \quad |j-j'| \ge C_3 \tag{4.11}$$

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 (4.9), we deduce

$$|\bar{X}_{j,l} - \bar{X}_{j',l'}| \le 2C_2\rho^2.$$

Then we compute

$$\begin{array}{rcl} |A(t)-(\hat{X}^*_{j,l}-\hat{X}^*_{j',l'})| &=& |t\varepsilon(\bar{X}_{j,l}-\bar{X}_{j',l'})| \\ &\leq& 2C_2\varepsilon\rho^2, \end{array}$$

and because $|\hat{X}^*_{j,l}-\hat{X}^*_{j',l'}|\geq \delta>0$ if $(j,l)\neq(j',l')$, we deduce for the choice $\varepsilon\rho^2\leq\varepsilon_1$ (for ε_1 small enough) that there exists a constant C_6 such that

$$|A(t)|\geq C_6.$$

Using moreover assumption (H0), there exists a constant $C_7>0$ such that

$$|D^2V(A(t))|\leq C_7\leq \frac{C_7}{|j-j'|^{p+2}}.$$

Using the conclusions of case 1 and case 2, we deduce that there exists a constant $C_8>0$ such that

$$\left|\int_0^1 D^2V(A(t))dt\right|\leq \frac{C_8}{|j-j'|^{p+2}}.$$

Moreover because of (4.9) and (4.10), we deduce that there exists a constant $C>0$ such that we have (4.8).

□

4.2 Proof of Theorem 4.1

Proof of Theorem 4.1

Step 1: Control of $\mathcal{N}_{\mathbb{Z}}(X)$ and $D_i(X,\theta_i,L_i)$

We apply our Saint-Venant principle (3.2) of Theorem 3.2 with $J=\mathbb{Z}$ and we get

$$\mathcal{N}_{\mathbb{Z}}(X)\leq\frac{C_1}{1-\mu}\sup_{j\in\mathbb{Z}}|f_j|.$$

We compute

$$\begin{array}{rcl} \sup_{j\in\mathbb{Z}}|f_j| &=& \sup_{j\in\mathbb{Z}}\sup_{0\leq l\leq K-1}|f_{j,l}| \\ &=& \sup_{j\in\mathbb{Z}}|\frac{1}{K}f^0_j| \\ &=& \frac{1}{K}\sup_{j\in\mathbb{Z}}|\int_{\varepsilon(j-\frac{1}{2})}^{\varepsilon(j+\frac{1}{2})}\bar{f}(x)dx| \\ &\leq& \frac{\varepsilon}{K}\sup_x|\bar{f}(x)|, \end{array}$$

where in the second line we have used (1.6) and in the third line we have used (1.14). Using (1.27) to bound $\bar{f}$, we deduce that for some constant $C_0>0$, we have

$$\mathcal{N}_{\mathbb{Z}}(X)\leq\bar{\varepsilon}\quad\text{with}\quad\bar{\varepsilon}:=C_0\varepsilon. \tag{4.12}$$

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 (4.12), we have

$$D_i(X,\theta_i,L_i) \le \bar{\varepsilon}. \tag{4.13}$$

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 (4.18)), we can apply (4.8) in Proposition 4.5 and deduce that there exists a constant C_2 such that for $|j-i|, |j'-i| \le \rho$:

$$|\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\widehat{X}^{*,i}_{j,l} - \widehat{X}^{*,i}_{j',l'})| \le \frac{C_2 \bar{\varepsilon}\rho^2}{|j-j'|^{p+2}}. \tag{4.14}$$

Then we compute

$$\begin{aligned}
|S_i(X) - S_i(\widehat{X}^{*,i})| &\le \sum_{\substack{i+1 \le j \le i+\rho \\ i-\rho \le j' \le i}} \sum_{0 \le l,l' \le K-1} |\nabla V(X_{j,l} - X_{j',l'}) - \nabla V(\widehat{X}^{*,i}_{j,l} - \widehat{X}^{*,i}_{j',l'})| \\
&\le \sum_{\substack{i+1 \le j \le i+\rho \\ i-\rho \le j' \le i}} \sum_{0 \le l,l' \le K-1} \frac{C_2 \bar{\varepsilon}\rho^2}{|j-j'|^{p+2}} \\
&\le \sum_{\substack{i+1 \le j \le i+\rho \\ i-\rho \le j' \le i}} \frac{K^2 C_2 \bar{\varepsilon}\rho^2}{|j-j'|^{p+2}} \\
&\le K^2 C_2 \bar{\varepsilon}\rho^2 \sum_{\substack{1 \le \bar{j} \le \rho \\ 0 \le \bar{j}' \le \rho}} \frac{1}{|\bar{j} + \bar{j}'|^{p+2}} \\
&\le K^2 C_2 \bar{\varepsilon}\rho^2 \sum_{\substack{\bar{j} \ge 1 \\ \bar{j}' \ge 0}} \frac{1}{|\bar{j} + \bar{j}'|^{p+2}},
\end{aligned}$$

where $\bar{j} := j - i$ and $\bar{j}' := i - j'$.
By Lemma 8.9 (with $\rho = 1$) with $p > 0$, there exists a constant C_3 such that we have

$$|S_i(X) - S_i(\widehat{X}^{*,i})| \leq C_3 \bar{\varepsilon} \rho^2. \tag{4.15}$$

Step 2-2: Error estimate on $F_i(X)$
By (1.27) we have

$$\sup_{j \in \mathbb{Z}} D_j(X, \theta^*, L^*) \leq \varepsilon_0.$$

Using (4.4) in Proposition 4.3, we deduce that there exists a constant $C_4 > 0$ such that

$$|\nabla V(X_{j,l} - X_{j',l'})| \leq \frac{C_4}{|j - j'|^{p+1}} \qquad \text{for } |j - j'| \geq \rho \geq 1. \tag{4.16}$$

Then
(4.17)

$$\begin{aligned} |F_i(X)| &\leq C_4 \Big(\sum_{\substack{j > i+\rho \\ j' \leq i}} \sum_{0 \leq l, l' \leq K-1} \frac{1}{|j - j'|^{p+1}} + \sum_{\substack{i+1 \leq j \leq i+\rho \\ j' < i - \rho}} \sum_{0 \leq l, l' \leq K-1} \frac{1}{|j - j'|^{p+1}} \Big) \\ &\leq K^2 C_4 \Big(\sum_{\substack{\bar{j} > \rho \\ \bar{j}' \geq 0}} \frac{1}{(\bar{j} + \bar{j}')^{p+1}} + \sum_{\substack{1 \leq \bar{j} \leq \rho \\ \bar{j}' > \rho}} \frac{1}{(\bar{j} + \bar{j}')^{p+1}} \Big) \\ &\leq 2K^2 C_4 \sum_{\substack{\bar{j} > \rho \\ \bar{j}' \geq 0}} \frac{1}{(\bar{j} + \bar{j}')^{p+1}}. \end{aligned}$$

where $\bar{j} := j - i$ and $\bar{j}' := i - j'$. By Lemma 8.9 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

$$\bar{\varepsilon} \rho^{p+1} = 1 \tag{4.18}$$

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 2.2 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 (4.3) with the mean fiber (see Definition 3.7)

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

We write (from Definition 2.9 and Proposition 2.10)

$$M_i[X] = M_i[X](0) = M_i[X](\tilde{a}_i) + \tilde{a}_i \times T_i[X] = \mathbb{S}_i(X - \tilde{a}_i) + \mathbb{F}_i(X - \tilde{a}_i) + \tilde{a}_i \times T_i[X], \tag{4.19}$$

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

$$\begin{aligned} \mathbb{F}_i(X - \tilde{a}_i) &= \sum_{\substack{j > i+\rho \\ j' \leq i}} \sum_{0 \leq l,l' \leq K-1} (X_{j,l} - \tilde{a}_i) \times \nabla V(X_{j,l} - X_{j',l'}) \\ &+ \sum_{\substack{i+1 \leq j \leq i+\rho \\ j' < i-\rho}} \sum_{0 \leq l,l' \leq K-1} (X_{j,l} - \tilde{a}_i) \times \nabla V(X_{j,l} - X_{j',l'}) \end{aligned}$$

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

$$\tilde{X}^{*,i} \in \mathcal{C}_*^{\theta_i, L_i}. \tag{4.20}$$

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 (4.13) we deduce

$$|X_i - \tilde{a}_i - \tilde{X}_i^{*,i}| \leq \bar{\varepsilon}, \tag{4.21}$$

and then (with $\tilde{b}_i^{*,i}$ the barycenter of $\tilde{X}_i^{*,i}$)

$$|b_i - \tilde{a}_i - \tilde{b}_i^{*,i}| \leq \bar{\varepsilon}. \tag{4.22}$$

Using (3.11) 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

$$|\tilde{X}_i^{*,i}| \le C_8. \tag{4.23}$$

Step 3-1: Error estimate on $\mathbb{S}_i(X - \tilde{a}_i)$
We compute (using the fact that $\tilde{X}_{j,l}^{*,i} - \tilde{X}_{j',l'}^{*,i} = \widehat{X}_{j,l}^{*,i} - \widehat{X}_{j',l'}^{*,i}$)

$$\begin{aligned}
&\mathbb{S}_i(X-\tilde{a}_i) - \mathbb{S}_i(\tilde{X}^{*,i})\\
=& \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} \left((X_{j,l}-\tilde{a}_i)\times\nabla V(X_{j,l}-X_{j',l'}) - \tilde{X}_{j,l}^{*,i}\times\nabla V(\tilde{X}_{j,l}^{*,i}-\tilde{X}_{j',l'}^{*,i})\right)\\
=& \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} \left((X_{j,l}-\tilde{a}_i)\times\nabla V(X_{j,l}-X_{j',l'}) - \tilde{X}_{j,l}^{*,i}\times\nabla V(\widehat{X}_{j,l}^{*,i}-\widehat{X}_{j',l'}^{*,i})\right)\\
=& \mathbb{S}_i^1+\mathbb{S}_i^2+\mathbb{S}_i^3,
\end{aligned}$$

with

$$\begin{cases}
\mathbb{S}_i^1 = \displaystyle\sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} (X_{j,l}-\tilde{a}_i-\tilde{X}_{j,l}^{*,i})\times\nabla V(X_{j,l}-X_{j',l'})\\
\mathbb{S}_i^2 = \displaystyle\sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} \left(R_{(j-i)\theta_i,\widehat{L}_i}(\tilde{X}_{i,l}^{*,i})\right)\times\left(\nabla V(X_{j,l}-X_{j',l'})-\nabla V(\widehat{X}_{j,l}^{*,i}-\widehat{X}_{j',l'}^{*,i})\right)\\
\mathbb{S}_i^3 = \displaystyle\sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} (j-i)L_i\times\left(\nabla V(X_{j,l}-X_{j',l'})-\nabla V(\widehat{X}_{j,l}^{*,i}-\widehat{X}_{j',l'}^{*,i})\right)
\end{cases}$$

where we have used (4.20).
Using (4.16) and (4.21), we deduce that there exists a constant C_9 such that we have

$$|\mathbb{S}_i^1| \le \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} \frac{C_4\bar{\varepsilon}}{|j-j'|^{p+1}} \le \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} C_4K^2\bar{\varepsilon} \le C_9\bar{\varepsilon}\rho^2.$$

Using (4.14) and (4.23), we deduce that

$$\begin{aligned}
|\mathbb{S}_i^2| &\le \sum_{\substack{i+1\le j\le i+\rho\\ i-\rho\le j'\le i}} \sum_{0\le l,l'\le K-1} \frac{C_8C_2\bar{\varepsilon}\rho^2}{|j-j'|^{p+1}} \le C_8C_2K^2\bar{\varepsilon}\rho^2 \sum_{\substack{1\le \bar{j}\le\rho\\ 0\le\bar{j}'\le\rho}} \frac{1}{|\bar{j}+\bar{j}'|^{p+1}}\\
&\le C_8C_2K^2\bar{\varepsilon}\rho^2 \sum_{\substack{\bar{j}\ge 1\\ \bar{j}'\ge 0}} \frac{1}{|\bar{j}+\bar{j}'|^{p+1}},
\end{aligned}$$

where $\bar{j} = j - i$ and $\bar{j}' = i - j'$. By Lemma 8.9 (with $\rho = 1$) with $p > 1$, we deduce that there exists a constant C_{10} such that

$$|\mathbb{S}_i^2| \le C_{10}\bar{\varepsilon}\rho^2.$$

Using (4.14), we deduce that there exists a constant C_{11} such that we have

$$|\mathbb{S}_i^3| \le C_{11}\bar{\varepsilon}\rho^2 \sum_{\substack{i+1\le j\le i+\rho \\ i-\rho\le j'\le i}} \frac{|j-i|}{|j-j'|^{p+2}} = C_{11}\bar{\varepsilon}\rho^2 \sum_{\substack{1\le \bar{j}\le \rho \\ 0\le \bar{j}'\le \rho}} \frac{\bar{j}}{(\bar{j}+\bar{j}')^{p+2}} \le C_{11}\bar{\varepsilon}\rho^2 \sum_{\substack{\bar{j}\ge 1 \\ \bar{j}'\ge 0}} \frac{\bar{j}}{(\bar{j}+\bar{j}')^{p+2}},$$

where $\bar{j} := j-i$ and $\bar{j}' := i-j'$.
By Lemma 8.9 (with $\rho = 1$) with $p > 1$, then there exists a constant C_{12} such that we have

$$|\mathbb{S}_i^3| \le C_{12}\bar{\varepsilon}\rho^2.$$

Finally we get

$$|\mathbb{S}_i(X-\tilde{a}_i) - \mathbb{S}_i(\tilde{X}^{*,i})| \le C_{13}\bar{\varepsilon}\rho^2, \tag{4.24}$$

with $C_{13} = C_9 + C_{10} + C_{12}$.
Step 3-2: Error estimate on $\mathbb{F}_i(X-\tilde{a}_i)$
Using (4.5), (4.21) and (4.23), we deduce that

$$\begin{aligned} |X_j - \tilde{a}_i| &\le |X_j - X_i| + |X_i - \tilde{a}_i - \tilde{X}_i^{*,i}| + |\tilde{X}_i^{*,i}| \\ &\le C_{14}(1+|j-i|), \end{aligned}$$

with $C_{14} > 0$. Using moreover (4.16), we get

$$\begin{aligned} |\mathbb{F}_i(X-\tilde{a}_i)| &= \left| \begin{array}{l} \displaystyle\sum_{\substack{j>i+\rho \\ j'\le i}} \sum_{0\le l,l'\le K-1} (X_{j,l}-\tilde{a}_i)\times \nabla V(X_{j,l}-X_{j',l'}) \\ + \displaystyle\sum_{\substack{i+1\le j\le i+\rho \\ j'<i-\rho}} \sum_{0\le l,l'\le K-1} (X_{j,l}-\tilde{a}_i)\times \nabla V(X_{j,l}-X_{j',l'}) \end{array} \right| \\ &\le K^2 C_4 \left(\sum_{\substack{j>i+\rho \\ j'\le i}} \frac{C_{14}(1+|j-i|)}{|j-j'|^{p+1}} + \sum_{\substack{i+1\le j\le i+\rho \\ j'<i-\rho}} \frac{C_{14}(1+|j-i|)}{|j-j'|^{p+1}} \right) \\ &\le K^2 C_4 C_{14} \left(\sum_{\substack{\bar{j}>\rho \\ \bar{j}'\ge 0}} \frac{1+\bar{j}}{(\bar{j}+\bar{j}')^{p+1}} + \sum_{\substack{1\le \bar{j}\le \rho \\ \bar{j}'>\rho}} \frac{1+\bar{j}}{(\bar{j}+\bar{j}')^{p+1}} \right), \end{aligned}$$

with $\bar{j} = j-i$ and $\bar{j}' = i-j'$. Using Lemmata 8.8 and 8.9 with $p > 2$, we deduce that there exists a constant C_{15} such that we have

$$|\mathbb{F}_i(X-\tilde{a}_i)| \le \frac{C_{15}}{\rho^{p-2}}.$$

Similarly, we have

$$|\mathbb{F}_i(\tilde{X}^{*,i})| \le \frac{C_{15}}{\rho^{p-2}}. \tag{4.25}$$

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 $C_{17}\bar{\varepsilon}^{\frac{p-2}{p}}$, we get

$$\left|M_i[X] - \tilde{a}_i \times T_i[X] - M_i[\tilde{X}^{*,i}]\right| \leq C_{17}\bar{\varepsilon}^{\frac{p-2}{p}}.$$

Finally using Lemma 2.11, 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 (4.19))

$$\left|M_i[X](\tilde{a}_i) - W'_\theta(\theta_i, L_i)\widehat{L}_i\right| \leq C\varepsilon^{\frac{p-2}{p}},$$

with $C \geq C_{17}C_0^{\frac{p-2}{p}}$, which means exactly (4.3).

$\square$

5 An estimate about the scalar line torsion

In order to use later (in Section 6) the estimates of Theorem 4.1 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 5.1 (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 3.7.

The main result of this section is the following estimate about the scalar line torsion

Theorem 5.2 (Almost constant scalar line torsion)
Let us consider a nanotube X under the assumptions of Theorem 1.12. Then there exist constants $\bar{m}_0 \in \mathbb{R}$ and $C > 0$ such that we have for all $i \in \mathbb{Z}$

$$|m_i - \bar{m}_0| \le C\varepsilon^\gamma \quad \text{with} \quad \gamma = \min\left(\frac{1}{3}, \frac{p-2}{p}\right). \tag{5.1}$$

Notice that (5.1) 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 5.2 we first need the following lemma:

Lemma 5.3 (Estimate on $m_i - m_{i-1}$)
Let us consider a nanotube X under the assumptions of Theorem 1.12. Then we have for all $i \in \mathbb{Z}$

$$m_i - m_{i-1} = -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times f_i^0) + O(\varepsilon^{1+\bar{\bar{\gamma}}}), \tag{5.2}$$

with $\bar{\bar{\gamma}} = \dfrac{p-2}{p}$.

Proof of Lemma 5.3
By Theorem 4.1, we have (4.1), i.e.

$$D_i(X, \theta_i, L_i) \le C\varepsilon. \tag{5.3}$$

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

$$\widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_i \cdot M_{i-1}(\tilde{a}_{i-1}) = -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_i) + (b_i - \tilde{a}_{i-1}) \cdot (\widehat{L}_i \times T_{i-1}). \tag{5.4}$$

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 (3.13), in the third line we have used (5.3), Lemma 3.4 and Lemma 8.5 ii), and in the fifth line we have used (4.2) and the fact that $W'_L(\theta_{i-1}, L_{i-1})$ is parallel to L_{i-1} (see Corollary 2.5). Therefore from (5.4), we get

$$\begin{aligned}
\widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_i \cdot M_{i-1}(\tilde{a}_{i-1}) &= -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_i) + (b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times T_{i-1}) + O(\varepsilon^{1+\bar{\gamma}}) \\
&= -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times (T_i - T_{i-1})) + O(\varepsilon^{1+\bar{\gamma}}) \\
&= -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times f_i^0) + O(\varepsilon^{1+\bar{\gamma}}).
\end{aligned}$$

On the other hand we compute

$$\begin{aligned}
(\widehat{L}_i - \widehat{L}_{i-1}) \cdot M_{i-1}(\tilde{a}_{i-1}) &= (\widehat{L}_i - \widehat{L}_{i-1}) \cdot (W'_\theta(\theta_{i-1}, L_{i-1})\widehat{L}_{i-1} + O(\varepsilon^{\bar{\bar{\gamma}}})) \\
&= W'_\theta(\theta_{i-1}, L_{i-1})(\widehat{L}_i \cdot \widehat{L}_{i-1} - 1) + O(\varepsilon^{1+\bar{\bar{\gamma}}}) \\
&= O(\varepsilon^2) + O(\varepsilon^{1+\bar{\bar{\gamma}}}) = O(\varepsilon^{1+\bar{\bar{\gamma}}}),
\end{aligned}$$

where in the first line we have used (4.3) and in the last line we have used the square of the relation $\widehat{L}_i - \widehat{L}_{i-1} = O(\varepsilon)$. We compute

$$\begin{aligned}
m_i - m_{i-1} &= \widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_{i-1} \cdot M_{i-1}(\tilde{a}_{i-1}) \\
&= \widehat{L}_i \cdot M_i(\tilde{a}_i) - \widehat{L}_i \cdot M_{i-1}(\tilde{a}_{i-1}) + (\widehat{L}_i - \widehat{L}_{i-1}) \cdot M_{i-1}(\tilde{a}_{i-1}) \\
&= -(b_i - \tilde{a}_i) \cdot (\widehat{L}_i \times f_i^0) + O(\varepsilon^{1+\bar{\gamma}}) + O(\varepsilon^{1+\bar{\bar{\gamma}}})
\end{aligned}$$

and finally, because $\bar{\bar{\gamma}} < \bar{\gamma}$, we deduce (5.2).

□

Proof of Theorem 5.2

We recall that by Lemma 3.4, there exists a constant $C_1 > 0$ such that we have

$$(5.5) \qquad \begin{cases} |\theta_{i+1} - \theta_i| \le C_1\varepsilon \\ |L_{i+1} - L_i| \le C_1\varepsilon. \end{cases}$$

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 (5.2) in Lemma 5.3, 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 (5.5) and Lemma 8.5 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 $0 \le i \le \dfrac{1}{\varepsilon}$

$$\begin{aligned}
m_i - m_{i-1} &= -(b_i - \tilde{a}_i) \cdot \big((\widehat{L}_0 + O(i\varepsilon)) \times (f_0^0 + O(i\varepsilon^2))\big) + O(\varepsilon^{1+\bar{\bar{\gamma}}}) \\
&= -(b_i - \tilde{a}_i) \cdot (\widehat{L}_0 \times f_0^0) + O(i\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}).
\end{aligned}$$

Step 2: A refined estimate on $b_i - \tilde{a}_i$
We already know from (3.11) 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 (3.15), 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 (3.11)) , $\theta_{i-1} = \theta_0 + O((i-1)\varepsilon)$, $L_{i-1} = L_0 + O((i-1)\varepsilon)$, using Lemma 8.4 and Lemma 8.5 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 $i \geq 1$

$$\begin{aligned} b_i - \tilde{a}_i &= R_{\theta_0,\widehat{L}_0}(b_{i-1} - \tilde{a}_{i-1}) + O(i\varepsilon) \\ &= R_{\theta_0,\widehat{L}_0}\big(R_{\theta_0,\widehat{L}_0}(b_{i-2} - \tilde{a}_{i-2}) + O((i-1)\varepsilon)\big) + O(i\varepsilon) \\ &= R_{2\theta_0,\widehat{L}_0}(b_{i-2} - \tilde{a}_{i-2})) + O((i-1)\varepsilon) + O(i\varepsilon) \\ &= R_{i\theta_0,\widehat{L}_0}(b_0 - \tilde{a}_0) + O(\frac{i(i+1)}{2}\varepsilon) \end{aligned}$$

and then we have for $i \geq 0$

$$b_i - \tilde{a}_i = R_{i\theta_0,\widehat{L}_0}(b_0 - \tilde{a}_0) + O(i^2\varepsilon). \tag{5.6}$$

Step 3: An estimate on $m_i - m_{i-1}$
By Step 1 and (5.6), 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 $j \in \mathbb{Z}$

$$m_{j+i} - m_{j+i-1} = -\big((b_j - \tilde{a}_j) \times \widehat{L}_j\big) \cdot (R_{-i\theta_j,\widehat{L}_j}(f_j^0))^{\perp_{\widehat{L}_j}} + O(i^2\varepsilon^2 + \varepsilon^{1+\bar{\bar{\gamma}}}). \tag{5.7}$$

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 everage of the scalar line torsion on a window of length N. We rewrite (5.7) 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

$$\begin{aligned}
B \ &= \ \frac{1}{N}\sum_{k=1}^{N} O(k^2\varepsilon^2+\varepsilon^{1+\bar{\bar\gamma}}) \\
&= \ \frac{1}{N}O\Big(\frac{N(N+1)(2N+1)}{6}\varepsilon^2+N\varepsilon^{1+\bar{\bar\gamma}}\Big) \\
&= \ O\Big(\frac{(N+1)(2N+1)}{6}\varepsilon^2+\varepsilon^{1+\bar{\bar\gamma}}\Big) \\
&= \ O\big(N^2\varepsilon^2+\varepsilon^{1+\bar{\bar\gamma}}\big)
\end{aligned}$$

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 $0 \leq j \leq \frac{1}{\varepsilon}$

$$\bar{m}_j = \bar{m}_0 + O(\varepsilon^{\gamma}). \tag{5.8}$$

Step 5: An estimate on m_i
Using (4.3) in Theorem 4.1, we get that

$$m_i = W'_\theta(\theta_i, L_i) + O(\varepsilon^{\bar{\bar{\gamma}}}). \tag{5.9}$$

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 (5.9) and in the fourth line we have used Proposition 1.2 which implies that W is C^2 using its definition (1.26) (i.e. W'' is C^0) in the closed set $\mathcal{U}_0$, i.e. W'' is bounded. Using (5.8) and the $\frac{1}{\varepsilon}$-periodicity, we get

$$m_i = \bar{m}_0 + O(\varepsilon^{\gamma}) \qquad \text{for all } i \in \mathbb{Z}.$$

□

6 Estimate between discrete and continuous forces

The goal of this section is to prove the following Theorem 6.1, giving an error estimate between the discrete and the continuous forces.

Theorem 6.1 (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 1.12 with $p > 2$ and $(\theta_i, L_i) \in \mathcal{U}_0$ as in Theorem 4.1. There exists $\varepsilon_1 > 0$, such that if

$$|\theta^0 - \theta^*| \leq \varepsilon_1 \quad \textit{and} \quad |L^0 - L^*| \leq \varepsilon_1,$$

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 $x \in [(i - \frac{1}{2})\varepsilon, (i + \frac{1}{2})\varepsilon]$

$$|\Sigma_0 + W'_L(\alpha'(x), \Phi'(x)) - W'_L(\theta_i, L_i)| \leq C\varepsilon^{\bar{\gamma}} \tag{6.1}$$

and

$$|\sigma_0 + W'_\theta(\alpha'(x), \Phi'(x)) - W'_\theta(\theta_i, L_i)| \leq C\varepsilon^{\gamma}. \tag{6.2}$$

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 6.1 we need the following Proposition 6.2 giving the existence of a solution of the Euler-Lagrange system (1.5).

Proposition 6.2 (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

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

satisfying the periodic conditions (1.1).
Moreover there exists a constant $C > 0$ such that

$$|(\alpha', \Phi') - (\theta^0, L^0)|_{L^\infty(\mathbb{R})} \leq C|\bar{f}|_{L^\infty(\mathbb{R})}. \tag{6.3}$$

Proof of Proposition 6.2
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

$$\Lambda(0) = 0. \tag{6.4}$$

Then let us define

$$\lambda^0 = (\theta^0, L^0)$$

and

$$\mathcal{V}_1 = \{\Lambda \in W^{1,\infty}(\mathbb{R},\mathbb{R}^4);\ \Lambda(x+1) = \Lambda(x) + \lambda^0 \quad \text{with (6.4)}\}$$
$$\mathcal{V}_2 = \{g = h' \text{ with } h \in L^\infty(\mathbb{R},\mathbb{R}^4);\ h(x+1) = h(x)\}\,.$$

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

$$\begin{aligned} |\Psi(\Lambda_2) - \Psi(\Lambda_1)|_{\mathcal{V}_2} &\leq |W'_\lambda(\Lambda'_2) - W'_\lambda(\Lambda'_1)|_{L^\infty(\mathbb{R})} \\ &\leq |D^2W|_{L^\infty(\mathcal{U}_0)}|\Lambda'_2 - \Lambda'_1|_{L^\infty(\mathbb{R})} \\ &\leq |D^2W|_{L^\infty(\mathcal{U}_0)}|\Lambda_2 - \Lambda_1|_{W^{1,\infty}(\mathbb{R})}. \end{aligned}$$

We compute

$$D_\Lambda\Psi(\Lambda)\cdot\bar\Lambda = (D^2W(\Lambda')\cdot\bar\Lambda')'.$$

Therefore

$$\begin{aligned} & |D_\Lambda\Psi(\Lambda_2)\cdot\bar\Lambda_2 - D_\Lambda\Psi(\Lambda_1)\cdot\bar\Lambda_1|_{\mathcal{V}_2} \\ \leq\ & |D^2W(\Lambda'_2)\cdot\bar\Lambda'_2 - D^2W(\Lambda'_1)\cdot\bar\Lambda'_1|_{L^\infty(\mathbb{R})} \\ \leq\ & |D^2W(\Lambda'_2) - D^2W(\Lambda'_1)|_{L^\infty(\mathcal{U}_0)}|\bar\Lambda'_2|_{L^\infty(\mathbb{R})} + |D^2W|_{L^\infty(\mathcal{U}_0)}|\bar\Lambda'_2 - \bar\Lambda'_1|_{L^\infty(\mathbb{R})} \\ & \longrightarrow 0 \quad \text{as} \quad |(\Lambda_2,\bar\Lambda_2) - (\Lambda_1,\bar\Lambda_1)|_{\mathcal{V}_1\times\mathcal{V}_1} \longrightarrow 0, \end{aligned}$$

where we have used the fact that W is C^2 by Proposition 1.7. 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

$$D_\Lambda\Psi(\Lambda_0)\cdot\bar\Lambda = g, \tag{6.5}$$

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 (6.5) satisfying (6.4). Moreover there exists a constant $C > 0$ such that

$$\begin{array}{rcl} |\bar{\Lambda}|_{W^{1,\infty}(\mathbb{R})} & \leq & C|(A^0)^{-1}|_{L^\infty}|h+k|_{L^\infty(\mathbb{R})} \\ & \leq & 2C|(A^0)^{-1}|_{L^\infty}|h|_{L^\infty(\mathbb{R})} \\ & \leq & 2C|(A^0)^{-1}|_{L^\infty}|g|_{\mathcal{V}_2}. \end{array}$$

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

$$\Psi(\Lambda_0) = 0. \tag{6.6}$$

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

$$\Psi(\Lambda) = (0, \bar{f}). \tag{6.7}$$

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 (6.3)
Because of (6.6) and (6.7) 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 (6.3).

$\square$

Proof of Theorem 6.1

By Proposition 6.2, 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 (6.1)

We have $(W'_{\Phi'}(\alpha', \Phi'))' = \bar{f}$, then there exists a constant $\tilde{\Sigma}_0 \in \mathbb{R}^3$ such that

$$W'_{\Phi'}(\alpha'(x), \Phi'(x)) = \tilde{\Sigma}_0 + \int_0^x \bar{f}(y)\, dy. \tag{6.8}$$

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 (4.2), 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 (6.8), 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^∞)

$$|T_0 - \tilde{\Sigma}_0 + W'_{\Phi'}(\alpha'(x), \Phi'(x)) - W'_L(\theta_i, L_i)| \leq C_2 \varepsilon^{\frac{p-1}{p+1}}. \tag{6.9}$$

This implies (6.1) with $\Sigma_0 = T_0 - \tilde{\Sigma}_0$.

Step 2: Proof of (6.2)

We have $(W'_{\alpha'}(\alpha', \Phi'))' = 0$, then there exists a constant $\tilde{\sigma}_0 \in \mathbb{R}$ such that

$$W'_{\alpha'}(\alpha', \Phi') = \tilde{\sigma}_0 \tag{6.10}$$

From (4.3), 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 (5.1), we get

$$|\bar{m}_0 - W'_\theta(\theta_i, L_i)| \leq C_4 \varepsilon^{\gamma}.$$

Using (6.10), we get for $x \in [(i - \frac{1}{2})\varepsilon, (i + \frac{1}{2})\varepsilon]$

$$|\bar{m}_0 - \tilde{\sigma}_0 + W'_{\alpha'}(\alpha'(x), \Phi'(x)) - W'_\theta(\theta_i, L_i)| \leq C_4 \varepsilon^{\gamma}. \tag{6.11}$$

which implies (6.2) with $\sigma_0 = \bar{m}_0 - \tilde{\sigma}_0$.

$\square$

7 Proof of the main results: Theorem 1.12 and Corollary 1.13

The goal of this section is to prove Theorem 1.12 and Corollary 1.13.

Proof of Theorem 1.12
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

$$(7.1) \qquad \left\{ \begin{array}{l} \tilde{\alpha}'(x) = (1-t)\theta_i + t\theta_{i+1} \\ \tilde{\Phi}'(x) = (1-t)L_i + tL_{i+1} \end{array} \right| \quad \text{with } t = \frac{x - i\varepsilon}{\varepsilon} \quad \text{for} \quad i\varepsilon \le x \le (i+1)\varepsilon.$$

where (θ_i, L_i) are given in Theorem 6.1. Notice that because of (1.7), we can choose (θ_i, L_i) and $\tilde{a}_i$ given in Theorem 3.8 such that we have

$$\left\{ \begin{array}{ccc} (\theta_{i+N_\varepsilon}, L_{i+N_\varepsilon}) & = & (\theta_i, L_i) \\ \tilde{a}_{i+N_\varepsilon} & = & \tilde{a}_i + N_\varepsilon L^0. \end{array} \right.$$

From (3.14) 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

$$(7.2) \qquad \int_0^1 \tilde{\Phi}'(x)\, dx = O(\varepsilon) + \varepsilon \sum_{i=0}^{N_\varepsilon - 1} L_i = L^0 + O(\varepsilon).$$

Similarly we have

$$(7.3) \qquad \int_0^1 \tilde{\alpha}'(x)\, dx = O(\varepsilon) + \varepsilon \sum_{i=0}^{N_\varepsilon - 1} \theta_i := \theta^0.$$

Step 1-2: Properties of (θ^0, L^0)
By (4.1) and (1.27) 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 3.4 and deduce for $\varepsilon \le \varepsilon_0$ with ε_0 small enough that

$$\text{(7.4)} \qquad \left\{ \begin{array}{l} |\theta_i - \theta^*| \le C\varepsilon_0 \\ |L_i - L^*| \le C\varepsilon_0. \end{array} \right.$$

Using (7.2) and (7.3), this implies (1.28), i.e.

$$\text{(7.5)} \qquad \left\{ \begin{array}{l} |\theta^0 - \theta^*| \le C\varepsilon_0 \\ |L^0 - L^*| \le C\varepsilon_0. \end{array} \right.$$

Step 1-3: Definition of (α, Φ)
For ε_0 small enough, we deduce from (7.5) that $|\theta^0 - \theta^*| \le \varepsilon_1$ and $|L^0 - L^*| \le \varepsilon_1$ and then we can apply Theorem 6.1 which shows the existence of a solution (α, Φ) of (1.1), (1.5). We get in particular

$$\text{(7.6)} \qquad \left\{ \begin{array}{l} \displaystyle\int_0^1 \tilde{\Phi}'(x)\,dx = \int_0^1 \Phi'(x)\,dx + O(\varepsilon) \\ \displaystyle\int_0^1 \tilde{\alpha}'(x)\,dx = \int_0^1 \alpha'(x)\,dx. \end{array} \right.$$

Step 2: Estimate on the differences of W'
By (7.1) 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 (4.1) and (3.5), 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 (6.1) and (6.2) that there exists a constant C_1 such that we have

$$\text{(7.7)} \qquad \left\{ \begin{array}{l} |\Sigma_0 + W'_L(\alpha'(x), \Phi'(x)) - W'_L(\tilde{\alpha}'(x), \tilde{\Phi}'(x))| \le C_1\varepsilon^{\bar{\gamma}} \\ |\sigma_0 + W'_\theta(\alpha'(x), \Phi'(x)) - W'_\theta(\tilde{\alpha}'(x), \tilde{\Phi}'(x))| \le C_1\varepsilon^{\gamma}. \end{array} \right.$$

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 $\lambda = (\theta, L)$

$$\text{(7.8)} \qquad |c_0 + W'_\lambda(u(x)) - W'_\lambda(\tilde{u}(x))| \le C_2\varepsilon^{\gamma}.$$

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

$$(7.9) \qquad |\tilde{u}(x) - u(x) - \big(D^2W(u(x))\big)^{-1}(c_0)| \le O\big(\varepsilon^\gamma + |\tilde{u}(x) - u(x)|\omega(|\tilde{u} - u|_{L^\infty})\big),$$

and then we deduce that there exists a constant C_3 such that we have

$$(7.10) \quad |\tilde{u}(x) - u(x) - \big(D^2W(u^0)\big)^{-1}(c_0)| \le C_3\left(\varepsilon^\gamma + |\tilde{u} - u|_{L^\infty}\omega(|\tilde{u} - u|_{L^\infty}) + |c_0|\,\omega(|u - u^0|_{L^\infty})\right).$$

Using (7.6), 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 (7.10) 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 (6.3), 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 (7.9) 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 (6.3) and (7.4), 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

$$(7.11) \qquad \begin{cases} |\theta_j - \alpha'(j\varepsilon)| \le C_6\varepsilon^\gamma \\ |L_j - \Phi'(j\varepsilon)| \le C_6\varepsilon^\gamma. \end{cases}$$

Using (3.11) and (3.12), we deduce that there exists a constant C_7 such that we have

$$(7.12) \qquad |X_j - \tilde{a}_j| \le C_7.$$

Using (3.15) and (3.16), 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 (7.11), (7.12), Lemma 8.4 and Lemma 8.5 ii), we deduce that there exists a constant C_9 such that we have

$$|X_{j+1} - \tilde{a}_{j+1} - R_{\alpha'(j\varepsilon),\widehat{\Phi'(j\varepsilon)}}(X_j - \tilde{a}_j)| \leq C_9\varepsilon^\gamma. \tag{7.13}$$

Using (3.14) and (7.11), we deduce that there exists a constant C_{10} such that we have

$$|\tilde{a}_{j+1} - \tilde{a}_j - \Phi'(j\varepsilon)| \leq C_{10}\varepsilon^\gamma. \tag{7.14}$$

Finally (7.13), (7.14),(7.12) and the choice $C = \max(C_7, C_9, C_{10})$ prove (1.30).

Step 5: Proof of (1.29)

By Theorem 4.1 we have (4.1), 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

$$\sup_{|\beta|\leq q} |X_{j+\beta} - \widehat{X}^{*,j}_{j+\beta}| \leq C_{11}\varepsilon. \tag{7.15}$$

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

$$\widehat{\bar{X}}_j^{*,j} = \bar{Y}_j^{*,j} + c_j \quad \text{with} \quad \bar{Y}_j^{*,j} := R_{\delta,\widehat{\bar{L}}_j}(\mathcal{X}_0^*(\bar{\theta}_j, \bar{L}_j)) \quad \text{and} \quad \left\{ \begin{array}{l} \bar{\theta}_j := \alpha'(j\varepsilon) \\ \bar{L}_j := \Phi'(j\varepsilon), \end{array}\right.$$

with

$$\widehat{\bar{X}}^{*,j} \in \widehat{\mathcal{C}}^{\bar{\theta}_j, \bar{L}_j}. \tag{7.16}$$

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 8.4 and (7.11), 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 (7.15), we deduce that there exists a constant $C > 0$ such that

$$\sup_{|\beta|\le q} |X_{j+\beta} - \widehat{\widehat{X}}^{*,j}_{j+\beta}| \le C\varepsilon^\gamma$$

which proves (1.29). This ends the proof of Theorem 1.12.

□

Proof of Corollary 1.13
Step 1: Proof of (7.17)
We recall the second line in (1.30)

$$|\tilde{a}_{j+1} - \tilde{a}_j - \Phi'(j\varepsilon)| \le C\varepsilon^\gamma.$$

Then we get

$$|\varepsilon\tilde{a}_{j+1} - \varepsilon\tilde{a}_j - \varepsilon\Phi'(j\varepsilon)| \le C\varepsilon^{1+\gamma}.$$

On the other hand we deduce by Proposition 6.2 that $\Phi \in W^{2,\infty}$, and then

$$|\Phi((j+1)\varepsilon) - \Phi(j\varepsilon) - \varepsilon\Phi'(j\varepsilon)| \le C\varepsilon^2.$$

Using the two last inequalities, we get

$$|e_{j+1} - e_j| \le C\varepsilon^{1+\gamma} \quad \text{with} \quad e_j := \varepsilon\tilde{a}_j - \Phi(j\varepsilon),$$

and then by iteration for $0 \le j \le \dfrac{1}{\varepsilon} - 1$, we get

$$|e_j - e_0| \le C\varepsilon^\gamma$$

i.e.

$$|\varepsilon\tilde{a}_j - \Phi(j\varepsilon) - a| \le C\varepsilon^\gamma, \tag{7.17}$$

with $a = e_0$.
Step 2: Conclusion
Using the first line of (1.30) and (7.17), we obtain (1.31).

□

8 Appendix

This appendix is composed of two independent subsections. In the first subsection, we recall some results about rotations. In the second subsection, we give a few estimates on some series.

8.1 Some results about rotations

Lemma 8.1 (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 8.1
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 8.2 (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 8.2
This is a straightforward consequence of Lemma 8.1.

□

Lemma 8.3 (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 8.3
We compute

$$\widehat{L} \cdot (x \times y) = (\widehat{L} \times x) \cdot y = (R_{\frac{\pi}{2},\widehat{L}}(x))^{\perp_{\widehat{L}}} \cdot y.$$

□

We now recall the following four results that are proven in the companion paper [25].

Lemma 8.4 (Control of rotations by angles and axes)
Let us consider two angles θ_1, $\theta_2 \in \mathbb{R}$ and two axes $\widehat{L}_1$, $\widehat{L}_2 \in \mathbb{R}^3$, then we have

$$|R_{\theta_2,\widehat{L}_2} - R_{\theta_1,\widehat{L}_1}| \leq |\theta_2 - \theta_1| + 5|\widehat{L}_2 - \widehat{L}_1|.$$

Lemma 8.5 (A control for axes)
Let us consider two axes L, $L' \in \mathbb{R}^3$ such that

$$|L| \geq \delta > 0 \qquad \text{for some} \quad \delta > 0. \tag{8.1}$$

If

$$|L - L'| \leq \varepsilon$$

then there exists a constant $C = C(\delta)$ such that we have
i) $\big||L| - |L'|\big| \leq \varepsilon$
ii) $|\widehat{L} - \widehat{L}'| \leq C\varepsilon$.

Lemma 8.6 (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

$$\nabla V(R(x)) = R(\nabla V(x)).$$

Lemma 8.7 (Derivative of rotations)
For $u \in \mathbb{R}^3$, we have

$$R_{\theta,\widehat{L}}(u) = (u.\widehat{L})\widehat{L} + (\cos\theta)(u - (u.\widehat{L})\widehat{L}) + (\sin\theta)(\widehat{L} \times u). \tag{8.2}$$

We also have

$$\bar{L}.\nabla_L(R_{\theta,\widehat{L}}(u)) = \big((u.\bar{\bar{L}})\widehat{L} + (u.\widehat{L})\bar{\bar{L}}\big)(1 - \cos\theta) + (\sin\theta)(\bar{\bar{L}} \times u) \tag{8.3}$$

with

$$\bar{\bar{L}} := \bar{L}.\nabla_L(\widehat{L}) = \frac{\bar{L}}{|L|} - \frac{L}{|L|^3}(L.\bar{L}). \tag{8.4}$$

Lemmata 8.4, 8.5, 8.6 and 8.7 correspond respectively to Lemmata 6.5, 6.6, 6.1 and 6.4 in [25].

8.2 Convergent series

Lemma 8.8 (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

$$\sum_{\substack{1 \leq j \leq \rho \\ j' \geq \rho}} \frac{1 + j^n}{(j + j')^{q+n}} \leq \frac{C}{\rho^{q-2}}.$$

Lemma 8.9 (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 8.9
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

$$\begin{aligned}\sum_{\substack{j\geq\rho\\ j'\geq 0}}\frac{1+j^n}{(j+j')^{q+n}} &\leq \sum_{\substack{j\geq\rho\\ j'\geq 0}}\int_{(j,j')+[0,1]^2}\frac{1+x^n}{(x+y-2)^{q+n}}dxdy\\ &= \int_{x\geq\rho,y\geq 0}\frac{1+x^n}{(x+y-2)^{q+n}}dxdy\\ &= \int_{x\geq\rho}\frac{1+x^n}{(q+n-1)(x-2)^{q+n-1}}dx\\ &\leq C_1\int_{\bar{x}\geq\rho-2}\frac{1}{(q+n-1)\bar{x}^{q-1}}d\bar{x}\\ &\leq \frac{C_2}{(\rho-2)^{q-2}}\\ &\leq \frac{C}{\rho^{q-2}},\end{aligned}$$

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.

□

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