Thomas-Fermi type theories for polymers and solid films

X. Blanc & C. Le Bris

CERMICS, Ecole Nationale des Ponts et Chaussées,

6 & 8, avenue Blaise Pascal, Cité Descartes,

Champs sur Marne, 77455 Marne-La-Vallée Cedex

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Abstract

We define a Thomas-Fermi-von Weizsäcker model for polymers and solid films through a thermodynamic limit process. Our argument makes use of standard techniques for elliptic PDEs, such as maximum principles or supersolution methods. In the course of our work, we establish some existence and uniqueness results for a system of non-linear PDE.

1 Introduction

In [5], I. Catto, P.L. Lions and one of us have studied the problem of thermodynamic limit for a three-dimensional crystal in the Thomas-Fermi-von Weizsäcker (TFW in short) setting. Given a finite set of nuclei represented by a set of points $\Lambda \subset \mathbf{R}^3$, each one of charge $+1$, the TFW model associates to this set an electronic density, denoted by ρ_Λ, which minimizes the so-called TFW energy, that is :

$$\begin{aligned} E_\Lambda(\rho) &= \int_{\mathbf{R}^3} |\nabla\sqrt{\rho}|^2 + \int_{\mathbf{R}^3} \rho^{5/3} - \sum_{k\in\Lambda} \int_{\mathbf{R}^3} \frac{\rho(x)}{|x-k|} dx \\ &+\frac{1}{2}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dxdy. \end{aligned} \tag{1.1}$$

In other words, the density ρ_Λ is a solution to the following minimization problem :

$$I_\Lambda = \inf\left\{ E_\Lambda(\rho) + \frac{1}{2}\sum_{k\neq j\in\Lambda} \frac{1}{|k-j|}, \rho \geq 0,\ \sqrt{\rho} \in H^1(\mathbf{R}^3), \int_{\mathbf{R}^3} \rho = |\Lambda| \right\}, \tag{1.2}$$

where $|\Lambda|$ denotes the cardinal of the set Λ. The case of smeared nuclei can be also considered ; that is when the measure defining the nuclei in (1.1) is replaced by a smooth measure m, having compact support and total mass one. In this latter case, (1.1) and (1.2) become :

$$\begin{aligned} E_\Lambda^m(\rho) &= \int_{\mathbf{R}^3} |\nabla\sqrt{\rho}|^2 + \int_{\mathbf{R}^3} \rho^{5/3} - \int_{\mathbf{R}^3} (m_\Lambda \star \frac{1}{|x|})\rho \\ &+ \frac{1}{2}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{\rho(x)\rho(y)}{|x-y|} dxdy, \end{aligned}$$

where $m_\Lambda = \sum_{k\in\Lambda} m(\cdot - k)$, and $\star$ is the convolution product over $\mathbf{R}^3$,

$$\begin{aligned} I_\Lambda^m &= \inf\left\{ E_\Lambda^m(\rho) + \frac{1}{2}\int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{m_\Lambda(x)m_\Lambda(y)}{|x-y|} dxdy, \right. \\ & \left. \rho \geq 0,\ \sqrt{\rho} \in H^1(\mathbf{R}^3),\ \int_{\mathbf{R}^3} \rho = |\Lambda| \right\}. \end{aligned} \tag{1.3}$$

It is well-known that the problem (1.2) (respectively (1.3)) has a unique minimizer (see for instance [2], [10] or [12]), basically because the energy functional E_Λ is convex with respect to ρ.

The thermodynamic limit problem is the following : letting Λ be a subset of a periodic lattice, determine the behaviour of I_Λ and ρ_Λ as Λ progressively fills in the entire lattice.

In order to tackle this problem mathematically, we introduce the notion of Van Hove sequences :

Let $\Lambda = (\Lambda_h)_{h\in\mathbf{N}}$ be a sequence of subsets of $\mathbf{Z}^n$, having cardinal $|\Lambda|$. Λ is a Van Hove sequence of $\mathbf{Z}^n$ if it satisfies the following :

(An) *For any finite subset A of $\mathbf{Z}^n$, there exists $h_0 \in \mathbf{N}$ such that for all $h \geq h_0$, $A \subset \Lambda_h$.*

(Bn) *Denoting by Γ the unit cube centered at the origin, by $\Gamma(\Lambda)$ the set $\cup_{k\in\Lambda}(\Gamma + k)$, by Λ^a the set $\{x \in \mathbf{R}^n \;/\; d(x, \partial\Gamma(\Lambda)) < a\}$, where d is the Euclidean distance in $\mathbf{R}^n$, and by $|\Lambda_h^a|$ the Lebesgue measure (in $\mathbf{R}^n$) of the set Λ_h^a, we have, for all $a > 0$, the Van Hove condition, that is :*

$$\lim_{h\to\infty} \frac{|\Lambda_h^a|}{|\Lambda_h|} = 0 \tag{1.4}$$

The thermodynamic limit problem studied in [5] consists then in answering the following questions, for any Van Hove sequence Λ of $\mathbf{Z}^3$:

(L1) *Does the energy per cell $\frac{I_\Lambda}{|\Lambda|}$ converge as $|\Lambda|$ goes to infinity ?*

(L2) *Does the density ρ_Λ converge to a limit ρ_∞ as $|\Lambda|$ goes to infinity ?*

(L3) *Does the limit ρ_∞ have the same periodicity as that of the lattice ?*

In this article, we study questions (L1), (L2), (L3) in two cases that do not satisfy conditions (A3) and (B3) :

(a) *The first case is the thermodynamic limit of a lineic molecule, that is $\Lambda = \{(0,0)\} \times \Lambda_3$ will be a subset of $\{(0,0)\} \times \mathbf{Z}$, such that Λ_3 is a Van Hove sequence of $\mathbf{Z}^1$,*

(b) *The second case is the same problem concerning a solid film : $\Lambda = \Lambda_2 \times \{0\}$ is a subset of $\mathbf{Z}^2 \times \{0\}$, and the sequence Λ_2 is a Van Hove sequence of $\mathbf{Z}^2$.*

1.1 Lineic molecules

In this case, to which Section 2 is devoted, we are going to answer affirmatively the questions (L1), (L2), and (L3). More precisely, we introduce the following notation :

(i) we denote by $\Gamma_0 = \mathbf{R}^2 \times]-\frac{1}{2}, \frac{1}{2}]$ the periodic cell of the problem, and by $\Gamma(\Lambda)$ the set $\cup_{k\in\Lambda}\Gamma_0 + k$.

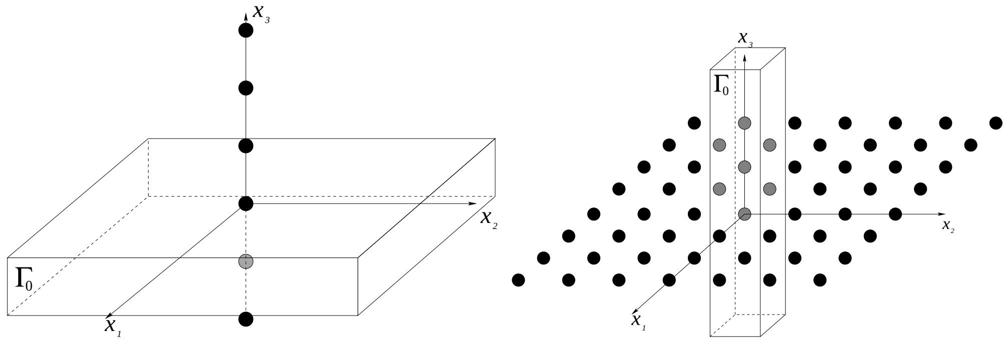

Figure 1: The set Λ in the case of polymers (on the left) and solid films (on the right)

(ii) For any functional space S, $S_{per}(\Gamma_0)$ denotes the set of elements of $S_{loc}(\mathbf{R}^3) \cap S(\Gamma_0)$ that are periodic with periodic cell Γ_0.

We introduce the following variational problem :

$$I_{per} = \inf\left\{ E_{per}(\rho), \rho \geq 0,\ \sqrt{\rho} \in X_{per},\ \int_{\Gamma_0} \rho = 1 \right\}, \tag{1.5}$$

where X_{per} is a subspace of $H^1_{per}(\Gamma_0)$ to be made precise later on (see formula 2.14), and E_{per} is defined by :

$$E_{per}(\rho) = \int_{\Gamma_0} |\nabla \sqrt{\rho}|^2 + \int_{\Gamma_0} \rho^{5/3} - \int_{\Gamma_0} G\rho + \frac{1}{2}\int_{\Gamma_0}\int_{\Gamma_0} \rho(x)\rho(y)G(x-y)dxdy. \tag{1.6}$$

The potential G, which is not to be confused with the potential G appearing in [5] (it is its 1-D analogue), is the periodic potential modeling the Coulombian interaction in the periodic lattice $\{(0,0)\} \times \mathbf{Z}$. (In the smeared nuclei case, the only necessary change is to take $G \star_{\Gamma_0} m$ instead of G in the third term of the energy.) From the conclusions of [11], it is natural to introduce :

$$G(x) = -2\log|x'| + \sum_{k\in\mathbf{Z}} \left(\frac{1}{|x-ke_3|} - \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dy}{|x-(y+k)e_3|} \right), \tag{1.7}$$

where we denote by x' the vector (x_1, x_2), and by (e_1, e_2, e_3) the canonical basis of $\mathbf{R}^3$. It is easy to check that G is periodic, with periodic cell Γ_0, and that it satisfies :

$$-\Delta G = 4\pi \sum_{k\in\mathbf{Z}} \delta_{ke_3}.$$

The constant M is defined by follows :

- In the point nuclei case, $M = \lim_{x \to 0} \big(G(x) - \frac{1}{|x|} \big)$.
- In the smeared nuclei case, $M = \int_{\Gamma_0} \int_{\Gamma_0} m(x) m(y) \big(G(x-y) - \frac{1}{|x-y|} \big)$.

The main result of Section 2 is the following theorem :

Theorem 1.1 *Let Λ be a Van Hove sequence in the third dimension, in the sense made precise above, and ρ_Λ the minimizing density of the TFW energy. Then we have :*

(i) $\lim_{\Lambda \to \infty} \frac{I_\Lambda}{|\Lambda|} = I_{per} + \frac{M}{2}$.

(ii) The density ρ_Λ converges to ρ_{per} uniformly on any subset of the form $\mathbf{R}^2 \times K$, K being a compact subset of $\mathbf{R}$.

The strategy of the proof is as follows : we first write down I_Λ's Euler-Lagrange equation, that is : (setting $\rho_\Lambda = u_\Lambda^2$ and $m_\Lambda = \sum_{k \in \Lambda} m(\cdot - k)$, m being either δ_0 in the point nuclei case, or a smooth function in the smeared nuclei case)

$$-\Delta u_\Lambda + \frac{5}{3} u_\Lambda^{7/3} - \left((m_\Lambda - u_\Lambda^2) \star \frac{1}{|x|} \right) u_\Lambda = -\theta_\Lambda u_\Lambda,$$

where θ_Λ denotes the Lagrange multiplier associated to the mass constraint in I_Λ. Hence, denoting by ϕ_Λ the function $(m_\Lambda - u_\Lambda^2) \star \frac{1}{|x|} - \theta_\Lambda$, we get a solution of the system :

$$\left\{ \begin{array}{l} -\Delta u_\Lambda + \frac{5}{3} u_\Lambda^{7/3} - u_\Lambda \phi_\Lambda = 0, \\ -\Delta \phi_\Lambda = 4\pi (m_\Lambda - u_\Lambda^2), \\ u_\Lambda \geq 0. \end{array} \right. \tag{1.8}$$

As in [5], we then establish bounds on u_Λ and ϕ_Λ, so that we can pass locally to the limit in the above system. Next, we show the following uniqueness result :

Theorem 1.2 *Let $\mu \not\equiv 0$ be a non-negative measure with compact support with respect to (x_1, x_2). Assume that μ is periodic with periodic cell Γ_0, and that $\mu(\Gamma_0) = 1$. Then the following system*

$$\left\{ \begin{array}{l} -\Delta u + \frac{5}{3} u^{7/3} - u \phi = 0, \\ -\Delta \phi = 4\pi (\mu - u^2), \\ u \geq 0 \end{array} \right. \tag{1.9}$$

has a unique solution $(u, \phi) \in \big(L^2_{unif} \cap L^{7/3}_{loc}(\mathbf{R}^3) \big) \times L^1_{unif}(\mathbf{R}^3)$. In addition, this solution satisfies the following properties :

(i) $u \in L^\infty(\mathbf{R}^3)$, *and* $u(x) \leq \frac{C}{1+(x_1^2+x_2^2)^{3/4}}$, $C > 0$ *being a constant independent of* x.

(ii) $\phi \in L^p_{unif}(\mathbf{R}^3)$ *for all* $p < 3$, *and there exists a constant* θ_{per} *such that* $\phi = G \star_{\Gamma_0} (\mu - u^2) - \theta_{per}$.

(iii) $\int_{\Gamma_0} u^2 = 1$.

The space $L^p_{unif}(\mathbf{R}^3)$ is $\{f \in L^p_{loc}(\mathbf{R}^3)\ /\ \sup_{x\in\mathbf{R}^3} \|f\|_{L^p(B_1+x)} < \infty\}$.

Once this result is established, applying it to the case $\mu = \sum_{k\in\mathbf{Z}^3} m(\cdot + k)$, we may therefore identify the limit of u_Λ as the unique solution of this system.

Concerning the proof of Theorem 1.2, the strategy consists in showing that any solution of system (1.9) is periodic, with periodic cell Γ_0, hence that $\rho = u^2$ is a critical point of I_{per}, with nuclei defined by $m = \mu$ on Γ_0, and next showing that this problem is strictly convex, so that ρ is necessarily its unique minimizer. In order to show that I_{per} is convex, we introduce the bilinear form D_G defined by :

$$D_G(f,g) = \int_{\Gamma_0}\int_{\Gamma_0} f(x)g(y)G(x-y)dxdy = \int_{\Gamma_0} (f \star_{\Gamma_0} G)g,$$

and we rewrite E_{per} as :

$$E_{per}(\rho) = \int_{\Gamma_0} |\nabla\sqrt{\rho}|^2 + \int_{\Gamma_0} \rho^{5/3} + \frac{1}{2}D_G(m-\rho, m-\rho) - \frac{1}{2}D_G(m,m).$$

Of course, this is possible only in the smeared nuclei case, or equivalently if m is smooth. If it is not, we introduce the characteristic function of the unite cube, denoted by 1_Q, and write :

$$\begin{aligned} E_{per}(\rho) \quad = \quad & \int_{\Gamma_0} |\nabla\sqrt{\rho}|^2 + \int_{\Gamma_0} \rho^{5/3} + \frac{1}{2}D_G(1_Q-\rho, 1_Q-\rho) - \frac{1}{2}D_G(1_Q, 1_Q) \\ & + \int_{\Gamma_0} \big((1_Q - m) \star_{\Gamma_0} G\big)\rho. \end{aligned}$$

In both cases, the point is that, by studying closely the potential G, we find that D_G is positive on a set that includes $m - \rho$ and $1_Q - \rho$ as far as $\sqrt{\rho}$ lies in X_{per} and ρ has total mass one over Γ_0. So D_G is a convex functional on that set. Hence I_{per} becomes a convex problem.

Those results answer questions (L2) and (L3). Next, we use them as in [5] to show the convergence of the energy, answering question (L1).

All these results give a TFW model for any molecule which nuclei are periodically ditributed with respect to x_3, and contained in a cylinder having vertical axis. This is the case for many polymers, and for DNA molecules.

1.2 Solid films

The second part of our work concerns problem (b).

As above, we denote by Γ_0 the periodic cell of the problem, which is now $]-\frac{1}{2},\frac{1}{2}]^2\times\mathbf{R}$, and by $\Gamma(\Lambda)$ the set $\cup_{k\in\Lambda}\Gamma_0+k$. The notation $H^1_{per}(\Gamma_0)$ follows as in the one-dimensional case.

Here again, we introduce a periodic potential, that we still denote by G, though it is neither the same as in [5] nor as in (1.7) :

$$G(x) = -2\pi|x_3| + \sum_{k\in\mathbf{Z}^2\times\{0\}}\left(\frac{1}{|x-k|} - \int_{K\times\{0\}}\frac{dy}{|x-y-k|}\right), \tag{1.10}$$

where K is the unit square of $\mathbf{R}^2$, namely $]-\frac{1}{2},\frac{1}{2}[^2$. We notice that G satisfies the equation

$$-\Delta G = 4\pi\sum_{k\in\mathbf{Z}^2\times\{0\}}\delta_k.$$

The energy E_{per} is defined by (1.6), and the problem I_{per} by (1.5). We also define the constant M exactly in the same way as in the polymers case.

We do not have here a convergence result as that of the preceding section, although we suspect it to hold. In fact, to be able to show a convergence theorem as Theorem 1.1, we need the additional assumption that Λ is symmetric with respect to x_1 and x_2. However, it is only a technical hypothesis, and the convergence result that is stated in Theorem 1.3 below is likely to be true for any Van Hove sequence.

Theorem 1.3 *Let Λ be a Van Hove sequence in the first two directions. Assume that Λ is symmetric with respect to x_1 and x_2. (In the smeared nuclei case, m is also supposed to be symmetric.) Then, we have :*

(i) $\lim_{|\Lambda|\to\infty}\frac{I_\Lambda}{|\Lambda|} = I_{per}+\frac{M}{2}$.

(ii) ρ_Λ uniformly converges to ρ_{per} on any set of the form $K\times\mathbf{R}$, K being a compact subset of $\mathbf{R}^2$.

As in the preceding section, we start by proving the second assertion of Theorem 1.3, the first one being a consequence of it. For this purpose, we use exactly the same strategy as above, showing first that the Euler-Lagrange passes to the limit, and then that such a solution is a critical point of I_{per}. The same positiveness property holds concerning D_G, and so the proof carries through. The only difference is that, for technical reasons, we are not able to show a uniqueness result similar to that of Theorem 1.2 : such a result would hold only (so far as we know) to a solution coming from the thermodynamic limit process for a sequence of symmetric domains.

Remark 1.1 *In all the results we have stated above, we have used the Coulombian interaction potential, that is $V(x) = \frac{1}{|x|}$. Another choice is possible, namely the Yukawa potential :*

$$V(x) = \frac{e^{-a|x|}}{|x|}, \tag{1.11}$$

where $a > 0$.

Then (1.1) and (1.8) become :

$$\begin{aligned} E_\Lambda(\rho) &= \int_{\mathbf{R}^3} |\nabla\sqrt{\rho}|^2 + \int_{\mathbf{R}^3} \rho^{5/3} - \sum_{k\in\Lambda} \int_{\mathbf{R}^3} \rho V(\cdot - k) \\ &\quad + \frac{1}{2}\int_{\mathbf{R}^3} (\rho \star V)\rho. \end{aligned} \tag{1.12}$$

$$\begin{cases} -\Delta u_\Lambda + \frac{5}{3}u_\Lambda^{7/3} - u_\Lambda\phi_\Lambda = 0, \\ -\Delta\phi_\Lambda + a^2\phi_\Lambda = 4\pi(m_\Lambda - u_\Lambda^2), \\ u_\Lambda \geq 0. \end{cases} \tag{1.13}$$

In this case, we have stronger results that are briefly exposed (without proofs) in Section 4, together with uniqueness results for some related semilinear PDEs.

2 Polymers

We study here the thermodynamic limit problem in one dimension, that is to say the limit of a line growing to infinity. More precisely, we consider a sequence $\Lambda = \{(0,0)\} \times \Lambda_3 \subset \{(0,0)\} \times \mathbf{Z}$, such that Λ_3 is a Van Hove sequence of $\mathbf{Z}$. We recall that Γ_0 is the periodic cell of the problem, i.e $\Gamma_0 = \mathbf{R}^2 \times]-\frac{1}{2}, \frac{1}{2}]$, and $\Gamma(\Lambda) = \bigcup_{k\in\Lambda} \Gamma_0 + k$. Putting $x = (x_1, x_2, x_3)$ a point in $\mathbf{R}^3$, we denote by $r = r(x)$ the quantity $\sqrt{x_1^2 + x_2^2}$. For all Λ, we denote by :

$$E_\Lambda(\rho) = \int_{\mathbf{R}^3} |\nabla\sqrt{\rho}|^2 + \int_{\mathbf{R}^3} \rho^{5/3} - \int_{\mathbf{R}^3} (m_\Lambda \star \frac{1}{|x|})\rho + \frac{1}{2}\int_{\mathbf{R}^3} (\rho \star \frac{1}{|x|})\rho \tag{2.1}$$

the Thomas-Fermi-von Weizsäcker energy. Here $m_\Lambda = \sum_{k\in\Lambda} \delta_k$. In the case of smeared nuclei, δ_k will be replaced by $m(\cdot - k)$, where m is the measure defining the shape of a nucleus. In this case, m will be considered to be in $\mathcal{D}(\mathbf{R}^3)$, such that its support lies in Γ_0. We will denote by I_Λ the minimization problem :

$$I_\Lambda = \inf\{E_\Lambda(\rho) + \sum_{k\neq j\in\Lambda} \frac{1}{|k-j|}, \rho \geq 0,\ \sqrt{\rho} \in H^1(\mathbf{R}^3), \int_{\mathbf{R}^3} \rho = |\Lambda|\}. \tag{2.2}$$

We will denote by ρ_Λ the solution of the problem I_Λ.

We also recall the Euler-Lagrange equation of problem (2.2) :

$$-\Delta u_\Lambda + \frac{5}{3} u_\Lambda^{7/3} - \phi_\Lambda u_\Lambda = 0, \tag{2.3}$$

where $u_\Lambda = \sqrt{\rho_\Lambda}$ and $\phi_\Lambda = (m_\Lambda - u_\Lambda^2) \star \frac{1}{|x|} - \theta_\Lambda$, $\theta_\Lambda \in \mathbf{R}$ being the Lagrange multiplier associated to the constraint in (2.2). Hence ϕ_Λ satisfies

$$-\Delta \phi_\Lambda = 4\pi (m_\Lambda - u_\Lambda^2). \tag{2.4}$$

Let us begin with some a priori estimates.

2.1 A priori estimates

2.1.1 Energy bounds

First of all, we establish some bounds on ρ_Λ and ϕ_Λ. For this purpose, we follow exactly the proof of [5], Chapter 3, Section 3.2, which carries through here since it does not depend on the sequence Λ, and we get :

Theorem 2.1 (Catto, Le Bris, Lions, [5]) *There exist various positive constants C such that, for any sequence $\Lambda \subset \mathbf{Z}^3$, we have :*

(i) $|I_\Lambda| \leq C|\Lambda|$,

(ii) $\int_{\mathbf{R}^3} |\nabla u_\Lambda|^2 \leq C|\Lambda|$,

(iii) $\|\rho_\Lambda\|_{L^p} \leq C|\Lambda|^{1/p}$ *for all* $p \leq \frac{5}{3}$,

(iv) $0 \leq \int_{\mathbf{R}^3} \phi_\Lambda \rho_\Lambda \leq C|\Lambda|$,

(v) $0 < \theta_\Lambda \leq C$,

(vi) $|\sum_{k \neq j \in \Lambda} \frac{1}{|k-j|} - \int_{\mathbf{R}^3} \rho_\Lambda (m_\Lambda \star \frac{1}{|x|})| \leq C|\Lambda|$.

In the case of smeared nuclei, we also have :

(vii) $D(m_\Lambda - \rho_\Lambda, m_\Lambda - \rho_\Lambda) \leq C|\Lambda|$, *i.e* $\int_{\mathbf{R}^3} |\nabla \phi_\Lambda|^2 \leq C|\Lambda|$.

2.1.2 L^∞ bounds

Next, we may obtain L^∞ bounds, still exactly as in [5], Section 3.2. Here again, the proof does not depend on the sequence Λ, so we have :

Theorem 2.2 (Catto, Le Bris, Lions, [5]) *There exist positive constants C independent of Λ such that, for all $\Lambda \subset \mathbf{Z}^3$, we have :*

(i) $\|\rho_\Lambda\|_{L^\infty(\mathbf{R}^3)} \leq C$.

(ii) In the smeared nuclei case, $\|\phi_\Lambda\|_{L^\infty(\mathbf{R}^3)} \leq C$.

In the point nuclei case, we have :

(ii') $\|\phi_\Lambda\|_{L^\infty(Q(\Lambda)^c)} \leq C$, where $Q(\Lambda) = \cup_{k\in\Lambda} Q + k$, Q being the unit cube of $\mathbf{R}^3$ and :

(iii') $\|\phi_\Lambda\|_{L^p_{unif}(\mathbf{R}^3)} \leq C$, for all $1 \leq p < 3$.

The norm $\|\cdot\|_{L^p_{unif}(\mathbf{R}^3)}$ is defined by $\sup_{x\in\mathbf{R}^3} \|\cdot\|_{L^p(x+B_1)}$.

Remark 2.1 *Let us point out that the proof of Theorem 2.2 is based only on the Euler equations (2.3)-(2.4), and the fact that the measure m is positive, bounded, and has compact support. Hence it holds for any such solutions, and in particular if m_Λ is replaced by $m_\infty = \sum_{k\in\mathbf{Z}} m(\cdot - ke_3)$, or by any Γ_0-periodic measure with compact support in the direction (x_1, x_2). This will be useful in the proof of the uniqueness Theorem 2.4 below.*

2.1.3 Asymptotic estimates

As the set of nuclei remains confined in a subset of $\mathbf{R}^3$ which is bounded with respect to r, we expect the above uniform bounds not to be optimal. More precisely, we expect, at least concerning the density ρ_Λ, a decay as r goes to infinity. For this purpose, we use Solovej's method [15] (see also [1]).

Let e_R be the ground state of the Laplacian with homogeneous Dirichlet boundary conditions on the ball B_R of radius R centered at the origin, normalized by the condition $\|e_R\|_{L^2} = 1$, and prolonged by 0 outside B_R. That is, $e_R(x) = \frac{sin(\pi|x|/R)}{|x|\sqrt{2\pi R}}$ on B_R. Then we have $\|\nabla e_R\|_{L^2} = \pi/R$. We set $g_R = e_R^2$.

Lemma 2.1 (Benguria, Lieb, [1]) *Let Ω be any open subset of $\mathbf{R}^3$. If $u_\Lambda \in H^1_0(\Omega)$ is positive and satisfies (2.3) with $\phi_\Lambda \in L^2(\Omega)+L^\infty(\Omega)$ satisfying (2.4), then for all $x \in \Omega$ such that $d(x, \partial\Omega) > R$, we have :*

$$g_R \star \phi_\Lambda \leq g_R \star u_\Lambda^{4/3} + \pi^2 R^{-2}. \tag{2.5}$$

And if $B_R + x$ does not contain any nuclei, i.e $m_\Lambda = 0$ in $B_R + x$, we have :

$$\phi_\Lambda(x) \leq g_R \star \phi_\Lambda(x). \tag{2.6}$$

Proof : For the sake of consistency, we reproduce here the proof of this lemma. Since u_Λ is positive, and u_Λ satisfies (2.3), it is the ground state of the operator $H = -\Delta + u_\Lambda^{4/3} - \phi_\Lambda$ with Dirichlet condition on Ω. Hence, for all $w \in H^1_0(\Omega)$, we have :

$$\int_\Omega |\nabla w|^2 + \int_\Omega (u_\Lambda^{4/3} - \phi_\Lambda) w^2 \geq 0. \tag{2.7}$$

We now apply this inequality to $w = e_R(x - \cdot)$, and we get (2.5), provided $d(x, \partial\Omega) > R$. Let us now show (2.6) : if ϕ_Λ satisfies (2.4) and $B_R + x$ contains no nuclei, ϕ_Λ is subharmonic on $B_R + x$, hence applying the mean-value inequality (see for instance [8]), we get :

$$g_R \star \phi_\Lambda(x) = \int_0^R \left(\int_{S_r} \phi_\Lambda(x-y)dy \right) g_R(r)dr \geq \int_0^R 4\pi r^2 \phi_\Lambda(x) g_R(r)dr = \phi_\Lambda(x)$$

because g_R is of total mass one. $\Diamond$

Now we turn to the estimate at infinity :

Theorem 2.3 *For any solution $(u_\Lambda, \phi_\Lambda)$ of the system (2.3)-(2.4) satisfying $u_\Lambda \geq 0$, we have :*

$$\begin{aligned} \phi_\Lambda &\leq \frac{C}{1+r^2}, \ \forall r \geq 1, \\ 0 \leq u_\Lambda &\leq \frac{C}{1+r^{3/2}} \quad , \end{aligned}$$

where C denotes various positive constants independent of the measure m_Λ.

Furthermore, in the smeared nuclei case, i.e when m in (2.4) is supposed to be smooth, the first inequality holds everywhere.

Remark 2.2 *The first estimate is not efficient for Λ fixed : $\phi_\Lambda = (m_\Lambda - u_\Lambda^2) \star \frac{1}{|x|} - \theta_\Lambda$ is negative at infinity, since θ_Λ is positive (see [15]). However, the point is that this estimate does not depend on the measure m_Λ, hence is independent of the sequence Λ, as far as it satisfies the hypotheses we have required at the beginning of this section.*

Proof :

We apply lemma 2.1, with $\Omega = \mathbf{R}^3$, and get :

$$g_R \star \phi_\Lambda \leq g_R \star u_\Lambda^{4/3} + \frac{\pi^2}{R^2},$$

for all $R > 0$. We define $\tilde{\phi} = g_R \star \phi_\Lambda - \frac{\pi^2}{R^2}$, and get, using Jensen's inequality :

$$\tilde{\phi} \leq g_R \star u_\Lambda^{4/3} \leq (g_R \star u_\Lambda^2)^{2/3}.$$

Now, convoluting (2.4) on both sides, we get :

$$-\Delta(g_R \star \phi_\Lambda) = 4\pi(m_\Lambda \star g_R - u_\Lambda^2 \star g_R),$$

that is,

$$-\Delta\tilde{\phi} + (\tilde{\phi})_+^{3/2} \leq 4\pi(m_\Lambda \star g_R).$$

Now, we may assume, without loss of generality, that the support of m_Λ lies in $\{r \leq 1\}$. So we have $m_\Lambda \star g_R = 0$ on $C_{R+1} = \{r \geq R+1\}$, hence $-\Delta\tilde{\phi} + (\tilde{\phi})_+^{3/2} \leq 0$ on that set.

We are going now to use a comparison argument on $\tilde{\phi}$, in the spirit of [3]. For that purpose, we fix an $R' > R+1$ and introduce the function

$$U = \frac{a}{(r^2 - R^2)^2} + \frac{bR'^4}{(R'^2 - |x|^2)^4},$$

where a and b are positive constants to be determined later on. In particular, we need U to be a supersolution of the differential inequality satisfied by $\tilde{\phi}$, that is, $-\Delta U + U_+^{3/2} \geq 0$. One easily computes :

$$-\Delta U = -8a\frac{R^2 + 2r^2}{(r^2 - R^2)^4} - 8bR'^4\frac{3R'^2 + 7|x|^2}{(R'^2 - |x|^2)^6}. \tag{2.8}$$

Using the inequality $(\alpha + \beta)^{3/2} \geq \alpha^{3/2} + \beta^{3/2}$, which is valid for all $\alpha, \beta > 0$, one finds :

$$-\Delta U + U^{3/2} \geq \frac{a(\sqrt{a} - 8\frac{R^2+2r^2}{r^2-R^2})}{(r^2 - R^2)^3} + \frac{bR'^4(\sqrt{b}R'^2 - 24R'^2 - 56|x|^2)}{(R'^2 - |x|^2)^6}. \tag{2.9}$$

We want this quantity to be positive on $C_{R+1} \cap B_{R'}$, which is true as soon as $a \geq (16 + \frac{24R^2}{2R+1})^2$ and $b \geq 80^2$. We also need that $U \geq \tilde{\phi}$ on $\partial C_{R+1} \cap B_{R'}$, i.e $\frac{a}{(2R+1)^2} \geq \|\tilde{\phi}\|_{L^\infty}$. The latter quantity exists because $\phi_\Lambda \in L^1_{unif}$ and g_R is smooth. So we can choose a large enough to ensure all those properties, together with $a \leq cR^2$, c being a universal constant.

We then have :

$$-\Delta(\tilde{\phi} - U) + (\tilde{\phi})_+^{3/2} - U^{3/2} \leq 0.$$

Hence, using Kato's inequality :

$$-\Delta(\tilde{\phi} - U)_+ \leq -\mathrm{sgn}^+(\tilde{\phi} - U)((\tilde{\phi})_+^{3/2} - U^{3/2}) \leq 0.$$

We use now the maximum principle to conclude that on the set $C_{R+1} \cap B_{R'}$,

$$\tilde{\phi} \leq \frac{cR^2}{(r^2 - R^2)^2} + \frac{bR'^4}{(R'^2 - |x|^2)^4}.$$

This holds for any $R' > R+1$, with c and b being universal constants. So, by letting R' go to infinity, we find :

$$\tilde{\phi} \leq \frac{cR^2}{(r^2 - R^2)^2}$$

on C_{R+1}.

Furthermore, from Lemma 2.1, we know that on this set, (2.6) holds. Therefore, we finally get :

$$\phi_\Lambda \leq \frac{CR^2}{(r^2-R^2)^2} + \frac{\pi^2}{R^2}.$$

This inequality holds whenever $R > 0$ and $r \geq R+1$. So if r is fixed and larger than 2, we may choose $R = r/2$, and we find

$$\forall r \geq 2,\ \phi_\Lambda \leq \frac{C}{r^2}.$$

Pointing out that $\phi_\Lambda \in L^\infty(\{r > 1\}$, we infer that

$$\forall r \geq 1,\ \phi_\Lambda \leq \frac{C}{1+r^2}.$$

And in the smeared nuclei case, we know that $\phi_\Lambda \in L^\infty$, so this inequality holds on $\mathbf{R}^3$.

We now turn to the second assertion, namely the estimate on u_Λ. For this purpose, we use the above inequality and (2.3), and write :

$$-\Delta u_\Lambda + \frac{5}{3} u_\Lambda^{7/3} \leq \frac{Cu_\Lambda}{r^2},\ \forall r \geq 1.$$

Now, there exists a constant c such that for all $a, b \geq 0$, $ab \leq \frac{1}{3}a^{7/3} + cb^{7/4}$. So we have, on the set $\{r \geq 1\}$:

$$-\Delta u_\Lambda + \frac{4}{3} u_\Lambda^{7/3} \leq \frac{C}{r^{7/2}}.$$

We are now going to use the same comparison argument as above, introducing the function $V = \frac{a}{r^{3/2}} + \frac{bR'^{3/2}}{(R'^2-|x|^2)^{3/2}}$. Computing $-\Delta V$, and using (here again) that $(\alpha+\beta)^{7/3} \geq \alpha^{7/3} + \beta^{7/3}$, we find that

$$-\Delta V + \frac{4}{3} V^{7/3} \geq \frac{a}{r^{7/2}} \left(\frac{4a^{4/3}}{3} - \frac{9}{4}\right) + \frac{bR'^{3/2}}{(R'^2-|x|^2)^{7/2}} \left(\frac{4}{3} b^{4/3} R'^2 - 9R'^2 - 6|x|^2\right).$$

Thus, choosing $a^{4/3} > \frac{27}{16}$ and $b^{4/3} > \frac{45}{4}$, we have :

$$-\Delta V + \frac{4}{3} V^{7/3} \geq -\Delta u_\Lambda + \frac{4}{3} u_\Lambda^{7/3}.$$

So by the same argument as above, we conclude that $u_\Lambda \leq V$ on the set $\{r \geq 1\}$. Since $u_\Lambda \in L^\infty(\mathbf{R}^3)$, this concludes the proof. $\Diamond$

2.1.4 Compactness

The next step consists in proving the compactness of the sequence ρ_Λ, i.e the fact that no electrons escape at infinity. Mathematically, this will be stated as :

$$\frac{1}{|\Lambda|}\int_{\Gamma(\Lambda)} \rho_\Lambda \longrightarrow 1 \quad \text{as} \quad \Lambda \to \infty. \tag{2.10}$$

We start with the smeared nuclei case, and next generalize the result to the point nuclei case :

Proposition 2.1 *In the smeared nuclei case, (2.10) holds.*

Proof : The key-point of the proof is, as in [5], that we have, for all $h \in H^1(\mathbf{R}^3)$,

$$|\int_{\mathbf{R}^3} (m_\Lambda - \rho_\Lambda) h| \leq \frac{1}{(2\pi)^3} D(m_\Lambda - \rho_\Lambda, m_\Lambda - \rho_\Lambda)^{1/2} \|\nabla h\|_{L^2(\mathbf{R}^3)}. \tag{2.11}$$

(We recall that $D(f,g) = \int_{\mathbf{R}^3}\int_{\mathbf{R}^3} \frac{f(x)g(y)}{|x-y|} dxdy$.) This inequality holds because $m_\Lambda - \rho_\Lambda \in L^{6/5}(\mathbf{R}^3) \subset H^{-1}(\mathbf{R}^3)$: it is exactly the Cauchy-Schwarz inequality in $H^{-1} \times H^1$, through the Fourier transform.

Now, we know from Theorem 2.3, that $D(m_\Lambda - \rho_\Lambda, m_\Lambda - \rho_\Lambda) \leq C|\Lambda|$.

Next, we choose $h = h_\Lambda$: we put $h_\Lambda(x) = f_\Lambda(r) g_\Lambda(x_3)$, where :

- $f_\Lambda(r) = 1 - (\frac{r}{R})^\alpha$ if $r \leq R$, 0 otherwise, with $1 > \alpha > 0$, and $R = R(\Lambda) > 0$ being chosen below.
- $g_\Lambda \in \mathcal{D}(\mathbf{R})$, $g_\Lambda = 1$ on the set $\{x \in \mathbf{R}/d(x,\Lambda_3) < \frac{1}{2}\}$, 0 on the set $\{x \in \mathbf{R}/d(x,\Lambda_3) > 1\}$, $0 \leq g_\Lambda \leq 1$ and $|g'_\Lambda| \leq 4$.

(We recall that $\Lambda = \{(0,0)\} \times \Lambda_3$, and that $|\Lambda_3^h| = \{t \in \mathbf{R},\ d(t, \partial(\cup_{k\in\Lambda_3}[k - 1/2, k+1/2])) < h\}$.)

For such an h_Λ, we compute :

$$\begin{aligned}
\int_{\mathbf{R}^3} |\nabla h_\Lambda|^2 &= \int_{\mathbf{R}^2\times[0,\infty[} g'_\Lambda(x_3)^2 f_\Lambda(r)^2 2\pi r dr dx_3 + \int_{\mathbf{R}^2\times[0,\infty[} g_\Lambda(x_3)^2 f'_\Lambda(r)^2 2\pi r dr dx_3 \\
&\leq C|\Lambda_3^1| \int_0^R (1 - (\frac{r}{R})^\alpha)^2 r dr + C|\Lambda| \int_0^R \alpha^2 \frac{r^{2\alpha-1}}{R^{2\alpha}} dr \\
&\leq C(R^2|\Lambda_3^1| + \alpha|\Lambda|).
\end{aligned}$$

We now choose $R = \left(\frac{|\Lambda|}{|\Lambda_3^1|}\right)^{1/4}$, so that we have $R \longrightarrow \infty$ as $|\Lambda| \to \infty$, together with $R|\Lambda_3^1|^{1/2} \ll |\Lambda|^{1/2}$. Thus, we find that $\|\nabla h_\Lambda\|_{L^2(\mathbf{R}^3)} \leq C(\sqrt{\alpha|\Lambda|} + o(\sqrt{|\Lambda|}))$, hence

$$\frac{1}{|\Lambda|} |\int_{\mathbf{R}^3} (m_\Lambda - \rho_\Lambda) h_\Lambda| \leq C\sqrt{\alpha} + o(1).$$

Now, because $h_\Lambda \leq 1$, $\int_{\mathbf{R}^3} m_\Lambda h_\Lambda \leq |\Lambda|$. On the other hand,

$$\int_{\mathbf{R}^3} m_\Lambda h_\Lambda \geq |\Lambda| - \int_{\mathbf{R}^3} m_\Lambda (\frac{r}{R})^\alpha.$$

And $\int_{\mathbf{R}^3} m_\Lambda (\frac{r}{R})^\alpha \leq C|\Lambda|/R^\alpha$, so we have :

$$\frac{1}{|\Lambda|}\int_{\mathbf{R}^3} m_\Lambda h_\Lambda \longrightarrow 1.$$

Furthermore,

$$\begin{aligned}\int_{\mathbf{R}^3} \rho_\Lambda h_\Lambda &= \int_{\Gamma(\Lambda)\cap\{r<R\}} \rho_\Lambda - \int_{\Gamma(\Lambda)\cap\{r<R\}} \rho_\Lambda (\frac{r}{R})^\alpha + \int_{\Gamma(\Lambda)^c} \rho_\Lambda h_\Lambda \\ &= \int_{\Gamma(\Lambda)} \rho_\Lambda + O(|\Lambda_3^1|) - \int_{\Gamma(\Lambda)\cap\{r<R\}} \rho_\Lambda (\frac{r}{R})^\alpha - \int_{\Gamma(\Lambda)\cap\{r>R\}} \rho_\Lambda,\end{aligned}$$

because $\int_{\Gamma(\Lambda)^c} h_\Lambda \rho_\Lambda \leq C|\Lambda_3^1| \int_0^R \frac{r dr}{1+r^3} \leq C|\Lambda_3^1|$, according to Theorem 2.3.

Concerning the remaining terms of the right-hand side of the above equality, we have :

$$0 \leq \int_{\Gamma(\Lambda)\cap\{r>R\}} \rho_\Lambda \leq C|\Lambda| \int_{r>R} \frac{dr}{r^2} \leq C\frac{|\Lambda|}{R} \ll |\Lambda|,$$

and :

$$0 \leq \int_{\Gamma(\Lambda)\cap\{r<R\}} \rho_\Lambda (\frac{r}{R})^\alpha \leq C\frac{|\Lambda|}{R^\alpha} \int_0^\infty \frac{r^{\alpha+1}}{1+r^3} dr \leq C\frac{|\Lambda|}{R^\alpha} \ll |\Lambda|,$$

because $3-\alpha-1>1$.

Collecting all those convergence results, we get :

$$|1 - \frac{1}{|\Lambda|}\int_{\Gamma(\Lambda)} \rho_\Lambda| \leq C\sqrt{\alpha} + o(1).$$

Letting $|\Lambda| \longrightarrow \infty$, this implies that

$$\limsup_{\Lambda\to\infty} |1 - \frac{1}{|\Lambda|}\int_{\Gamma(\Lambda)} \rho_\Lambda| \leq C\sqrt{\alpha}.$$

Here C does not depend on $\alpha > 0$, so letting $\alpha \to 0$, we find (2.10). $\diamondsuit$

Let us now turn to the point nuclei case. The only difference between this case and the preceding one is that $D(m_\Lambda - \rho_\Lambda, m_\Lambda - \rho_\Lambda)$ does not exist. So we are going to replace m_Λ by $1_{Q(\Lambda)}$, $Q(\Lambda)$ denoting $\bigcup_{k\in\Lambda} Q+k$, where Q is the unit cube in $\mathbf{R}^3$. $1_{Q(\Lambda)}$ lies in $L^1 \cap L^\infty(\mathbf{R}^3)$ and have compact support, so that the existence of $\frac{1}{|\Lambda|}D(1_{Q(\Lambda)} - \rho_\Lambda, 1_{Q(\Lambda)} - \rho_\Lambda)$ is ensured. The point is then to prove that this quantity is bounded independently of Λ, so that the smeared nuclei case proof will apply. Since this is only a technical adaptation of [5], Section 3.3.4, we skip this proof.

Proposition 2.2 *In the point nuclei case, (2.10) holds.*

2.2 Uniqueness for the system of PDE-Identification of the limit

Now that we have bounds on the sequence ρ_Λ, we may pass locally to the limit (up to a subsequence) in the system (2.3)-(2.4). Denoting by $\rho_\infty = u_\infty^2$ and ϕ_∞ the corresponding limits, we get a solution to the system :

$$\begin{cases} -\Delta u_\infty + \frac{5}{3} u_\infty^{7/3} - u_\infty \phi_\infty = 0, \\ -\Delta \phi_\infty = 4\pi (m_\infty - u_\infty^2), \end{cases} \tag{2.12}$$

where the measure m_∞ is either equal to $\sum_{k\in\mathbf{Z}} \delta_{ke_3}$ in the point nuclei case, or to $\sum_{k\in\mathbf{Z}} m(\cdot - ke_3)$ in the smeared nuclei case. In both cases, m_∞ is periodic and its periodic cell is Γ_0.

The aim of this section is to show a uniqueness result on the system, so as to identify the limit (u_∞, ϕ_∞) as the solution of the system (2.12). The first step will be the periodicity of the solution. Next, when the solution is shown to be periodic, we will compare it with the solution of the periodic variational problem :

$$I_{per} = \inf\{E_{per}(\rho), \rho \geq 0, \sqrt{\rho} \in X_{per}, \int_{\Gamma_0} \rho = 1\}, \tag{2.13}$$

X_{per} being defined by :

$$X_{per} = \{u \in H^1_{per}(\Gamma_0),\ \big(\log(2 + |x|)\big)^{1/2} u \in L^2(\Gamma_0)\}, \tag{2.14}$$

The energy E_{per} is defined by :

$$\begin{aligned} E_{per}(\rho) = \ & \textstyle\int_{\Gamma_0} |\nabla \sqrt{\rho}|^2 \ + \displaystyle\int_{\Gamma_0} \rho^{5/3} - \int_{\Gamma_0} (G \star_{\Gamma_0} m)\rho \\ + \ & \int_{\Gamma_0}\int_{\Gamma_0} G(x-y)\rho(x)\rho(y)dxdy. \end{aligned} \tag{2.15}$$

(We denote by $f \star_{\Gamma_0} g$ the convolution product over Γ_0 for periodic functions, that is, $f \star_{\Gamma_0} g(x) = \int_{\Gamma_0} f(x-y)g(y)dy$.)

The potential G is the periodic potential defined by (1.7).

We first study this periodic potential.

2.2.1 The potential G

We recall that in this section,

$$G(x) = -2\log(r) + \sum_{k\in\mathbf{Z}} \left(\frac{1}{|x - ke_3|} - \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dy}{|x - (y+k)e_3|} \right).$$

Lemma 2.2 *We have :*

(o) G *is smooth on* $\mathbf{R}^3 \setminus \mathbf{Z}e_3$.

(i) $G(x) = \frac{1}{|x|} + C + O(|x|)$ as $x \to 0$.

(ii) $G(x) = -2\log(r) + O(\frac{1}{r})$ as $r \to \infty$, *uniformly with respect to* x_3.

Proof :

First of all, we prove that the sum defining G does exist on $\mathbf{R}^3 \setminus \{r = 0\}$: indeed, denoting by $f(x)$ the quantity $\frac{1}{|x|} - \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dt}{|x-te_3|}$, we have, for $|x| \longrightarrow \infty$, and $r \neq 0$:

$$\begin{aligned} f(x) &= \frac{1}{|x|} - \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dt}{\sqrt{|x|^2 - 2tx_3 + t^2}} \\ &= \frac{1}{|x|} - \frac{1}{|x|} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dt}{\sqrt{1 - \frac{2tx_3}{|x|^2} + \frac{t^2}{|x|^2}}} \\ &= \frac{1}{|x|} - \frac{1}{|x|} \int_{-\frac{1}{2}}^{\frac{1}{2}} (1 + \frac{tx_3}{|x|^2} + O(\frac{1}{|x|^2}))dt \\ &= O(\frac{1}{|x|^3}), \end{aligned} \tag{2.16}$$

so this shows that $\sum_{k\in\mathbf{Z}} f(x + ke_3)$ is normally convergent on any compact subset of $\mathbf{R}^3 \setminus \{r = 0\}$. This proves our claim, and that G is smooth on this set, and periodic with periodic cell Γ_0.

We now turn to the proof of (i) : we isolate the interesting terms, and write G as :

$$\begin{aligned} G(x) = \quad & -2\log(r) \quad + \frac{1}{|x|} - \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dt}{|x - te_3|} \\ + \quad & \sum_{k\in\mathbf{Z}^*} \left(\frac{1}{|x - ke_3|} - \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dt}{|x - (t+k)e_3|} \right). \end{aligned} \tag{2.17}$$

Now, we compute, with $x \longrightarrow 0$, $x \neq 0$:

$$\begin{aligned} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{dt}{|x - te_3|} &= \operatorname{Argsh}(\frac{\frac{1}{2} - x_3}{r}) + \operatorname{Argsh}(\frac{\frac{1}{2} + x_3}{r}) \\ &= \log\left(\frac{x_3 + \frac{1}{2} + \sqrt{r^2 + (x_3 + \frac{1}{2})^2}}{x_3 - \frac{1}{2} + \sqrt{r^2 + (x_3 - \frac{1}{2})^2}} \right) \\ &= \log\left(\frac{x_3 + \frac{1}{2} + \sqrt{r^2 + (x_3 + \frac{1}{2})^2}}{x_3 - \frac{1}{2} + \frac{1}{2}(1 - 2x_3 + 2|x|^2 - 2x_3^2 + O(|x|^3))} \right), \end{aligned}$$

because

$$\begin{aligned}\sqrt{r^2+(x_3-\frac{1}{2})^2} &= \frac{1}{2}\sqrt{1-4x_3+4|x|^2}\\ &= \frac{1}{2}(1-2x_3+2|x|^2-\frac{1}{8}(4x_3)^2)+O(|x|^3).\end{aligned}$$

Hence

$$\begin{aligned}\int_{-\frac{1}{2}}^{\frac{1}{2}}\frac{dt}{|x-te_3|} &= \log\left(\frac{1+O(|x|)}{r^2+O(|x|^3)}\right)\\ &= -2\log(r)+O(|x|).\end{aligned}$$

So we may write

$$G(x)=\frac{1}{|x|}+\sum_{k\in\mathbf{Z}^*}\left(\frac{1}{|x-ke_3|}-\int_{-\frac{1}{2}}^{\frac{1}{2}}\frac{dt}{|x-(t+k)e_3|}\right)+O(|x|)$$

as $|x|\longrightarrow 0$.

Now, all the terms of the remaining sum are clearly defined on Γ_0, so using the estimate (2.16) on f, we conclude that this series defines a smooth function on Γ_0. With the periodicity of G, this shows (o) and (i), with $C=\sum_{k\in\mathbf{Z}^*}\left(\frac{1}{|k|}-\int_{-\frac{1}{2}}^{\frac{1}{2}}\frac{dt}{|k+t|}\right)$.

We now turn to the proof of (ii), which results only in showing that :

$$\sum_{k\in\mathbf{Z}}\left|\frac{1}{|x-ke_3|}-\int_{-\frac{1}{2}}^{\frac{1}{2}}\frac{dt}{|x-(k+t)e_3|}\right|\leq\frac{C}{r} \tag{2.18}$$

as $r\longrightarrow\infty$, uniformly with respect to x_3.

Considering the function f defined above, this expression may be written as : $\sum_{k\in\mathbf{Z}}f(x-ke_3)$. So, as we know that

$$|f(x)|\leq\frac{C}{|x|^3},$$

we have :

$$|\sum_{k\in\mathbf{Z}}f(x-ke_3)|\leq\sum_{k\in\mathbf{Z}}\frac{1}{r^3+|k|^3},$$

for r sufficiently large. Now, we have

$$\sum_{k\in\mathbf{Z}}\frac{1}{r^3+|k|^3}\leq\frac{1}{r^3}+\sum_{k\in\mathbf{Z}^*}\frac{1}{r^{3/2}|k|^{3/2}}\leq\frac{C}{r^{3/2}}.$$

This proves (2.18). $\diamondsuit$

Now that we know the behaviour of G, we turn to a positiveness property for D_G. We recall that :

$$D_G(f,g) = \int_{\Gamma_0}\int_{\Gamma_0} f(x)g(y)G(x-y)dxdy. \tag{2.19}$$

Since D_G appears in the expression of the energy and is a bilinear form, its positiveness (in the sense of bilinear forms) will ensure its convexity, hence the convexity of the energy.

In the following Proposition, we assume that $\mathrm{Supp}(m) \subset \{r < 1\}$, since this may be done without loss of generality

Proposition 2.3 *The bilinear form D_G is positive on the set $Y_{per} = \{f \in L^1_{per}(\Gamma_0)/ \sqrt{|f|} \in H^1_{per}(\Gamma_0 \cap \{r > 1\}),\ \int_{\Gamma_0} f = 0$ and $\log(2+|x|)f \in L^1(\Gamma_0)\}$.*

Where the space $H^1_{per}(\Gamma_0 \cap \{r > 1\})$ is defined as the set of functions lying in $H^1_{loc}(\{r > 1\}) \cap H^1(\Gamma_0 \cap \{r > 1\})$ that are periodic with respect to x_3, of period 1.

Proof :

We define on $\mathcal{S}_{per}(\Gamma_0)$, that is, the set of functions that are C^∞ on $\mathbf{R}^3$, periodic with periodic cell Γ_0, and decaying faster than any power of r as $r \to \infty$, the Fourier transform $f \longmapsto \widehat{f}$ as :

$$\widehat{f}(\xi, n) = \int_{\Gamma_0} f(x)e^{-i2\pi(x'\cdot\xi + x_3 n)}dx, \tag{2.20}$$

where $x = (x', x_3)$, $x', \xi \in \mathbf{R}^2$, and $n \in \mathbf{Z}$. It is easy to check out that this Fourier transform has the isometry-property of the classical Fourier transform, that is :

$$\int_{\Gamma_0} f(x)\overline{g(x)}dx = \sum_{n\in\mathbf{Z}} \int_{\mathbf{R}^2} \widehat{f}(\xi,n)\overline{\widehat{g}(\xi,n)}d\xi. \tag{2.21}$$

Hence it may be prolonged to $\mathcal{S}'_{per}(\Gamma_0)$. We also have :

$$\forall f \in \mathcal{S}'_{per}(\Gamma_0),\ \widehat{\partial_j f}(\xi,n) = i2\pi\xi_j \widehat{f}(\xi,n), \quad j = 1,2.$$

And

$$\forall f \in \mathcal{S}'_{per}(\Gamma_0) \text{ and } g \in \mathcal{S}_{per}(\Gamma_0),\ \widehat{f \star_{\Gamma_0} g} = \widehat{f}\widehat{g}.$$

So, since we know that $-\Delta G = 4\pi\delta_0$ on Γ_0, we deduce :

$$4\pi^2(|\xi|^2 + n^2)\widehat{G}(\xi,n) = 4\pi.$$

Hence when $n \neq 0$, $\widehat{G}(\xi,n) = \frac{1}{\pi(|\xi|^2+n^2)}$. Now for $n=0$, $\widehat{G}$ becomes the classical Fourier transform of $\log|x'|$ on $\mathbf{R}^2$. Indeed, we have, putting $G_0(x) = G(x) + 2\log(r)$,

$$\int_{-\frac{1}{2}}^{\frac{1}{2}} G_0(x)dx_3 = 0. \tag{2.22}$$

Because computing $-\Delta\int_{-\frac{1}{2}}^{\frac{1}{2}} G_0(x)dx_3$, with $x \in \Gamma_0$, one finds :

$$\begin{aligned}
-\Delta \int_{-\frac{1}{2}}^{\frac{1}{2}} G_0(x)dx_3 &= \int_{-\frac{1}{2}}^{\frac{1}{2}} -\Delta(G_0(x))dx_3 \\
&= 4\pi \int_{-\frac{1}{2}}^{\frac{1}{2}} \big(\delta_0 - \delta_{r=0}\big)dx_3 \\
&= 4\pi(\delta_{r=0} - \delta_{r=0}) = 0.
\end{aligned}$$

So the left-hand side of (2.22) is the expression of a harmonic function, which lies in L^∞ because of Lemma 2.2, hence is a constant. But, still because of Lemma 2.2, G_0 goes to 0 as r goes to infinity, so (2.22) holds.

The classical Fourier transform of $\log|x|$ on $\mathbf{R}^2$ is equal to $\mathrm{vp}(\frac{1}{|x|^2}) + a\delta_0$, with $a > 0$, and where $\mathrm{vp}(\frac{1}{|x|^2})$ is defined as follows (see [14]) :

$$< \mathrm{vp}(\frac{1}{|x|^2}), \varphi >= \lim_{\varepsilon \to 0^+}\Big(\int_{|x|>\varepsilon} \frac{\varphi(x)}{|x|^2}dx + \frac{\log\varepsilon}{\varepsilon}\int_{|x|=\varepsilon} \varphi\Big). \tag{2.23}$$

(In fact, $\mathrm{vp}(\frac{1}{|x|^2}) = \mathrm{div}(\frac{\log|x|}{|x|^2}x)$ in $\mathcal{D}'(\mathbf{R}^2)$.)

So we have :

$$\widehat{G}(\xi, 0) = \mathrm{vp}(\frac{1}{|\xi|^2}) + a\delta_0.$$

Now, we compute, for all $f \in Y_{per}$:

$$\begin{aligned}
D_G(f,f) &= \int_{\Gamma_0} (G \star_{\Gamma_0} f)f \\
&= \sum_{n\in\mathbf{Z}} \int_{\mathbf{R}^2} \widehat{G \star_{\Gamma_0} f}(\xi,n)\widehat{f}(\xi,n)d\xi \\
&= \sum_{n\in\mathbf{Z}^*} \int_{\mathbf{R}^2} \frac{(\widehat{f}(\xi,n))^2}{4\pi^2(|\xi|^2+n^2)}d\xi + < \mathrm{vp}(\frac{1}{|\xi|^2}), (\widehat{f}(\xi,0))^2 >,
\end{aligned}$$

since $\widehat{f}(0) = \int_{\Gamma_0} f = 0$. So Proposition 2.3 will be proved if we show that when $f \in Y_{per}$, $< \mathrm{vp}(\frac{1}{|\xi|^2}), (\widehat{f}(\xi,0))^2 > \geq 0$.

From the fact that $f \in Y_{per}$, we have :

$$
\begin{aligned}
|\widehat{f}(\xi,0)| &= \left| \int_{\Gamma_0} (e^{-2i\pi x'\xi} - 1) f(x) dx \right| \\
&\leq \int_{\Gamma_0 \cap \{r > \frac{1}{\sqrt{|\xi|}}\}} |e^{-2i\pi x'\xi} - 1||f(x)|dx + \int_{\Gamma_0 \cap \{r < \frac{1}{\sqrt{|\xi|}}\}} |e^{-2i\pi x'\xi} - 1||f(x)|dx \\
&\leq \frac{2}{\log(2 + \frac{1}{\sqrt{|\xi|}})} \int_{\Gamma_0 \cap \{r > \frac{1}{\sqrt{|\xi|}}\}} \log(2+r)|f(x)|dx \\
&\quad + \int_{\Gamma_0 \cap \{r < \frac{1}{\sqrt{|\xi|}}\}} |x'||\xi||f(x)|dx \\
&\leq \frac{4}{\big|\log|\xi|\big|} \int_{\Gamma_0} \log(2+|x|)|f(x)|dx + \sqrt{|\xi|} \int_{\Gamma_0} |f(x)|dx \\
&\leq \frac{C}{\big|\log|\xi|\big|}
\end{aligned}
\tag{2.24}
$$

as $|\xi| \longrightarrow 0$.

Hence, (2.24) implies that $\frac{\widehat{f}(\xi,0)}{|\xi|} \in L^2_{loc}(\Gamma_0)$, and that $\frac{\log\varepsilon}{\varepsilon}\int_{|\xi|=\varepsilon} \widehat{f}(\xi,0)^2$ vanishes as $\varepsilon \to 0$. Since $\widehat{f}(\cdot,0) \in L^2(\mathbf{R}^2)$, we conclude from (2.23) that we have :

$$
< \mathrm{vp}(\frac{1}{|\xi|^2}), (\widehat{f}(\xi,0))^2 >= \int_{\Gamma_0} \frac{\widehat{f}(\xi,0)^2}{|\xi|^2} d\xi \geq 0.
$$

This concludes the proof. $\diamondsuit$

Remark 2.3 *Let us point out that the important property of f is that its integral vanishes. For example, if $f = \delta_{ke_1} + \delta_{-ke_1}$ on Γ_0, f being periodic with periodic cell Γ_0, one may compute that, for $k > 0$ large enough, we have $D_G(f,f) \sim -\log k < 0$. And we may even convolute f with a regularizing kernel, so as to get a C^∞ function g, having compact support, and such that $D_G(g,g) < 0$.*

We now turn to our main result : the uniqueness of the solution of the system (2.12), which will be stated more precisely in Theorem 2.4 below. We consider a positive measure μ with compact support, periodic with periodic cell Γ_0, such that $\mu \not\equiv 0$, and the system :

$$
\left\{
\begin{array}{l}
-\Delta u + \frac{5}{3} u^{7/3} - u\phi = 0, \\
-\Delta \phi = 4\pi(\mu - u^2), \\
u \geq 0,
\end{array}
\right.
\tag{2.25}
$$

and intend to prove a uniqueness result for this system.

We write

$$\mu = \sum_{k\in\mathbf{Z}} m(\cdot - ke_3),$$

with m having its support in Γ_0. With no loss of generality, we may assume that $\mathrm{Supp}\, m \subset \{r < 1\}$, and that $m(\Gamma_0) = 1$. We first need some a priori estimates on the solution of the system. It is the aim of the following section.

2.2.2 A priori bounds

Proposition 2.4 *Let (u, ϕ) be a solution of (2.25), with $u \in L^\infty(\mathbf{R}^3)$ and $\phi \in L^1_{unif}(\mathbf{R}^3)$. Then for any $R > 0$, there exists a constant $\nu > 0$ such that $\inf_{r<R} u \geq \nu$.*

Proof : First of all, we remark that, by elliptic regularity, the fact that $\phi \in L^1_{unif}$ implies that $u \in W^{2,1}_{unif}$, hence belongs to $H^1_{unif}(\mathbf{R}^3)$. So $\phi \in H^3_{unif}(\{r > 1\}) \subset L^\infty(\{r > 1\}$, and u lies in $L^\infty \cap C^{0,\alpha}(\{r > 1\})$ for some $\alpha > 0$. Moreover, the fact that $\phi \in L^1_{unif}(\mathbf{R}^3)$ and $\Delta\phi$ is a uniformly locally bounded measure, we deduce that $\phi \in L^p(\mathbf{R}^3)$, for all $p < 3$.

We argue by contradiction, and suppose that the above property is false, i.e that there exists $R > 0$ such that :

$$\inf_{r<R} u = 0. \tag{2.26}$$

This means in particular that there exists a sequence $(x_n)_{n\geq 0}$ such that $r(x_n) \leq R$ and $u(x_n) \longrightarrow 0$ as $n \to \infty$. So, denoting by u_n and ϕ_n the functions $u(\cdot + x_n)$ and $\phi(\cdot + x_n)$ respectively, we have that

$$u_n(0) \longrightarrow 0 \text{ as } n \to \infty. \tag{2.27}$$

Now, we may write $x_n = k_n + x_n^0$, with $k_n \in \mathbf{Z}e_3$ and $x_n^0 \in \Gamma_0$. Since $r(x_n) = r(x_n^0) \leq R$, we may extract a subsequence so as to have $x_n^0 \longrightarrow x^0$, for some $x^0 \in \overline{\Gamma}_0$, satisfying $r(x^0) \leq R$.

But from (2.25), (2.27) and Harnack's inequality (see for instance [8]), we deduce that $u_n \longrightarrow 0$ uniformly on any compact subset of $\mathbf{R}^3$. Considering the bounds on u and ϕ, we may pass locally to the limit, up to a subsequence, in (2.25). We then get $\overline{\phi} \in L^1_{unif}$ a solution to :

$$-\Delta\overline{\phi} = 4\pi\mu(\cdot + x^0). \tag{2.28}$$

Hence, denoting by ψ the function $\overline{\phi}(\cdot - x^0)$, we have $\psi \in L^1_{unif}$, satisfying :

$$-\Delta\psi = 4\pi\mu. \tag{2.29}$$

With no loss of generality, we may assume that $r(x^0) = 0$, so that $-\Delta\psi$ has its support in $\{r < 1\}$.

We are now going to use a scaling argument to show that the fact that ψ is a solution to (2.29) is in contradiction with its belonging to L^1_{unif}. The first thing is that ψ is harmonic on the set $\{r > 1\}$, hence continuous on this set, and thus belongs to $L^\infty(\{r > 1\})$.

Let $\xi_0 \in C^\infty(\mathbf{R})$, such that $\xi_0 = 1$ on $[-1, 1]$, $\xi_0 = 0$ on $[-2, 2]^c$, and $|\xi_0''| \leq 4$. Let $\alpha \in]0, 1[$ and $\eta_R : \mathbf{R}^2 \longrightarrow \mathbf{R}$ be the solution of $-\Delta\eta = 0$ on $\{1 < |x| < R^\alpha\}$ with boundary conditions $\eta = 1$ on $\{1 = |x|\}$, $\eta = 0$ on $\{|x| = R^\alpha\}$. Namely, we have

$$\eta_R(x) = 1 - \frac{\log|x|}{\alpha \log R}$$

on the set $\{1 < |x| < R^\alpha\}$. We prolong it by 1 on $\{1 > |x|\}$, 0 on $\{|x| > R^\alpha\}$. We set $\xi_R(x) = \eta_R(x')\xi_0(\frac{x_3}{R})$, for all $x \in \mathbf{R}^3$.

And we compute :

$$\begin{aligned}
< -\Delta\psi, \xi_R > &= 4\pi < \mu, \xi_R > \\
&= \sum_{k\in\mathbf{Z}} < m(\cdot + ke_3), \xi_R > \\
&= \sum_{k\in\mathbf{Z}, |k|\leq 2R} \int_{\Gamma_0} \xi_0(\frac{x_3 - k}{R}) m(x) dx \\
&\geq \sum_{k\in\mathbf{Z}, |k|\leq R} \int_{\Gamma_0} m.
\end{aligned}$$

So we conclude that :

$$< -\Delta\psi, \xi_R > \geq 2R. \tag{2.30}$$

On the other hand, we have, denoting by Ω_R the set $\{r < R^\alpha, |x_3| < 2R\}$ and by ω_R the set $\{r < 1, |x_3| < R\}$,

$$\begin{aligned}
\int_{\mathbf{R}^3} -\Delta\psi\xi_R &= \int_{\Omega_R} -\Delta\psi\xi_R \\
&= \int_{\Omega_R\setminus\omega_R} \nabla\psi\nabla\xi_R \\
&= -\int_{\Omega_R\setminus\omega_R} \psi\Delta\xi_R - \int_{r=R^\alpha, |x_3|<2R} \psi\frac{\partial\xi_R}{\partial r} + \int_{r=1, |x_3|<2R} \psi\frac{\partial\xi_R}{\partial r}.
\end{aligned}$$

We know that $\Delta\xi_R = \frac{1}{R^2}\eta_R(r)\xi_0''(\frac{x_3}{R})$ on the set $\Omega_R \setminus \omega_R$, so we have :

$$\begin{aligned}\left|\int_{\Omega_R\setminus\omega_R}\psi\Delta\xi_R\right| &= \frac{1}{R^2}\left|\int_{\Omega_R\setminus\omega_R}\psi\eta_R(r)\xi_0''(\frac{x_3}{R})\right| \\ &\leq \frac{4}{R^2}\left|\int_{\Omega_R}\psi\right| \\ &\leq \frac{C}{R^2}|\Omega_R| = CR^{2\alpha-1} \ll R,\end{aligned}$$

because $\psi \in L^1_{unif}$ and $\alpha < 1$.

Next, we compute that

$$\frac{\partial\xi_R}{\partial r} = -\frac{\xi_0(\frac{x_3}{R})}{\alpha r\log R},$$

so we also have, using the fact that ψ belongs to $L^\infty(\{r>1\})$ and is smooth on this set :

$$\left|\int_{r=R^\alpha,|x_3|<2R}\psi\frac{\partial\xi_R}{\partial r}\right| \leq \frac{CR^{\alpha+1}}{\alpha R^\alpha\log R} = \frac{CR}{\log R} \ll R. \tag{2.31}$$

And :

$$\left|\int_{r=1,|x_3|<2R}\psi\frac{\partial\xi_R}{\partial r}\right| \leq \frac{CR}{\log R} \ll R. \tag{2.32}$$

So we conclude that

$$\left|< -\Delta\psi, \xi_R >\right| \ll R,$$

reaching a contradiction with (2.30). This concludes the proof. ◊

We now have a lower bound on u, and intend to get upper bounds :

Proposition 2.5 *Let (u,ϕ) be a solution of (2.25), satisfying $u \in L^\infty$ and $\phi \in L^1_{unif}$. Then we have :*

(i) $\phi \leq \frac{C}{1+r^2}\ \forall r>1;$ *and*

(ii) $u \leq \frac{C}{1+r^{3/2}}$.

Proof : The proof follows exactly the same pattern as that of Theorem 2.3. Indeed, this proof only uses the fact that the measure m_Λ has its support in $\{r<1\}$ and that the functions u_Λ, ϕ_Λ are solutions of the system (2.3)-(2.4). So the whole proof carries through to this case. ◊

2.2.3 Periodicity of the solutions

We are now going to show that the solutions of the system (2.25) are necessarily periodic.

For this purpose, we denote, for any function f defined on $\mathbf{R}^3$,

$$\tau f(x) = f(x+e_3). \tag{2.33}$$

We then have, if (u,ϕ) is a solution to (2.25),

$$-\Delta(\tau\phi - \phi) = 4\pi(u^2 - \tau u^2). \tag{2.34}$$

Hence, from elliptic regularity, $(\tau\phi-\phi) \in C^0 \cap L^\infty(\mathbf{R}^3)$.

Proposition 2.6 *Let $(u,\phi) \in L^\infty(\mathbf{R}^3) \times L^1_{unif}(\mathbf{R}^3)$ be a solution of (2.25). Then*

$$\tau\phi - \phi = u^2 \star (\frac{1}{|x|} - \tau\frac{1}{|x|}).$$

And

$$|\tau\phi-\phi| \leq \frac{C}{1+r} \ ,$$

for some constant C independent of x_3.

Proof : The first thing is to check out if this convolution product exists : Since we have

$$u^2 \leq \frac{C}{1+r^3}$$

and

$$\begin{aligned} |\frac{1}{|x|} - \tau\frac{1}{|x|}| &\leq \frac{|2x_3+1|}{|x||x+e_3|(|x|+|x+e_3|)} \\ &\leq \frac{1}{|x|(|x|+|x+e_3|)} + \frac{1}{|x+e_3|(|x|+|x+e_3|)}, \end{aligned}$$

this is easy to check. Moreover, we have :

$$\begin{aligned} \left|u^2 \star (\tau\frac{1}{|x|} - \frac{1}{|x|})\right| &\leq \int_{\mathbf{R}^3} \frac{1}{1+r(y)^3} \frac{dy}{|x-y+e_3|(|x-y|+|x-y+e_3|)} \\ &\quad + \int_{\mathbf{R}^3} \frac{1}{1+r(y)^3} \frac{dy}{|x-y|(|x-y|+|x-y+e_3|)} \\ &\leq 2\int_{\mathbf{R}^3} \frac{1}{1+r(y)^3} \frac{dy}{|x-y|(|x-y|+|x-y+e_3|)}. \end{aligned}$$

We split this integral into two others, and write, with $r(x) > 2$:

$$\begin{aligned}
\int_{\mathbf{R}^3} & \frac{1}{1+r(y)^3} \frac{dy}{|x-y|(|x-y|+|x-y+e_3|)} \\
&= \int_{|x-y|<2} \frac{1}{1+r(y)^3} \frac{dy}{|x-y|(|x-y|+|x-y+e_3|)} \\
&\qquad + \int_{|x-y|>2} \frac{1}{1+r(y)^3} \frac{dy}{|x-y|(|x-y|+|x-y+e_3|)}.
\end{aligned}$$

So that we have, denoting by $A(x)$ and $B(x)$ respectively the terms of this sum,

$$A(x) \leq \frac{C}{1+r(x)^3}, \tag{2.35}$$

because

$$\int_{|x-y|<2} \frac{dy}{|x-y||x-y+e_3|} = \int_{|y|<2} \frac{dy}{|y||y+e_3|} \leq C,$$

and because the fact that $|x-y|<2$ together with $r(x)>2$ imply that $\frac{1}{1+r(y)^3} \leq \frac{C}{1+r(x)^3}$, where C does not depend on x.

Concerning B, we have, for an $R < r(x) = |x'|$ that will be chosen later on :

$$\begin{aligned}
B(x) &\leq \int_{\mathbf{R}^3} \frac{C}{1+r(y)^3} \frac{dy}{1+|x-y|^2} \\
&\leq \int_{\mathbf{R}^2} \frac{C}{1+|y'|^3} \left(\int_{\mathbf{R}} \frac{dy_3}{1+|x'-y'|^2+|x_3-y_3|^2} \right) dy' \\
&\leq \int_{\mathbf{R}^2} \frac{1}{1+|y'|^3} \frac{C}{|x'-y'|} dy' = \int_{\mathbf{R}^2} \frac{C}{(1+|x'-y'|^3)} \frac{dy'}{|y'|} \\
&\leq \int_{|y'|<R} \frac{C}{(1+|x'-y'|^3)} \frac{dy'}{|y'|} + \int_{|y'|>R} \frac{C}{(1+|x'-y'|^3)} \frac{dy'}{|y'|} \\
&\leq \int_{|y'|<R} \frac{dy'}{|y'|} \frac{1}{1+(|x'|-R)^3} + \frac{1}{R} \int_{|y'|>R} \frac{dy'}{1+|x'-y'|^3} \\
&\leq \frac{CR}{1+(|x'|-R)^3} + \frac{C}{R} ,
\end{aligned}$$

where C is a constant independent of x. Finally, we choose $R = \frac{|x'|}{2}$, so as to have :

$$B(x) \leq \frac{C}{r(x)} . \tag{2.36}$$

Now, collecting (2.35) and (2.36), we get :

$$\left|u^2 \star (\tau \frac{1}{|x|} - \frac{1}{|x|})\right| \le \frac{C}{r} \ . \tag{2.37}$$

Finally, since $u^2 \star (\tau \frac{1}{|x|} - \frac{1}{|x|})$ is continuous, (2.37) implies :

$$\left|u^2 \star (\tau \frac{1}{|x|} - \frac{1}{|x|})\right| \le \frac{C}{1+r} \ . \tag{2.38}$$

So there only remains to prove that this expression is indeed equal to $\tau\phi - \phi$. In order to do so, we compute its Laplacian, and find :

$$-\Delta(u^2 \star (\tau \frac{1}{|x|} - \frac{1}{|x|})) = u^2 \star (-\Delta(\tau \frac{1}{|x|} - \frac{1}{|x|})) = u^2 \star (\delta_{e_3} - \delta_0) = \tau u^2 - u^2.$$

So the function $\tau\phi - \phi - u^2 \star (\tau \frac{1}{|x|} - \frac{1}{|x|})$ is harmonic. But since, from (2.38), it lies in $L^\infty(\mathbf{R}^3)$, it must be a constant. Hence

$$\tau\phi - \phi = u^2 \star (\tau \frac{1}{|x|} - \frac{1}{|x|}) + a. \tag{2.39}$$

Now, considering (2.38), we know that for some R large enough,

$$|u^2 \star (\tau \frac{1}{|x|} - \frac{1}{|x|})| < \frac{|a|}{2}$$

on the set $\{r > R\}$. So we have

$$a - \frac{|a|}{2} \le \tau\phi - \phi \le a + \frac{|a|}{2}$$

on this set, which implies that, for all $n \in \mathbf{N}$, we have :

$$|\tau^n \phi - \phi| \ge n\frac{|a|}{2}$$

on $\{r > R\}$. So

$$2\|\phi\|_{L^1_{unif}} \ge \int_{B_1 + 2Re_1} |\tau^n\phi - \phi| \ge n\frac{|a|}{2}|B_1|.$$

This is valid for all $n \in \mathbf{N}$, so we reach a contradiction with the fact that $\phi \in L^1_{unif}$, unless $a = 0$. This concludes the proof. $\diamondsuit$

Next we turn to a uniqueness result that will ensure the periodicity of u, hence of ϕ.

Lemma 2.3 *Let (u,ϕ) and (v,ψ) be two solutions of system (2.25), both lying in $L^\infty \times L^1_{unif}$, such that $|\phi-\psi| \le \frac{C}{1+r}$ for some constant C. Then $u=v$ and $\phi=\psi$.*

Proof : The proof follows exactly the same pattern as the uniqueness Theorem of [5], Section 5.3 : we are going to collect all the former results, and then use a scaling argument on u and ϕ.

First of all, we know from Proposition 2.4 that there exists a positive function η, independent of x_3, such that :

$$u, v \ge \eta. \tag{2.40}$$

Next, denoting by w the function $u-v$, we get, substracting the two systems :

$$-\Delta w + u^{7/3} - v^{7/3} - (\phi u - \psi v) = 0. \tag{2.41}$$

and :

$$-\Delta(\phi-\psi) = v^2 - u^2. \tag{2.42}$$

Hence, for any $\xi \in \mathcal{D}(\mathbf{R}^3)$, we have :

$$\int_{\mathbf{R}^3} \nabla w \nabla(w\xi^2) + \int_{\mathbf{R}^3} (u^{7/3} - v^{7/3}) w\xi^2 - \int_{\mathbf{R}^3} (\phi u - \psi v) w \xi^2 = 0. \tag{2.43}$$

The first term of this sum may be rewritten as :

$$\int_{\mathbf{R}^3} \nabla w \nabla(w\xi^2) = \int_{\mathbf{R}^3} |\nabla(w\xi)|^2 - \int_{\mathbf{R}^3} w^2 |\nabla \xi|^2. \tag{2.44}$$

Now, from (2.40), we deduce that there exists a positive function $\nu(r)$ such that :

$$(u^{7/3} - v^{7/3})(u-v) \ge \frac{1}{2}(u^{4/3} + v^{4/3})(u-v)^2 + \nu(u-v)^2.$$

That is,

$$(u^{7/3} - v^{7/3}) w \ge \frac{1}{2}(u^{4/3} + v^{4/3}) w^2 + \nu w^2. \tag{2.45}$$

On the other hand, we write :

$$\phi u - \psi v = \frac{1}{2}(\phi+\psi) w + \frac{1}{2}(\phi-\psi)(u+v). \tag{2.46}$$

We denote by L the operator $-\Delta+\frac{1}{2}(u^{4/3}+v^{4/3})-\frac{1}{2}(\phi+\psi)$, and deduce from (2.43), (2.45) and (2.46) that :

$$< L(w\xi), w\xi > + \int_{\mathbf{R}^3} \nu w^2\xi^2 \leq \frac{1}{2}\int_{\mathbf{R}^3} (\phi-\psi)(u^2-v^2)\xi^2 + \int_{\mathbf{R}^3} w^2|\nabla\xi|^2. \tag{2.47}$$

We claim that the operator L (with homogeneous Dirichlet boundary conditions on a bounded set) is positive. Indeed, we may write it as

$$L = \frac{1}{2}\big((-\Delta+u^{4/3}-\phi)+(-\Delta+v^{7/3}-\psi)\big) = \frac{1}{2}(L_1+L_2),$$

and the only thing to prove is that L_1 and L_2 are positive. This comes from the first equation of (2.25) : denoting by λ_1 the first eigenvalue of L_1 on Ω, and by f_1 the associated eigenvector, satisfying $f_1>0$ on Ω, we have :

$$\int_\Omega -\Delta f_1 u + \int_\Omega u^{4/3} f_1 u - \int_\Omega \phi f_1 u = \int_\Omega \lambda_1 f_1 u.$$

Integrating by parts and using the first equation of (2.25), we find :

$$-\int_{\partial\Omega} u\frac{\partial f_1}{\partial n} + \int_{\partial\Omega} f_1\frac{\partial u}{\partial n} = \lambda_1\int_\Omega f_1 u.$$

Since the second term of the left-hand side is 0, and because of Hopf's Lemma, which shows that $\frac{\partial f_1}{\partial n}<0$ on $\partial\Omega$, we infer that $\lambda_1>0$, hence that L_1 is positive. L_2 may be dealt with exactly in the same way, so our claim is proved.

So the equation (2.47) implies :

$$\int_{\mathbf{R}^3} \nu w^2\xi^2 \leq \frac{1}{2}\int_{\mathbf{R}^3} (\phi-\psi)(u^2-v^2)\xi^2 + \int_{\mathbf{R}^3} w^2|\nabla\xi|^2. \tag{2.48}$$

We now go back to (2.42), and use it to rewrite the first term of (2.48)'s right-hand side as :

$$\frac{1}{2}\int_{\mathbf{R}^3} (\phi-\psi)\Delta(\phi-\psi)\xi^2 = -\frac{1}{2}\int_{\mathbf{R}^3} |\nabla(\phi-\psi)\xi|^2 + \frac{1}{2}\int_{\mathbf{R}^3} (\phi-\psi)^2|\nabla\xi|^2.$$

So the inequality (2.48) becomes :

$$\int_{\mathbf{R}^3} \nu w^2\xi^2 + \int_{\mathbf{R}^3} |\nabla((\phi-\psi)\xi)|^2 \leq \int_{\mathbf{R}^3} w^2|\nabla\xi|^2 + \frac{1}{2}\int_{\mathbf{R}^3} (\phi-\psi)^2|\nabla\xi|^2. \tag{2.49}$$

Since this holds for any $\xi\in\mathcal{D}(\mathbf{R}^3)$, we may apply it to a sequence ξ_n converging to

$$\xi(x) = \frac{1}{(1+x_3^2)^{\alpha/2}(1+r^2)^{\beta/2}}.$$

With $\alpha > \frac{1}{2}$, $\beta > 0$ and $\alpha + \beta < 1$. We then get (2.49) for this choice of ξ. Now, for this function ξ, it is clear, from the hypotheses on α and β, and from Proposition 2.5, (ii) that we have $\int_{\mathbf{R}^3} w^2\xi^2 < \infty$ and $\int_{\mathbf{R}^3} (\phi - \psi)^2\xi^2 < \infty$.

We are now going to use a scaling argument on the inequality (2.49). We define ξ_ε as :

$$\xi_\varepsilon(x) = \xi(\varepsilon x). \tag{2.50}$$

We then compute :

$$\begin{aligned}
|\nabla \xi_\varepsilon|^2 &= \left|\beta \frac{\varepsilon^2 x'}{(1+\varepsilon^2 r^2)^{(\frac{\beta}{2}+1)}(1+x_3^2)^{\frac{\alpha}{2}}}\right|^2 + \left|\alpha \frac{\varepsilon^2 x_3}{(1+\varepsilon^2 r^2)^{\frac{\beta}{2}}(1+\varepsilon^2 x_3^2)^{(\frac{\alpha}{2}+1)}}\right|^2 \\
&= \beta^2 \frac{\varepsilon^4 r^2}{(1+\varepsilon^2 r^2)^{(\beta+2)}(1+x_3^2)^{\alpha}} + \alpha^2 \frac{\varepsilon^4 x_3^2}{(1+\varepsilon^2 r^2)^{\beta}(1+\varepsilon^2 x_3^2)^{(\alpha+2)}} \\
&\leq \beta^2 \frac{\varepsilon^2}{(1+\varepsilon^2 r^2)^{\beta}(1+\varepsilon^2 x_3^2)^{\alpha}} + \alpha^2 \frac{\varepsilon^2}{(1+\varepsilon^2 r^2)^{\beta}(1+\varepsilon^2 x_3^2)^{\alpha}} \\
&\leq \frac{C\varepsilon^{2-2\alpha-2\beta}}{(1+x_3^2)^{\alpha}(1+r^2)^{\beta}} = C\varepsilon^{2-2\alpha-2\beta}\xi^2.
\end{aligned} \tag{2.51}$$

Now we consider inequality (2.49) together with (2.51), and find :

$$\int_{\mathbf{R}^3} \nu w^2 \xi_\varepsilon^2 \leq C\varepsilon^{2-2\alpha-2\beta}.$$

Fixing $R > 0$, we also have :

$$\int_{\mathbf{R}^3} \nu w^2 \xi_\varepsilon^2 \geq \frac{\inf_{B_R} \nu}{1+\varepsilon^2 R^2} \int_{B_R} w^2 \geq \inf_{B_R} \nu \int_{B_R} w^2.$$

Letting ε go to 0, and using the fact that $\alpha + \beta < 1$, we deduce that

$$\int_{B_R} w^2 = 0,$$

hence $w = 0$. Now, since $u, v > 0$, we also conclude, from the first equation of (2.25), that $\phi = \psi$. $\Diamond$

This Lemma, together with Proposition 2.4, Proposition 2.5 and proposition 2.6, allows us to assert that any solution of (2.25) is periodic, with periodic cell Γ_0. Now, we are going to complete the proof of our uniqueness theorem.

2.2.4 Uniqueness for the system

We intend to prove the following theorem :

Theorem 2.4 *Let μ be a periodic positive measure, with periodic cell $\Gamma_0 = \mathbf{R}^2 \times]-\frac{1}{2}, \frac{1}{2}]$ such that :*

(a) $\operatorname{Supp} \mu \subset \{r < 1\}$.

(b) $\mu(\Gamma_0) = 1$.

Then the system (2.25), that is :

$$\left\{ \begin{array}{l} -\Delta u + \frac{5}{3} u^{7/3} - u\phi = 0, \\ -\Delta \phi = 4\pi(\mu - u^2), \\ u \geq 0. \end{array} \right. \tag{2.52}$$

has a unique solution (u, ϕ) in $\left(L^2_{unif} \cap L^{7/3}_{loc}(\mathbf{R}^3)\right) \times L^1_{unif}(\mathbf{R}^3)$. Moreover, this solution is periodic with respect to x_3, of period 1, and we have :

(i) $u \in L^\infty(\mathbf{R}^3)$, and there exists a constant $C > 0$ and a positive function ν depending only on r, such that $0 < \nu \leq u \leq \frac{C}{1+r^{3/2}}$; and

(ii) there exists a constant θ such that $\phi = G \star_{\Gamma_0} (\mu - u^2) + \theta$; and

(iii) $\int_{\Gamma_0} u^2 = 1$.

Remark 2.4 *Of course, in properties (a)-(b), the number 1 may be replaced by any positive real. That is, those assumptions could be replaced by :*

(a') μ has compact support with respect to (x_1, x_2).

(b') $\mu \neq 0$.

And in this case, the conclusion (iii) would become :

(iii') $\int_{\Gamma_0} u^2 = \mu(\Gamma_0)$.

Remark 2.5 *In the three-dimensional case, that is if Λ is a Van Hove sequence of $\mathbf{Z}^3$, this uniqueness result holds provided μ satisfies weaker condition of the kind $(H_1) - (H_2)$ of Theorem 4.1. Here we are not able to adapt our proof to those kind of μ's. The periodicity is a necessary condition of our proof. However, in the Yukawa case, such a result holds (see Section 4).*

Proof : We give here two technical results that we will need in the course of the proof, their proof being postponed until the end of the present one :

Lemma 2.4 *Let $\psi \in L^2_{unif}(\mathbf{R}^2) \cap H^{3/2}_{loc}(B^c_{R_0})$ for some $R_0 > 0$, and denote by ψ_R the function $\psi - \frac{1}{2\pi R} \int_{|x|=R} \psi$. Assume that $(-\Delta\psi)\psi_R$ is bounded in $L^1(B^c_{R_0})$ independently of R. Then $\nabla\psi \in L^2(B^c_{R_0})$.*

Lemma 2.5 *Let $v \in Z_{per} = \{g \in \mathcal{S}'(\Gamma_0),\ \int_{\Gamma_0} \log(2+|x|)|g| < \infty,\ \int_{\Gamma_0} g = 0\}$, such that $v \in L^1_{loc}(\Gamma_0 \cap \{r > 1\})$ and $|v| \leq \frac{C}{1+r^3}$ on $\{r > 1\}$. Then $G \star_{\Gamma_0} v \in L^1_{unif}(\Gamma_0)$.*

The proof of the existence is a straight-forward adaptation of the thermodynamic limit process, using the measure m instead of a smooth function or δ_0. One checks easily that the point nuclei case proofs generalizes to any bounded measure with compact support. And the associated variational problem I_Λ has been studied in [10].

We refer the reader to [5], Section 5.3.2 for the belonging of u to L^∞. The proof also gives the information that $\phi \in L^p_{unif}(\mathbf{R}^3) \cap L^\infty(\{r > 1\})$, for all $1 \leq p < 3$. This comes from elliptic regularity results.

Now, we know that whenever $u \in L^\infty(\mathbf{R}^3)$ and $\phi \in L^1_{unif}(\mathbf{R}^3)$ satisfy (2.25), Lemma 2.3 and Propositions 2.4, 2.5 and 2.6 show that u and ϕ are periodic, with periodic cell Γ_0, and that (i) holds.

Now that the periodicity of u and ϕ is ensured, we introduce the variational problem (2.13), that is :

$$I_{per} = \inf\{E_{per}(\rho),\ \sqrt{\rho} \in X_{per},\ \int_{\Gamma_0} \rho = 1\}.$$

Where E_{per} is defined by (2.15), i.e

$$\begin{aligned} E_{per}(\rho) = \ & \int_{\Gamma_0} |\nabla\sqrt{\rho}|^2 + \int_{\Gamma_0} \rho^{5/3} - \int_{\Gamma_0} (G \star_{\Gamma_0} \mu)\rho \\ + \ & \frac{1}{2}\int_{\Gamma_0}\int_{\Gamma_0} \rho(x)\rho(y)G(x-y)dxdy. \end{aligned}$$

Here G is the periodic potential defined in (1.7), and X_{per} is the functional space :

$$X_{per} = \{v \in H^1_{per}(\Gamma_0),\ \big(\log(2+|x|)\big)^{1/2} v \in L^2(\Gamma_0)\}.$$

The first observation is that $u \in X_{per}$. Indeed, we already know from (i),the second equation of (2.25) and the fact that $\phi \in L^1_{unif}$, that :

$$\|-\Delta u\|_{L^p(B_1+x)} = \|-u^{7/3} + \phi u\|_{L^p(B_1+x)} \leq \frac{C}{1+r(x)^{3/2}}.$$

(We recall that $r(x) = |x'| = \sqrt{x_1^2 + x_2^2}$.) The same inequality holds for u instead of Δu, so by standard elliptic regularity results, and taking p large enough, we deduce that

$$|\nabla u| \leq \frac{C}{1+r^{3/2}}. \tag{2.53}$$

Hence $u \in H^1(\Gamma_0)$. Since u is periodic, this shows that

$$u \in X_{per}.$$

The next step is to show that u is a critical point of the problem I_{per}. So we write the Euler-Lagrange equation of this problem :

$$-\Delta u + \frac{5}{3}u^{7/3} - (G \star_{\Gamma_0} (\mu - u^2))u = \theta u, \tag{2.54}$$

for some $\theta \in \mathbf{R}$. The point is then to show that

$$\phi = G \star_{\Gamma_0} (\mu - u^2) + d, \tag{2.55}$$

with $d \in \mathbf{R}$. We set :

$$\psi = \int_{-1/2}^{1/2} \phi(x) dx_3,$$

and

$$f = \int_{-1/2}^{1/2} (\mu - u^2) dx_3.$$

Those functions are defined on $\mathbf{R}^2$, and since we have $-\Delta\psi = \int_{-1/2}^{1/2} -\Delta\phi = \int_{-1/2}^{1/2} \mu - u^2$, from the periodicity of ϕ, the first Laplacian being a two-dimensional one, and the second one a three-dimensional one, we have :

$$-\Delta\psi = f$$

on $\mathbf{R}^2$.

We want here to apply Lemma 2.4 with $R_0 = 1$. For that purpose, we only need to show that $\|(-\Delta\psi)\psi_R\|_{L^1(B_1^c)}$ is bounded independently of R. So, denoting by Q the unit cube of $\mathbf{R}^3$, we write :

$$\begin{aligned}
\int_{B_1^c} |f\psi_R| &= \sum_{k\in(\mathbf{Z}^2)^*} \int_{(Q+k)\cap B_1^c} |f\psi_R| \\
&\leq \sum_{k\in(\mathbf{Z}^2)^*} \|f\|_{L^\infty(Q+k)} \|\psi_R\|_{L^1_{unif}(B_1^c)} \\
&\leq C \sum_{k\in(\mathbf{Z}^2)^*} \frac{\|\psi_R\|_{L^1_{unif}(B_1^c)}}{1+|k|^3} \\
&\leq C\|\psi\|_{L^1_{unif}(B_1^c)} + C \sup_{R>1} \left| \frac{\int_{|x|=R} \psi}{2\pi R} \right| \\
&\leq C\|\phi\|_{L^1_{unif}(\{r>1\})} + C\|\phi\|_{L^\infty(\{r>1\})}.
\end{aligned}$$

So we may apply Lemma 2.4 to ψ, deducing that $\nabla\psi \in L^2(\mathbf{R}^2)$. Knowing this, we are going now to prove that :

$$\int_{\Gamma_0} u^2 = 1. \tag{2.56}$$

This will follow from :

$$\int_{\Gamma_0} -\Delta\phi = 0.$$

And, since this last property may be written as :

$$\int_{\mathbf{R}^2} -\Delta\psi = 0, \tag{2.57}$$

we focus on this last equation. Let ζ_R be a cut-off function, in the following sense :

$$\zeta_R(x) = \zeta(\frac{|x|}{R}), \text{ with :}$$

- $\zeta \in \mathcal{D}(\mathbf{R})$, $0 \leq \zeta \leq 1$, $|\zeta'| \leq 2$.
- $\zeta(t) = 1 \; \forall t \in [-1, 1]$.
- $\zeta(t) = 0 \; \forall t \in [-2, 2]^c$.

We have, for all $R > 1$:

$$\begin{aligned} \int_{\mathbf{R}^2} -\Delta\psi\zeta_R &= \int_{\mathbf{R}^2} \nabla\psi\nabla\zeta_R. \\ \left|\int_{\mathbf{R}^2} -\Delta\psi\zeta_R\right| &\leq \left(\int_{R<r<2R} |\nabla\psi|^2\right)^{1/2} \left(\int_{R<r<2R} |\nabla\zeta_R|^2\right)^{1/2}. \end{aligned}$$

And, since

$$|\nabla\zeta_R|^2 = \frac{1}{R^2}\left|\zeta'\left(\frac{|x|}{R}\right)\right|^2 \leq \frac{C}{R^2},$$

we conclude that

$$\left|\int_{\mathbf{R}^2} -\Delta\psi\zeta_R\right| \leq C\left(\int_{r>R} |\nabla\psi|^2\right)^{1/2}.$$

The right-hand side of this inequality vanishes as R goes to infinity, since $\nabla\psi \in L^2(B_1^c)$. Hence we get (2.57), that is (2.56), or (iii).

Now, we are going to prove (2.55). In order to do so, we compute the Laplacian of $\phi - G \star_{\Gamma_0} (\mu - u^2)$, and find, from the equality

$$-\Delta G = \sum_{k\in\mathbf{Z}} \delta_{ke_3}$$

that $\phi - G \star_{\Gamma_0} (\mu - u^2)$ is harmonic. On the other hand, we set $v = \mu - u^2$, hence we have $\int_{\Gamma_0} v = 0$, $v \in \mathcal{S}'_{per}(\Gamma_0)$ and v is smooth on $\{r > 1\}$, satisfying $|v| \leq \frac{C}{1+r^3}$. Hence, applying Lemma 2.5, we deduce that

$$G \star_{\Gamma_0} (\mu - u^2) \in L^1_{unif}. \tag{2.58}$$

Now, since a harmonic function belonging to L^1_{unif} is necessarily a constant, we conclude that (2.55) holds.

Thus, we know that $u \in X_{per}$, that u^2 has total mass one on Γ_0, and that it satisfies the Euler-Lagrange equation of I_{per}. Since this problem is convex, because the quadratic form D_G is positive, hence convex with respect to ρ, we conclude that u must be a solution of I_{per}. Hence u is unique, and so is ϕ. $\Diamond$

We now give proofs of the two lemmas that we have stated at the beginning of our proof :

Proof of Lemma 2.4 : This result seems to be a standard one, but since we have found no proof in the literature, we provide one for the convenience of the reader.

We first notice that $\psi_R \in L^2_{unif}(\mathbf{R}^2)$, since $\psi \in L^2_{unif}(\mathbf{R}^2)$.

We fix an $R > R_0$. Let ξ_R be a cut-off function, that is, $\xi_R \in \mathcal{D}(\mathbf{R}^2)$, such that $\xi_R(x) = 1$ on $B_R \setminus B_{2R_0}$ and 0 on $B^c_{R+1} \cup B_{R_0}$, $0 \leq \xi_R \leq 1$, and $\|\nabla \xi_R\|_{L^\infty} \leq 1 + \frac{2}{R_0}$.

We have :

$$\begin{aligned} \left| \int_{\mathbf{R}^2} -\Delta\psi_R \psi_R \xi_R^2 \right| &\leq C \\ \left| \int_{\mathbf{R}^2} \nabla\psi_R \nabla(\xi_R^2 \psi_R) \right| &\leq C. \end{aligned} \tag{2.59}$$

This implies :

$$\begin{aligned} \int_{\mathbf{R}^2} |\nabla(\psi_R \xi_R)|^2 &\leq C + \int_{\mathbf{R}^2} \psi_R^2 |\nabla \xi_R|^2 \\ &\leq C + CR, \end{aligned} \tag{2.60}$$

We also have :

$$\begin{aligned}
\int_{\mathbf{R}^2} |\nabla(\psi_R\xi_R)|^2 &\geq \int_{\mathbf{R}^2} |\nabla\psi_R|^2\xi_R^2 + 2\int_{\mathbf{R}^2} \psi_R\nabla\psi_R\xi_R\nabla\xi_R \\
&\geq \int_{\mathbf{R}^2} |\nabla\psi_R|^2\xi_R^2 \\
&\quad -2\Big(\int_{\mathbf{R}^2} |\nabla\psi_R|^2\xi_R^2\Big)^{1/2}\Big(\int_{\mathbf{R}^2} |\nabla\xi_R|^2\psi_R^2\Big)^{1/2} \\
&\geq \int_{\mathbf{R}^2} |\nabla\psi_R|^2\xi_R^2 - 2C\sqrt{R}\Big(\int_{\mathbf{R}^2} |\nabla\psi_R|^2\xi_R^2\Big)^{1/2} \\
&\geq \frac{1}{2}\int_{\mathbf{R}^2} |\nabla\psi_R|^2\xi_R^2 - CR.
\end{aligned}$$

This, together with (2.60), shows that

$$\int_{B_R\setminus B_{2R_0}} |\nabla\psi|^2 = \int_{B_R\setminus B_{2R_0}} |\nabla\psi_R|^2 \leq \int_{\mathbf{R}^2} |\nabla\psi_R|^2\xi_R^2 \leq CR, \tag{2.61}$$

for some constant C independent of R. We also have, integrating by parts over $B_R \setminus B_{2R_0}$,

$$\int_{B_R\setminus B_{2R_0}} (-\Delta\psi_R)\psi_R = \int_{B_R\setminus B_{2R_0}} |\nabla\psi_R|^2 - \int_{|x|=R} \psi_R\frac{\partial\psi_R}{\partial r} + \int_{|x|=2R_0} \psi_R\frac{\partial\psi_R}{\partial r}. \tag{2.62}$$

And from Poincaré inequality, we know that :

$$\Big(\int_{|x|=R} {\psi_R}^2\Big)^{1/2} \leq \frac{1}{R}\Big(\int_{|x|=R}\Big|\frac{\partial\psi_R}{\partial\theta}\Big|^2\Big)^{1/2}. \tag{2.63}$$

This, together with (2.62) and (2.59), gives :

$$\begin{aligned}
\int_{B_R\setminus B_{2R_0}} |\nabla\psi|^2 - C_0 &\leq R\Big(\int_{|x|=R}\Big|\frac{\partial\psi_R}{\partial r}\Big|^2\Big)^{1/2}\frac{1}{R}\Big(\int_{|x|=R}\Big|\frac{\partial\psi_R}{\partial\theta}\Big|^2\Big)^{1/2} \\
&\leq \frac{R}{2}\int_{|x|=R} |\nabla\psi_R|^2 = \frac{R}{2}\int_{|x|=R} |\nabla\psi|^2,
\end{aligned}$$

C_0 being a constant bounding $\left|\int_{|x|=2R_0} \psi_R\frac{\partial\psi}{\partial r} + \int_{B_R\setminus B_{2R_0}} (-\Delta\psi_R)\psi_R\right|$.

So, letting g be the function

$$g(R) = \int_{B_R\setminus B_{2R_0}} |\nabla\psi|^2 - C_0,$$

we get the differential inequality :

$$g(R) \leq \frac{R}{2} g'(R).$$

Hence

$$\frac{d}{dR}\Big(\frac{1}{R^2} g(R)\Big) = \frac{1}{R^3}(Rg'(R) - 2g(R)) \geq 0.$$

So, integrating from $R_1 > R_0$ to R, we get, for all $R > R_1$,

$$g(R) \geq \frac{g(R_1)}{R_1^2} R^2.$$

If there exists at least one R_1 such that $g(R_1) > 0$, we reach a contradiction with (2.61). Hence $g \leq 0$, that is

$$\int_{B_R \setminus B_{2R_0}} |\nabla \psi|^2 \leq C_0.$$

Which implies that $\nabla\psi \in L^2(B_{R_0}^c)$. $\diamondsuit$

Proof of Lemma 2.5 : We already know that $G \star_{\Gamma_0} v$ lies in $L^1_{loc}(\Gamma_0)$, so the only thing to check out is that it is bounded as $r \to \infty$.

We now write :

$$\begin{aligned} G \star_{\Gamma_0} v &= \int_{\Gamma_0} v(y)(G(x-y) + 2\log(r(x-y)))dy \\ &\quad - \int_{\Gamma_0} 2v(y)(\log(r(x-y)) - \log(r(x)))dy. \end{aligned}$$

We first consider the first term of this expression : from Lemma 2.2, we know that

$$|G(x) + 2\log(r)| \leq \frac{C}{r} \ ,$$

for $x \in 2\Gamma_0$. Hence :

$$\begin{aligned} \left| \int_{\Gamma_0} v(y)(G(x-y) + 2\log(r(x-y)))dy \right| &\leq C \int_{\Gamma_0} \frac{|v(y)|}{r(x-y)} dy \\ &\leq C \int_{\Gamma_0 \cap \{r(x-y) > 1\}} |v(y)| dy \\ &\quad + C \int_{\Gamma_0 \cap \{r(x-y) < 1\}} \frac{|v(y)|}{r(x-y)} dy \\ &\leq C + C \int_{|y_3| < \frac{1}{2}, r(y) < 1} \frac{dy}{r(y)} \\ &\leq C. \end{aligned} \tag{2.64}$$

Now we rewrite the second term as :

$$\int_{\Gamma_0} 2|v(y)||\log(r(x-y)) - \log(r(x))|dy \leq C\int_{\Gamma_0} |v(y)|\left|\log\left|\frac{x'}{|x'|} - \frac{y'}{|x'|}\right|\right|dy \tag{2.65}$$

$$\leq C\int_{\Gamma_0\cap\{|y'|<R\}} |v(y)|\left|\log\left|\frac{x'}{|x'|} - \frac{y'}{|x'|}\right|\right|dy + C\int_{\Gamma_0\cap\{|y'|>R\}} |v(y)|\left|\log\left|\frac{x'}{|x'|} - \frac{y'}{|x'|}\right|\right|dy. \tag{2.66}$$

Where $R = R(x)$ satisfies $R \ll |x'|$. So we may write, for $|y'| < R$:

$$\left|\log\left|\frac{x'}{|x'|} - \frac{y'}{|x'|}\right|\right| = \frac{1}{2}\left|\log\left(1 - \frac{2x'y'}{|x'|^2} + \frac{|y'|^2}{|x'|^2}\right)\right| = O(\frac{R}{|x'|}).$$

Which implies :

$$\begin{aligned}\int_{\Gamma_0\cap\{|y'|<R\}} |v(y)|\left|\log\left|\frac{x'}{|x'|} - \frac{y'}{|x'|}\right|\right|dy \ &\leq \ \frac{CR}{|x'|}\int_{\Gamma_0\cap\{|y'|<R\}} |v(y)|dy \\ &\leq \ \frac{CR}{|x'|}\int_R^\infty \frac{rdr}{r^3} \leq \frac{C}{|x'|}.\end{aligned}$$

Concerning the remaining term of (2.66), we integrate first over the set

$$\Gamma_0 \cap \{|y'| > R\} \cap \{|x'-y'| > 1\} = D_R,$$

then over the set

$$\Gamma_0 \cap \{|y'| > R\} \cap \{|x'-y'| < 1\} = E_R.$$

On the first one, we have :

$$|\log\left|\frac{x'}{|x'|} - \frac{y'}{|x'|}\right|| \leq C\log\left(1 + \frac{|y'|}{|x'|}\right). \tag{2.67}$$

The second one is a compact subset of $\mathbf{R}^3$, so, as $\log|x'| \in L^1_{loc}(\mathbf{R}^3)$, we may bound the integral of $|v(y)|\left|\log\left|\frac{x'}{|x'|} - \frac{y'}{|x'|}\right|\right|$ over E_R by $\frac{C}{R^3}$.

And coming back to (2.67), we write :

$$\begin{aligned}
\int_{\Gamma_0\cap\{|y'|>R\}} |v(y)|\left|\log\left|\frac{x'}{|x'|}-\frac{y'}{|x'|}\right|\right|dy &\leq \int_{D_R}|v(y)|\left|\log\left(1+\frac{|y'|}{|x'|}\right)\right|dy+\frac{C}{R^3} \\
&\leq C\int_R^\infty \frac{|\log(1+\frac{r}{|x'|})|}{r^2}dr+\frac{C}{R^3} \\
&\leq \frac{C}{|x'|}\int_{R/|x'|}^\infty \frac{|\log(1+t)|}{t^2}dt+\frac{C}{R^3} \\
&\leq \frac{C}{|x'|}\left(\frac{|x'|\log(1+\frac{R}{|x'|})}{R}\right) \\
&\quad +\frac{C}{|x'|}\int_{R/|x'|}^\infty \frac{dt}{t(1+t)}+\frac{C}{R^3} \\
&\leq \frac{C}{|x'|}+\frac{C}{R}+\frac{C}{R^3}. \qquad (2.68)
\end{aligned}$$

All this is bounded as $|x'| \longrightarrow \infty$, so this ends the proof. $\diamondsuit$

Remark 2.6 *Looking closely at inequality (2.68), we notice that the bound may be $\frac{C}{|x'|^\alpha}$, for any $\alpha < 1$. (Just take $R = |x'|^\alpha$.) On the other hand, the same kind of computation could be done in (2.64), by developing $\frac{1}{|x'-y'|}$ as $|x'| \longrightarrow \infty$. One would find the same kind of inequality, namely C in (2.64) would be replaced by $\frac{C}{|x'|^\alpha}$. So we may in fact assert that $\phi = \phi_0 + d$, with $d \in \mathbf{R}$ and $\phi_0 \in L^1_{unif}$, satisfying*

$$|\phi_0| \leq \frac{C}{|x'|^\alpha}, \ \forall \alpha < 1.$$

We may also notice that, in the course of our proof, we have found a solution to the problem I_{per}, and hence ensured that this problem is well-posed :

Remark 2.7 *As a corollary of Theorem 2.4, one may state the result that the periodic problem I_{per} is well-posed. Of course, this result could be proved without using the above theorem, by using standard variational methods, but it is not our point here.*

2.2.5 Convergence and identification of the limit

Now that we have a uniqueness result for the system (2.25), we are able to show the convergence of the sequence ρ_Λ :

Proposition 2.7 *The sequence u_Λ converges to u_{per} in $H^1(\Gamma_0)$.*

Proof : The proof only consists in collecting the preceding results, as pointed out above. ◊

Actually, as in [5], we establish in Theorem 2.5 below a much stronger convergence result. In order to do so, we introduce what we will in this context call interior domains :

Definition 2.1 *Let $\Lambda \subset \{(0,0)\} \times \mathbf{Z}$ be a Van Hove sequence in the third direction. Λ' will be said to be a sequence of interior domains, denoted by $\Lambda' \subset\subset \Lambda$, if it satisfies the following properties :*

(i) $\Lambda' \subset \Lambda$.

(ii) For any finite subset A of $\mathbf{Z}e_3$, there exists an $h_0 \in \mathbf{N}$ such that $\forall h \geq h_0$, $A \subset \Lambda'_h$.

(iii) $\frac{|\Lambda'|}{|\Lambda|} \longrightarrow 1$ *as* $\Lambda \to \infty$.

(iv) $d(\Lambda', \partial\Gamma(\Lambda)) \longrightarrow \infty$ *as* $\Lambda \to \infty$.

Theorem 2.5 *For any sequence $\Lambda' \subset\subset \Lambda$ and any $R > 0$, we have :*

$$\|u_\Lambda - u_{per}\|_{L^\infty(\Gamma(\Lambda'))}, \longrightarrow 0 \tag{2.69}$$

$$\|\phi_\Lambda - \phi_{per}\|_{L^\infty(\Gamma(\Lambda')\cap\{r<R\})} \longrightarrow 0, \tag{2.70}$$

as $\Lambda \longrightarrow \infty$. (We recall that $\phi_{per} = G \star_{\Gamma_0} (m - u_{per}^2) - \theta_{per}$)

Proof : We follow step by step, here again, the proof of [5]. We only provide a proof of (2.69), the proof of (2.70) following exactly the same pattern. We argue by contradiction, and suppose that (2.69) does not hold. This implies that there exists, extracting a subsequence if necessary, a sequence x_Λ in $\Gamma(\Lambda')$, such that :

$$|u_\Lambda(x_\Lambda) - u_{per}(x_\Lambda)| > \frac{\varepsilon}{2}, \tag{2.71}$$

for some $\varepsilon > 0$. On the other hand, we have :

$$|u_\Lambda(x_\Lambda) - u_{per}(x_\Lambda)| \leq \frac{C}{1 + r(x_\Lambda)^{3/2}}.$$

Hence $r(x_\Lambda)$ is necessarily bounded. Now we write $x_\Lambda = y_\Lambda + k_\Lambda e_3$, with $y_\Lambda \in \Gamma_0$ and $k_\Lambda \in \mathbf{Z}$. Since the sequence $r(x_\Lambda)$ is bounded, so is y_Λ. We then may assume that this sequence is convergent, and that the limit $\overline{y}$ lies in $\overline{\Gamma}_0$. We then have, using (2.71), and taking $|\Lambda|$ large enough,

$$|u_\Lambda(x_\Lambda) - u_{per}(\overline{y})| > \frac{\varepsilon}{4}. \tag{2.72}$$

We denote by $\overline{u}_\Lambda$ the function $u_\Lambda(\cdot+x_\Lambda)$, and by $\overline{\phi}_\Lambda$ the function $\phi_\Lambda(\cdot+x_\Lambda)$. One may then rewrite (2.3)-(2.4) as :

$$\left\{ \begin{array}{l} -\Delta\overline{u}_\Lambda + \frac{5}{3}\overline{u}_\Lambda^{7/3} - \overline{u}_\Lambda\overline{\phi}_\Lambda = 0, \\ -\Delta\overline{\phi}_\Lambda = 4\pi(m_\Lambda(\cdot+x_\Lambda) - \overline{u}_\Lambda^2). \end{array} \right. \tag{2.73}$$

The bounds on u_Λ and ϕ_Λ hold for $\overline{u}_\Lambda$ and $\overline{\phi}_\Lambda$, so we may pass locally to the limit in the system (2.73) above, and denoting by $\overline{u}$ and $\overline{\phi}$ the corresponding limits, we have :

$$\left\{ \begin{array}{l} -\Delta\overline{u} + \frac{5}{3}\overline{u}^{7/3} - \overline{\phi}\overline{u} = 0, \\ -\Delta\overline{\phi} = 4\pi(m_\infty(\cdot+\overline{y}) - \overline{u}^2), \end{array} \right. \tag{2.74}$$

because $m_\Lambda(\cdot+x_\Lambda) \longrightarrow m_\infty(\cdot+\overline{y})$ in $\mathcal{D}'(\mathbf{R}^3)$ as $\Lambda \to \infty$. Indeed, we have, for any $\varphi \in \mathcal{D}(\mathbf{R}^3)$, K being its support :

$$\begin{aligned} < m_\Lambda(\cdot+x_\Lambda),\varphi > &= \sum_{k\in\Lambda} < m(\cdot+x_\Lambda+k),\varphi > \\ &= \sum_{k\in\Lambda\cap(\Gamma_0-K-x_\Lambda)} < m,\varphi(\cdot-x_\Lambda-k) > . \end{aligned}$$

Using Definition 2.1-(iv), we have that the set $\Lambda\cap(\Gamma_0-K-x_\Lambda)$ becomes $\mathbf{Z}e_3\cap(\Gamma_0-K-x_\Lambda)$ when Λ is large enough, because in this case, Γ_0-K-x_Λ comes to be included in Λ. Hence,

$$\begin{aligned} < m_\Lambda(\cdot+x_\Lambda),\varphi > &= \sum_{k\in\mathbf{Z}e_3} < m,\varphi(\cdot-x_\Lambda-k) > \\ &= < m_\infty,\varphi(\cdot-y_\Lambda) > \longrightarrow < m_\infty(\cdot+\overline{y}),\varphi > . \end{aligned}$$

Now, from Theorem 2.4, we know that (2.74) implies that

$$\overline{u} = u_{per}(\cdot+\overline{y}).$$

Hence

$$\overline{u}_\Lambda \longrightarrow u_{per}(\cdot+\overline{y})$$

in $L^2_{loc}(\mathbf{R}^3)$. On the other hand, from the bounds we have on ∇u_Λ (see formula (2.53)), we deduce that the above convergence is point-wise, reaching a contradiction with (2.72).

Now, concerning (2.70), the only change is the fact that we do not need to show that y_Λ is bounded, all the other steps of the proof carrying through. $\diamondsuit$

2.2.6 Convergence of the energy

We are now going to answer the only question of the problem of thermodynamic limit that we have left aside so far, namely the convergence of the energy per unit volume.

Theorem 2.6 *For any Van Hove sequence, we have :*

$$\frac{I_\Lambda}{|\Lambda|} \longrightarrow I_{per} + \frac{M}{2}$$

as $\Lambda \to \infty$.

Proof : Here again, our proof is an adaptation of [5]'s, using the compactness result (2.10), and the decay we have obtained on ∇u in (2.53), that is :

$$|\nabla u_\Lambda| \leq \frac{C}{1 + r^{3/2}}.$$

The strategy of proof is to study one by one the terms of the energy, and to split the integrals over $\mathbf{R}^3$ into integrals over $\Gamma(\Lambda')$, $\Gamma(\Lambda) \setminus \Gamma(\Lambda')$ and $\Gamma(\Lambda)^c$, for some $\Lambda' \subset\subset \Lambda$, the first being dealt with using the convergence result of Theorem 2.5, the second using the bounds we have on u_{per} and u_Λ, and the third one using the compactness result (2.10). We refer the reader to [5] for more details. $\diamondsuit$

3 Solid films

This section is devoted to the thermodynamic limit problem in two dimension, that is to say, the problem of the thermodynamic limit concerning solid films. Throughout this section, $\Lambda = \Lambda_2 \times \{0\} \subset \mathbf{Z}^2 \times \{0\}$ will denote a Van Hove sequence in the first two dimensions, i.e such that Λ_2 is a Van Hove sequence of $\mathbf{Z}^2$. Γ_0 will denote the periodic cell of the problem, that is, $]-\frac{1}{2}, \frac{1}{2}]^2 \times \mathbf{R}$, and $\Gamma(\Lambda) = \bigcup_{k\in\Lambda} \Gamma_0 + k$. For such a Λ, we define as in the preceding section the energy $E_\Lambda(\rho)$ and the minimizing problem I_Λ by formulas (2.1) and (2.2).

The unique minimizer $\rho_\Lambda = u_\Lambda^2$ satisfies here again :

$$-\Delta u_\Lambda + \frac{5}{3} u_\Lambda^{7/3} - \phi_\Lambda u_\Lambda = 0, \tag{3.1}$$

where $\phi_\Lambda = (m_\Lambda - u_\Lambda^2) \star \frac{1}{|x|} - \theta_\Lambda$ satisfies :

$$-\Delta \phi_\Lambda = 4\pi(m_\Lambda - u_\Lambda^2). \tag{3.2}$$

Following exactly the steps of Section 2, we start with some a priori estimates.

3.1 A priori estimates

3.1.1 Energy bounds and L^∞ bounds

We have exactly the same results as in Section 2, namely Theorems 2.1 and 2.2. Here again, as in Section 2, we notice that the proof of theorem 2.2 is only based on equations (3.1)-(3.2), and on the fact that the measure m_Λ is non-negative, bounded and has compact support with respect to x_3. Hence it will hold for any such solutions, and in particular if we replace m_Λ by $m_\infty = \sum_{k\in\mathbf{Z}} m(\cdot - ke_3)$, or by any Γ_0-periodic measure having compact support with respect to x_3.

3.1.2 Asymptotic estimates

As in Section 2, we now derive bounds at infinity, that is estimates of the decay of u_Λ as $|x_3| \longrightarrow \infty$, which are uniform with respect to Λ. As in Section 2, we use Lemma 2.1 to prove the following estimates :

Theorem 3.1 *For any solution $(u_\Lambda, \phi_\Lambda)$ of the system (3.1)-(3.2) satisfying $u_\Lambda \geq 0$, we have :*

$$\begin{aligned} \phi_\Lambda &\leq \frac{C}{1+|x_3|^2}, \quad \forall\,|x_3| \geq 1, \\ 0 \leq u_\Lambda &\leq \frac{C}{1+|x_3|^{3/2}}, \end{aligned}$$

where C denotes various positive constants independent of the measure m_Λ.

Furthermore, in the smeared nuclei case, i.e when m in (3.2) is supposed to be smooth, the first inequality holds everywhere.

Proof : The proof is only a copy of that of Theorem 2.3. We only point out the necessary changes in that proof : the function g_R is unchanged, and so is $\tilde{\phi}$. In all the inequalities and definition of sets, r becomes $|x_3|$. Hence C_{R+1} is now the set $\{|x_3| > R+1\}$, and U is the function :

$$U = \frac{a}{(|x_3|^2 - R^2)^2} + \frac{bR'^4}{(R'^2 - |x_3|^2)^4}.$$

Computations follow exactly the same pattern, and we find in U the desired supersolution, the only change being the constants $\frac{a}{(2R+1)^2}$ and b. The whole proof carries through, and we finally get the desired conclusion. $\diamondsuit$

3.1.3 Compactness

We now study the compactness of the sequence ρ_Λ, namely we are going to show that :

Proposition 3.1 *For any sequence $\Lambda \subset \mathbf{Z}^2 \times 0$, being a Van Hove sequence in the first two dimensions, we have :*

$$\frac{1}{|\Lambda|}\int_{\Gamma(\Lambda)} \rho_\Lambda \longrightarrow 1 \quad \text{as} \quad \Lambda \to \infty. \tag{3.3}$$

Proof : Here again, we provide only a smeared nuclei case proof, referring to [5] for the generalization to the point nuclei case. We start exactly as in Proposition 2.1, writing that for all $h \in H^1(\mathbf{R}^2)$, we have :

$$|\int_{\mathbf{R}^3} (m_\Lambda - \rho_\Lambda) h| \leq \frac{1}{(2\pi)^3} D(m_\Lambda - \rho_\Lambda, m_\Lambda - \rho_\Lambda)^{1/2} \|\nabla h\|_{L^2(\mathbf{R}^3)}. \tag{3.4}$$

We then choose $h = h_\Lambda$: we set $h_\Lambda(x) = f_\Lambda(x_3) g_\Lambda(x_1, x_2)$, with :

- $f_\Lambda(t) = 1 - \frac{|t|}{R}$ if $|t| < R$, 0 otherwise, where $R = R(\Lambda)$ will be chosen later on.
- $g_\Lambda \in \mathcal{D}(\mathbf{R}^2)$, $0 \leq g_\Lambda \leq 1$, $g_\Lambda = 1$ on the set $\{x \in \mathbf{R}^2 / d(x, \Lambda_2) < \frac{1}{\sqrt{2}}\}$, 0 on the set $\{x \in \mathbf{R}^2 / d(x, \Lambda_2) > 1\}$, and satisfying $|\nabla g_\Lambda| \leq 4$.

(We recall that $\Lambda = \Lambda_2 \times \{0\}$, that $\Lambda_2^1 = \{t \in \mathbf{R}^2,\ d(t, \cup_{k \in \Lambda_2}(k +] - \frac{1}{2}, \frac{1}{2}]^2)) < 1\}$, and that the Van-Hove hypotheses imply $|\Lambda_2^1| \ll |\Lambda|$.)

We have, for such an h_Λ :

$$\begin{aligned}
\int_{\mathbf{R}^3} |\nabla h_\Lambda|^2 &= \int_{\mathbf{R}^3} f_\Lambda'(x_3)^2 g_\Lambda(x')^2 dx' dx_3 + \int_{\mathbf{R}^3} f_\Lambda(x_3)^2 |\nabla g_\Lambda|^2(x') dx' dx_3 \\
&\leq C|\Lambda| \int_0^R \frac{dt}{R^2} + C|\Lambda_2^1| \int_0^R (1 - \frac{t}{R})^2 dt \\
&\leq C\frac{|\Lambda|}{R} + CR|\Lambda_2^1|.
\end{aligned}$$

We now choose $R = \left(\frac{|\Lambda|}{|\Lambda_2^1|}\right)^{1/2}$, so that we have $\frac{|\Lambda|}{R} \ll |\Lambda|$, and $R|\Lambda_2^1| \ll |\Lambda|$. Hence, we have :

$$\|\nabla h_\Lambda\|_{L^2(\mathbf{R}^3)} = o(|\Lambda|). \tag{3.5}$$

Thus, since we already know from Theorem 2.1 (vii) that $D(m_\Lambda - \rho_\Lambda, m_\Lambda - \rho_\Lambda) \leq C|\Lambda|$, (3.5) implies :

$$\frac{1}{|\Lambda|}\int_{\mathbf{R}^3} (m_\Lambda - \rho_\Lambda) h_\Lambda \longrightarrow 0 \tag{3.6}$$

as $\Lambda \to \infty$.

On the other hand, since $h_\Lambda \leq 1$, we have $\int_{\mathbf{R}^3} m_\Lambda h_\Lambda \leq |\Lambda|$. We also have :

$$\int_{\mathbf{R}^3} m_\Lambda h_\Lambda \geq |\Lambda| - \int_{\mathbf{R}^3} m_\Lambda \frac{|x_3|}{R},$$

and $0 \leq \int_{\mathbf{R}^3} m_\Lambda \frac{|x_3|}{R} \leq \frac{|\Lambda|}{R}$, hence we infer that :

$$\frac{1}{|\Lambda|} \int_{\mathbf{R}^3} m_\Lambda h_\Lambda \longrightarrow 1. \tag{3.7}$$

Next, we compute :

$$\begin{aligned} \int_{\mathbf{R}^3} \rho_\Lambda h_\Lambda \;&=\; \int_{\Gamma(\Lambda)} \rho_\Lambda - \int_{\Gamma(\Lambda)\cap\{|x_3|<R\}} \rho_\Lambda \frac{|x_3|}{R} + \int_{\Gamma(\Lambda)^c} \rho_\Lambda h_\Lambda \\ &\quad - \int_{\Gamma(\Lambda)\cap\{|x_3|>R\}} \rho_\Lambda. \end{aligned} \tag{3.8}$$

Concerning the second term of the right-hand side, we write :

$$\left| \int_{\Gamma(\Lambda)\cap\{|x_3|<R\}} \rho_\Lambda \frac{|x_3|}{R} \right| \leq C \frac{|\Lambda|}{R} \int_0^R \frac{tdt}{1+t^3} \leq C \frac{|\Lambda|}{R} \ll |\Lambda|.$$

We then deal with the third term as follows :

$$\left| \int_{\Gamma(\Lambda)^c} \rho_\Lambda h_\Lambda \right| \leq C \frac{|\Lambda^{\frac{1}{2}}|}{R} \int_0^R \frac{tdt}{1+t^3} \leq C \frac{|\Lambda^{\frac{1}{2}}|}{R} \ll |\Lambda|.$$

Turning to the fourth one, we have :

$$\int_{\Gamma(\Lambda)\cap\{|x_3|>R\}} \rho_\Lambda \leq C|\Lambda| \int_R^\infty \frac{tdt}{1+t^3} \leq C \frac{|\Lambda|}{R} \ll |\Lambda|.$$

Hence (3.8) implies :

$$\frac{1}{|\Lambda|} \int_{\mathbf{R}^3} \rho_\Lambda h_\Lambda = \frac{1}{|\Lambda|} \int_{\Gamma(\Lambda)} \rho_\Lambda + o(1). \tag{3.9}$$

Thus, collecting (3.6), (3.7) and (3.9), we conclude that (3.3) holds. $\diamondsuit$

3.2 Identification of the limit

Following the steps of Section 2, and we are now able to pass locally to the limit in the system (3.1)-(3.2), getting solutions u_∞ and ϕ_∞ of the system :

$$\begin{cases} -\Delta u_\infty + \frac{5}{3}u_\infty^{7/3} - u_\infty\phi_\infty = 0, \\ -\Delta\phi_\infty = 4\pi(m_\infty - u_\infty^2). \end{cases} \tag{3.10}$$

m_∞ being the measure $\sum_{k\in\mathbf{Z}^2} m(\cdot - k)$, and in particular a periodic measure. We suspect a uniqueness result similar to that of Section 2 to be true in this case, but we did not manage to prove it. However, we are going to prove a convergence result for the sequence ρ_Λ.

We first need some preliminary results on the periodic potential G.

3.2.1 The potential G

In this section, we denote by G the function

$$G(x) = -2\pi|x_3| + \sum_{k\in\mathbf{Z}^2}\left(\frac{1}{|x-k|} - \int_K \frac{dy}{|x-y-k|}\right).$$

Where K denotes the unit square of $\mathbf{R}^2$, that is, $K =]-\frac{1}{2}, \frac{1}{2}[^2$.

First of all, we check out that this sum clearly defines G :

Proposition 3.2 *The sum defining G is convergent over the set $\mathbf{R}^3 \setminus (\mathbf{Z}^2 \times \{0\})$, and normally convergent on any compact subset of this set.*

Proof : Here again, we develop the integrand as $|x| \longrightarrow \infty$:

$$\begin{aligned} f(x) &= \frac{1}{|x|} - \int_K \frac{dy}{|x-y|} \\ &= \frac{1}{|x|} - \int_K \frac{dy}{\sqrt{|x|^2 - 2xy + |y|^2}} \\ &= \frac{1}{|x|} - \frac{1}{|x|}\int_K \frac{dy}{\sqrt{1 - 2\frac{xy}{|x|^2} + \frac{|y|^2}{|x|^2}}} \\ &= \frac{1}{|x|} - \frac{1}{|x|}\int_K \left(1 + \frac{xy}{|x|^2} + O(\frac{1}{|x|^2})\right)dy \\ &= \frac{1}{|x|} - \frac{1}{|x|} + O(\frac{1}{|x|^3}). \end{aligned}$$

And this concludes our proof, since $\sum_{k\in\mathbf{Z}^2} \frac{1}{1+|k|^3}$ does converge. ◊

We now prove the analogue of Lemma 2.2 :

Lemma 3.1 *We have :*

(i) $G(x) = \frac{1}{|x|} + C + o(1)$ *as* $|x| \longrightarrow 0$.

(ii) $G(x) = -2\pi|x_3| + O(\frac{1}{|x_3|^\alpha})$ *as* $|x_3| \longrightarrow \infty$*, for any* $\alpha < 1$*, uniformly with respect to* $x' = (x_1, x_2)$*.*

Proof : We rewrite G as :

$$G(x) = -2\pi|x_3| + \frac{1}{|x|} - \int_K \frac{dy}{|x-y|} + \sum_{k\in(\mathbf{Z}^2)^*} \left(\frac{1}{|x-k|} - \int_K \frac{dy}{|x-y-k|} \right). \tag{3.11}$$

From the computation of the preceding proposition's proof, we know that the remaining sum converges normally on a neighborhood of 0. Hence it is continuous on that neighborhood. On the other hand, $x \mapsto \int_K \frac{dy}{|x-y|}$ is continuous on $\mathbf{R}^3$, and this concludes the proof of (i).

We now turn to (ii). We intend to show that :

$$\sum_{k\in(\mathbf{Z}^2)^*} \left| \frac{1}{|x-k|} - \int_K \frac{dy}{|x-k-y|} \right| \leq \frac{C}{|x_3|^\alpha}. \tag{3.12}$$

Considering the function f defined above, we know that $|f(x)| \leq \frac{C}{|x|^3}$. So we may write :

$$\sum_{k\in(\mathbf{Z}^2)^*} |f(x-k)| \leq \sum_{k\in(\mathbf{Z}^2)^*} \frac{C}{|x-k|^3} \leq \sum_{k\in(\mathbf{Z}^2)^*} \frac{C}{|k|^3 + |x_3|^3}.$$

We now use Young's inequality, finding that for all $\alpha < 1$, we have :

$$|k|^3 + |t|^3 \geq C|k|^{3-\alpha}|t|^\alpha.$$

So we infer that :

$$\sum_{k\in(\mathbf{Z}^2)^*} |f(x-k)| \leq \frac{C}{|x_3|^\alpha} \sum_{k\in(\mathbf{Z}^2)^*} \frac{C}{|k|^{3-\alpha}}.$$

Since $\alpha < 1$ implies $3 - \alpha > 2$, we conclude that (3.12) holds. $\diamondsuit$

Let us now establish a positiveness property on the operator D_G (We recall that it is defined by $D_G(f,g) = \int_{\Gamma_0}\int_{\Gamma_0} f(x)g(y)G(x-y)dxdy = \int_{\Gamma_0}(G\star_{\Gamma_0} f)g)$. We assume here that the support of m is contained in $\{r < 1\}$. (This implies no loss of generality).

Proposition 3.3 *The bilinear form* D_G *is positive on the set* $Y_{per} = \{f \in L^1_{per}(\Gamma_0)/\sqrt{|f|} \in H^1_{per}(\Gamma_0 \cap \{|x_3| > 1\}), \int_{\Gamma_0} f = 0,$ *and* $(1+|x|)f \in L^1(\Gamma_0)\}$.

Where the space $H^1_{per}(\Gamma_0 \cap \{|x_3| > 1\})$ is defined by the set of all functions belonging to $H^1_{loc}(\{|x_3| > 1\}) \cap H^1(\Gamma_0 \cap \{|x_3| > 1\})$ that are periodic of periodic cell Γ_0.

Proof : We introduce, as in Section 2, the Fourier transform on Γ_0, defined by :

$$\widehat{f}(n,\xi) = \int_{\Gamma_0} f(x) e^{-i2\pi(x_3\xi + nx')} dx, \tag{3.13}$$

where $\xi \in \mathbf{R}$, $n \in \mathbf{Z}^2$ and $x = (x', x_3)$. By a straightforward computation, one finds that for this Fourier transform, Parceval's and Plancherel's formulas hold, so that we may prolong it to $\mathcal{S}'_{per}(\Gamma_0)$. We also have :

$$\forall f \in \mathcal{S}'_{per}(\Gamma_0),\ \widehat{\partial_3 f}(n,\xi) = i2\pi\xi \widehat{f}(n,\xi). \tag{3.14}$$

And

$$\forall f \in \mathcal{S}'_{per}(\Gamma_0),\ \forall g \in \mathcal{S}_{per}(\Gamma_0),\ \widehat{f \star_{\Gamma_0} g} = \widehat{f}\widehat{g}.$$

So, since $-\Delta G = 4\pi\delta_0$ on Γ_0, we deduce :

$$4\pi^2(\xi^2 + |n|^2)\widehat{G}(n,\xi) = 4\pi.$$

Thus, when $n \neq 0$, we have $\widehat{G}(n,\xi) = \frac{1}{\pi(|n|^2+\xi^2)}$. Concerning the case $n = 0$, we notice that $\widehat{G}(0,\xi)$ is exactly equal to the classical Fourier transform of $-2\pi|x_3|$ over $\mathbf{R}$. Indeed, putting $G_0(x) = G(x) + 2\pi|x_3|$, we notice that $\int_K G_0(x)dx'$ is a harmonic function, which goes to zero as $|x_3| \longrightarrow \infty$, from Lemma 3.1. So it is necessarily 0.

Furthermore, the Fourier transform of $-2\pi|x_3|$ is shown to be $4\pi \mathrm{vp}(\frac{1}{\xi^2}) + a\delta_0$ in [14], where $\mathrm{vp}(\frac{1}{\xi^2})$ is defined by :

$$\begin{aligned} < \mathrm{vp}(\frac{1}{\xi^2}), \varphi > \quad &= \quad \lim_{\varepsilon \to 0^+} \Bigg(\int_{|\xi|>\varepsilon} \frac{\varphi(\xi)}{\xi^2} d\xi - \frac{1}{\varepsilon}\big(\varphi(\varepsilon) + \varphi(-\varepsilon)\big) \\ &\qquad + (\log\varepsilon)\big(\varphi'(\varepsilon) - \varphi'(-\varepsilon)\big) \Bigg). \end{aligned} \tag{3.15}$$

In fact, $\mathrm{vp}(\frac{1}{x^2}) = -(\log|x|)''$ in $\mathcal{D}'(\mathbf{R})$. Now let $f \in Y_{per}$. We have :

$$\begin{aligned} D_G(f,f) \quad &= \quad \int_{\Gamma_0} (G \star_{\Gamma_0} f) f \\ &= \quad \sum_{k \in \mathbf{Z}^2} \int_{\mathbf{R}} \widehat{G \star_{\Gamma_0}} f(k,\xi) \widehat{f}(k,\xi) d\xi \\ &= \quad \sum_{k \in (\mathbf{Z}^2)^*} \int_{\mathbf{R}} \frac{(\widehat{f}(k,\xi))^2}{4\pi^2(|k|^2+\xi^2)} d\xi + 4\pi < \mathrm{vp}(\frac{1}{\xi^2}), (\widehat{f}(0,\xi))^2 > . \end{aligned}$$

So the only thing to show is that $< \mathrm{vp}(\frac{1}{\xi^2}), (\widehat{f}(0,\xi))^2 > \geq 0$. We notice that the belonging of f to Y_{per} implies that $|\widehat{f}(0,\xi)| \leq C|\xi|$ as $\xi \to 0$, so that $\frac{(\widehat{f}(0,\xi))^2}{\xi^2} \in L^1(\mathbf{R})$, and (3.15) implies that

$$< \mathrm{vp}(\frac{1}{\xi^2}), (\widehat{f}(0,\xi))^2 >= \int_{\mathbf{R}} \frac{(\widehat{f}(0,\xi))^2}{\xi^2} d\xi \geq 0.$$

This concludes the proof. ◊

3.2.2 Periodicity of the limit

We will say from now on that a function u is symmetric with respect to x_1 if it satisfies the equality :

$$u(x_1, x_2, x_3) = u(-x_1, x_2, x_3). \tag{3.16}$$

And the sequence Λ will be said to be symmetric if $1_{\Gamma(\Lambda)}$ is.

For all function f, we denote by $\tau_1 f$ the function :

$$\tau_1 f(x) = f(x + e_1). \tag{3.17}$$

Proposition 3.4 *Assume that Λ is symmetric with respect to x_1, in addition to the hypotheses we have required so far. In the smeared nuclei case, m is also required to be symmetric. Let (u, ϕ) be the limit of $(u_\Lambda, \phi_\Lambda)$. Then $u \in L^\infty(\mathbf{R}^3)$, $\phi \in L^1_{unif}(\mathbf{R}^3)$, and we have :*

$$|\tau_1 \phi - \phi| \leq \frac{C}{1 + |x_3|}. \tag{3.18}$$

Proof : The belonging of (u, ϕ) to $L^\infty(\mathbf{R}^3) \times L^1_{unif}(\mathbf{R}^3)$ comes directly from the bounds of Theorem 2.2. Moreover, we have :

$$-\Delta(\tau_1 \phi - \phi) = 4\pi(u^2 - \tau_1 u^2).$$

Hence $(\tau_1 \phi - \phi) \in W^{2,p}_{unif}(\mathbf{R}^3)$ for all $p > 1$, and in particular it lies in $L^\infty(\mathbf{R}^3)$, so the bound (3.18) need only to be shown on the set $\{|x_3| > 2\}$. Hereafter, we assume that $|x_3| > 2$.

Now we are going to show this estimate for $(u_\Lambda, \phi_\Lambda)$, uniformly with respect to Λ, and hence deduce it for (u, ϕ).

From the uniqueness of u_Λ, we know that $v_\Lambda = m_\Lambda - u_\Lambda^2$ is symmetric with respect to x_1. Hence we have :

$$\int_{B_R} v_\Lambda(y) \frac{y_1}{|y|^k} dy = 0, \tag{3.19}$$

for all $k < 4$ and $R > 0$.

We split the expression of $\psi_\Lambda = \tau_1 \phi_\Lambda - \phi_\Lambda$ into two terms :

$$
\begin{aligned}
\psi_\Lambda(x) &= \int_{|x-y|<R} v_\Lambda(y)\left(\frac{1}{|x-y+e_1|}-\frac{1}{|x-y|}-\frac{y_1}{|y|^3}\right)dy \\
&\quad+\int_{|x-y|>R} v_\Lambda(y)\left(\frac{1}{|x-y+e_1|}-\frac{1}{|x-y|}-\frac{y_1}{|y|^3}\right)dy,
\end{aligned}
$$

where $R=\frac{|x_3|}{2}$. We call $a(x)$ the first term, $b(x)$ the second one. We notice that

$$
\int_{|x-y|<2}|v_\Lambda(y)|\left|\frac{1}{|x-y+e_1|}-\frac{1}{|x-y|}-\frac{y_1}{|y|^3}\right|dy\le\frac{C}{|x_3|^3},
$$

because $\frac{1}{|x-y+e_1|}-\frac{1}{|x-y|}+\frac{y_1}{|y|^3}$ lies in $L^1(B_2+x)$ and is bounded independently of x in this space. So we may as well restrict ourselves to integrals over $|x-y|>2$, which is equivalent to replacing $|x-y|$ by $1+|x-y|$ in the integrals. The same remark holds concerning terms of the form $\frac{1}{|y|}$, which will be replaced by $\frac{1}{1+|y|}$.

On the other hand, we may bound $|\frac{1}{|x+e_1|}-\frac{1}{|x|}|$ by $\frac{C|x_1|}{|x|^3}$ on $\{|x|>2\}$, for a universal constant C. Hence we have, x' and y' denoting the variables (x_1,x_2) and (y_1,y_2) respectively :

$$
\begin{aligned}
|a(x)| &\le \int_{|x-y|<R}\frac{C}{1+|y_3|^3}\left|\frac{1}{|x-y+e_1|}-\frac{1}{|x-y|}-\frac{y_1}{|y|^3}\right|dy \\
&\le \int_{|x-y|<R}\frac{C}{1+|y_3|^3}\frac{|x_1-y_1|}{1+|x-y|^3}dy \\
&\quad+\int_{|x-y|<R}\frac{C}{1+|y_3|^3}\frac{|y_1|}{1+|y|^3}dy \\
&\le \frac{C}{(|x_3|-R)^3}R\int_{|y'|<R}\frac{dy'}{1+|y'|^2} \\
&\quad+\frac{CR}{(|x_3|-R)^3}\int_{|x'-y'|<R}\frac{dy'}{1+|y'|^2} \\
&\le \frac{CR\log R}{(|x_3|-R)^3}+\frac{CR^3}{(|x_3|-R)^3}\frac{1}{(|x|-R)^2} \\
&\le \frac{C}{|x_3|}. \qquad (3.20)
\end{aligned}
$$

Concerning $b(x)$, we split it again into two terms, writing :

$$
\begin{aligned}
b(x) &= \int_{|x-y|>R,|y|<R'} v_\Lambda(y)\left(\frac{1}{|x-y+e_1|}-\frac{1}{|x-y|}-\frac{y_1}{|y|^3}\right)dy \\
&\quad+\int_{|x-y|>R,|y|>R'} v_\Lambda(y)\left(\frac{1}{|x-y+e_1|}-\frac{1}{|x-y|}-\frac{y_1}{|y|^3}\right)dy,
\end{aligned}
$$

where $R' = |x|^\alpha$, for some $\alpha < 1$.

We call respectively $c(x)$ and $d(x)$ those two terms. In order to bound $c(x)$, we write, for $|y| < R' \ll |x|$:

$$\frac{1}{|x-y+e_1|} - \frac{1}{|x-y|} = \frac{-x_1}{|x|^3} + \frac{3}{2}\left(\frac{1-2x_1}{|x|^4}\right) + \frac{2y_1-1}{|x|^2} + O(\frac{R'^3}{|x|^3}). \quad (3.21)$$

This implies :

$$\left|\frac{1}{|x-y+e_1|} - \frac{1}{|x-y|}\right| \leq \frac{CR'}{|x|^2} + \frac{CR'^3}{|x|^3}.$$

On the other hand, we notice that (3.19) allows us to convert the term containing $\frac{y_1}{|y|^3}$ into

$$-\int_{|x-y|<R,|y|<R'} v_\Lambda(y)\frac{y_1}{|y|^3}dy,$$

and we have already bounded such a term when dealing with $a(x)$. So we have :

$$\begin{aligned}
|c(x)| &\leq \int_{|y|<R'} \frac{1}{1+|y_3|^3}\frac{CR'}{|x|^2}dy + \int_{|y|<R'} \frac{1}{1+|y_3|^3}\frac{CR'^3}{|x|^3}dy \\
&\leq \frac{CR'}{|x|^2}\int_{|y'|<R'} dy' + \frac{CR'^3}{|x|^3}\int_{|y'|<R'} dy' \\
&\leq C(\frac{R'^3}{|x|^2} + \frac{R'^5}{|x|^3}) \\
&\leq \frac{C}{|x|^{2-3\alpha}} + \frac{C}{|x|^{3-5\alpha}}. \quad (3.22)
\end{aligned}$$

We now turn to $d(x)$. Knowing that we have

$$\left|\frac{1}{|x-y+e_1|} - \frac{1}{|x-y|} + \frac{x_1-y_1}{|x-y|^3}\right| \leq \frac{C}{2+|x-y|^3}$$

on the set $\{|x-y| > R, |y| > R'\}$, we infer that :

$$\begin{aligned}
|d(x)| \leq & \int_{|x-y|>R,|y|>R'} \frac{C}{(1+|y_3|^3)(2+|x-y|^3)}dy \\
& + \int_{|x-y|>R,|y|>R'} \frac{C}{1+|y_3|^3}\frac{|x_1|}{|x-y|^3}dy \\
& + \int_{|x-y|>R,|y|>R'} \frac{C}{1+|y_3|^3}\left|\frac{y_1}{|x-y|^3} - \frac{y_1}{|y|^3}\right|dy. \quad (3.23)
\end{aligned}$$

Here we point out that bounding the second term, which we denote by $d_1(x)$, will be sufficient to bound the first one. In order to bound $d_1(x)$, we use the inequality $|x-y| \geq \big||x|-|y|\big|$, and write :

$$\begin{aligned} |d_1(x)| &\leq |x_1| \int_{|x-y|>R,|y|>R'} \frac{C\,dy}{(1+|y_3|^3)(1+\big||x|-|y|\big|^3)} \\ &\leq \frac{|x|}{|x|^3} \int_{|\frac{x}{|x|}-z|>\frac{R}{|x|},|z|>\frac{R'}{|x|}} \frac{C\,dz}{(1+|z_3|^3)(1+\big|1-|z|\big|^3)} \\ &\leq \frac{C}{|x|^2}, \end{aligned} \tag{3.24}$$

where we have set $y=|x|z$.

We now bound the third term of (3.23), which we call $d_2(x)$. In order to do so, we write :

$$\begin{aligned} \left|\frac{y_1}{|x-y|^3}-\frac{y_1}{|y|^3}\right| &\leq |y_1|\left|\frac{|x-y|^4-|y|^4}{|x-y|^3|y|^3(|x-y|+|y|)}\right| \\ &\leq \frac{\big||x-y|^2-|y|^2\big|(|x-y|^2+|y|^2)}{|y|^2|x-y|^3(|x-y|+|y|)} \\ &\leq C\frac{|2xy-|x|^2|(|x-y|+|y|)}{|y|^2|x-y|^3} \\ &\leq C\frac{|x|(|y|+|x-y|)^2}{|y|^2|x-y|^3} \\ &\leq C|x|\left(\frac{1}{|x-y|^3}+\frac{1}{|y|^2|x-y|}\right). \end{aligned}$$

Hence we see that $d_2(x)$ may be bounded by the sum of two terms, the first one being equivalent to $d_1(x)$, and the second one, which we call $d_3(x)$, being dealt with as follows :

$$\begin{aligned} |d_3(x)| &\leq \int_{|x-y|>R,|y|>R'} \frac{C}{1+|y_3|^3}\frac{|x|}{1+|y|^2|x-y|}dy \\ &\leq \frac{|x|}{|x|^3}\int_{|\frac{x}{|x|}-z|>\frac{R}{|x|},|z|>\frac{R'}{|x|}} \frac{C}{1+|z_3|^3}\frac{dz}{1+|z|^2\big|1-|z|\big|} \\ &\leq \frac{C}{|x|^2}. \end{aligned} \tag{3.25}$$

Hence, collecting (3.23), (3.24) and (3.25), we find that

$$|d(x)| \leq \frac{C}{|x|^2}. \tag{3.26}$$

Thus, gathering (3.26) and (3.22), we find that

$$|b(x)| \leq \frac{C}{|x|^{2-3\alpha}} + \frac{C}{|x|^{3-5\alpha}} + \frac{C}{|x|^2}.$$

Choosing now an α such that $\alpha \leq \frac{1}{3}$ and $\alpha \leq \frac{2}{5}$, we find that

$$|b(x)| \leq \frac{C}{|x|}. \tag{3.27}$$

There only remains to collect (3.20) and (3.27) to conclude that (3.18) holds for ϕ_Λ. Now, since this bound is uniform with respect to Λ, ϕ inherits it. $\diamondsuit$

We now need a lower bound on u, which is the aim of the following proposition :

Proposition 3.5 *Let (u, ϕ) be a solution of (3.10), such that $u \in L^\infty(\mathbf{R}^3)$, $u \geq 0$, and $\phi \in L^1_{unif}(\mathbf{R}^3)$. Then for any $R > 0$, there exists a constant $\nu > 0$ such that* $\inf_{|x_3|<R} u \geq \nu$.

Proof : We follow exactly the steps of Proposition 2.4, and arguing by contradiction, build $\psi \in L^1_{unif}(\mathbf{R}^3)$ solution to :

$$-\Delta\psi = 4\pi\mu(\cdot + x^0). \tag{3.28}$$

This is exactly where the proof differs : we are going to use here again a scaling argument, but the scaling function needs to be chosen differently.

Let $\xi_0 \in C^\infty(\mathbf{R})$, such that $\xi_0 = 1$ on $[-1, 1]$, $\xi_0 = 0$ on $[-2, 2]^c$, $|\xi_0''| \leq 4$, and $0 \leq \xi_0 \leq 1$. Let $\eta_R : \mathbf{R} \longrightarrow \mathbf{R}$ be defined by follows :

- $\eta_R = 1$ on [-1,1].
- $\eta_R(t) = 1 + \frac{1-|t|}{R-1}$ if $1 < |t| < R$.
- $\eta_R = 0$ on $[-R, R]^c$.

We denote by ξ_R the function $\xi_R(x) = \eta_R(x_3)\xi_0(\frac{r}{R})$. And we compute :

$$\begin{aligned} < -\Delta\psi, \xi_R > &= 4\pi < m_\infty, \xi_R > \\ &= 4\pi \sum_{k\in\mathbf{Z}^2} < m(\cdot + k), \xi_0(\frac{r}{R}) > \\ &\geq 4\pi \sum_{k\in\mathbf{Z}^2, |k|\leq 2R} < m(\cdot + k), \xi_0(\frac{r}{R}) > \\ &\geq CR^2. \end{aligned} \tag{3.29}$$

On the other hand, we have, denoting by Ω_R the set $\{r < 2R, |x_3| < R\}$ and by ω_R the set $\{r < R, |x_3| < 1\}$:

$$
\begin{aligned}
< -\Delta\psi, \xi_R > &= \int_{\Omega_R \setminus \omega_R} \nabla\psi\nabla\xi_R \\
&= \int_{\Omega_R \setminus \omega_R} \psi(-\Delta\xi_R) + \int_{|x_3|=R, r<2R} \psi\frac{\partial\xi_R}{\partial n} + \int_{|x_3|=1, r<R} \psi\frac{\partial\xi_R}{\partial n}.
\end{aligned}
$$

Since $-\Delta\xi_R = -\eta_R(x_3)\Delta\xi_0(\frac{r}{R}) = \eta_R(x_3)(\frac{1}{rR}\xi_0'(\frac{r}{R}) - \frac{1}{R^2}\xi_0''(\frac{r}{R}))$, the first term may be dealt with as follows :

$$
\begin{aligned}
\left|\int_{\Omega_R \setminus \omega_R} \psi(-\Delta\xi_R)\right| &\leq \frac{1}{R^2}\int_{\Omega_R} |\psi| + \int_{\Omega_R \setminus \omega_R} \frac{|\psi(x)|}{rR} dx \\
&\leq C\frac{R^3}{R^2} + \frac{C}{R}\left(\int_{\Omega_R \setminus \omega_R} |\psi|^2\right)^{1/2} \left(\int_R^{2R} R\frac{dr}{r}\right)^{1/2} \\
&\leq CR + C\frac{R^{3/2}}{R}(R\log 2)^{1/2} \ll R^2. \qquad (3.30)
\end{aligned}
$$

Concerning the remaining terms, we have :

$$
\left|\int_{|x_3|=R, r<2R} \psi\frac{\partial\xi_R}{\partial x_3}\right| \leq \int_{|x_3|=R, r<2R} |\psi|\frac{C}{R} \leq C\frac{R^2}{R} \ll R^2. \qquad (3.31)
$$

And :

$$
\left|\int_{|x_3|=1, r<R} \psi\frac{\partial\xi_R}{\partial x_3}\right| \leq \int_{|x_3|=1, r<R} |\psi|\frac{C}{R} \leq C\frac{R^2}{R} \ll R^2. \qquad (3.32)
$$

Hence, collecting (3.29), (3.30), (3.31) and (3.32), we infer that (3.28) is in contradiction with the belonging of ψ to L^1_{unif}. $\diamondsuit$

We now state a uniqueness lemma that will allow us to conclude that u and ϕ are periodic.

Lemma 3.2 *Let (u, ϕ) and (v, ψ) be solutions to the system (3.10), satisfying the following :*

(i) $u, v \in L^\infty(\mathbf{R}^3)$, and $\phi, \psi \in L^1_{unif}(\mathbf{R}^3)$.

(ii) There exists a function $U \in L^2(\mathbf{R})$ such that $|\phi - \psi| + |u - v| \leq U(x_3)$.

Then $u = v$ and $\phi = \psi$.

Proof : The firsts steps of the proof are exactly those of Lemma 2.3. We thereby skip it, and start with equation (2.49), that is :

$$\int_{\mathbf{R}^3} \nu w^2 \xi^2 \leq \int_{\mathbf{R}^3} w^2 |\nabla \xi|^2 + \frac{1}{2} \int_{\mathbf{R}^3} (\phi - \psi)^2 |\nabla \xi|^2, \tag{3.33}$$

where ν is a positive function depending only on x_3, $w = u - v$, and ξ is any smooth function with compact support.

We apply inequality (3.33) to a sequence ξ_n converging to ξ defined by follows :

- $\xi(x) = 1 - \frac{r^\alpha}{R^\alpha}$ on the set $\{r < R\}$.
- $\xi(x) = 0$ elsewhere.

where $R > 0$ and $\alpha > 0$. Hence (3.33) is valid for this choice of ξ. For such a ξ, we compute that

$$|\nabla \xi|^2 = \alpha^2 \frac{r^{2\alpha - 2}}{R^{2\alpha}}.$$

So we have :

$$\begin{aligned} \int_{\mathbf{R}^3} \nu w^2 \xi^2 &\leq \frac{3}{2} \int_{\mathbf{R}^3} \alpha^2 \frac{r^{2\alpha-2}}{R^{2\alpha}} U(x_3)^2 \\ &\leq \frac{3}{2} \|U\|_{L^2(\mathbf{R})} \int_0^R \alpha^2 \frac{r^{2\alpha-1}}{R^{2\alpha}} 2\pi dr \\ &\leq \frac{3}{2} \|U\|_{L^2(\mathbf{R})} \alpha \pi. \end{aligned} \tag{3.34}$$

We let now R go to infinity, deducing, from the monotone convergence theorem, that we have :

$$\int_{\mathbf{R}^3} \nu w^2 \leq \frac{3}{2} \pi \alpha \|U\|_{L^2(\mathbf{R})}.$$

Since this holds for any $\alpha > 0$, we let now α go to zero, and find that :

$$\int_{\mathbf{R}^3} \nu w^2 = 0.$$

This implies that $w = 0$, since ν is positive, hence that $\phi = \psi$. $\Diamond$

3.2.3 Convergence and identification of the limit

We recall the periodic variational problem I_{per} :

$$I_{per} = \inf\{E_{per}(\rho),\ \sqrt{\rho} \in X_{per},\ \int_{\Gamma_0} \rho = 1\}, \tag{3.35}$$

where E_{per} and X_{per} are defined as follows :

$$X_{per} = \{v \in H^1_{per}(\Gamma_0),\ (1+|x|)^{\frac{1}{2}} v \in L^2(\Gamma_0)\}.$$

$$\begin{aligned} E_{per}(\rho) = \quad & \textstyle\int_{\Gamma_0} |\nabla \sqrt{\rho}|^2 + \int_{\Gamma_0} \rho^{5/3} - \int_{\Gamma_0} (G \star_{\Gamma_0} m_\infty)\rho \\ + \quad & \frac{1}{2}\int_{\Gamma_0}\int_{\Gamma_0} \rho(x)\rho(y)G(x-y)dxdy. \end{aligned}$$

We are now able to state the following theorem :

Theorem 3.2 *Let $\Lambda = \Lambda_2 \times \{0\}$ be a Van Hove sequence in the first two directions, that is, Λ_2 is supposed to be a Van Hove sequence of $\mathbf{Z}^2$. Assume in addition that Λ is symmetric both with respect to x_1 and with respect to x_2 (in the smeared nuclei case, we also assume that the measure m is symmetric with respect to x_1 and x_2). Denote by $\rho_\Lambda = u_\Lambda^2$ the solution of I_Λ. Then u_Λ converges to u_{per} in $H^1(\Gamma_0)$, $\rho_{per} = u_{per}^2$ being the minimizer of the periodic problem I_{per}. Moreover, we have the following estimates :*

(i) $u_{per}(x) \leq \frac{C}{1+|x_3|^{3/2}}$ *for some constant $C > 0$.*

(ii) There exists a positive function ν depending only on x_3 such that we have : $\nu \leq u_{per}$.

Proof : We know that $(u_\Lambda, \phi_\Lambda)$ is bounded in $H^1(\Gamma_0) \times L^p_{unif}(\mathbf{R}^3)$, for all $p < 3$. Hence we may pass locally to the limit in the system (3.1)-(3.2). Denoting by $(u,\phi) \in H^1(\Gamma_0) \times L^p_{unif}(\mathbf{R}^3)$ the corresponding limit, we find a solution to the system (3.10), that is :

$$\begin{cases} -\Delta u + \frac{5}{3}u^{7/3} - u\phi = 0, \\ -\Delta \phi = 4\pi(m_\infty - u^2). \end{cases}$$

From the a priori bounds shown in Theorem 3.1, which shows in particular that $u \leq \frac{C}{1+|x_3|^{3/2}}$, and from Proposition 3.4, we know that, applying Lemma 3.2, we find :

$$\tau_1 \phi = \phi.$$

On the other hand, all the symmetries being also satisfied with respect to x_2, we deduce, denoting by $\tau_2\phi$ the function $\phi(\cdot + e_2)$,

$$\tau_2 \phi = \phi.$$

This implies that ϕ, hence u, are periodic with periodic cell Γ_0.

From the estimate of Theorem 3.1, we also deduce that $u \in X_{per}$. We are now going to prove that

$$\int_{\Gamma_0} u^2 = 1. \tag{3.36}$$

In order to do so, we introduce the functions :

$$\psi(x_3) = \int_{[-\frac{1}{2},\frac{1}{2}]^2} \phi(x) dx_1 dx_2.$$

and

$$f(x_3) = \int_{[-\frac{1}{2},\frac{1}{2}]^2} 4\pi(m_\infty(x) - u(x)^2) dx_3.$$

Those functions satisfy the differential equation

$$-\psi'' = f,$$

since $\int_{[-\frac{1}{2},\frac{1}{2}]^2} \left(\frac{\partial^2\phi}{\partial x_1^2} + \frac{\partial^2\phi}{\partial x_2^2}\right) dx_1 dx_2 = 0$ from the periodicity of ϕ.

Furthermore, $\phi \in L^\infty(\{|x_3| > 1\})$, hence $\psi \in L^\infty([-1,1]^c)$, so from the estimates on u, we deduce that

$$\psi\psi'' \in L^1([-1,1]^c).$$

On the other hand, $\psi'(t) - \psi'(1) = \int_1^t f$, for all $t > 1$. Hence we infer that

$$\psi' \in L^\infty([1,\infty)).$$

Those two properties, together with the equality

$$\int_1^t \psi\psi'' = \psi(t)\psi'(t) - \psi(1)\psi'(1) - \int_1^t \psi'^2,$$

show that

$$\psi' \in L^2([1,\infty)).$$

Repeating the same argument for $t < -1$, replacing 1 by -1, we conclude that

$$\psi' \in L^2([-1,1]^c).$$

But ψ' has a limit at infinity, namely $\psi'(1) + \int_1^\infty f$, so this limit must be 0. The same results holds concerning its limit at $-\infty$, so that we have :

$$\int_{\mathbf{R}} \psi'' = \lim_{\infty} \psi' - \lim_{-\infty} \psi' = 0.$$

This implies $\int_{\Gamma_0} -\Delta\phi = 0$, hence (3.36).

The next step is to show that

$$\phi = G \star_{\Gamma_0} (m_\infty - u^2) + d, \tag{3.37}$$

for some $d \in \mathbf{R}$. Noticing that $\phi - G \star_{\Gamma_0} (m_\infty - u^2)$ is harmonic over $\mathbf{R}^3$, and periodic with periodic cell Γ_0, we conclude that it is sufficient to show that $G \star_{\Gamma_0} (m_\infty - u^2) \in L^1_{unif}(\Gamma_0)$. And from Lemma 2.2, we know that

$$\left(G(x) - \frac{1}{|x|} + 2\pi |x_3| \right) \in L^\infty(\Gamma_0).$$

So we only need to prove that

$$\frac{1}{|x|} \star_{\Gamma_0} (m_\infty - u^2) \in L^1_{unif}(\Gamma_0) \tag{3.38}$$

and

$$|x_3| \star_{\Gamma_0} (m_\infty - u^2) \in L^1_{unif}(\Gamma_0). \tag{3.39}$$

(3.38) has been shown in the course of Lemma 2.5, so we only provide a proof of (3.39) :

Since we already know that the convolution product arising in (3.39) lies in $L^1_{loc}(\Gamma_0)$, we only need to bound it as $|x_3| \to \infty$. (3.36) implies that we have :

$$\int_{\Gamma_0} (m_\infty - u^2)(y) |x_3 - y_3| dy = \int_{\Gamma_0} (m_\infty - u^2)(y) (|x_3 - y_3| - |x_3|) dy.$$

Letting $R = \sqrt{|x_3|}$, we have, for $|y_3| < R$, and $|x_3| \to \infty$,

$$|x_3 - y_3| - |x_3| = -y_3 + O(\frac{R^2}{|x_3|}) = -y_3 + O(1).$$

Hence we may write :

$$\begin{aligned} \big| |x_3| \star_{\Gamma_0} (m_\infty - u^2) \big| &\leq \int_{\Gamma_0 \cap \{|y_3| > R\}} |m_\infty - u^2|(y) \big| |x_3 - y_3| - |x_3| \big| dy \\ &\quad + \int_{\Gamma_0 \cap \{|y_3| < R\}} |m_\infty - u^2|(y) (|y_3| + C) dy \\ &\leq \int_{\Gamma_0 \cap \{|y_3| > R\}} |m_\infty - u^2|(y) |y_3 - x_3 + x_3| dy \\ &\quad + \int_{\Gamma_0 \cap \{|y_3| < R\}} C |m_\infty - u^2|(y) (1 + |y_3|) dy. \end{aligned}$$

Those two terms are bounded because $u \in X_{per}$, so this concludes the proof of (3.39), hence of (3.37).

Now, this implies that u^2 is a solution of the Euler-Lagrange equation of the problem I_{per}, namely :

$$-\Delta\sqrt{\rho}+\frac{5}{3}\rho^{7/6}-\Big(G\star_{\Gamma_0}(m_\infty-\rho)+\theta_{per}\Big)\sqrt{\rho}=0.$$

(θ_{per} is the Lagrange multiplier associated with the constraint in I_{per}.)

On the other hand, the problem I_{per} is convex because D_G is, since it is bilinear and positive, on the set of the test-functions of I_{per}. So u is the solution of I_{per}, which is unique. Thus, the convergence does not only occur for a subsequence of u_Λ, but for the whole sequence. $\Diamond$

3.2.4 Convergence of the energy

This paragraph is the exact analog of the corresponding one in Section 2. We start with the definition of interior domains, which is exactly the same as in Section 2.

Definition 3.1 *Let $\Lambda \subset \mathbf{Z}^2\times\{0\}$ be a Van Hove sequence in the first two directions. Λ' will be said to be a sequence of interior domains, denoted by $\Lambda' \subset\subset \Lambda$, if it satisfies the following properties :*

(i) $\Lambda' \subset \Lambda$.

(ii) For any finite subset A of $\mathbf{Z}^2$, there exists an $h_0 \in \mathbf{N}$ such that $\forall h \geq h_0$, $A \subset \Lambda'_h$.

(iii) $\frac{|\Lambda'|}{|\Lambda|} \longrightarrow 1$ *as* $\Lambda \to \infty$.

(iv) $d(\Lambda', \partial\Gamma(\Lambda)) \longrightarrow \infty$ *as* $\Lambda \to \infty$.

For now on, we assume that the sequence Λ satisfies the hypotheses of Theorem 3.2, that is, in addition to the Van Hove hypotheses, Λ is supposed to be symmetric with respect to x_1 and x_2, and so is m.

Next, we state the following theorem :

Theorem 3.3 *For any sequence $\Lambda' \subset\subset \Lambda$ and any $R > 0$, we have :*

$$||u_\Lambda - u_{per}||_{L^\infty(\Gamma(\Lambda'))} \longrightarrow 0, \tag{3.40}$$

$$||\phi_\Lambda - \phi_{per}||_{L^\infty(\Gamma(\Lambda')\cap\{|x_3|<R\})} \longrightarrow 0, \tag{3.41}$$

as $\Lambda \longrightarrow \infty$. (We recall that $\phi_{per} = G\star_{\Gamma_0}(m-u_{per}^2)-\theta_{per}$)

Proof : The proof starts exactly as that of Theorem 2.5, except that Theorem 2.4 is not available here. Hence, we slightly modify the proof in the following way : $\overline{u}_\Lambda$ will not be $u_\Lambda(\cdot + x_\Lambda)$, but :

$$\overline{u}_\Lambda = u_\Lambda(\cdot + (x_\Lambda)_3 e_3).$$

Hence, the same convergence argument hold, except that we notice that $\overline{m}_\Lambda = m_\Lambda(\cdot + (x_\Lambda)_3 e_3)$ defines a Van Hove sequence, since $x_\Lambda \in \Gamma(\Lambda')$, and that it is symmetric with respect to both x_1 and x_2. Hence the proof carries through, replacing the use of Theorem 2.4 by that of Theorem 3.2, or (equivalently) by the fact that I_{per} has a unique solution. $\diamondsuit$

We end up by stating the energy convergence Theorem for solid films :

Theorem 3.4 *For any Van Hove sequence, symmetric with respect to x_1 and x_2, we have :*

$$\frac{I_\Lambda}{|\Lambda|} \longrightarrow I_{per} + \frac{M}{2}$$

as $\Lambda \to \infty$.

Proof : Here again, the proof is not different from that of Theorem 2.6, the only thing to check being that we have :

$$|\nabla u_\Lambda| \leq \frac{C}{1 + |x_3|^{3/2}}.$$

And this easy to prove from elliptic regularity, together with the bounds we have on u_Λ and ϕ_Λ. $\diamondsuit$

4 The Yukawa case

We give here without proof some results that can be obtained on the Yukawa case.

Replacing the Coulombian interaction potential $\frac{1}{|x|}$ by the Yukawa potential defined in (1.11), we get :

$$\begin{cases} -\Delta u_\Lambda + \frac{5}{3} u_\Lambda^{7/3} - u_\Lambda \phi_\Lambda = 0, \\ -\Delta \phi_\Lambda + a^2 \phi_\Lambda = 4\pi(m_\Lambda - u_\Lambda^2), \\ u_\Lambda \geq 0. \end{cases} \tag{4.1}$$

The limit system (1.9) being modified in an analogous way. Next, we notice that in this system, we have added a coercive term in the second equation. This fundamental difference allows us to show stronger uniqueness results, as the following one :

Theorem 4.1 *Let μ be a nonnegative measure, having its support in the set $\{|x_3| < 1\}$, and satisfying the following :*

(H_1) $\sup_{x\in\mathbf{R}^2\times\{0\}} \mu(B_1 + x) < +\infty$.

(H_2) $\lim_{R\to\infty} \inf_{x\in\mathbf{R}^2\times\{0\}} \frac{\mu(B_R+x)}{R} = +\infty$.

Then the system

$$\begin{cases} -\Delta u + \frac{5}{3}u^{7/3} - \phi u = 0, \\ -\Delta\phi + a^2\phi = 4\pi(\mu - u^2), \\ u \geq 0. \end{cases} \tag{4.2}$$

has a unique solution (u, ϕ) in the set

$$\{(u,\phi) \in L^{7/3}_{loc} \cap L^2_{unif}(\mathbf{R}^3) \times L^1_{unif}(\mathbf{R}^3),\ \forall h > 0, \inf_{\{|x_3|<h\}} u > 0\}.$$

Furthermore, this solution belongs to $W^{2,p}_{unif}(\mathbf{R}^3) \times L^p_{unif}(\mathbf{R}^3)$ for all $p < 3$, and there exists a constant C such that $u \leq \frac{C}{1+|x_3|^{3/2}}$.

A similar theorem is also valid in the one-dimensional case. This implies that we have convergence results in both cases (namely solid films and polymers), at least for the density, provided the finite problem I_Λ with Yukawa potential has a unique solution ρ_Λ. This is the case for instance (see [5]) if a is small enough.

On the other hand, the use of the Yukawa potential destroys the compactness of the sequence ρ_Λ (in the sense of (2.10) and (3.3)). In fact, this potential is too weak at infinity to prevent some of the electrons from escaping at infinity. Thus, the periodic variational problems I_{per}, in addition to the potential change, will bear a different mass constraint.

Alternatively, in the spirit of the results displayed in [5], Chapter 4, we have :

Theorem 4.2 *(Here Γ_0 denotes $]-\frac{1}{2},\frac{1}{2}]^2 \times \mathbf{R}$, and r the cylindrical radius $\sqrt{x_1^2 + x_2^2}$.) Let $p > 1$, Γ a Γ_0-periodic potential lying in $L^q_{loc}(\mathbf{R}^3)$ for some $q > \frac{3p}{2p-2}$, such that $\Gamma^+ \leq \frac{C}{|x_3|^2}$ as $|x_3| \to \infty$. Assume that there exists $R > 0$ such that the first eigenvalue of the operator $-\Delta - \Gamma$ with periodic boundary conditions with respect to (x_1, x_2) and homogeneous Dirichlet conditions with respect to x_3 on $\Gamma_0 \cap \{|x_3| < R\}$ is negative. Then the equation*

$$-\Delta u + u^p - \Gamma u = 0 \tag{4.3}$$

has a unique nonnegative non trivial solution in the set

$$\{u \in H^1_{loc}(\mathbf{R}^3) \,/\, \forall x \in \mathbf{R}^3, u \in H^1(\Gamma_0 + x)\}.$$

This solution satisfies :

$$u(x) \leq \frac{C}{1+|x_3|^{\frac{2}{p-1}}},$$

for some constant $C > 0$.

Here again, a similar result may be stated in the one-dimensional case.

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References

[1] R. Benguria & E.H. Lieb, *The most negative ion in the Thomas-Fermi-von-Weizsäcker theory of atoms and molecules.*, J. Phys., B 18, pp 1045-1059, 1985.

[2] R. Benguria, H. Brezis & E. H. Lieb, *The Thomas-Fermi-von Weizsäcker theory of atoms and molecules*, Comm. Math. Phys., 79, pp 167-180.

[3] H. Brézis, *Semilinear equations in* $\mathbf{R}^n$ *without condition at infinity*, App. Math. & Opt., 12, pp 271-282, 1984.

[4] I. Catto, C. Le Bris & P-L. Lions, *Limite thermodynamique pour des modèles de type Thomas-Fermi*, C. R. Acad. Sci. Paris, t. 322, Série I, p 357-364, 1996.

[5] I. Catto, C. Le Bris & P-L. Lions, *Mathematical Theory of thermodynamic limits : Thomas-Fermi type models*, Oxford Mathematical Monographs, Oxford University Press, 1998.

[6] I. Catto, C. Le Bris & P-L. Lions, *Sur la limite thermodynamique des modèles de type Hartree et Hartree-Fock*, C. R. Acad. Sci. Paris, t. 327, Série I, pp 259-266, 1998.

[7] I. Catto, C. Le Bris & P-L. Lions, *On the Thermodynamic limit for Hartree and Hartree-Fock type models*, work in preparation.

[8] D. Gilbarg & N.S. Trudinger *Elliptic Partial Differential Equations of Second Order*, 2nd edition, Springer, 1997

[9] E. H. Lieb, *Thomas-Fermi and related theories of atoms and molecules*, Rev. Modern Phys., 53, 4, pp 603-641.

[10] E. H. Lieb & B. Simon, *The Thomas-Fermi theory of atoms, molecules and solids*, Adv. in Maths., 23, 1977, pp 22-116.

[11] P.-L. Lions, *Solutions of Hartree-Fock equations for Coulomb systems*, Comm. Math. Phys., 109, 1987, pp 33-97.

[12] L. Schwartz, *Théorie des distributions*, Hermann, 1973

[13] J.P. Solovej, *Universality in the Thomas-Fermi-von Weizsäcker Model of Atoms and Molecules*, Comm. Math. Phys. 129, 1990, pp. 561-598