Geometry optimization for crystals in Thomas-Fermi type theories of solids

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Abstract

We study here the problem of geometry optimization for a crystal in the TFW solid-state setting, i.e the problem of minimizing the TFW energy with respect to the periodic lattice defining the positions of the nuclei. We show the existence of such a minimum, and use for that purpose the TFW models of polymers and thin films defined in a previous work [5].

Contents

1 Introduction

We are interested here in the Thomas-Fermi-Von Weizscker (TFW) theory of solids, and more precisely in the geometry optimization problem, which may be stated in the following way : given the energy functional which to a periodic lattice associates its TFW energy (defined in [9]), does there exist a periodic lattice minimizing this energy ?

Let ℓ be a proper periodic lattice of $\mathbf{R}^3$, that is, a subgroup of $(\mathbf{R}^3,+)$ generated by three linearly independent vectors a, b, and c. We define the TFW energy of this lattice with respect to basis (a,b,c), i.e the TFW energy of a neutral crystal of lattice ℓ, with each nucleus of charge $+1$:

$$\mathcal{E}(\ell) = \inf\left\{ E^{TFW}_{(a,b,c)}(\rho), \quad \rho \geq 0, \quad \sqrt{\rho} \in H^1_{per}(\ell), \quad \int_{\Gamma_{(a,b,c)}} \rho = 1 \right\}, \tag{1.1}$$

where we used the following notation :

$$\Gamma_{(a,b,c)} = \left\{ ta + sb + rc, \quad t, r, s \in [-\frac{1}{2}, \frac{1}{2}[\right\}, \tag{1.2}$$

$$H^1_{per}(\ell) = \left\{ f \in H^1_{loc}(\mathbf{R}^3), \quad f \quad \text{is} \quad \ell - \text{periodic} \right\}, \tag{1.3}$$

and, skipping here the subscript (a, b, c) for $\Gamma_{(a,b,c)} = \Gamma$:

$$E^{TFW}_{(a,b,c)}(\rho) = \int_\Gamma |\nabla\sqrt{\rho}|^2 + \int_\Gamma \rho^{5/3} - \int_\Gamma G_\ell \rho + \int_\Gamma \int_\Gamma \rho(x)\rho(y)G_\ell(x-y)dxdy, \tag{1.4}$$

the potential G_ℓ being the ℓ-periodic solution of :

$$\begin{cases} -\Delta G_\ell = 4\pi\big((\sum_{k\in\ell} \delta_k) - \frac{1}{|\Gamma_{(a,b,c)}|}\big), \\ \lim_{x\to 0}\big(G_\ell(x) - \frac{1}{|x|}\big) = 0. \end{cases} \tag{1.5}$$

A preliminary observation is that these notations do not depend on the choice of the basis (a, b, c). This is stated in Proposition 2.1 below : equations (1.1), (1.4) and (1.5) do not depend on the choice of a basis of ℓ, but only on ℓ.

We now make precise the problem we are studying : denoting by $\mathcal{L}_3(\mathbf{R}^3)$ the set of proper periodic lattices of $\mathbf{R}^3$, does the problem

$$\mathcal{I} = \inf\left\{ \mathcal{E}(\ell), \quad \ell \in \mathcal{L}_3(\mathbf{R}^3) \right\} \tag{1.6}$$

have a solution ?

Our main result is :

Theorem 1.1 *Any minimizing sequence of problem (1.6) is relatively compact. Therefore, this problem has at least one solution.*

In order to show this result, we begin with recalling in Section 3 the definition and basic properties of what we call degenerate cases of the above solid state theory (1.1)-(1.4), namely the atomic model (3.1)-(3.2), and the linear polymer (3.6)-(3.8) and thin film (3.37)-(3.39) models. We refer to [3] and [7] for a study of the atomic model, and to [5] for a study of polymer and thin film models. Moreover, we show in Section 3 some further results similar to those of [7] : in particular we show the positiveness of the associated Lagrange multiplier, and give sharp estimates on the decay at infinity of the density. These estimates will be of crucial importance in the sequel.

In Section 4, we investigate the behavior of the minimizing sequences of problem (1.6). Up to rather technical complications that will be dealt with below but that we prefer to skip in this simplified presentation, it is sufficient to consider minimizing sequences of the form :

$$\ell_n = \left\{ iR^n_1 a + jR^n_2 b + kR^n_3 c, \quad i, j, k \in \mathbf{Z} \right\}, \tag{1.7}$$

with $0 < R_1^n \le R_2^n \le R_3^n$, and (a, b, c) is a fixed basis such that $|a| = |b| = |c| = 1$.

Hence, showing Theorem 1.1 amounts to prove that R_i^n is bounded both from above and away from 0, for all $i = 1, 2, 3$. For this purpose, we show the following proposition :

Proposition 1.2

(i) If R_1^n goes to infinity as n goes to infinity, then the energy $\mathcal{E}(\ell_n)$ converges to the atomic TFW energy.

(ii) If R_1^n converges to some $R_1 > 0$, and R_2^n goes to infinity as n goes to infinity, then $\mathcal{E}(\ell_n)$ converges to the TFW energy of a linear polymer defined by $R_1 a$.

(iii) If (R_1^n, R_2^n) goes to (R_1, R_2), with $R_1, R_2 > 0$, and R_3^n goes to infinity as n goes to infinity, then $\mathcal{E}(\ell_n)$ converges to the TFW energy of a thin film defined by $(R_1 a, R_2 b)$.

Once this proposition is proved, we show with the help of the results of Section 3 that for any of the atomic, polymer and solid film TFW energies, there exists a proper lattice having strictly lower energy than those limits. This is done in Section 5, through the fact that the limits of Proposition 1.2 are asymptotically approached from below. Note that the positiveness of the Lagrange multiplier plays a key-role here. We also show in this Section, in order to complete the proof of Theorem 1.1, that the radii R_i^n are bounded away from 0, with the help of Teller's Lemma [13]. As a by-product of these proofs, we finally prove that in TF theory, any proper lattice has greater energy than the atomic TF energy, which shows that the analogue of problem (1.6) in the TF setting has no solution. This corroborates the fact that our whole argument in the TFW case is based on the positiveness of the Lagrange multiplier in the degenerate problems (atomic, polymer and solid film cases). Indeed, one may check that in the atomic TF model, the Lagrange multiplier is 0.

Remark 1.3 *Let us point out that here, we have used a different normalization than in [13] and [8, 9] for the potential G_ℓ. This is due to the fact that the constant M appearing in [13] and [8, 9] depends in fact on ℓ. Our renormalization (1.5) cancels M, or more precisely includes it in the expression of G_ℓ. This allows us to write $\mathcal{E}(\ell)$ as the exact limit of the energy per nuclei in the thermodynamic limit process, as may be seen in (5.2).*

Let us mention that the results detailed here have been announced in [6].

2 Notation and representation of lattices

Throughout this paper, we will use the following notation :

Definition 2.1

(i) A subset ℓ of $\mathbf{R}^3$ will be said to be a proper lattice, or a lattice of dimension 3 (or of rank 3), if there exists three independent vectors (a, b, c) such that $\ell = \{ia+jb+kc, \quad i, j, k \in \mathbf{Z}\}$. We denote by $\mathcal{L}_3(\mathbf{R}^3)$ the set of proper lattices of $\mathbf{R}^3$.

(ii) A subset of $\mathbf{R}^3$ of the form $\{ia + jb, \quad i, j \in \mathbf{Z}\}$, with a, b linearly independent will be called a lattice of dimension 2. The set of 2-dimensional lattices will be denoted by $\mathcal{L}_2(\mathbf{R}^3)$.

(iii) A subset ℓ of $\mathbf{R}^3$ will be said to be a lattice of dimension 1 if there exists $a \in \mathbf{R}^3 \setminus \{0\}$ such that $\ell = \{ia, \ i \in \mathbf{Z}\}$. We denote by $\mathcal{L}_1(\mathbf{R}^3)$ the set of lattices of dimension 1.

Identifying $\mathcal{L}_3(\mathbf{R}^3)$ with the quotient group $GL_3(\mathbf{R})/GL_3(\mathbf{Z})$, we define on $\mathcal{L}_3(\mathbf{R}^3)$ a topology. (We denote by $GL_3(\mathbf{Z})$ the set of matrices belonging to $GL_3(\mathbf{R})$, having integer entries, and such that their inverse have integer entries.) For this topology, $\mathcal{L}_3(\mathbf{R}^3)$ is a separated locally compact manifold. After having checked out that $\mathcal{E}$ is well-defined on $\mathcal{L}_3(\mathbf{R}^3)$, we then study its continuity on this manifold :

Proposition 2.1 *The function $\mathcal{E}$ defined in (1.1) and the potential defined in (1.5) do not depend on the choice of the basis (a, b, c).*

Proof : We choose two different basis (a, b, c) and (a', b', c') of the same proper lattice ℓ, and denote respectively by $\mathcal{E}$ and $\mathcal{E}'$ the associated energy. We know that there exists M in $GL_3(\mathbf{Z})$ such that $a' = Ma$, $b' = Mb$, and $c' = Mc$. M being invertible in the set $M_3(\mathbf{Z})$ of integer 3×3-matrices, its determinant must be invertible in $\mathbf{Z}$, so we have :

$$|\det M| = 1.$$

This implies in particular that $|\Gamma_{(a,b,c)}| = |\Gamma_{(a',b',c')}|$, so that the potential defined from (a, b, c) in (1.5) must be equal to the one defined by (a', b', c'). Next, we notice that for any ℓ-periodic function f, we have :

$$\int_{\Gamma_{(a,b,c)}} f = \int_{\Gamma_{(a',b',c')}} f.$$

This implies, for any $\rho \geq 0$ such that $\sqrt{\rho} \in H^1_{per}(\ell)$:

$$E^{TFW}_{(a,b,c)}(\rho) = E^{TFW}_{(a',b',c')}(\rho), \tag{2.1}$$

and

$$\int_{\Gamma_{(a,b,c)}} \rho = \int_{\Gamma_{(a',b',c')}} \rho. \tag{2.2}$$

(2.1) and (2.2) then imply that $\mathcal{E} = \mathcal{E}'$. $\diamondsuit$

Remark 2.2 *Note that one easily proves in the same fashion that for any orthogonal matrix M, the energy is unchanged under M, that is, $\mathcal{E}(\ell) = \mathcal{E}(M\ell)$. This will be useful in the sequel.*

Note also that up to minor modifications, Proposition 2.1 also holds for polymers and thin films models defined in Section 3.

Now that the function $\mathcal{E}$ is well-defined, we may show that it is continuous :

Proposition 2.3 *The function $\mathcal{E}$ is continuous with respect to the quotient topology of $\mathcal{L}_3(\mathbf{R}^3)$.*

Proof : The only thing to show here is that $\mathcal{E}$ is continuous as a function defined on $GL_3(\mathbf{R})$. This is easy to do by changing variables in the expression of $E^{TFW}_{(a,b,c)}$ and noticing that if (a,b,c) is close enough to (a',b',c'), then the norm $\|G_\ell - G_{\ell'}\|_{L^1(\Gamma_{(a,b,c)}\cup\Gamma_{(a',b',c')})}$ is small. (Here we denote by ℓ and ℓ' respectively the lattices of basis (a,b,c) and (a',b',c').) $\diamondsuit$

We now state a result on the representation of a lattice by one of its basis, referring to [10] for its proof :

Theorem 2.4 (Engel, [10]) *For any periodic lattice ℓ of rank 3, there exists a basis (a,b,c) of ℓ such that :*

$$\left\{\begin{array}{l} |a| \le |b| \le |c|, \\ \widehat{(a,b)}, \widehat{(a,c)}, \widehat{(b,c)} \in [\frac{\pi}{3}, \frac{\pi}{2}], \end{array}\right. \tag{2.3}$$

where $\widehat{(x,y)}$ denotes the angle between x and y.

We thus see that, according to Proposition 2.1 and Theorem 2.4, we may reduce any minimizing sequence to the form (1.7), up to the fact that (a,b,c) will not be fixed but satisfy conditions (2.3).

3 Preliminary results on the degenerate cases

We recall in this section the definitions of what we call here the degenerate models, namely thin film models, polymers models and atomic model in the TFW setting. We refer to [5] concerning precisions on the first two models, and to [13] and [7] for the latter. In the thin film and polymer cases, we also show further results, mainly on the asymptotic behavior of the density far away from the nuclei.

3.1 TFW theory of atoms

We first recall the definition and the main properties of the TFW theory of atoms : the ground state of an atom consisting of a point nucleus of charge +1 located at 0 and of an electron is determined by its electronic density, unique solution of the problem :

$$I^{TFW}_{at} = \inf\left\{ E^{TFW}_{at}(\rho), \quad \rho \ge 0, \quad \sqrt{\rho} \in H^1(\mathbf{R}^3), \quad \int_{\mathbf{R}^3} \rho = 1 \right\}, \tag{3.1}$$

where the energy functional E^{TFW}_{at} is defined by :

$$E^{TFW}_{at}(\rho) = \int_{\mathbf{R}^3} |\nabla\sqrt{\rho}|^2 + \int_{\mathbf{R}^3} \rho^{5/3} - \int_{\mathbf{R}^3} \frac{\rho}{|x|} + \frac{1}{2}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dxdy. \tag{3.2}$$

Problem (3.1) has a unique solution ρ_{at} (see [13] or [3]), which is positive, and which square root $u_{at} = \sqrt{\rho_{at}}$ satisfies the following Euler-Lagrange equation, with a Lagrange multiplier $\theta = \theta_{at} > 0$:

$$-\Delta u_{at} + \frac{5}{3}u_{at}^{7/3} + \big(-\frac{1}{|x|} + u_{at}^2 \star \frac{1}{|x|}\big)u_{at} + \theta_{at}u_{at} = 0. \tag{3.3}$$

It is shown in [7] that the following estimates hold :

$$\rho_{at}(x) \sim \frac{a}{|x|^2}e^{-2\sqrt{\theta}|x|}, \quad \text{as} \quad |x| \longrightarrow \infty, \tag{3.4}$$

where a is a positive constant. The effective potential $\phi_{at} = \frac{1}{|x|} - \rho_{at} \star \frac{1}{|x|}$ satisfies :

$$\phi_{at}(x) \sim \frac{\pi a}{\theta|x|^2}e^{-2\sqrt{\theta}|x|}, \quad \text{as} \quad |x| \longrightarrow \infty. \tag{3.5}$$

3.2 TFW theory of polymers

We now consider the TFW model of polymers, as defined in [5], and which we recall here. Considering a periodic lattice of rank 1, that is some $\ell \in \mathcal{L}_1(\mathbf{R}^3)$, we may assume with no loss of generality that it is located on the vertical axis; that is, $\ell = \mathbf{Z}Re_3$, with $R \in \mathbf{R}_+^*$. We define its TFW energy as follows :

$$\begin{aligned}\mathcal{E}(\ell) = I_{pol}^{TFW}(\ell) &= \inf\Big\{E_\ell^{TFW}(\rho), \quad \rho \geq 0, \quad \sqrt{\rho} \in H^1_{per}(\ell), \\ &\qquad \log(2+|x|)\rho \in L^1(\Gamma(\ell)), \quad \int_{\Gamma(\ell)} \rho = 1\Big\},\end{aligned} \tag{3.6}$$

where $\Gamma(\ell) = \{x \in \mathbf{R}^3, \quad x_3 \in [-\frac{R}{2}, \frac{R}{2}[\}$,

$$H^1_{per}(\ell) = \Big\{f \in H^1_{loc}(\mathbf{R}^3) \cap H^1(\Gamma(\ell)), \quad f \quad \text{is} \quad \ell-\text{periodic}\Big\},$$

and the energy E_ℓ^{TFW} reads :

$$\begin{aligned}E_\ell^{TFW}(\rho) &= \int_{\Gamma(\ell)} |\nabla\sqrt{\rho}|^2 + \int_{\Gamma(\ell)} \rho^{5/3} - \int_{\Gamma(\ell)} G_\ell\rho \\ &+ \int_{\Gamma(\ell)}\int_{\Gamma(\ell)} \rho(x)\rho(y)G_\ell(x-y)dxdy,\end{aligned} \tag{3.7}$$

the periodic potential G_ℓ being defined by :

$$\begin{aligned}G_\ell(x) &= C_\ell - \frac{2}{R}\log|x'| + \sum_{k\in\ell}\left(\frac{1}{|x-ke_3|} - \frac{1}{R}\int_{-\frac{R}{2}}^{\frac{R}{2}} \frac{dt}{|x-(k+t)e_3|}\right) \\ &= C_\ell - \frac{2}{R}\log|x'| + \frac{1}{\pi R}\sum_{k\in\mathbf{Z}\setminus\{0\}}\int_{\mathbf{R}^2}\end{aligned}$$

$\mathrm{e}^{2i\pi(\frac{k}{R}x_3+x'\cdot\xi)}\frac{}{\frac{k^2}{R^2}+|\xi|^2 d\xi,(3.8)}$ the constant C_ℓ being chosen so that we have $\lim_{x\to 0}(G_\ell(x)-\frac{1}{|x|})=0$, and x' denoting the vector (x_1,x_2). We recall a few properties of the potential G_ℓ shown in [5] :

Proposition 3.1 *We have :*

(i) G_ℓ *is smooth on* $\mathbf{R}^3\setminus\ell$*,*

(ii) $G_\ell(x)=\frac{1}{|x|}+O(|x|)$ *as* $x\to 0$*,*

(iii) $G_\ell(x)=-\frac{2}{R}\log|x'|+C_\ell+O(\frac{1}{|x'|})$ *as* $|x'|\to\infty$*, uniformly with respect to* x_3*.*

We now show the following :

Proposition 3.2 *For any* $R>0$*, the problem (3.6) has a unique solution* ρ_ℓ*. The function* $u_\ell=\sqrt{\rho_\ell}$ *is a solution of :*

$$-\Delta u_\ell+\frac{5}{3}u_\ell^{7/3}+(u_\ell^2\star_{\Gamma(\ell)}G_\ell-G_\ell)u_\ell+\theta_\ell u_\ell=0, \tag{3.9}$$

where $\star_{\Gamma(\ell)}$ *denotes the convolution product over the set* $\Gamma(\ell)$*. Moreover, the Lagrange multiplier* θ_ℓ *is positive.*

Proof : We refer to [5] for the proof of the existence and uniqueness of ρ_ℓ. Moreover, we recognize in (3.9) the Euler-Lagrange equation of problem (3.6). We now prove that θ_ℓ is positive.

Denoting by ϕ_ℓ the function

$$\phi_\ell=G_\ell-u_\ell^2\star_{\Gamma_\ell}G_\ell,$$

it is possible to show the following a priori estimates (see [5], Proposition 2.5) :

$$0<u_\ell\leq\frac{C}{1+|x'|^{3/2}}, \tag{3.10}$$

$$\phi_\ell-\theta_\ell\leq\frac{C}{1+|x'|^2}\quad\text{on}\quad\{|x'|>1\}. \tag{3.11}$$

We claim that

$$\phi_\ell\longrightarrow 0\quad\text{as}\quad|x'|\to\infty. \tag{3.12}$$

In order prove our claim, we denote by G_ℓ^0 the potential $G_\ell-C_\ell$, and notice that we have :

$$\phi_\ell=G_\ell^0-u_\ell^2\star_{\Gamma(\ell)}G_\ell^0.$$

Hence, we have :

$$\begin{aligned}\phi_\ell(x) &= \int_{\Gamma(\ell)} (G^0_\ell(x) - G^0_\ell(x-y))u^2_\ell(y)dy,\\ &= \int_{\Gamma(\ell)\cap\{|y'|<|x'|^{1/2}\}} (G^0_\ell(x) - G^0_\ell(x-y))u^2_\ell(y)dy\\ &\quad + \int_{\Gamma(\ell)\cap\{|y'|>|x'|^{1/2}\}} (G^0_\ell(x) - G^0_\ell(x-y))u^2_\ell(y)dy.\end{aligned}$$

If $|y'| < |x'|^{1/2} \ll |x'|$ as $|x'| \to \infty$, we have, from Proposition 3.1-(iii) :

$$G^0_\ell(x) - G^0_\ell(x-y) = -\frac{2}{R}\Big(\log(|x'|) - \log(|x'-y'|)\Big) + O(\frac{1}{|x'|}).$$

Developing this expression with respect to $\frac{|y|}{|x'|}$, we find :

$$\left|\int_{\Gamma(\ell)\cap\{|y'|<|x'|^{1/2}\}} \Big(G^0_\ell(x) - G^0_\ell(x-y)\Big)u^2_\ell(y)dy\right| \leq \frac{C}{|x'|^{1/2}}. \tag{3.13}$$

In order to deal with the second term, we use (3.10) and show that :

$$\left|\int_{\Gamma(\ell)\cap\{|y'|>|x'|^{1/2}\}} \Big(G^0_\ell(x) - G^0_\ell(x-y)\Big)u^2_\ell(y)dy\right| \leq \frac{C\log|x'|}{|x'|}.$$

This, together with (3.13), proves (3.12). Using estimate (3.11), we infer that

$$\theta_\ell \geq 0.$$

We assume from now on that we have $\theta_\ell = 0$, and try to reach a contradiction, which will conclude the proof.

Since there is no ambiguity here, we skip the subscript ℓ for the rest of the proof. From the uniqueness of u and the definition of ϕ, these functions depend on x' only through $|x'| = r$. We set

$$\overline{\phi}(r) = \frac{1}{R}\int_{-\frac{R}{2}}^{\frac{R}{2}} \phi(r, x_3)dx_3,$$

and

$$\overline{\rho}(r) = \frac{1}{R}\int_{-\frac{R}{2}}^{\frac{R}{2}} \rho(r, x_3)dx_3.$$

From the definition of ϕ, we have :

$$-\overline{\phi}'' - \frac{1}{r}\overline{\phi}' = -4\pi\overline{\rho}$$

on $\mathbf{R}_+ \setminus \{0\}$. Hence, using (3.10) :

$$0 \leq (r\overline{\phi}')' \leq \frac{C}{r^2}. \tag{3.14}$$

This shows that $(r\overline{\phi}')'$ is integrable on a neighborhood of $+\infty$. We now integrate (3.14) from $r > 0$ to ∞, and get :

$$r\overline{\phi}'(r) - \lim_{t\to\infty}(t\overline{\phi}'(t)) \leq 0.$$

Denoting by l the limit $\lim_{t\to\infty}(t\overline{\phi}'(t))$, which exists in virtue of (3.14), and assuming it to be different from 0, we deduce that $\overline{\phi}'(t) \sim \frac{l}{t}$ as t goes to infinity. This implies that $\overline{\phi}$ goes to $\pm\infty$ at infinity, which is a contradiction with estimate (3.11). Hence, $\overline{\phi}'$ is non-positive at infinity, which implies, in view of (3.12), that

$$\overline{\phi} \geq 0 \quad \text{for} \quad r \geq r_0. \tag{3.15}$$

It follows that :

$$\exists R_0 > 0, \quad \forall r \geq R_0, \quad \exists x_3 \in [-\frac{R}{2}, \frac{R}{2}[, \quad \phi(r, x_3) \geq 0. \tag{3.16}$$

On the other hand, we have, using Hlder estimates, for any ball B of radius 1, and any $v \in C^{2,\alpha}(B)$ for some $\alpha > 0$, (see [12] or [11])

$$\|\nabla v\|_{C^0(\frac{1}{2}B)} \leq \gamma\Big(\|\Delta v\|_{C^0(B)} + \|v\|_{C^0(B)}\Big),$$

where $\frac{1}{2}B$ denotes the ball of radius $\frac{1}{2}$ having the same center as B, and γ being a universal constant. Hence, from a scaling argument, we deduce that for any ball B_a of radius $a > 0$, and any $v \in C^{2,\alpha}(B_a)$,

$$\|\nabla v\|_{C^0(\frac{1}{2}B_a)} \leq \gamma\Big(a\|\Delta v\|_{C^0(B_a)} + \frac{1}{a}\|v\|_{C^0(B_a)}\Big). \tag{3.17}$$

Applying this inequality to ϕ, we find, for any ball B_a of radius $a > 0$ not containing 0 :

$$\|\nabla \phi\|_{C^0(\frac{1}{2}B_a)} \leq \gamma\Big(a\|\rho\|_{C^0(B_a)} + \frac{1}{a}\|\phi\|_{C^0(B_a)}\Big). \tag{3.18}$$

Using estimate (3.10) and the fact that ϕ is periodic and bounded as $r \to \infty$, and applying (3.18) with $a = \frac{|x|}{2}$, B_a centered at x, we thus find :

$$|\nabla \phi| \leq \frac{C}{r} \quad \text{as} \quad r \longrightarrow \infty.$$

In particular, we have this bound on $|\partial_3 \phi|$. Hence, from property (3.16), we infer that :

$$\phi(x) \geq -\frac{CR}{r} \quad \text{as} \quad r \longrightarrow \infty.$$

Inserting this information in (3.18), and using again (3.16), we find that $\phi \geq -\frac{C}{r^2}$ for sufficiently large r, hence, again from (3.11) :

$$|\phi(x)| \leq \frac{C}{r^2} \quad \text{as} \quad r \longrightarrow \infty.$$

We now apply again (3.18) on ϕ, but with $B_a = B_{\sqrt{r}}(x)$, and find that $\phi \geq -\frac{C}{r^{5/2}}$. Hence, using (3.11), we have :

$$-\frac{C}{r^{5/2}} \leq \phi(x) \leq \frac{C}{r^2} \quad \text{as} \quad r \to \infty. \tag{3.19}$$

With this result, we are going to show that $V = \frac{5}{3}u^{4/3} - \phi \leq \frac{1}{r^2}$.

This estimate, in the spirit of a work by Benguria and Yarur [2], will imply that $u \geq \frac{C}{r}$, which contradicts (3.10).

In view of equations (3.9) and (3.19), and the fact that $\theta = 0$, we infer that

$$-\Delta u + \frac{5}{3}u^{7/3} \geq -\frac{C}{r^4},$$

on the set $\{r > r_0\}$, for some $r_0 > 0$. Hence, denoting by u_0 the function $\frac{3}{10r^{3/2}}$, one computes easily :

$$-\Delta(u - u_0) + \frac{5}{3}(u^{7/3} - {u_0}^{7/3}) \geq (\frac{9}{4} - \frac{5}{3}(\frac{3}{10})^{7/3})\frac{1}{r^{7/2}} - \frac{C}{r^4}. \tag{3.20}$$

Since $\frac{9}{4} - \frac{5}{3}(\frac{3}{10})^{7/3} > 0$, it is then clear that there exists an $r_1 > 0$ such that on the set $\{r > r_1\}$, $v = u - u_0$ satisfies the following :

$$\Delta v \leq \frac{5}{3}(u^{7/3} - {u_0}^{7/3}).$$

Defining $F = \{r > r_1\} \cap \{v < 0\}$, we now show the following assertions :

(a) F is unbounded,

(b) F has no bounded connected component strictly included in $\{r > r_1\}$.

In order to show (a), we assume that F is bounded, and notice that then there exists r_2 such that $v \geq 0$ on $\{r > r_2\}$. Hence, on this set,

$$\Delta\phi \geq \frac{6\pi}{5r^3}.$$

This means in particular :

$$(r\overline{\phi}')' \geq \frac{6\pi}{5r^2}.$$

Integrating this inequality from r to $+\infty$, one finds $\overline{\phi}' \leq -\frac{6\pi}{5r^2}$, hence

$$\overline{\phi} \geq \frac{6\pi}{5r},$$

which is in contradiction with estimate (3.11).

We now show (b) by supposing that F has at least one bounded connected component F_0 such that $\{r = r_1\} \cap F_0 = \emptyset$. On F_0, $\Delta v < 0$, and $v = 0$ on ∂F_0. Hence from the maximum principle, v must be non-negative on F_0, which is contradictory.

Using (a) and (b), we deduce that (3.16) holds for $-v$:

$$\exists R_0 > 0, \quad \forall r \geq R_0, \quad \exists x_3 \in [-\frac{R}{2}, \frac{R}{2}[, \quad u(r, x_3) \leq \frac{3}{10r^{3/2}}.$$

Now, from the equation satisfied by u, it is clearly possible to show, using the same Hlder estimate as for ϕ, that

$$|\partial_3 u| \leq \frac{C}{r^{5/2}}.$$

This implies that, as $r \to \infty$, $u \leq \frac{3}{5r^{3/2}}$, and in particular :

$$V = \frac{5}{3}u^{4/3} - \phi \leq \frac{1}{r^2}.$$

The final step of the proof is merely a copy of Benguria and Yarur's proof [2] : $\overline{u}(r) = \int_{-\frac{R}{2}}^{\frac{R}{2}} u(r, x_3)dx_3$ satisfies :

$$-\overline{u}'' - \frac{1}{r}\overline{u}' + \frac{1}{r^2}\overline{u} \geq 0,$$

whenever $r > R_1$, for some $R_1 > 0$. Denoting by w the function $\overline{u} - \frac{\alpha}{r}$, where α is chosen so that $w > 0$ somewhere in $]R_1, \infty[$, we see that

$$-w'' - \frac{1}{r}w' + \frac{1}{r^2}w \geq 0 \tag{3.21}$$

on this set. And if w is negative at some point of $]R_1, \infty[$, it must have a negative minimum, which is in contradiction with (3.21). This shows that $u \geq \frac{C}{r}$. This is in contradiction with (3.10). $\Diamond$

Proposition 3.3 *The unique solution ρ_ℓ of problem (3.6) satisfies the following, where $a_\ell > 0$ depends only on ℓ :*

$$\rho_\ell(r, x_3) \sim a_\ell \frac{e^{-2\sqrt{\theta_\ell} r}}{r}, \quad as \quad r \longrightarrow \infty. \tag{3.22}$$

Moreover, setting $\phi_\ell = G_\ell - G_\ell \star_{\Gamma(\ell)} \rho_\ell$ the effective potential, there exists a finite set of complex numbers λ_k depending only on ℓ such that :

$$\left| \phi_\ell(r, x_3) - \sum_{0 < \pi|k| \leq R\sqrt{\theta_\ell}} \lambda_k e^{2i\pi \frac{k}{R} x_3} W_{2\pi \frac{|k|}{R}}(r) \right| \leq b_{\ell,\epsilon} \frac{e^{-(2\sqrt{\theta_\ell} - \epsilon) r}}{\sqrt{r}}, \quad as \quad r \longrightarrow \infty, \tag{3.23}$$

for all $\epsilon > 0$. The constant $b_{\ell,\epsilon} > 0$ depends only on ℓ and ϵ, and W_a denotes the Yukawa potential of parameter $a > 0$ in $\mathbf{R}^2$, i.e the solution of $-\Delta f + a^2 f = 4\pi\delta_0$ in $\mathbf{R}^2$ vanishing at infinity.

Proof : We begin with a few properties of the Yukawa potential W_a of $\mathbf{R}^2$, with $a > 0$: W_a is the unique solution vanishing at infinity of :

$$-\Delta W_a + a^2 W_a = 4\pi\delta_0. \tag{3.24}$$

The potential W_a is spherically symmetric and satisfies the differential equation :

$$W_a'' + \frac{1}{r}W_a' - a^2 W_a = 0$$

on $\mathbf{R}_*^+$. Here $'$ denotes the radial derivative in $\mathbf{R}^2$. For all the following properties, we use the notation of [1], in which one may find these results. We refer to [17] concerning their proofs. The modified Bessel functions I_0 and K_0 are defined by :

$$I_0(t) = \sum_{n\geq 0}\left(\frac{t^n}{2^n n!}\right)^2,$$

$$K_0(t) = -\big(\log(\frac{t}{2}) + \gamma\big)I_0(t) + \sum_{n\geq 1}\left(\sum_{j=1}^{n}\frac{1}{j}\right)\left(\frac{t^n}{2^n n!}\right)^2,$$

where $\gamma = \lim_{n\to\infty}(\sum_{j=1}^n \frac{1}{j} - \log n)$ denotes the Euler constant. We have :

(a) The potential W_a is equal to the modified Bessel function K_0 :

$$W_a(t) = 2K_0(at).$$

(b) We denote by $\overline{W}_a$ the potential

$$\overline{W}_a(t) = 2K_0(at) + 2\pi I_0(at).$$

It is a solution of (3.24).

(c) The functions W_a and $\overline{W}_a$ are respectively decreasing and increasing, and satisfy the following estimates :

$$\begin{cases} W_a(t) \sim \sqrt{\frac{2\pi}{a}}\frac{e^{-at}}{\sqrt{t}} & \text{as} \quad t\to\infty, \\ W_a(t) \sim -2\log(t) & \text{as} \quad t\to 0. \end{cases} \tag{3.25}$$

$$\begin{cases} \overline{W}_a(t) \sim \sqrt{\frac{2\pi}{a}}\frac{e^{at}}{\sqrt{t}} & \text{as} \quad t\to\infty, \\ \overline{W}_a(t) \sim -2\log(t) & \text{as} \quad r\to 0. \end{cases} \tag{3.26}$$

$$\overline{W}_a' W_a - W_a'\overline{W}_a = \frac{4\pi}{t}. \tag{3.27}$$

Keeping these results in mind, we may now begin our proof.

We denote by V_ℓ the ℓ-periodic Yukawa potential with parameter $\sqrt{\theta_\ell}$:

$$V_\ell(x) = \sum_{k\in\ell} \frac{e^{-\sqrt{\theta_\ell}|x-k|}}{|x-k|}. \tag{3.28}$$

Comparing it with $W_{\sqrt{\theta_\ell}}(r)$, where $r = \sqrt{x_1^2 + x_2^2}$, and noticing that

$$W_{\sqrt{\theta_\ell}}(r) = \int_{\mathbf{R}} \frac{e^{-\sqrt{\theta}_\ell(r^2+z^2)}}{\sqrt{r^2+z^2}} dz,$$

one shows through a basic computation that $\frac{V_\ell}{W_{\sqrt{\theta_\ell}}} \to 1$ as $r \to \infty$, hence :

$$V_\ell(x) \sim \left(\sqrt{\frac{2\pi}{\sqrt{\theta_\ell}}}\right) \frac{e^{-\sqrt{\theta}_\ell r}}{\sqrt{r}}, \tag{3.29}$$

as r goes to infinity.

Denoting by f_ℓ the function $\frac{5}{3}{u_\ell}^{4/3} - \phi_\ell$, and using the bounds we have on u_ℓ and ϕ_ℓ, namely (3.10) and (3.19), we deduce that

$$|f_\ell| \le \frac{C}{r^2}, \tag{3.30}$$

on $\{r > R_0\}$, for some $R_0 > 0$. Hence, we have there

$$-\Delta u_\ell + (\theta_\ell - \frac{C}{r^2})u_\ell \le -\Delta u_\ell + (f_\ell + \theta_\ell)u_\ell = 0.$$

Now, denoting by v the function $\frac{e^{-\sqrt{\theta_\ell} r}}{\sqrt{r}} e^{-\mu/r}$, one easily finds that :

$$-\Delta v + (\theta_\ell - \frac{C}{r^2})v = (\frac{2\mu\sqrt{\theta_\ell} - \frac{1}{4} - C}{r^2} + \frac{2\mu}{r^3} - \frac{\mu^2}{r^4})v.$$

Hence, choosing $\mu > \frac{4C+1}{8\sqrt{\theta_\ell}}$, we have :

$$-\Delta v + (\theta_\ell - \frac{C}{r^2})v \ge 0$$

on some set $\{r > R_1\}$. Next, by a similar computation, setting $w(x) = \sqrt{R}\frac{e^{\sqrt{\theta_\ell}(|x|-R)}}{|x|} e^{-\frac{\mu}{|x|}}$, one easily shows w satisfies the same estimate. Hence, taking $v + w$ as a supersolution, and letting then R go to infinity, one can show that this implies :

$$u_\ell \le Cv,$$

for some constant $C > 0$. In particular, we have

$$u_\ell \le \frac{a}{\sqrt{r}} e^{-\sqrt{\theta_\ell} r}, \quad \text{at} \quad \text{infinity}, \tag{3.31}$$

for some $a > 0$. Now, an easy computation, in the spirit of [7], Proposition A.1, shows that, from this estimate, together with (3.29) and (3.30), we have :

$$(-f_\ell u_\ell) \star_{\Gamma(\ell)} V_\ell \sim \sqrt{a}_\ell \frac{e^{-\sqrt{\theta_\ell} r}}{\sqrt{r}}, \quad \text{as} \quad r \to \infty,$$

with $\sqrt{a}_\ell = \frac{1}{2\pi} \int_0^{2\pi} e^{\sqrt{\theta_\ell} \cos\theta} d\theta \int_{\Gamma(\ell)} -f_\ell u_\ell$, which is positive since $-f_\ell u_\ell = -\Delta u_\ell + \theta_\ell u_\ell$. Hence, convoluting $-\Delta u_\ell + \theta_\ell u_\ell = -f_\ell u_\ell$ on both sides with V_ℓ, one finds (3.22).

We now prove (3.23) : we define a partial periodic Fourier transform by :

$$\tilde{f}(x', k) = \int_{-\frac{R}{2}}^{\frac{R}{2}} f(x) e^{-2i\pi \frac{k}{R} x_3} dx_3, \tag{3.32}$$

for any L^2_{loc} and ℓ-periodic function f. Applying this to ϕ_ℓ, and using the fact that $-\Delta\phi_\ell = 4\pi(\delta_0 - \rho_\ell)$ in $\Gamma(\ell)$, one finds :

$$-\Delta_T \tilde{\phi}_\ell(x', k) + 4\pi^2 \frac{k^2}{R^2} \tilde{\phi}_\ell(x', k) = 4\pi(\delta_{r=0} - \tilde{\rho}_\ell(x', k)), \tag{3.33}$$

for all $k \in \mathbf{Z}$, where Δ_T denotes the Laplacian with respect to x'. We first notice that

$$|\tilde{\phi}_\ell(x', 0)| \le C \frac{e^{-2\sqrt{\theta_\ell} r}}{r}, \tag{3.34}$$

since it is a radially symmetric function in $\mathbf{R}^2$ satisfying $(r\tilde{\phi}_\ell(r, 0)')' \sim a_\ell e^{-2\sqrt{\theta_\ell} r}$. Moreover, if $|k| \neq 0$, convoluting (3.33) with $W_{2\pi\frac{|k|}{R}}$, we have :

$$\tilde{\phi}_\ell = W_{2\pi\frac{|k|}{R}} - W_{2\pi\frac{|k|}{R}} \star_{\mathbf{R}^2} \tilde{\rho}_\ell.$$

We use here the following Lemma, which proof is postponed until the end of the present one :

Lemma 3.4 *Let a be a positive real, and let W_a and $\overline{W}_a$ be the potentials defined in (a) and (b) above. Then, for any spherically symmetric function $v \in L^1_{loc}(\mathbf{R}^2)$ such that $vW_a \in L^1(\mathbf{R}^2)$ and v has a trace on any circle of $\mathbf{R}^2$, we have :*

$$v \star W_a(x) = 8\pi^2 \left[\overline{W}_a(x) \int_{|y|>|x|} vW_a + W_a(x) \left(\int_{|y|<|x|} v\overline{W}_a - \int_{\mathbf{R}^2} vW_a \right) \right]. \tag{3.35}$$

Applying this result to $a = 2\pi\frac{|k|}{R}$ and $v = \tilde{\rho}_\ell(\cdot, k)$, which is spherically symmetric in $\mathbf{R}^2$, and using estimates (3.22), (3.25) and (3.26), one easily finds :

$$\Big(W_{2\pi\frac{|k|}{R}} \star_{\mathbf{R}^2} \tilde{\rho}_\ell\Big)(r) = \Big(\int_{\mathbf{R}^2} \tilde{\rho}_\ell \overline{W}_{2\pi\frac{|k|}{R}}\Big) W_{2\pi\frac{|k|}{R}}(r) + O\Big(\int_{|x'|>r} \tilde{\rho}_\ell\Big),$$

whenever $2\pi\frac{|k|}{R} < 2\sqrt{\theta_\ell}$. Thus, for such a k, setting $\lambda_k = \frac{1}{R} - \frac{1}{R}\int_{\mathbf{R}^2} \tilde{\rho}_\ell \overline{W}_{2\pi\frac{|k|}{R}}$,

$$\begin{aligned} \tilde{\phi}_\ell(x', k) &= R\lambda_k W_{2\pi\frac{|k|}{R}}(r) e^{2i\pi\frac{kx_3}{R}} + O\Big(\int_{|x'|>r} \tilde{\rho}_\ell\Big) \\ &= R\lambda_k W_{2\pi\frac{|k|}{R}}(r) e^{2i\pi\frac{kx_3}{R}} + O\Big(\frac{e^{-2\sqrt{\theta_\ell}r}}{\sqrt{r}}\Big). \end{aligned}$$

We next use Plancherel's formula and write :

$$\begin{aligned} \phi_\ell(x) &= \sum_{k\in\mathbf{Z}} \frac{1}{R}\tilde{\phi}_\ell(x', k) e^{2i\pi\frac{kx_3}{R}} \\ &= \sum_{0<\pi|k|\le R\sqrt{\theta_\ell}} \lambda_k W_{2\pi\frac{|k|}{R}}(r) e^{2i\pi\frac{kx_3}{R}} + \sum_{\pi|k|>R\sqrt{\theta_\ell}} \frac{1}{R}\tilde{\phi}_\ell(x', k) e^{2i\pi\frac{kx_3}{R}} + O\Big(\frac{e^{-2\sqrt{\theta_\ell}r}}{\sqrt{r}}\Big). \end{aligned}$$

Denoting by ψ_ℓ the function

$$\psi_\ell = \sum_{\pi|k|>R\sqrt{\theta_\ell}} \frac{1}{R}\tilde{\phi}_\ell(x', k) e^{2i\pi\frac{k}{R}x_3},$$

proving (3.23) amounts to show that

$$|\psi_\ell| \le C_\epsilon \frac{e^{-(2\sqrt{\theta_\ell}-\epsilon)r}}{\sqrt{r}},$$

for all $\epsilon > 0$. For this purpose, we notice that, using (3.35) again, we have, for all $|k| > \frac{R\sqrt{\theta_\ell}}{\pi}$:

$$|\tilde{\psi}_\ell(x', k)| = |\tilde{\phi}_\ell(x', k)| \le C\frac{e^{-2\sqrt{\theta_\ell}r}}{\sqrt{r}}.$$

On the other hand, from the fact that $\Delta\psi_\ell$ is smooth and that ψ_ℓ is bounded on $\{r > 1\}$, ψ_ℓ is bounded in $C^p(\Gamma(\ell) \cap \{r > 1\})$, for all $p \in \mathbf{N}$, so that we have :

$$|\tilde{\psi}_\ell(x', k)| \le C_p \frac{1}{|k|^p},$$

for all $p > 0$, with C_p depending only on p. Those two bounds, together with the definition of ψ_ℓ, allow to write, for any $\beta < 1$:

$$\begin{aligned} \int_{r=R_0} |\psi_\ell|^2 dx_3 &= \frac{1}{R} \sum_{\pi|k|>R\sqrt{\theta_\ell}} |\tilde{\psi}(R_0, k)|^2 \\ &\le C\frac{e^{-4\beta\sqrt{\theta_\ell}R_0}}{R_0} \sum_{\pi|k|>\sqrt{\theta_\ell}} \frac{C_p^{(2-2\beta)}}{|k|^{p(2-2\beta)}} + O(\frac{e^{-4\sqrt{\theta_\ell}R_0}}{R_0}). \end{aligned}$$

This is valid for all R_0 sufficiently large. We then choose $\beta = 1 - \frac{\epsilon}{2\sqrt{\theta_\ell}}$ and $p > \frac{1}{2-2\beta}$, and finally conclude through elliptic regularity and the fact that $|\Delta\psi_\ell| \leq C\frac{e^{-\sqrt{\theta_\ell}r}}{\sqrt{r}}$. $\diamondsuit$

Proof of Lemma 3.4 : We denote by $F(x)$ the function defined in (3.35). F is spherically symmetric, and using estimates (c) above, one easily shows that F vanishes at infinity. Hence, it is sufficient to prove that $-\Delta F + a^2 F = 8\pi^2 v$. For this purpose, we notice that :

$$-\Delta F = -F'' - \frac{1}{|x|}F'.$$

We then compute :

$$F'(|x|) = \overline{W}_a'(|x|)\int_{|y|>|x|} vW_a + W_a'(|x|)\left(\int_{|y|<|x|} v\overline{W}_a - \int_{\mathbf{R}^n} vW_a\right).$$

Thus, we have :

$$\begin{aligned}-\Delta F \quad &= \quad -\Delta\overline{W}_a\int_{|y|>|x|} vW_a - \Delta W_a\left(\int_{|y|<|x|} v\overline{W}_a - \int_{\mathbf{R}^n} vW_a\right) \\ &\quad\quad +\overline{W}_a'\int_{|y|=|x|} vW_a - W_a'\int_{|y|=|x|} v\overline{W}_a.\end{aligned}$$

This implies the following :

$$-\Delta F + a^2 F = v2\pi|x|(\overline{W}_a' W_a - W_a'\overline{W}_a).$$

We then use (3.27) and conclude the proof. $\diamondsuit$

Estimate (3.23) has been proved for ϕ_ℓ, but what will be really useful is the same estimate on the partial derivative $\partial_r\phi_\ell$, with $r = \sqrt{x_1^2 + x_2^2}$. Since the estimates we have used on ρ_ℓ also hold for $\partial_r\rho_\ell$, an easy adaptation of Proposition 3.3 shows :

Proposition 3.5 *Let ρ_ℓ be the unique solution of problem (3.6), and $\phi_\ell = G_\ell - G_\ell \star_{\Gamma(\ell)} \rho_\ell$. There exists a finite set of complex numbers μ_k depending only on ℓ such that :*

$$\left|\partial_r\phi_\ell(r, x_3) - \sum_{0<\pi|k|\leq R\sqrt{\theta_\ell}} \mu_k e^{2i\pi\frac{k}{R}x_3} W_{2\pi\frac{|k|}{R}}(r)\right| \leq b'_{\ell,\epsilon}\frac{e^{-(2\sqrt{\theta_\ell}-\epsilon)r}}{\sqrt{r}}, \quad as \quad r \to \infty, \qquad (3.36)$$

for all $\epsilon > 0$, the constant $b'_{\ell,\epsilon}$ depending only on ℓ and ϵ.

3.3 TFW theory of thin films

We recall the TFW model for thin films defined in [5] : considering a periodic lattice ℓ of rank 2, we may assume that it is included in the plane generated by the two first vectors of the canonical basis (e_1, e_2, e_3). In other words, there exists $R_1 > 0$ and $b = b_1e_1 + b_2e_2$, such that $a = R_1e_1$ and b generate ℓ :

$$\ell = \{ia + jb, \quad i, j \in \mathbf{Z}^2\}.$$

We define its TFW energy by :

$$\begin{aligned}\mathcal{E}(\ell) = I_{film}^{TFW} &= \Big\{E_\ell^{TFW}(\rho), \quad \rho \geq 0, \quad , \sqrt{\rho} \in H^1_{per}(\ell),\\ &\qquad (1+|x_3|)\rho \in L^1(\Gamma(\ell)), \quad \int_{\Gamma(\ell)} \rho = 1\Big\},\end{aligned} \tag{3.37}$$

where $\Gamma(\ell) = \{ua + vb + we_3, \quad u, v \in [-\frac{1}{2}, \frac{1}{2}[, \quad w \in \mathbf{R}\}$,

$$H^1_{per}(\ell) = \Big\{f \in H^1_{loc}(\mathbf{R}^3) \cap H^1(\Gamma(\ell)), \quad f \quad \text{is} \quad \ell-\text{periodic}\Big\},$$

and the energy E_ℓ^{TFW} reads :

$$\begin{aligned}E_\ell^{TFW}(\rho) &= \int_{\Gamma(\ell)} |\nabla\sqrt{\rho}|^2 + \int_{\Gamma(\ell)} \rho^{5/3} - \int_{\Gamma(\ell)} G_\ell \rho\\ &+ \int_{\Gamma(\ell)}\int_{\Gamma(\ell)} \rho(x)\rho(y)G_\ell(x-y)dxdy,\end{aligned} \tag{3.38}$$

the periodic potential G_ℓ being the analogue of (3.8), with $a \wedge b$ denoting the inner product of the two vectors a and b :

$$\begin{aligned}G_\ell(x) &= C_\ell - \frac{2\pi}{|a\wedge b|}|x_3| + \sum_{k\in\ell}\left(\frac{1}{|x-k|} - \frac{1}{|a\wedge b|}\int_{\Gamma(\ell)\cap\{x_3=0\}}\frac{dy}{|x-k-y|}\right)\\ &= C_\ell - \frac{2\pi}{|a\wedge b|}|x_3| + \frac{1}{\pi|a\wedge b|}\sum_{k\in\ell^*\setminus\{0\}}\int_{\mathbf{R}}\frac{e^{2i\pi(k\cdot x + x_3\xi)}}{|k|^2+\xi^2}d\xi,\end{aligned} \tag{3.39}$$

where C_ℓ is chosen so that $\lim_{x\to 0}(G_\ell(x) - \frac{1}{|x|}) = 0$, and ℓ^* is the reciprocal lattice to ℓ in the plane (e_1, e_2), that is, ℓ^* is the periodic lattice generated by the basis (a', b') of $\{x_3 = 0\}$ defined by $a \cdot a' = b \cdot b' = 1$, and $a \cdot b' = b \cdot a' = 0$.

Here again, we have the analogue of Proposition 3.1, proven in [5] :

Proposition 3.6 *We have :*

(i) G_ℓ *is smooth on* $\mathbf{R}^3 \setminus \ell$,

(ii) $G_\ell(x) = \frac{1}{|x|} + O(|x|)$ *as* $x \to 0$,

(iii) $G_\ell(x) = -\frac{2\pi}{|a\wedge b|}|x_3| + C_\ell + O(\frac{1}{|x_3|})$ *as* $|x_3| \to \infty$, *uniformly with respect to* (x_1, x_2).

We also have the following :

Proposition 3.7 *For any basis (a, b) of the plane generated by (e_1, e_2), the problem (3.37) has a unique solution ρ_ℓ. Setting $u_\ell = \sqrt{\rho_\ell}$, u_ℓ is a solution of :*

$$-\Delta u_\ell + \frac{5}{3} u_\ell^{7/3} + (u_\ell^2 \star_{\Gamma(\ell)} G_\ell - G_\ell) u_\ell + \theta_\ell u_\ell = 0, \tag{3.40}$$

with $\theta_\ell > 0$.

Proof : We skip this proof, since it is a straightforward adaptation of Proposition 3.2's. $\diamondsuit$

Next, we mimic the proof of Proposition 3.3 and find :

Proposition 3.8 *The solution ρ_ℓ of problem (3.37) satisfies the following estimate, where a_ℓ is a positive constant depending only on ℓ :*

$$\rho_\ell(x) \sim a_\ell e^{-2\sqrt{\theta_\ell}|x_3|}, \quad \textit{as} \quad |x_3| \longrightarrow \infty. \tag{3.41}$$

Denoting by $\phi_\ell = G_\ell - G_\ell \star_{\Gamma(\ell)} \rho_\ell$ the effective potential, there exists complex numbers μ_k such that, for all $\epsilon > 0$,

$$\left| \partial_3 \phi_\ell(r, x_3) - \sum_{0 < \pi|k| \leq \sqrt{\theta_\ell}, k \in \ell^*} \mu_k e^{2i\pi k \cdot x'} e^{-2\pi|k||x_3|} \right| \leq b_{\ell,\epsilon} e^{-(2\sqrt{\theta_\ell} - \epsilon)|x_3|}, \quad \textit{as} \quad |x_3| \to \infty, \tag{3.42}$$

with $b_{\ell,\epsilon} > 0$ depending only on ℓ and ϵ.

Proof : The only necessary change is to show the above estimate for the Yukawa potential :

$$V_\ell(x) = \sum_{k \in \ell} \frac{e^{-\sqrt{\theta_\ell}|x-k|}}{|x-k|} \sim \frac{2\pi}{\sqrt{\theta_\ell}} e^{-\sqrt{\theta_\ell}|x_3|} \quad \text{as} \quad |x_3| \to \infty,$$

which is easy to prove by comparing it to the one-dimensional Yukawa potential with respect to x_3, namely $\frac{2\pi}{\sqrt{\theta_\ell}} e^{-\sqrt{\theta_\ell}|x_3|}$. The partial Fourier transform defined in (3.32) is adapted as follows :

$$\tilde{f}(k, t) = \int_{\Gamma(\ell) \cap \{x_3 = t\}} f(x) e^{-2i\pi k \cdot x'} dx', \tag{3.43}$$

for all $k \in \ell^*$. And the role of $\overline{W}_a$ is played here by $e^{a|x_3|}$. $\diamondsuit$

4 Behaviour of unbounded sequences

We investigate in this section the behavior of the TFW energy of unbounded sequences. By unbounded sequences, we mean sequences of periodic lattices for which some sequence of basis satisfying (2.3) is unbounded.

We first establish some bounds on the electronic density ρ_ℓ that are uniform with respect to ℓ.

4.1 Bounds on ρ_ℓ for $\ell \in \mathcal{L}_3(\mathbf{R}^3)$

Throughout this section, ℓ denotes a proper lattice, and $\Gamma(\ell)$ is a cell of ℓ associated to a basis $(a_i)_{1\leq i\leq 3}$ satisfying (2.3), and the following :

$$0 < R_0 \leq \min_{i=1,2,3} |a_i| = \min_{i=1,2,3} R_i. \tag{4.1}$$

In the spirit of [4] and [16], we define, for a radius $R > 0$, the ground state e_R of the Laplace operator with Dirichlet condition on B_R, and set $g_R = e_R^2$.

Lemma 4.1 *For all $R > 0$, u_ℓ and ϕ_ℓ denoting the solutions of the Euler-Lagrange equation of (1.1), namely*

$$\left\{ \begin{array}{l} -\Delta u_\ell + \frac{5}{3}{u_\ell}^{7/3} - \phi_\ell u_\ell = 0, \\ -\Delta\phi_\ell = 4\pi(\sum_{k\in\ell}\delta_k - {u_\ell}^2), \end{array} \right. \tag{4.2}$$

we have, $\star$ denoting a convolution product over $\mathbf{R}^3$:

$$g_R \star \phi_\ell(x) \leq \frac{5}{3} g_R \star {u_\ell}^{4/3}(x) + \frac{\pi^2}{R^2}, \tag{4.3}$$

for all $x \in \Gamma(\ell)$. Moreover, if $0 \notin x + B_R$, i.e if $|x| > R$, $\phi_\ell(x) \leq (g_R \star \phi_\ell)(x)$.

Proof : We simply copy here the proof of [16], pointing out that it does not depend on ℓ. Since u_ℓ is non-negative and satisfies (4.2), the operator $-\Delta + \frac{5}{3}{u_\ell}^{4/3} - \phi_\ell$, with homogeneous Dirichlet boundary conditions on $B_R + x$, is positive. Hence, for all $\chi \in H_0^1(B_R + x)$,

$$\int_{\Gamma(\ell)} |\nabla\chi|^2 + \int_{\Gamma(\ell)} (\frac{5}{3}{u_\ell}^{4/3} - \phi_\ell)\chi^2 \geq 0.$$

We apply this inequality with $\chi = e_R(x - \cdot)$, and find (4.3).

Assuming that $|x| > R$, ϕ_ℓ is then subharmonic on $B_R + x$, hence from the mean-value inequality and the fact that $\int_{\mathbf{R}^3} g_R = 1$, $\phi_\ell(x) \leq (g_R \star \phi_\ell)(x)$. $\Diamond$

Proposition 4.2 *For any solution (u_ℓ, ϕ_ℓ) of (4.2), we have the following estimate, valid in $\Gamma(\ell) \cap \{|x| > 2\}$:*

$$\phi_\ell(x) \leq \frac{b}{|x|^2} + \sum_{k\in\ell} \frac{a}{|x-k|^4}, \tag{4.4}$$

$a, b > 0$ being universal constants.

Proof : Here again, we merely check out that [16]'s proof carries through this case, with minor modifications. Using estimate (4.3), together with Hlder inequality, we have :

$$g_R \star \phi_\ell - \frac{\pi^2}{R^2} \leq \frac{5}{3}\left(g_R \star {u_\ell}^2\right)^{2/3}.$$

Denoting by $\tilde{\phi}_\ell$ the function $\tilde{\phi}_\ell = g_R \star \phi_\ell - \frac{\pi^2}{R^2}$, we then have $-\Delta\tilde{\phi}_\ell = 4\pi(\sum_{k\in\ell} g_R(\cdot - k) - g_R \star {u_\ell}^2)$, hence :

$$-\Delta\tilde{\phi}_\ell + (\frac{3}{5}\tilde{\phi}_\ell)_+^{3/2} \leq 4\pi \sum_{k\in\ell} g_R(\cdot - k).$$

We now introduce the corresponding periodic TF-potential $\widehat{\phi}_\ell$, that is, the positive solution of :

$$-\Delta\widehat{\phi}_\ell + \frac{5}{3}\widehat{\phi}_\ell^{\,3/2} = 4\pi \sum_{k\in\ell} g_R(\cdot - k).$$

It is thus clear, from a comparison argument, that we have : $\tilde{\phi}_\ell \leq \widehat{\phi}_\ell$. Now, on the one hand, from Theorem V.12 of [14], we know that $\widehat{\phi}_\ell \leq \sum_{k\in\ell} \widehat{\phi}(\cdot - k)$, where $\widehat{\phi}$ is the solution of :

$$-\Delta\widehat{\phi} + \frac{5}{3}(\widehat{\phi})^{3/2} = 4\pi g_R.$$

On the other hand, Lemma 11 of [16] shows that

$$\widehat{\phi} \leq \frac{a}{|x|^4} \quad \text{on} \quad \{|x| > R+1\},$$

where $a > 0$ is a universal constant. Collecting those results and taking, for $|x| > 2$, $R = \frac{1}{2}|x|$, we find (4.4). $\diamondsuit$

Proposition 4.3 *For any solution (u_ℓ, ϕ_ℓ) of (4.2), we have the following estimate, for $x \in \Gamma(\ell) \cap \{|x| > 2\}$:*

$$u_\ell^{4/3} \leq \frac{b'}{|x|^2} + a' \sum_{k\in\ell} \frac{1}{|x-k|^4}, \tag{4.5}$$

where $a', b' > 0$ depend only on R_0 defined in (4.1), and not on the R_i.

Proof : We first remark that the proof of Propositions 3.5 and 3.10 of [9] do not in fact depend on the periodic lattice, as far as its radii R_i satisfy (4.1), and that we thus have :

$$0 < u_\ell \leq c,$$

where $c > 0$ is a constant depending on R_0, and not on ℓ. We define the function :

$$f(x) = \beta \sum_{k\in\ell} \frac{1}{|x-k|^4} + \frac{\gamma}{|x|^2} + \frac{\delta R'^2}{(|x|^2 - R'^2)^2}.$$

An easy but tedious computation shows that :

$$-\Delta f \geq \beta \sum_{k\in\ell} \frac{-12}{|x-k|^6} - \frac{2\gamma}{|x|^4} - 12\delta R'^2 \frac{|x|^2 + R'^2}{(|x|^2 - R'^2)^4}.$$

We also have :

$$f(x)^2 \geq \beta^2 \sum_{k\in\ell} \frac{1}{|x-k|^8} + \frac{\gamma^2}{|x|^4} + 2\beta\gamma \sum_{k\in\ell} \frac{1}{|x-k|^4|x|^2} + \frac{\delta^2 R'^4}{(|x|^2 - R'^2)^4}.$$

Hence, choosing $\gamma \geq 6$, $\beta \geq 12$ and $\delta \geq 24$, we have, in $B_{R'}$:

$$-\Delta f + f^2 \geq 0. \tag{4.6}$$

Now, we also have : $\Delta(u_\ell^{4/3}) \geq \frac{4}{3}(\frac{5}{3}u_\ell^{4/3} - \phi_\ell)u_\ell^{4/3}$. Thus, denoting by S the set $S = \{u_\ell^{4/3} > f\}$, which is open, bounded and included in $\{|x| > 2\} \cap B_{R'}$ as far as $\beta \geq 16c$, from the definition of f and (4.4), we notice that on S, $u_\ell^{4/3} \geq \frac{\inf(\beta,\gamma)}{\sup(a,b)}\phi_\ell$. Hence

$$\Delta u_\ell^{4/3} \geq \frac{4}{3}\left(\frac{5}{3} - \frac{\sup(a,b)}{\inf(\beta,\gamma)}\right)(u_\ell^{4/3})^2.$$

In addition to the above conditions on β and γ, we may impose the inequality $\beta, \gamma > 2\sup(a,b)$, so that, on S :

$$\Delta(u_\ell^{4/3} - f) \geq (u_\ell^{4/3})^2 - f^2 > 0.$$

The function $u_\ell^{4/3} - f$ is thus subharmonic on S, and cancels on ∂S. From the maximum principle, we infer that $u_\ell^{4/3} - f$ is non-positive on S, which is impossible. Hence, $S = \emptyset$. Letting then R' go to infinity, we find (4.5). $\diamondsuit$

4.2 Convergence of G_ℓ

Considering unbounded sequences, we investigate here the behavior of the associated potential G_ℓ.

4.2.1 The Thin film case

We consider here the case of a sequence $(\ell_n)_{n\geq 0}$ such that only one of its radii R_i^n is unbounded, and the others are bounded away from 0 as well as bounded from above. That is, we consider a sequence $(\ell_n)_{n\in\mathbf{N}}$ such that for all $n \in \mathbf{N}$, ℓ_n has a basis $(a_i^n)_{1\leq i\leq 3}$ satisfying the conclusion of Theorem 2.4 together with :

(1) $a_1^n \longrightarrow a_1 \neq 0$ as n goes to infinity,

(2) $a_2^n \longrightarrow a_2 \neq 0$ as n goes to infinity,

(3) $|a_3^n| = R_3^n \longrightarrow \infty$ as n goes to infinity.

Moreover, we may assume, changing the system of coordinates if necessary, that for all $n \geq 0$, the plane generated by (a_1^n, a_2^n) as well as the one generated by (a_1, a_2), is included in (hence equal to) the one generated by (e_1, e_2). Note that since the angle between a_1^n and a_2^n is confined in $[\frac{\pi}{3}, \frac{\pi}{2}]$, so is the angle between a_1 and a_2, and these two vectors must be linearly independent.

We denote by G_n the periodic potential associated to ℓ_n, defined in (1.5), and which may be written as :

$$G_n(x) = C_n + \frac{1}{\pi|\Gamma(\ell_n)|} \sum_{k \in \ell_n^* \setminus \{0\}} \frac{e^{2i\pi k \cdot x}}{|k|^2}, \tag{4.7}$$

where $C_n = \frac{1}{|\Gamma(\ell_n)|} \int_{\Gamma(\ell_n)} G_n$ is such that $\lim_{x \to 0}(G_{\ell_n}(x) - \frac{1}{|x|}) = 0$, and ℓ_n^* is the periodic lattice reciprocal to ℓ_n, i.e the lattice of basis (b_1^n, b_2^n, b_3^n) satisfying :

$$a_i^n \cdot b_j^n = \delta_{ij}, \quad \forall i, j \in \{1, 2, 3\}.$$

The potential G_∞ denotes the potential associated to the lattice ℓ_∞ generated by (a_1, a_2), as defined in (3.39). We now show the following :

Proposition 4.4 *The potentials G_n and G_∞ satisfy, for all $x \in \Gamma(\ell_n)$:*

$$|G_n(x) - G_\infty(x)| \leq C(1 + |x_3|), \tag{4.8}$$

where $C > 0$ is a constant independent of n.

Proof : The strategy of the proof is the following : writing G_n through its Fourier series, we isolate singular terms, and deal with them separately, whereas in the remaining terms, we recognize a Riemann sum converging to the Fourier coefficients of G_∞, as defined in (3.39).

We denote by $(\tilde{a}_i^n)$ the renormalized basis associated to (a_i^n), that is, $\tilde{a}_i^n = \frac{a_i^n}{R_i^n} = \frac{a_i^n}{|a_i^n|}$. We thus have, setting $\delta_n = |\tilde{a}_1^n \cdot (\tilde{a}_2^n \wedge \tilde{a}_3^n)| = |\det(\tilde{a}_1^n, \tilde{a}_2^n, \tilde{a}_3^n)|$:

$$G_n(x) = C_n + \frac{1}{\pi R_1^n R_2^n R_3^n \delta_n} \sum_{k \in \mathbf{Z}^3 \setminus \{0\}} \frac{e^{2i\pi(k_1 b_1^n + k_2 b_2^n + k_3 b_3^n) \cdot x}}{|k_1 b_2^n + k_2 b_2^n + k_3 b_3^n|^2}. \tag{4.9}$$

Hence, isolating the terms where $k_1 = k_2 = 0$, and denoting by $\tilde{b}_3^n$ the vector $\tilde{b}_3^n = R_3^n b_3^n$:

$$\begin{aligned} G_n(x) &= C_n + \frac{R_3^n}{\pi R_1^n R_2^n \delta_n} \sum_{k_3 \neq 0} \frac{e^{2i\pi k_3 \frac{\tilde{b}_3^n \cdot x}{R_3^n}}}{k_3^2 |\tilde{b}_3^n|^2} \\ &+ \frac{1}{\pi R_1^n R_2^n R_3^n \delta_n} \sum_{(k_1,k_2) \in \mathbf{Z}^2 \setminus \{0\}} \sum_{k_3 \in \mathbf{Z}} \frac{e^{2i\pi(k_1 b_1^n + k_2 b_2^n + k_3 \frac{\tilde{b}_3^n}{R_3^n}) \cdot x}}{|k_1 b_1^n + k_2 b_2^n + k_3 \frac{\tilde{b}_3^n}{R_3^n}|^2}. \end{aligned}$$

Next, considering the fact that (a_1, a_2) is a basis of the plane generated by (e_1, e_2), together with the definition of b_i^n, we infer that $\tilde{b}_3^n = \lambda_n e_3$, with $\lambda_n \in \mathbf{R}$ bounded away from 0 as well as bounded from above. Next, we notice that the first sum is easily computable, since $\sum_{k\in\mathbf{Z}\setminus\{0\}} \frac{e^{2i\pi kt}}{k^2} = \frac{\pi^2}{3} + 2\pi^2|t|(|t|-1)$ for $|t| \le \frac{1}{2}$. Hence, for all $x \in \Gamma(\ell)$:

$$\begin{aligned} G_n(x) &= C_n + \frac{\pi R_3^n}{3R_1^n R_2^n \delta_n \lambda_n^2} + \frac{2\pi x_3^2}{\delta_n R_1^n R_2^n R_3^n} - \frac{2\pi|x_3|}{R_1^n R_2^n \delta_n \lambda_n} \\ &+ \frac{1}{\pi R_1^n R_2^n R_3^n \delta_n} \sum_{(k_1,k_2)\in\mathbf{Z}^2\setminus\{0\}} \sum_{k_3\in\mathbf{Z}} \frac{e^{2i\pi((k_1 b_1^n + k_2 b_2^n)\cdot x + \frac{\lambda_n x_3}{R_3^n})}}{|k_1 b_1^n + k_2 b_2^n + k_3 \frac{\lambda_n e_3}{R_3^n}|^2}. \end{aligned}$$

We denote by $G_{(a_1^n,a_2^n)}$ the thin film potential associated to the lattice of basis (a_1^n, a_2^n). Denoting by $\overline{G}_n$ the function

$$\overline{G}_n(x) = \overline{C}_n - \frac{2\pi}{R_1^n R_2^n \lambda_n \delta_n}|x_3| + \frac{1}{\pi R_1^n R_2^n \lambda_n \delta_n} \sum_{k\in\mathbf{Z}^2\setminus\{0\}} \int_{\mathbf{R}} \frac{e^{2i\pi((k_1 b_1^n + k_2 b_2^n)\cdot x + \xi x_3)}}{|k_1 b_1^n + k_2 b_2^n + \xi e_3|^2},$$

with $\overline{C}_n$ chosen so that $\overline{G}_n(x) - \frac{1}{|x|}$ cancels at 0, and computing its Laplacian, we find that $\overline{G}_n - G_{(a_1^n,a_2^n)}$ is harmonic, bounded (from Proposition 3.6-(iii)), has value 0 at the origin. Thus, $\overline{G}_n = G_{(a_1^n,a_2^n)}$. We then have, denoting by F_n the function $G_n - G_\infty$:

$$\begin{aligned} F_n(x) &= G_{(a_1^n,a_2^n)}(x) - G_\infty(x) - \overline{C}_n + C_n \\ &+ \frac{\pi R_3^n}{3R_1^n R_2^n \delta_n \lambda_n^2} + \frac{2\pi x_3^2}{\delta_n R_1^n R_2^n R_3^n} \\ &- \frac{1}{\pi R_1^n R_2^n \delta_n \lambda_n} \sum_{(k_1,k_2)\neq(0,0)} e^{2i\pi(k_1 b_1^n + k_2 b_2^n)\cdot x} \Bigg(\int_{\mathbf{R}} \frac{e^{2i\pi\xi x_3}}{|k_1 b_1^n + k_2 b_2^n + \xi e_3|^2} \\ &- \frac{\lambda_n}{R_3^n} \sum_{k_3\in\mathbf{Z}} \frac{e^{2i\pi\frac{\lambda_n k_3 x_3}{R_3^n}}}{|k_1 b_1^n + k_2 b_2^n + k_3 \frac{\lambda_n e_3}{R_3^n}|^2} \Bigg). \end{aligned} \tag{4.10}$$

Using estimate (ii) and (iii) of Proposition 3.6, it is clear that

$$\left| G_{(a_1^n,a_2^n)}(x) - G_\infty(x) \right| \le C(1 + |x_3|) \tag{4.11}$$

in $\Gamma(\ell_n)$, for n sufficiently large. We now deal with the sum appearing in (4.10) : we denote it by $F_n'(x)$, omitting the factor $\frac{1}{\pi R_1^n R_2^n \delta_n \lambda_n}$ since it is bounded, and write $F_n' = F_n^1 + F_n^2$, where :

$$F_n^1(x) = \sum_{(k_1,k_2)\neq(0,0)} \sum_{k_3\in\mathbf{Z}} \frac{\left(\frac{\lambda_n}{R_3^n} - \int_{(k_3-\frac{1}{2})\frac{\lambda_n}{R_3^n}}^{(k_3+\frac{1}{2})\frac{\lambda_n}{R_3^n}} e^{2i\pi x_3(\xi - \frac{\lambda_n k_3}{R_3^n})} d\xi \right) e^{2i\pi(k_1 b_1^n + k_2 b_2^n + \frac{k_3\lambda_n}{R_3^n} e_3)\cdot x}}{|k_1 b_1^n + k_2 b_2^n + \frac{k_3\lambda_n}{R_3^n} e_3|^2}, \tag{4.12}$$

$$\begin{aligned} F_n^2(x) &= \sum_{(k_1,k_2)\neq(0,0)} e^{2i\pi(k_1 b_1^n + k_2 b_2^n)\cdot x} \sum_{k_3\in\mathbf{Z}} \int_{(k_3-\frac{1}{2})\frac{\lambda_n}{R_3^n}}^{(k_3+\frac{1}{2})\frac{\lambda_n}{R_3^n}} \Bigg(\frac{1}{|k_1 b_1^n + k_2 b_2^n + \frac{k_3\lambda_n}{R_3^n} e_3|^2} \\ &- \frac{1}{|k_1 b_1^n + k_2 b_2^n + \xi e_3|^2} \Bigg) e^{2i\pi\xi x_3} d\xi. \end{aligned} \tag{4.13}$$

And we have $F_n^1(x) = \overline{F}_n^1(x)(\frac{\lambda_n}{R_3^n} - \frac{\sin(\pi\frac{\lambda_n x_3}{R_3^n})}{\pi x_3})$, with

$$\overline{F}_n^1(x) = \sum_{(k_1,k_2)\neq(0,0)} \sum_{k_3\in\mathbf{Z}} \frac{e^{2i\pi(k_1b_1^n+k_2b_2^n+\frac{k_3\lambda_n}{R_3^n}e_3)\cdot x}}{|k_1b_1^n+k_2b_2^n+\frac{k_3\lambda_n}{R_3^n}e_3|^2}.$$

One computes easily :

$$\|\overline{F}_n^1\|^2_{L^2(\Gamma(\ell_n))} = C(R_3^n)^2 \sum_{(k_1,k_2)\neq(0,0)} \frac{1}{R_3^n} \sum_{k_3\in\mathbf{Z}} \frac{1}{|k_1b_1^n+k_2b_2^n+\frac{k_3\lambda_n}{R_3^n}e_3|^4},$$

and since the sum over k_3 is a Riemann sum converging to $\int_{\mathbf{R}} \frac{d\xi}{|k_1b_1^n+k_2b_2^n+\xi e_3|^4} \leq \frac{C}{|k_1b_1^n+k_2b_2^n|^3}$ as R_3^n goes to infinity, we infer that :

$$\|\overline{F}_n^1\|_{L^2(\Gamma(\ell_n))} \leq CR_3^n,$$

where C does not depend on n. This implies :

$$\|F_n^1\|_{L^2(\Gamma(\ell_n))} \leq C, \tag{4.14}$$

with C independent of n. We now turn to F_n^2 : noticing that

$$\left|\int_{(k_3-\frac{1}{2})\frac{\lambda_n}{R_3^n}}^{(k_3+\frac{1}{2})\frac{\lambda_n}{R_3^n}} \left(\frac{1}{|k_1b_1^n+k_2b_2^n+\frac{k_3\lambda_n}{R_3^n}e_3|^2} - \frac{1}{|k_1b_1^n+k_2b_2^n+\xi e_3|^2}\right) e^{2i\pi\xi x_3} d\xi\right|$$
$$\leq C\big(\frac{\lambda_n}{R_3^n}\big)^2 \frac{1}{|k_1b_1^n+k_2b_2^n+\frac{k_3\lambda_n}{R_3^n}e_3|^3},$$

we deduce, according to (4.13), that we have :

$$\begin{aligned}\|F_n^2\|^2_{L^2(\Gamma(\ell))} &\leq CR_3^n \sum_{(k_1,k_2)\neq(0,0)} \left(\sum_{k_3\neq 0} \big(\frac{\lambda_n}{R_3^n}\big)^2 \frac{1}{|k_1b_1^n+k_2b_2^n+\frac{k_3\lambda_n}{R_3^n}e_3|^3}\right)^2 \\ &\leq C\frac{\lambda_n^4}{(R_3^n)^2} \sum_{(k_1,k_2)\neq(0,0)} \frac{1}{(k_1^2+k_2^2)^2}.\end{aligned}$$

This shows that

$$\|F_n^2\|_{L^2(\Gamma(\ell_n))} \leq \frac{C}{R_3^n}, \tag{4.15}$$

with C independent of n. With (4.14), we get :

$$\|F_n'\|_{L^2(\Gamma(\ell_n))} \leq C, \tag{4.16}$$

the constant C not depending on n. Next, since F_n' is harmonic in $\Gamma(\ell_n)$, standard elliptic regularity results show that F_n' is necessarily bounded in $L^\infty(\Gamma(\ell_n))$. Since $F_n(0)=0$, this also shows that $C_n - C_{(a_1^n,a_2^n)} + \frac{\pi R_3^n}{3R_1^n R_2^n \lambda_n \delta_n}$ is bounded, and we finally get (4.8). $\diamondsuit$

Next, looking closely at F_n', we notice that its $L^\infty(\Gamma(\ell_n)\cap\{|x_3|\leq R\})$ norm satisfies (4.15), for any fixed $R>0$. Indeed, if $|x_3|\leq R$, $|\frac{\lambda_n}{R_3^n} - \frac{\sin(\pi\frac{\lambda_n x_3}{R_3^n})}{\pi x_3}| \leq \frac{CR^2}{(R_3^n)^3}$, so that (4.14) then becomes :

$$\|F_n^1\|_{L^2(\Gamma(\ell_n))} \leq \frac{C}{(R_3^n)^2}.$$

Hence, with the help of (4.10),the last bound we have obtained may be improved :

$$C_n - \overline{C}_n + \frac{\pi R_3^n}{3R_1^n R_2^n \lambda_n \delta_n} \longrightarrow 0. \tag{4.17}$$

This implies the following :

Proposition 4.5 *As n goes to infinity, we have, for any fixed $R>0$:*

$$\|G_n - G_\infty\|_{L^\infty(\Gamma(\ell_n)\cap\{|x_3|<R\})} \longrightarrow 0 \quad \text{as} \quad n\to\infty.$$

Proof : From the above remark (4.17), we only need to improve (4.11), and show that this quantity is not only bounded, but goes to zero as n goes to infinity when $|x_3|$ is bounded. In order to do so, we only need to show it for the Fourier series, since the term of the form $\alpha_n|x_3|$ does converge. And the Fourier series may be dealt with in the same way as F_n'. This completes the proof. $\diamondsuit$

Remark 4.6 *In all the above bounds, we have omitted for simplicity the factor $\frac{1}{R_1^n R_2^n}$, since it is bounded from above. Rigorously, it should appear in all bounds, so that in fact (4.8) may very well read :*

$$|G_n(x) - G_\infty(x)| \leq C\left(1 + \frac{|x_3|}{R_1^n R_2^n}\right), \tag{4.18}$$

with C independent of n. This will be useful in the sequel.

4.2.2 The polymer case

We use here the same notation as in Section 4.2.1, except that only R_1^n is bounded. In other words, we have :

(1) $a_1^n \longrightarrow a_1 \neq 0$ as n goes to infinity,

(2) $R_2^n \longrightarrow \infty$ as n goes to infinity,

(3) $R_3^n \longrightarrow \infty$ as n goes to infinity.

Changing coordinates if necessary, we may assume that a_1^n is collinear to e_3, for all $n \in \mathbf{N}$. Next, we may rotate the system of coordinates so that the angle between a_2^n and e_1 is lower than $\frac{\pi}{6}$. Hence, from (2.3), the angle between a_3^n and e_2 is necessarily bounded, and there exists a constant C independent of n such that :

$$|a_2^n \cdot e_1| \geq C R_2^n, \quad \text{and} \quad |a_3^n \cdot e_2| \geq C R_3^n.$$

Here the lattice ℓ_∞ is the one generated by $a_1 = R_1 e_3$, and G_∞ is thus defined by (3.8).

Proposition 4.7 *There exists a constant C independent of n such that for all x in $\Gamma(\ell_n)$, we have :*

$$|G_n(x) - G_\infty(x)| \leq C\left(1 + \frac{|x_2|}{R_2^n} + \log(2 + |x'|)\right). \tag{4.19}$$

Moreover, $G_n - G_\infty$ goes to 0 in $L^\infty(\Gamma(\ell_n) \cap \{r < R\})$, for any $R > 0$.

Proof : Writing G_n through its Fourier coefficients, we argue exactly as in the proof of Proposition 4.4 concerning the Fourier series F_n'. The argument carries through this case. Hence, we only study the residual term, that is,

$$A_n(x) = C_n - C_{a_1^n} + \frac{1}{\pi \delta_n R_1^n R_2^n R_3^n} \sum_{(k_2,k_3) \neq (0,0)} \frac{e^{2i\pi(k_2 b_2^n + k_3 b_3^n)\cdot x}}{|k_2 b_2^n + k_3 b_3^n|^2} + \frac{2}{R_1^n} \log|x'| + G_{a_1^n}(x) - G_\infty(x),$$

where $G_{a_1^n}$ is the polymer potential associated to a lattice of basis (a_1^n), and $C_{a_1^n}$ the corresponding constant appearing in (3.8). We use estimates (ii)-(iii) of Proposition 3.1 to deal with $G_{a_1^n}(x) - G_\infty(x)$, finding :

$$\left| G_{a_1^n}(x) - G_\infty(x) \right| \leq C(1 + \log(2 + |x'|)), \tag{4.20}$$

in $\Gamma(\ell_n)$. Next, we need a bound on the remaining term. Unfortunately, we do not have, as in the preceding case, an exact expression of this Fourier series. But we know that it depends only on $x' = (x_1, x_2)$, since a_1^n is collinear to e_3, and we may compute its Laplacian in the plane $\{x_3 = 0\}$:

$$-\Delta\left(\frac{1}{\pi R_1^n R_2^n} \sum_{(k_2,k_3)\neq(0,0)} \frac{e^{2i\pi(k_2 b_2^n + k_3 b_3^n)\cdot x}}{|k_2 b_2^n + k_3 b_3^n|^2}\right) = 4\pi(\delta_0 - \frac{1}{R_1^n R_2^n}),$$

and this function is periodic. Its periodic cell is defined by the basis $(\overline{a}_2^n, \overline{a}_3^n)$ reciprocal to (b_2^n, b_3^n). It is thus clear that $\overline{a}_2^n$ and $\overline{a}_3^n$ are respectively the projection of a_2^n and a_3^n on the plane $\{x_3 = 0\}$, so that their norms $\tilde{R}_2^n$ and $\tilde{R}_3^n$ go to infinity as n goes to infinity. Two cases are then possible :

Case 1 : $\tilde{R}_2^n/\tilde{R}_3^n$ is bounded. We reduce this case to $\tilde{R}_2^n = \tilde{R}_3^n = R^n$, the general case being a rather technical adaptation of this one. We then have, denoting by $B_n(x')$ the above function,

$$B_n(x') = B(\frac{x'}{R^n}),$$

where B is the function B_n with $R^n = 1$. Hence, we have, denoting by $\tilde{\Gamma}_n$ the set $\{t\tilde{a}_1^n + u\tilde{a}_2^n, \quad -\frac{1}{2} < t, u \leq \frac{1}{2}\}$:

$$\|B_n + 2\log\frac{|x'|}{R^n}\|_{L^\infty(\tilde{\Gamma}_n)} = \|B + 2\log|x'|\|_{L^\infty(\frac{1}{R^n}\tilde{\Gamma}_n)} \leq C,$$

C being a constant independent of n. This gives a bound on $A_n(x) - C_n + C_{a_1^n} - \log(R^n)$ in $L^\infty(\Gamma(\ell_n))$, hence on $G_n - G_\infty - C_n + C_{a_1^n} - \log(R^n)$. Pointing out that $G_n - G_\infty$ cancels at 0, we thus deduce a bound on $-C_n + C_{a_1^n} - \log(R^n)$, and conclude the proof of (4.19).

If now $\tilde{R}_2^n \neq \tilde{R}_3^n$, we may re-scale by $\tilde{R}_2^n$ in the same way as above, and thus get a periodic Green function on a periodic cell of the form $\frac{1}{\tilde{R}_n^2}\tilde{\Gamma}_n$. The above bounds are then still valid, since the domain is bounded independently of n.

Case 2 : $\tilde{R}_2^n/\tilde{R}_3^n$ is unbounded. We may then assume that this quotient goes to infinity. Re-scaling by $\tilde{R}_2^n$ as in Case 1, we then have a problem of the same kind as Proposition 4.5's, except that it is in two dimensions and not in three. Nevertheless, it may be dealt with in the same way. As pointed out in Remark 4.6, we then get the right coefficient with $|x_2|$. This concludes the proof of (4.19).

The L^∞ convergence is then proved by pointing out that the same remarks as in Proposition 4.5's proof are available. ◊

Remark 4.8 *Here again, we have omitted the coefficient $\frac{1}{R_1^n}$ in front of all terms, but it will be useful to keep in mind that it is implicit in the constant C of (4.19).*

4.2.3 The atomic case

We now consider the case when all radii go to infinity :

$$R_3^n \geq R_2^n \geq R_1^n \longrightarrow \infty.$$

We assume (changing coordinates if necessary, here again) that a_1^n is collinear to e_1, and that the angle between a_2^n and e_2 is not larger than $\frac{\pi}{6}$. This also implies that the angle between a_3^n and e_3 is bounded, and that :

$$|a_2^n \cdot e_2| \geq CR_2^n, \quad \text{and} \quad |a_3^n \cdot e_3| \geq CR_3^n.$$

In this case, we have the following :

Proposition 4.9 *There exists a constant C independent of n such that :*

$$|G_n(x) - \frac{1}{|x|}| \leq C(1 + \frac{\log(2 + |x'|)}{R_1^n} + \frac{|x_3|}{R_1^n R_2^n}). \tag{4.21}$$

Moreover, $G_n - \frac{1}{|x|}$ converges to 0 in $L^\infty_{loc}(\mathbf{R}^3)$.

Proof : We first assume that $\frac{R_3^n}{R_1^n}$ is bounded. In this case, we may assume that this ratio, together with $\frac{R_2^n}{R_1^n}$, converge. Thus, denoting by $\overline{G}_n$ the function

$$\overline{G}_n(x) = R_1^n G_n(R_1^n x), \tag{4.22}$$

a direct computation shows that $\overline{G}_n$ is the periodic potential associated to the lattice of basis $(\frac{a_1^n}{R_1^n}, \frac{a_2^n}{R_1^n}, \frac{a_3^n}{R_1^n})$. Next, we notice that $\overline{G}_n - \frac{1}{|x|}$ has its Laplacian identically equal to 1 in $\frac{1}{R_1^n}\Gamma(\ell_n)$ and that G_n is bounded in $L^2(\Gamma(\ell_n))$ (from its Fourier coefficients), independently of n, so that we have :

$$\left\|\overline{G}_n - \frac{1}{|x|}\right\|_{L^\infty(\frac{1}{R_1^n}\Gamma(\ell_n))} \leq C.$$

This implies :

$$\left\|G_n - \frac{1}{|x|}\right\|_{L^\infty(\Gamma(\ell_n))} \leq \frac{C}{R_1^n},$$

and (4.21) follows, as well as the L^∞_{loc} convergence.

We next consider the possibility :

$$\frac{R_3^n}{R_1^n} \longrightarrow \infty, \quad \text{with} \quad \frac{R_2^n}{R_1^n} \quad \text{bounded.}$$

Here again, we rescale the potential G_n with respect to R_1^n, according to (4.22), and find ourselves in the case of Proposition 4.4, and using the same tricks, we show (4.8) for $\overline{G}_n$ and $R_1^n G_\infty(R_1^n x)$. Next, we notice that, from the same reasons as in the first case,

$$\left| R_1^n G_\infty(R_1^n x) - \frac{1}{|x|}\right| \leq \frac{C}{R_1^n}$$

in $\Gamma(\ell_n)$. Therefore :

$$|G_n(x) - \frac{1}{|x|}| \leq C(\frac{1}{R_1^n} + \frac{|x_3|}{R_1^n R_2^n}).$$

Here again, this shows (4.21) as well as the L^∞_{loc} convergence.

The last case is the following :

$$\frac{R_3^n}{R_1^n} \longrightarrow \infty, \quad \text{and} \quad \frac{R_2^n}{R_1^n} \longrightarrow \infty.$$

Here again, we rescale and find the polymer case. Adapting the corresponding proof, our Proposition is proved. ◊

Remark 4.10 *Formally, the above estimates assert that the convergence of G_n to G_∞ is a good one if it is isotropic. When it is not, the convergence defect behaves like the corresponding intermediate potential. For example, in the case of the convergence towards $\frac{1}{|x|}$, it $G_n - \frac{1}{|x|}$ converges to 0 in $L^\infty(\Gamma(\ell_n))$ if $R_1^n = R_2^n = R_3^n$, whereas if $R_1^n = R_2^n \ll R_3^n$, a residual term appears, which has the same behavior as the thin film potential associated to the basis (a_1^n, a_2^n).*

4.3 Convergence of the energy

According to the bounds we have shown in the preceding sections, we are now in position to show the following :

Theorem 4.11 *Let ℓ_n be a sequence of proper lattices, with basis (a_i^n) satisfying conclusions of Theorem 2.4. Assume in addition that there exists an R_0 such that*

$$\forall n \geq 0, \quad \forall i = 1,2,3, \quad R_i^n = |a_i^n| \geq R_0.$$

Then we have :

(i) If $R_3^n \longrightarrow \infty$ and $a_i^n \longrightarrow a_i$, $i \neq 3$, as $n \to \infty$, then the energy $\mathcal{E}(\ell_n)$ converges to $\mathcal{E}(\ell_\infty)$, where ℓ_∞ is the periodic lattice of rank 2 generated by (a_1, a_2),

(ii) If $R_2^n \longrightarrow \infty$ as $n \to \infty$, and if a_1^n converges to some $a_1 \neq 0$, then $\mathcal{E}(\ell_n)$ converges to the energy $\mathcal{E}(\ell_\infty)$ of the polymer defined by a_1,

(iii) If $R_1^n \longrightarrow \infty$ as $n \to \infty$, then $\mathcal{E}(\ell_n)$ converges to the atomic energy I_{at}^{TFW}.

Proof : We first prove (i) : in this case, we may assume (as has been done in the proof of Proposition 4.4) that a_1^n and a_2^n belong to the plane $\{x_3 = 0\}$. We first show that :

$$\limsup_{n\to\infty} \mathcal{E}(\ell_n) \leq \mathcal{E}(\ell_\infty). \tag{4.23}$$

For this purpose, we fix a $\rho \geq 0$, such that $\sqrt{\rho} \in C^\infty(\mathbf{R}^3)$, $\sqrt{\rho}$ has compact support with respect to x_3, and is ℓ_∞-periodic, and has total mass one over $\Gamma(\ell_\infty)$. We denote by M_n the unique matrix satisfying :

$$M_n a_i^n = a_i, \quad i = 1,2, \quad \text{and} \quad M_n e_3 = e_3.$$

It is clear that M_n converges to the identity matrix as n goes to infinity. Moreover, if n is large enough to ensure that $\mathrm{Supp}\rho \subset \{|x_3| \leq R_3^n\}$, $\rho_n = |\det M_n| \rho \circ M_n$ is a test-function for the variational problem I_n defining $\mathcal{E}(\ell_n)$. Hence :

$$E_{\ell_n}^{TFW}(\rho_n) \geq \mathcal{E}(\ell_n).$$

We then study separately the four terms appearing in $E_{\ell_n}^{TFW}(\rho_n)$.

Considering the term $\int_{\Gamma(\ell_n)} |\nabla\sqrt{\rho}_n|^2$, we notice that $\nabla\sqrt{\rho}_n = |\det M_n|^{1/2} M_n \cdot \nabla(\sqrt{\rho}) \circ M_n$, so that, changing variables in this term, we have :

$$\int_{\Gamma(\ell_n)} |\nabla\sqrt{\rho}_n|^2 = \int_{\Gamma(\ell_\infty)} \left|M_n \cdot \nabla\sqrt{\rho}\right|^2,$$

which converges to $\int_{\Gamma(\ell_\infty)} |\nabla\sqrt{\rho}|^2$ as n goes to infinity. The second term may be dealt with exactly in the same way, and we then turn to the electrostatic terms :

$$\begin{aligned}
\int_{\Gamma(\ell_n)} \rho_n G_n &= \int_{\Gamma(\ell_\infty)} \rho\, G_n \circ M_n^{-1} \\
&= \int_{\Gamma(\ell_\infty)} \rho(G_n \circ M_n^{-1} - G_\infty \circ M_n^{-1}) + \int_{\Gamma(\ell_\infty)} \rho G_\infty \circ M_n^{-1}.
\end{aligned}$$

Since $\int_{\Gamma(\ell_\infty)} \rho G_\infty \circ M_n^{-1} = \int_{\Gamma(\ell_n)} |\det M_n| (\rho \circ M_n) G_\infty$, the fact that G_∞ is bounded in $L^2_{loc}(\Gamma(\ell_n))$ together with the convergence of ρ_n towards ρ in $L^2(\Gamma(\ell_\infty))$ and the fact that ρ has compact support with respect to x_3, shows that

$$\int_{\Gamma(\ell_\infty)} \rho\, G_\infty \circ M_n^{-1} \longrightarrow \int_{\Gamma(\ell_\infty)} \rho\, G_\infty.$$

On the other hand, we have, choosing R so that $\mathrm{Supp}\rho \subset \{|x_3| < R\}$:

$$\begin{aligned} \int_{\Gamma(\ell_\infty)} \left|\rho (G_n \circ M_n^{-1} - G_\infty \circ M_n^{-1})\right| &\leq \|(G_n - G_\infty) \circ M_n^{-1}\|_{L^\infty(\Gamma(\ell_\infty) \cap \{|x_3| \leq R\})} \\ &\leq \|G_n - G_\infty\|_{L^\infty(\Gamma(\ell_n) \cap \{|x_3| \leq R\})}, \end{aligned}$$

which vanishes as $n \to \infty$ from Proposition 4.5. Since the remaining term of the energy follows then exactly in the same way, we have proved that

$$\limsup_{n \to \infty} \mathcal{E}(\ell_n) \leq E^{TFW}_{\ell_\infty}(\rho).$$

This is valid for all ℓ_∞-periodic ρ such that $\sqrt{\rho} \in C^\infty(\mathbf{R}^3)$ and $\mathrm{Supp}\rho$ is compact with respect to x_3. Since this subspace of $H^1_{per}(\ell_\infty)$ is dense, we conclude that (4.23) holds.

The next step consists in showing :

$$\liminf_{n \to \infty} \mathcal{E}(\ell_n) \geq \mathcal{E}(\ell_\infty). \tag{4.24}$$

We denote by ρ_n the unique solution of problem (1.1) defining $\mathcal{E}(\ell_n)$, and by $u_n = \sqrt{\rho_n}$ its square root. From (4.23), we know that the energy $E^{TFW}_{\ell_n}(\rho_n)$ is bounded. Moreover, if we fix an $R > 2$ and choose n large enough to have $\Gamma(\ell_n) \cap \{|x_3| > R\} \neq \emptyset$, we have :

$$\int_{\Gamma(\ell_n)} \rho_n |G_n - G_\infty| \leq \|G_n - G_\infty\|_{L^\infty(\Gamma(\ell_n) \cap \{|x_3| < R\})} + \int_{\Gamma(\ell_n) \cap \{|x_3| > R\}} \rho_n |G_n - G_\infty|.$$

We infer from Propositions 4.3 and 4.4 :

$$\rho_n \leq C \left(\frac{1}{|x|^2} + \sum_{k \in \ell_n} \frac{1}{|x - k|^4} \right)^{3/2} \leq C \left(\frac{1}{|x|^2} + \sum_{j \in \mathbf{Z}} \frac{1}{|x - j R_3^n e_3|^2} \right)^{3/2},$$

in $\Gamma(\ell_n) \cap \{|x_3| > R\}$, hence :

$$\int_{\Gamma(\ell_n)} \rho_n |G_n - G_\infty| \leq \|G_n - G_\infty\|_{L^\infty(\Gamma(\ell_n) \cap \{|x_3| < R\})} + C \int_R^{R_3^n} t \left(\frac{1}{t^2} + \sum_{j \neq 0} \frac{1}{t^2 + j^2 {R_3^n}^2} \right)^{3/2} dt.$$

Using the convergence result of Proposition 4.5, we thus have :

$$\begin{aligned} \int_{\Gamma(\ell_n)} \rho_n |G_n - G_\infty| &\leq o(1) + C \int_R^{R_3^n} t \left(\frac{1}{t^2} + \frac{1}{t R_3^n} \right)^{3/2} dt \\ &\leq o(1) + C \int_R^{R_3^n} t \left(\frac{1}{t^{3/2}} + \frac{1}{(R_3^n t)^{3/4}} \right)^2 \\ &\leq o(1) + \frac{C}{R} + \frac{C}{R_3^n}, \end{aligned}$$

where $o(1)$ denotes a function which goes to 0 as n goes to infinity. Letting n, then R, go to infinity, this shows that :

$$\int_{\Gamma(\ell_n)} \rho_n (G_n - G_\infty) \longrightarrow 0. \tag{4.25}$$

Repeating exactly the same kind of argument, one easily shows :

$$\int_{\Gamma(\ell_n)} \int_{\Gamma(\ell_n)} \rho_n(x)\rho_n(y)(G_n(x-y) - G_\infty(x-y))dxdy \longrightarrow 0. \tag{4.26}$$

Now, it is not difficult, from estimate (4.5) of Proposition 4.3 together with Proposition 3.6-(ii)-(iii), to show that $\int_{\Gamma(\ell_n)} \rho_n G_\infty$ and $\int_{\Gamma(\ell_n)} \int_{\Gamma(\ell_n)} \rho_n(x)\rho_n(y)G_\infty(x-y)dxdy$ are bounded independently of n. With the fact that $E^{TFW}_{\ell_n}(\rho_n)$ is bounded, this implies that u_n is bounded in $H^1_{loc}(\mathbf{R}^3)$. Extracting a subsequence if necessary, u_n then converges weakly to some $\sqrt{\rho} = u \in H^1_{loc}(\mathbf{R}^3)$. Then, letting $\Omega \subset\subset \Gamma(\ell_\infty)$, we have, taking n large enough to have $\Omega \subset \Gamma(\ell_n)$,

$$\int_{\Gamma(\ell_n)} |\nabla u_n|^2 \geq \int_\Omega |\nabla u_n|^2,$$

so that

$$\liminf_{n\to\infty} \int_{\Gamma(\ell_n)} |\nabla u_n|^2 \geq \liminf_{n\to\infty} \int_\Omega |\nabla u_n|^2 \geq \int_\Omega |\nabla u|^2.$$

This is valid for any $\Omega \subset\subset \Gamma(\ell_\infty)$, so that :

$$\liminf_{n\to\infty} \int_{\Gamma(\ell_n)} |\nabla u_n|^2 \geq \int_{\Gamma(\ell_\infty)} |\nabla u|^2. \tag{4.27}$$

With a slight adaptation of this argument, we have :

$$\liminf_{n\to\infty} \int_{\Gamma(\ell_n)} \rho_n^{5/3} \geq \int_{\Gamma(\ell_\infty)} \rho^{5/3}. \tag{4.28}$$

The weak convergence in H^1_{loc} implies a strong one in L^2_{loc}, up to extracting a subsequence, so that, with estimate (4.5), it is easy to show that :

$$\int_{\Gamma(\ell_n)} \rho_n G_\infty \longrightarrow \int_{\Gamma(\ell_\infty)} \rho G_\infty, \tag{4.29}$$

with a similar result concerning the convolution term. Hence, collecting (4.25), (4.26), (4.27), (4.28) and (4.29), and pointing out that the total mass of ρ_n is conserved from the L^2_{loc} convergence and estimate (4.5), we prove (4.24). This concludes the proof of (i).

The proofs of (ii) and (iii) follow exactly the same pattern : we show (4.23), by the very same argument. Showing (4.24) in cases (ii)-(iii) requires sharper estimates, precisely those shown in Propositions 4.7 and 4.9. $\diamondsuit$

5 Compactness of the minimizing sequences

We show in this Section our main result, namely Theorem 1.1, that we recall here :

Theorem 5.1 *Let $\mathcal{E}$ be the functional defined by (1.1), and denote by $\mathcal{I}$ the minimization problem (1.6), that is :*

$$\mathcal{I} = \inf\left\{\mathcal{E}(\ell), \quad \ell \in \mathcal{L}_3(\mathbf{R}^3)\right\}.$$

Then any minimizing sequence of $\mathcal{I}$ is relatively compact in $\mathcal{L}_3(\mathbf{R}^3)$, so that this problem has at least one solution.

In order to show this compactness result, we consider a minimizing sequence ℓ_n, and intend to prove that there exists a basis (a_i^n) of ℓ_n satisfying (2.3), together with :

(a) The sequences $R_i^n = |a_i^n|$ are bounded from below : $\exists R_0 > 0$, s.t $\forall i = 1,2,3$, $\forall n \in \mathbf{N}$, $R_i^n \geq R_0$.

(b) The sequences R_i^n are bounded from above, i.e $\exists R_1 > 0$, s.t $\forall i = 1,2,3$, $\forall n \in \mathbf{N}$, $R_i^n \leq R_1$.

We start with the proof of assertion (a).

5.1 Bound from below

Proposition 5.2 *Let $\ell \in \mathcal{L}_3(\mathbf{R}^3)$, and $(a_i)_{i=1,2,3}$ one of its basis. Denote by $R_i = |a_i|$ the associated radii, and assume that $R_1 \leq R_2 \leq R_3$. Then we have the following :*

$$\mathcal{E}(\ell) \geq \frac{1}{4R_1} + a, \tag{5.1}$$

the constant $a \in \mathbf{R}$ being independent of ℓ.

Proof : We go back to the thermodynamic limit process (see [9, 8]), and recall that taking $\Lambda_n = \left\{\sum_{i=1}^3 k_i a_i, k_i \in \{-n, -n+1, \ldots, n, n+1\}\right\}$, we have :

$$\mathcal{E}(\ell) = \lim_{n\to\infty} \frac{I_{\Lambda_n}^{TFW}}{|\Lambda_n|}, \tag{5.2}$$

where $|\Lambda_n| = (2n+2)^3$ is the cardinal of Λ_n, and $I_{\Lambda_n}^{TFW}$ is the TFW energy defined by :

$$I_{\Lambda_n}^{TFW} = \inf\left\{E_{\Lambda_n}^{TFW}(\rho) + \frac{1}{2}\sum_{k\neq j\in\Lambda_n} \frac{1}{|k-j|}, \quad \rho \geq 0, \quad \sqrt{\rho} \in H^1(\mathbf{R}^3), \quad \int_{\mathbf{R}^3} \rho = (2n+2)^3\right\},$$

with

$$E_{\Lambda_n}^{TFW}(\rho) = \int_{\mathbf{R}^3} |\nabla\sqrt{\rho}|^2 + \int_{\mathbf{R}^3} \rho^{5/3} - \sum_{k\in\Lambda_n} \int_{\mathbf{R}^3} \frac{\rho(x)}{|x-k|}dx + \frac{1}{2}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}dxdy.$$

In particular, we may bound this energy from below by the corresponding TF energy :

$$E^{TFW}_{\Lambda_n}(\rho) \geq E^{TF}_{\Lambda_n}(\rho) = \int_{\mathbf{R}^3} \rho^{5/3} - \sum_{k\in\Lambda} \int_{\mathbf{R}^3} \frac{\rho(x)}{|x-k|}dx + \frac{1}{2}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\rho(x)\rho(y)}{|x-y|}dxdy,$$

so that

$$I^{TFW}_{\Lambda_n} \geq I^{TF}_{\Lambda_n},$$

$I^{TF}_{\Lambda_n}$ being defined by

$$I^{TF}_{\Lambda_n} = \inf\left\{ E^{TF}_{\Lambda_n}(\rho) + \frac{1}{2}\sum_{k\neq j\in\Lambda_n} \frac{1}{|k-j|}, \quad \rho \geq 0, \quad \rho \in L^1 \cap L^{5/3}(\mathbf{R}^3), \quad \int_{\mathbf{R}^3} \rho = (2n+2)^3 \right\}.$$

We now invoke Teller's Lemma [14], which we recall here :

Lemma 5.3 (Teller) *Let $\Lambda = \Lambda_a \cup \Lambda_b$ be a finite subset of $\mathbf{R}^3$, with (Λ_a, Λ_b) a partition of Λ. Then we have :*

$$I^{TF}_{\Lambda} > I^{TF}_{\Lambda_a} + I^{TF}_{\Lambda_b}.$$

Figure 1: The set Λ_n and its subdivision into diatomic molecules (in only two dimensions).

Separating Λ_n into $4(n+1)^3$ sets of two points which distance is equal to R_1, as shown in Figure 5.1 we then have :

$$I^{TFW}_{\Lambda_n} \geq I^{TF}_{\Lambda_n} > 4(n+1)^3 I^{TF}_{\Lambda_0},$$

with $\Lambda_0 = \{0, a_1\}$. Hence considering (5.2), it is sufficient to prove (5.1) for $I^{TF}_{\Lambda_0}$, i.e :

$$E^{TF}_{\{0,a_1\}}(\rho) \geq a, \quad \forall \rho \in L^1 \cap L^{5/3}, \quad \int_{\mathbf{R}^3} \rho = 2, \tag{5.3}$$

with a independent of a_1. In order to do so, we notice that $\frac{1}{|x|} \in L^{5/2}_{loc}(\mathbf{R}^3)$, and thus :

$$\int_{\mathbf{R}^3} \frac{1}{|x|}\rho \leq \int_{|x|>1} \rho + (8\pi)^{2/5}\left(\int_{|x|<1} \rho^{5/3}\right)^{3/5} \leq 2 + (8\pi)^{2/5}\left(\int_{\mathbf{R}^3} \rho^{5/3}\right)^{3/5}.$$

This implies that :

$$E^{TF}_{\Lambda_0}(\rho) \geq \int_{\mathbf{R}^3} \rho^{5/3} - 2(8\pi)^{2/5}\left(\int_{\mathbf{R}^3} \rho^{5/3}\right)^{3/5} - 4 \geq a,$$

for some universal constant $a \in \mathbf{R}$. This implies (5.3), and thus concludes the proof. $\diamondsuit$

At this stage, we would like to make some comment on the Thomas-Fermi case (see [13, 14]). It is worth noticing that we may use directly Teller's Lemma on the TF energy, in order to obtain (since the analogous result to (5.2) is valid in the TF setting, see [14]), that

$$\mathcal{E}^{TF}(\ell) = \lim_{n\to\infty} \frac{I^{TF}_{\Lambda_n}}{|\Lambda_n|} \geq \frac{1}{2} I^{TF}_{\Lambda_0} > I^{TF}_{at},$$

where $I^{TF}_{\Lambda_0}$ is the TF energy of the diatomic molecule with nuclei at positions 0 and a_1, and I^{TF}_{at} is the atomic TF energy (defined exactly as in (3.1)-(3.2), but without the gradient term). Since the same convergence results as those of Theorem 4.11 may be shown in the TF setting, we have the following :

Theorem 5.4 *In the Thomas-Fermi case, problem (1.6) has no solution. Moreover, for any $\ell \in \mathcal{L}_3(\mathbf{R}^3)$, $\mathcal{E}(\ell) > I^{TFW}_{at}$.*

A direct consequence of Proposition 5.2 is the following :

Proposition 5.5 *For any minimizing sequence $(\ell_n)_{n\in\mathbf{N}}$ of problem (1.6), any sequence of basis (a^n_i) of ℓ_n satisfy :*

$$\exists R_0 > 0, \quad |a^n_i| \geq R_0.$$

5.2 Bound from above

We now turn to the proof of (b). We assume that there exists an unbounded minimizing sequence $(\ell_n)_{n\in\mathbf{N}}$, and try to reach a contradiction. For that purpose, we denote by (a^n_i) a basis of ℓ_n given by Theorem 2.4, by $R^n_i = |a^n_i|$ the corresponding radii, and notice that, up to extracting a subsequence, only three cases may occur :

(1) R^n_1 goes to infinity as n goes to infinity,

(2) a^n_1 converges to some a_1 and R^n_2 goes to infinity as n goes to infinity,

(3) (a^n_1, a^n_2) converges to some (a_1, a_2) and R^n_3 goes to infinity as n goes to infinity.

Using Theorem 4.11, we know that respectively in case (1), (2), (3), $\mathcal{E}(\ell_n)$ converges to the atomic energy, the polymer energy associated to a_1, or the thin film energy associated to (a_1, a_2). It is thus sufficient to prove that in all three cases, there exists a proper lattice having a lower energy than those limits. This is our aim in the following subsections.

5.2.1 The thin film case

We show here that for any $\ell \in \mathcal{L}_2(\mathbf{R}^3)$, $\mathcal{E}(\ell)$ cannot be a minimum of $\mathcal{E}$, therefore excluding occurrence (3).

Proposition 5.6 *For any $\ell \in \mathcal{L}_2(\mathbf{R}^3)$, there exists an $\ell_0 \in \mathcal{L}_3(\mathbf{R}^3)$ such that :*

$$\mathcal{E}(\ell_0) < \mathcal{E}(\ell).$$

Proof : We fix an $\ell \in \mathcal{L}_2(\mathbf{R}^3)$, of basis (a_1, a_2), that we may assume to be in the plane $\{x_3 = 0\}$. For any $R > 0$, we define $\ell_R \in \mathcal{L}_3(\mathbf{R}^3)$ the proper lattice of basis (a_1, a_2, Re_3). We intend to show the following :

$$\mathcal{E}(\ell_R) \leq \mathcal{E}(\ell) - Ce^{-\sqrt{\theta_\ell}R} + o(e^{-\sqrt{\theta_\ell}R}), \quad \text{as} \quad R \longrightarrow \infty, \tag{5.4}$$

with $C > 0$, and where $\theta_\ell > 0$ is the Lagrange multiplier of problem (3.37). For this purpose, we denote by ρ the unique electronic density associated to the lattice ℓ, and set $\rho_R = \frac{\rho_{|\Gamma(\ell_R)}}{\|\rho\|_{L^1(\Gamma(\ell_R))}}$. Since ρ is even with respect to x_3, ρ_R is ℓ_R-periodic, thus is a test function for the variational problem defining $\mathcal{E}(\ell_R)$. Denoting by $\varepsilon_R = \int_{\Gamma(\ell)\cap\{|x_3|>R\}} \rho$, we have, from Proposition 3.8,

$$\varepsilon_R \sim a_\ell \frac{|a_1 \wedge a_2|}{2\sqrt{\theta_\ell}} e^{-\sqrt{\theta_\ell}R} = \alpha e^{-\sqrt{\theta_\ell}R}, \quad \text{as} \quad R \longrightarrow \infty.$$

We now study each terms of the energy functional :

$$\int_{\Gamma(\ell_R)} |\nabla\sqrt{\rho}_R|^2 \leq \frac{1}{1-\varepsilon_R} \int_{\Gamma(\ell)} |\nabla\sqrt{\rho}|^2 \leq (1+\varepsilon_R) \int_{\Gamma(\ell)} |\nabla\sqrt{\rho}|^2 + o(\varepsilon_R). \tag{5.5}$$

Likewise,

$$\int_{\Gamma(\ell_R)} \rho_R^{5/3} \leq (1 + \frac{5}{3}\varepsilon_R) \int_{\Gamma(\ell)} \rho^{5/3} + o(\varepsilon_R). \tag{5.6}$$

We then turn to the electrostatic terms : setting

$$E_{\ell_R}^{TFW,el}(\rho_R) = -\int_{\Gamma(\ell_R)} \rho_R G_{\ell_R} + \frac{1}{2} \int_{\Gamma(\ell_R)} \int_{\Gamma(\ell_R)} \rho_R(x)\rho_R(y) G_{\ell_R}(x-y)dxdy,$$

and denoting by h_R the function $G_\ell - G_{\ell_R}$, we have :

$$\begin{aligned} E_{\ell_R}^{TFW,el}(\rho_R) \quad = \quad & -\int_{\Gamma(\ell_R)} \rho_R G_\ell + \frac{1}{2} \int_{\Gamma(\ell_R)} \int_{\Gamma(\ell_R)} \rho_R(x)\rho_R(y) G_\ell(x-y)dxdy \\ & + \int_{\Gamma(\ell_R)} \rho_R h_R - \frac{1}{2} \int_{\Gamma(\ell_R)} \int_{\Gamma(\ell_R)} \rho_R(x)\rho_R(y) h_R(x-y)dxdy + o(\varepsilon_R). \end{aligned}$$

Hence, developing in the same fashion as above :

$$\begin{aligned} E^{TFW,el}_{\ell_R}(\rho_R) &= -(1+\varepsilon_R)\int_{\Gamma(\ell_R)}\rho G_\ell + (\frac{1}{2}+\varepsilon_R)\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)}\rho(x)\rho(y)G_\ell(x-y)dxdy \\ &\quad + \int_{\Gamma(\ell_R)}\rho_R h_R - \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)}\rho_R(x)\rho_R(y)h_R(x-y)dxdy + o(\varepsilon_R). \end{aligned}$$

We are now going to show that :

$$\begin{aligned} -\int_{\Gamma(\ell_R)}\rho G_\ell \;&+\; \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)}\rho(x)\rho(y)G_\ell(x-y)dxdy \le \\ &-\int_{\Gamma(\ell)}\rho G_\ell + \frac{1}{2}\int_{\Gamma(\ell)}\int_{\Gamma(\ell)}\rho(x)\rho(y)G_\ell(x-y)dxdy \end{aligned} \tag{5.7}$$

and

$$\int_{\Gamma(\ell_R)}\rho_R h_R - \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)}\rho_R(x)\rho_R(y)h_R(x-y)dxdy \le o(\varepsilon_R) \tag{5.8}$$

We begin with (5.7), and write the difference of these two expressions as :

$$\begin{aligned} -\int_{\Gamma(\ell_R)}\rho G_\ell \;&+\; \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)}\rho(x)\rho(y)G_\ell(x-y)dxdy \\ +\int_{\Gamma(\ell)}\rho G_\ell \;&-\; \frac{1}{2}\int_{\Gamma(\ell)}\int_{\Gamma(\ell)}\rho(x)\rho(y)G_\ell(x-y)dxdy \\ &= \int_{\Gamma(\ell)\setminus\Gamma(\ell_R)}\rho\big(G_\ell - \frac{1}{2}G_\ell\star_{\Gamma(\ell)}(\rho_{|\Gamma(\ell_R)}+\rho)\big). \end{aligned}$$

Hence, proving that $G_\ell - \frac{1}{2}G_\ell\star_{\Gamma(\ell)}(\rho_{|\Gamma(\ell_R)}+\rho) \le 0$ on $\Gamma(\ell)\setminus\Gamma(\ell_R)$, for R sufficiently large, will conclude the proof of (5.7). For this purpose, we use Proposition 3.6 and write :

$$-\alpha|x_3| + \beta - \frac{\gamma}{|x|} \le G_\ell(x) \le -\alpha|x_3| + \beta + \frac{\gamma}{|x|} \tag{5.9}$$

in $\Gamma(\ell)$, where α, β and γ are positive constants independent of R. From this and the fact that $\frac{1}{2}(\rho+\rho_{|\Gamma(\ell_R)})$ has total mass $1-\frac{\varepsilon_R}{2}$ over $\Gamma(\ell)$, we deduce that :

$$-\alpha(1-\frac{\varepsilon_R}{2})|x_3| + \beta(1-\frac{\varepsilon_R}{2}) - \frac{\gamma'}{|x|} \le \frac{1}{2}G_\ell\star_{\Gamma(\ell)}(\rho+\rho_{|\Gamma(\ell_R)}) \le -\alpha(1-\frac{\varepsilon_R}{2})|x_3| + \beta(1-\frac{\varepsilon_R}{2}) + \frac{\gamma'}{|x|},$$

with a constant $\gamma' > 0$ independent of R. This, together with (5.9), proves that

$$G_\ell - \frac{1}{2}G_\ell\star_{\Gamma(\ell)}(\rho_{|\Gamma(\ell_R)}+\rho) \le (1-\frac{\varepsilon_R}{2})(\beta - \alpha|x_3|) \le 0$$

whenever $|x_3|$ is sufficiently large. This proves our claim, and thus completes the proof of (5.7).

We now turn to (5.8), and set $\phi_R = G_\ell - G_\ell \star_{\Gamma(\ell)} \rho_R$. We have :

$$-\Delta \phi_R = 4\pi(\delta_0 - \rho_R).$$

Since h_R cancels at 0, we have :

$$\begin{aligned}
-\int_{\Gamma(\ell_R)} \rho_R h_R &+ \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)} \rho_R(x)\rho_R(y)h_R(x-y)dxdy \\
&= \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)} h_R(x-y)\Big(\rho_R(x)-\delta_0(x)\Big)\Big(\rho_R(y)-\delta_0(y)\Big)dxdy \\
&= \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)} h_R(x-y)\Big(-\Delta\phi_R(x)\Big)\Big(-\Delta\phi_R(y)\Big)dxdy.
\end{aligned}$$

We now integrate by parts this expression, and find :

$$\begin{aligned}
-\int_{\Gamma(\ell_R)} \rho_R h_R &+ \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)} \rho_R(x)\rho_R(y)h_R(x-y)dxdy \\
&= \frac{1}{2}\int_{\partial\Gamma(\ell_R)}\int_{\partial\Gamma(\ell_R)} \frac{\partial\phi_R}{\partial n}(x)\frac{\partial\phi_R}{\partial n}(y)h_R(x-y)dx'dy'.
\end{aligned}$$

From the ℓ-periodicity of ϕ_R, this boundary integral reduces to an integral over the set $\partial\Gamma(\ell_R)\cap\{|x_3| = \frac{R}{2}\}$. And using the fact that ϕ_R and h_R are even with respect to x_3, we thus have :

$$\begin{aligned}
-\int_{\Gamma(\ell_R)} \rho_R h_R &+ \frac{1}{2}\int_{\Gamma(\ell_R)}\int_{\Gamma(\ell_R)} \rho_R(x)\rho_R(y)h_R(x-y)dxdy \\
&= \int_{\{x_3=\frac{R}{2}\}\cap\overline{\Gamma(\ell)}}\int_{\{y_3=\frac{R}{2}\}\cap\overline{\Gamma(\ell)}} \partial_3\phi_R(x)\partial_3\phi_R(y)h_R(x-y)dx'dy' \\
&\quad -\int_{\{x_3=\frac{R}{2}\}\cap\overline{\Gamma(\ell)}}\int_{\{y_3=-\frac{R}{2}\}\cap\overline{\Gamma(\ell)}} \partial_3\phi_R(x)\partial_3\phi_R(y)h_R(x-y)dx'dy'.
\end{aligned}$$

In order to bound this term, we write :

$$\phi_R = \phi + \frac{1}{1-\varepsilon_R}\rho_{|\Gamma(\ell_R)^c}\star G_\ell - \frac{\varepsilon_R}{1-\varepsilon_R}\rho\star G_\ell = \phi + \hat{\phi}_R,$$

where the convolution products are over $\Gamma(\ell)$, and $\phi = G_\ell - \rho\star G_\ell$. We are going to prove (5.8) for all those terms. The second one may be dealt with as follows : we first notice that

$$|\rho\star G_\ell(x_3 = \pm\frac{R}{2})| \le CR, \tag{5.10}$$

and

$$\begin{aligned}
|(\rho_{|\Gamma(\ell_R)^c}\star G_\ell)(x_3 = \pm\frac{R}{2})| &= \left|\int_{\{|y_3|\ge\frac{R}{2}\}\cap\Gamma(\ell_R)} \rho(y)G_\ell(x-y)dy\right|(x_3 = \pm\frac{R}{2}) \\
&\le \int_{\{|y_3|\ge\frac{R}{2}\}\cap\Gamma(\ell_R)} \frac{\rho(y)}{|x-y|}dy + \int_{\{|y_3|\ge\frac{R}{2}\}\cap\Gamma(\ell_R)} \rho(y)|x-y|dy \\
&\le CR\varepsilon_R. \qquad (5.11)
\end{aligned}$$

(5.10) and (5.11) imply that :

$$|\hat{\phi}_R(x_3 = \pm\frac{R}{2})| \leq CR\varepsilon_R. \tag{5.12}$$

On the other hand, $|-\Delta\hat{\phi}_R(x_3 = \pm\frac{R}{2})| \leq |\rho_R(x_3 = \pm\frac{R}{2})| \leq C\varepsilon_R$, so that we have :

$$|\nabla\hat{\phi}_R(x_3 = \pm\frac{R}{2})| \leq CR\varepsilon_R.$$

Since we also know that $|\nabla\phi(x_3 = \pm\frac{R}{2})| \leq Ce^{-aR}$, for some $a > 0$ independent of R, (5.8) is proved for $\hat{\phi}_R$ and for the crossing term. Thus, the proof of (5.8) amounts to show :

$$\begin{aligned} &\int_{\{x_3=\frac{R}{2}\}\cap\Gamma(\ell)}\int_{\{y_3=\frac{R}{2}\}\cap\Gamma(\ell)} \partial_3\phi(x)\partial_3\phi(y)h_R(x-y)dx'dy' \\ -&\int_{\{x_3=\frac{R}{2}\}\cap\Gamma(\ell)}\int_{\{y_3=-\frac{R}{2}\}\cap\Gamma(\ell)} \partial_3\phi(x)\partial_3\phi(y)h_R(x-y)dx'dy' \quad \geq \quad o(\varepsilon_R). \end{aligned} \tag{5.13}$$

To prove this, we expand h_R as a Fourier series with respect to x'. Using (3.39) and (4.7), one easily computes :

$$h_R(x) = H_R(x_3) - c_\ell \sum_{k\in\ell^*\setminus\{0\}} \frac{e^{2i\pi k\cdot x'}}{|k|} \sum_{k_3\in\mathbf{Z}\setminus\{0\}} e^{-|k|2\pi|x_3-k_3R|}, \tag{5.14}$$

with $|H_R(t)| \leq C(1+|t|)$, C being independent of R, and $c_\ell > 0$. Here we have used the fact that

$$\int_{\mathbf{R}} \frac{e^{2i\pi x_3\xi}}{|k|^2+\xi^2}d\xi = \frac{2\pi}{|k|}e^{-2\pi|k||x_3|},$$

and the corresponding periodic equality, that is :

$$\frac{2\pi}{|k|}\sum_{k_3\in\mathbf{Z}} \frac{e^{2i\pi\frac{k_3}{R}x_3}}{|k|^2+\frac{k_3^2}{R^2}} = \sum_{k_3\in\mathbf{Z}} e^{-|k|2\pi|x_3-k_3R|}.$$

We then insert (5.14) into the left-hand side of (5.13), which we denote by A_R, and find :

$$\begin{aligned} A_R \;=\; &\int_{x_3=\frac{R}{2}}\int_{y_3=\frac{R}{2}} \partial_3\phi(x)\partial_3\phi(y)H_R(x_3-y_3)dx'dy' \\ &-\int_{x_3=\frac{R}{2}}\int_{y_3=-\frac{R}{2}} \partial_3\phi(x)\partial_3\phi(y)H_R(x_3-y_3)dx'dy' \\ &-c_\ell\sum_{k\in\ell^*}\left(\tilde{\partial_3\phi}(k,\frac{R}{2})\tilde{\partial_3\phi}(-k,\frac{R}{2})\sum_{k_3\neq 0} e^{-2\pi|k||k_3|R}\right) \\ &+c_\ell\sum_{k\in\ell^*}\left(\tilde{\partial_3\phi}(k,\frac{R}{2})\tilde{\partial_3\phi}(-k,-\frac{R}{2})\sum_{k_3\neq 0}(e^{-2\pi|k||1-k_3|R})\right), \end{aligned}$$

where the $\tilde{}$ -transform is defined by (3.43). We next use estimate (3.42)of Proposition 3.8, with $\epsilon < \sqrt{\theta_\ell}$ to show that the first two integrals of the above sum may be bounded by $O(R^2 e^{-2(\sqrt{\theta_\ell}-\epsilon)R}) = o(\varepsilon_R)$, and that up to terms of the same order, the sum reduces to a sum over $K = \ell^* \cap \{0 < \pi|k| < \sqrt{\theta_\ell}\}$. We thus have, μ_k being defined in (3.42) :

$$\begin{aligned} A_R &= -c_\ell \sum_{k \in K} \sum_{k_3 \neq 0} \mu_k \mu_{-k} e^{-2\pi|k|R} (e^{-2\pi|k||k_3|R} - e^{-2\pi|k||1-k_3|R}) + o(\varepsilon_R) \\ &= -c_\ell \sum_{k \in K} \mu_k \mu_{-k} e^{-2\pi|k|R} (-1 + e^{-2\pi|k|R}) + o(\varepsilon_R). \end{aligned}$$

Then, noticing that since $\partial_3 \phi$ is a real-valued function, we infer that $\mu_{-k} = \overline{\mu}_k$, so that we may write the above sum as :

$$A_R = c_\ell \sum_{k \in K} |\mu_k|^2 e^{-2\pi|k|R} (-e^{-2\pi|k|R} + 1) \geq 0,$$

for R large enough, since K does not depend on R. This proves (5.13), hence (5.8).

We now collect (5.5), (5.6), (5.7) and (5.8), and find :

$$\begin{aligned} E_{\ell_R}^{TFW}(\rho_R) \leq \; & E_\ell^{TFW}(\rho) + \varepsilon_R \left(\int_{\Gamma(\ell)} |\nabla \rho|^2 + \frac{5}{3} \int_{\Gamma(\ell)} \rho^{5/3} \right. \\ & \left. - \int_{\Gamma(\ell)} G_\ell \rho + \int_{\Gamma(\ell)} \int_{\Gamma(\ell)} \rho(x)\rho(y) G_\ell(x-y)\,dx\,dy \right) + o(\varepsilon_R). \end{aligned}$$

Integrating the Euler-Lagrange equation of the minimization problem defining $\mathcal{E}(\ell)$, we find that :

$$\int_{\Gamma(\ell)} |\nabla \rho|^2 + \frac{5}{3} \int_{\Gamma(\ell)} \rho^{5/3} - \int_{\Gamma(\ell)} G_\ell \rho + \int_{\Gamma(\ell)} \int_{\Gamma(\ell)} \rho(x)\rho(y) G_\ell(x-y)\,dx\,dy = -\theta_\ell,$$

so that we infer that :

$$\mathcal{E}(\ell_R) \leq \mathcal{E}(\ell) - \varepsilon_R \theta_\ell + o(\varepsilon_R).$$

This concludes the proof. $\diamondsuit$

5.2.2 The polymer case

We now turn to case (2) :

Proposition 5.7 *For any $\ell \in \mathcal{L}_1(\mathbf{R}^3)$, there exists $\ell_0 \in \mathcal{L}_3(\mathbf{R}^3)$ such that :*

$$\mathcal{E}(\ell_0) < \mathcal{E}(\ell).$$

Proof : We use exactly the same trick as for Proposition 5.6, defining ℓ_R as the lattice of basis (Re_1, Re_2, a), where a is the basis of ℓ, and is collinear to e_3 (this is always possible to do by change of coordinates). We intend to show estimate (5.4) in this case. We define ρ_R

and ε_R exactly in the same way, so that (5.5) and (5.6) follow immediately. (Note that from Proposition 3.3, ε_R satisfies exactly the same estimate as in the thin film case.)

A straightforward adaptation of (5.7)'s proof shows that this estimate also holds (just replace $|x_3|$ by $\log|x'|$). To prove (5.8), the same ϕ_R-trick works, and we are here again reduced to show bounds on integrals over the set $\{|x_1| = \frac{R}{2}\} \cup \{|x_2| = \frac{R}{2}\}$. Here again, the same type of estimates are available, namely (3.8), (4.7) and (3.36), so that the above proof can be easily adapted, replacing the function $e^{-a|x_3|}$ by $W_a(x')$ defined in (3.24) $\diamondsuit$

5.2.3 The atomic case

We deal here with case (3) :

Proposition 5.8 *There exists an $\ell \in \mathcal{L}_3(\mathbf{R}^3)$ satisfying the following :*

$$\mathcal{E}(\ell) < I_{at}^{TFW}.$$

Proof : We follow step by step the proof of Proposition 5.6, with $\ell_R = R\mathbf{Z}^3$, and find out that difficulties might only occur in the electrostatic terms. We introduce here again the function $\phi_R = \frac{1}{|x|} - \frac{1}{|x|} \star \rho_{R|\Gamma(\ell_R)}$, and using the same tricks, conclude the proof. Note that here, the proof is simpler since the eigenmodes appearing in the polymer and thin film case with coefficients μ_k vanish, so that the proof of (5.8) is simplified. $\diamondsuit$

This concludes the proof of Theorem 1.1, since, considering a minimizing sequence ℓ_n of problem (1.6), Proposition 5.5 shows that there exists an $R_0 > 0$ such that for any basis $(a_i^n)_{i=1,2,3}$ of ℓ_n, we have :

$$|a_i^n| \geq R_0, \quad \forall i \in \{1,2,3\}, \forall n \in \mathbf{N}.$$

On the other hand, Theorem 4.11 together with Propositions 5.6, 5.7 and 5.8, show that there exists a sequence of basis of ℓ_n which is bounded in $\mathbf{R}^3$, and hence is relatively compact.

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