Screening of an Applied Electric Field Inside a Metallic Layer Described by the Thomas-Fermi-von Weizsäcker Model.

X. Blanc* & R. Monneau*

Abstract

We are interested in the effect of a constant electric field on the electronic structure of a crystal. We model it by a density-functional theory, and derive from this microscopic model macroscopic features of the system by letting the ratio ε between atomic spacing and the size of the crystal go to zero. Although many aspects are disregarded in this approach, we show that the effect of the electric field is negligible inside the crystal and estimate its vanishing rate with respect to the distance from the boundary of the crystal.

AMS Classification: 35A15, 35J20, 35J50, 35Q40.
Keywords: Thomas-Fermi-von Weizsäcker theory, variational methods, electric field, exponential decay.

1 Introduction

We consider a band of crystal immersed in a constant electric field perpendicular to the surface of the crystal. Modeling the electrons by a quantum (hence microscopic) theory, namely the Thomas-Fermi-von Weizsäcker theory, we aim at deriving a macroscopic description of the effect of the electric field on this crystal. In order to do so, we let the ratio ε between the interatomic distance and the width of the crystal band go to zero, accounting for the fact that the first is physically of some orders of magnitude lower than the second.

The main feature of this limiting model is that the effect of the electric field is confined to the boundary of the crystal. Studying this aspect further, we give an estimate of the decaying of this effect in the crystal with respect to ε. However, some non-physical features are also evidenced.

These non-physical features are mainly due to the fact that the model describing the electrons is a static one, thereby preventing the description of any dynamical features. And even static macroscopic phenomena may very well originate from dynamical microscopic ones. Although the type of model we use here has proved to be relevant in some cases related to this one [4, 3], it surely misses some important aspects.

In the following we start by presenting a simplified one-dimensional version of our results, describing in section 2 the full three-dimensional Thomas-Fermi-von Weiszäcker model and the corresponding results. We will drop the proofs of the one-dimensional results which are easy adaptations of the more involved three-dimensional problem. A priori bounds are given in section 4 and the three-dimensional proofs are presented in sections 3 and 4.2. We add in Appendix 5 a homogenization approach by two scale convergence which gives more limited results in our context.

*CERMICS, École Nationale des Ponts et Chaussées, 6 & 8, avenue Blaise Pascal, Cité Descartes, Champs-sur-Marne, 77455 Marne-La-Vallée Cedex 2, FRANCE

1.1 A one-dimensional microscopic model

1.1.1 Physical description

We consider a one-dimensional crystal. Let us denote by $x \in \mathbf{R}$ the one-dimensional coordinate. We assume that the crystal fills the macroscopic segment:

$$[-1,1] \subset \mathbf{R},$$

and this crystal is submitted to a constant exterior electric field E. By symmetry considerations, we may assume that this electric field is oriented in the positive direction $x>0$, i.e. $E \geq 0$ (see fig. 1).

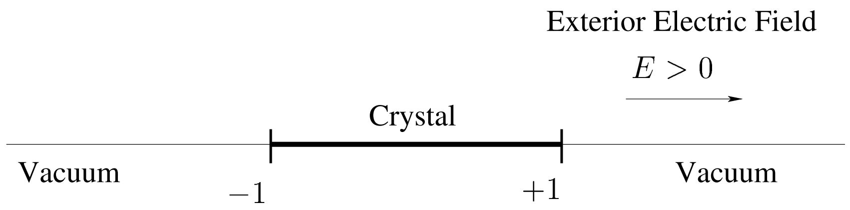

Figure 1: A one-dimensional crystal submitted to a constant exterior electric field

We assume that the crystal is physically described by nuclei and electrons. The nuclei are supposed to be fixed, and to stand at the positions $\{\varepsilon i, \quad i \in \mathbf{Z}, \quad |\varepsilon i| < 1\}$, where ε is the interatomic distance of the crystal. Mathematically, they should be described by Dirac masses, but in order to simplify our presentation, we use a Jellium-like approximation [11], replacing $\varepsilon \sum \delta_{\varepsilon i}$ by $m = \mathbf{1}_{[-1,1]}$. (Note that the first one converges to the second one in the sense of measures.) The density m can be understood as a collection of $\frac{2}{\varepsilon}$ nuclei. Furthermore, each nucleus has a renormalized charge equal to $+\varepsilon$. In particular the charge of the whole set of nuclei is $\int m = 2$ which is equal to the number of nuclei times the elementary renormalized charge ε. As it will be clear in subsection 2.3, the choice of the renormalized charge equal to ε is natural according to physical considerations.

For the examples that we have in mind the microscopic size ε is much smaller than the macroscopic size 1. Typically $\varepsilon \sim 10^{-10}$, so that we expect the limit $\varepsilon \to 0$ to be a good model.

The electrons are described by a renormalized density ρ which satisfies

$$\rho(x) \geq 0 \quad \text{on} \quad \mathbf{R}.$$

In this model we define the usual charge density by the ratio of $m-\rho$ and the charge ε of a nucleus:

$$\sigma = \frac{m-\rho}{\varepsilon}. \tag{1.1}$$

In particular $\int \sigma = +1$ means that there is one more nucleus than electrons, and $\int \sigma = -1$ means that there is one more electron than nuclei.

We define the Green function of the operator $-\Delta$ as a solution to $-\Delta G = \delta_0$. In the following, the one-dimensional Green function is chosen to be equal to

$$G(x) = -\frac{1}{2}|x|.$$

As a consequence of this choice, the electric potential (up to addition of a constant) is given by $G \star \sigma - Ex$ where we recall that the convolution is defined by $G \star \sigma(x) = \displaystyle\int_{-\infty}^{+\infty} dy \quad G(x-y)\sigma(y)$. Then the total electric field is

$$E_{tot} = -\frac{d}{dx}\left(G \star \sigma - Ex\right). \tag{1.2}$$

1.1.2 The mathematical model

We now present the mathematical microscopic model defining the electronic density ρ as the solution of a minimization problem. In this simplified version of the Thomas-Fermi-von Weiszäcker (TFW) model (see [6, 5, 7] for a presentation of this model and the related mathematical results), we assume that the density ρ minimizes an energy

$$\mathcal{E}_\varepsilon(\rho) = \int_{-\infty}^{+\infty} \varepsilon^4 \left(\frac{d}{dx}(\sqrt{\rho})\right)^2 + \varepsilon^2 \rho^{\frac{5}{3}} + \rho \cdot G \star \left(\frac{1}{2}\rho - m\right) + \varepsilon E x \rho$$

on the convex set K_λ defined by $(\lambda > 0)$

$$K_\lambda = \left\{ \rho \geq 0, \quad \sqrt{\rho} \in H^1(\mathbf{R}), \quad |x_3|\rho \in L^1(\mathbf{R}), \qquad \int_{-\infty}^{+\infty} \rho = \lambda \right\}.$$

The point is, $\mathcal{E}_\varepsilon$ is strictly convex on K_λ. The functional $\mathcal{E}_\varepsilon$ is a particular version of the thin film TFW energy presented in [7]. The coefficients in the energy originate from physical constants which may be expressed in terms of ε, as shown in section 2.3. The first term in the integral is a kind of kinetic energy, the second term is a Fermi pressure term, the third term contains the coulombian (in one dimension) interaction of the electrons with themselves and of the electrons with the nuclei, and the last term is the interaction between the electrons and the exterior electric field.

Remark 1.1 *The scaling in ε is such that for $\overline{x} = x/\varepsilon$, $\overline{\rho}(\overline{x}) = \rho(x)$, $\overline{m}(\overline{x}) = m(x)$, we have ρ minimizes $\mathcal{E}_\varepsilon$ if and only if $\overline{\rho}$ minimizes the energy $\mathcal{E}_1$ with $\varepsilon = 1$ and $\overline{m}$ in place of m.*

1.2 Results for the one-dimensional model

Our first result is the

Theorem 1.2 (Crystal Ionized by the Electric Field)
Assume that $0 \leq E < \frac{1}{\varepsilon}$. Then, setting

$$\lambda_c = (1 - \varepsilon E)\left(\int_{\mathbf{R}} m\right)$$

we have:

(i) If $\lambda > \lambda_c$, $\inf_{K_\lambda} \mathcal{E}_\varepsilon = -\infty$.

(ii) If $0 \leq \lambda \leq \lambda_c$, $\inf_{K_\lambda} \mathcal{E}_\varepsilon > -\infty$, and this energy admits a unique minimizer $\rho_\lambda \in K_\lambda$.

From the fact that $\lambda_c < \int m$ we see that every solution describes a ionized crystal when $E \neq 0$. This fact was already known for the TFW model (as well as in any quantum chemistry model): every molecular system submitted to a constant exterior electric has no stable state. Therefore our model can not give a globally neutral solution in an exterior electric field, so far as ground states are considered. In fact physically such a neutral solution is not the minimizer of an energy: every neutral solution in an exterior electric field is metastable.

Because $\int m = 2$, the ionization is equal to $2\varepsilon E$ but is not negligible at all. Let us recall that the charge in this model is obtained after a division by ε (see (1.1)). We deduce that the charge corresponding to the ionization is equal to $2E$ (see fig. 2).

In fig. 3 we have represented the situation for a perfect conductor: the electric field vanishes inside the material, but contrarily to the TFW crystal, the material is globally neutral and the charge $E\delta_1(x)$ is compensated by a negative charge $-E\delta_{-1}(x)$ on the other side of the material. As we explained, this compensation is impossible in a TFW model, because the electrons are unstable in the position $x = -1$ and can decrease their energy if they go to $-\infty$.

In the following, we will then consider the closest solution to the neutral one, namely the solution for $\lambda = \lambda_c$ that we simply denote by ρ. For this solution we prove the

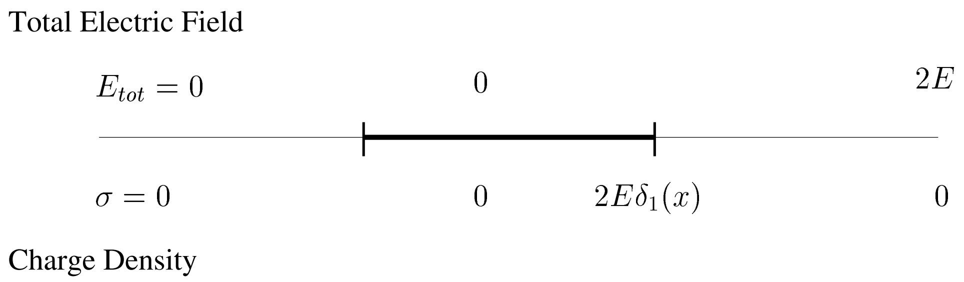

Figure 2: A TFW crystal at the limit $\varepsilon = 0$

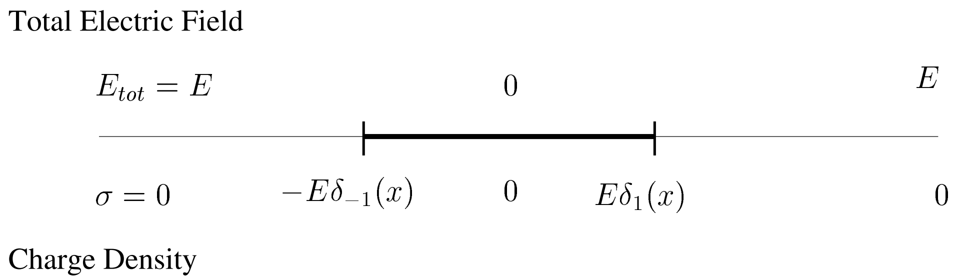

Figure 3: A perfect conductor submitted to a constant exterior electric field

Theorem 1.3 (Exponential Decay of the Electric Field Inside the Crystal)
Let $0 \leq E < \frac{1}{\varepsilon}$ and $\lambda = \lambda_c$. Then there exist two positive constants C_1, C_2 (which only depend on a bound on E and not on ε) such that the minimizing density ρ and the total electric field E_{tot} (given by equation (1.2)) satisfy

$$\left.\begin{array}{l} |\rho(x) - 1| \\ |E_{tot}(x)| \end{array}\right\} \quad \leq \quad C_1 e^{-C_2 \frac{d(x)}{\varepsilon}} \tag{1.3}$$

where $d(x) = d\left(x, [-1,1]^c\right)$ is the distance of a point x in the crystal to the boundary of the crystal.

This result shows that the interior of the crystal has a behavior of a perfect conductor far enough from its boundaries. In particular the penetration length of the electric field is essentially of the order of a few ε (the size of a cell of the crystal in this simple model).

This result is optimal in the sense that the constants C_1, C_2 can not depend on a bound on εE, because for $E = \frac{1}{\varepsilon}$ the only solution is $\rho = 0$ and (1.3) would be clearly wrong. Even in the case $E = 0$, this exponential decay result for a TFW-type model seems relevant.

2 The three-dimensional model

2.1 Setting of the problem

We study a band of crystal filling the following subregion of $\mathbf{R}^3$

$$\mathbf{R}^2 \times [-1, 1],$$

and submitted to a constant exterior electric field orthogonal to the crystal

$$E_{ext} = Ee_3,$$

where e_3 is the third vector of the canonical basis.

The nuclei are supposed to be fixed at their positions on a subset of the lattice $\varepsilon\mathbf{Z}^3$. The underlying thin film structure is present through its periodic lattice ℓ_ε:

$$\ell_\varepsilon = \varepsilon\mathbf{Z}^2 \times \{0\},$$

and, unless otherwise stated, all the functions we consider here will be assumed to be ℓ_ε-periodic. We introduce the (periodic) unit cell Γ_ε of the periodic lattice ℓ_ε:

$$\Gamma_\varepsilon = \mathbf{R}^3/\ell_\varepsilon = \left[-\frac{\varepsilon}{2}, \frac{\varepsilon}{2}\right)^2 \times \mathbf{R}.$$

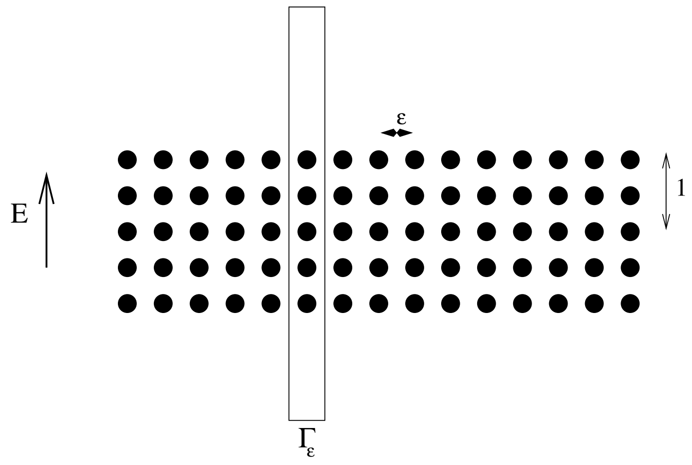

Figure 4: The set of nuclei together with the unit cell Γ_ε (projected on the plane $\{x_2 = 0\}$).

In this three-dimensional model, each nucleus carries a renormalized charge which is fixed equal to ε^3 such that the charge density generated by the nuclei in a cell Γ_ε is defined by

$$m(x) = \sum_{k=-N}^{N} \varepsilon^3 \delta(x - k\varepsilon e_3).$$

for some integer N. In particular we have $2N+1$ nuclei in each cell Γ_ε. As it will be clear is subsection 2.3, the choice of the renormilazed charge ε^3 is natural from physical considerations.

To simplify the presentation we restrict our study to the particular values of ε given by $\varepsilon = \frac{1}{N+\frac{1}{2}}$. For these values, we have $\frac{1}{\varepsilon^2}\int_{\Gamma_\varepsilon} m = 2$ where ε^2 has to be interpreted as the area of a section of Γ_ε, and the nuclei fill the set

$$\varepsilon\mathbf{Z}^3 \cap \Big(\mathbf{R}^2 \times [-1, 1]\Big).$$

The electrons are represented by their density ρ, which is a positive ℓ_ε-periodic function. In particular we define the usual volumic charge density on a cell Γ_ε by the ratio of $m - \rho$ by the charge of a nucleus divided by the area of a section of Γ_ε, i.e. $\varepsilon^3/\varepsilon^2 = \varepsilon$:

$$\sigma = \frac{m - \rho}{\varepsilon}$$

The ℓ_ε-periodic Green function G_ε satisfies $-\Delta G_\varepsilon = \delta_0(x)$ on Γ_ε and is chosen to be equal to

$$G_\varepsilon(x) = -\frac{1}{2\varepsilon^2}|x_3| + \frac{1}{4\pi}\sum_{k\in\varepsilon\mathbf{Z}^2\times\{0\}}\left(\frac{1}{|x-k|} - \frac{1}{\varepsilon^2}\int_{[-\frac{\varepsilon}{2},\frac{\varepsilon}{2}[\times\{0\}}\frac{dy}{|x-y-k|}\right) + \frac{M}{\varepsilon}, \tag{2.1}$$

where the constant M is chosen so that $G_\varepsilon(x) - \frac{1}{4\pi|x|} \to 0$ as $x \to 0$. From the definition of G_ε, M is independent of ε. With this definition of the Green function, the electric potential (up to addition of a constant) is given by $G_\varepsilon \star \sigma - Ex_3$ where the convolution product is defined by $G_\varepsilon \star \sigma(x) = \int_{\Gamma_\varepsilon} dy \quad G_\varepsilon(x-y)\sigma(y)$. Then the total electric field is

$$E_{tot} = -\nabla \left(G_\varepsilon \star \sigma - Ex_3\right) \tag{2.2}$$

The electronic density is moreover assumed to minimize an energy

$$\mathcal{E}_\varepsilon(\rho) = \int_{\Gamma_\varepsilon} \varepsilon^4 \left|\nabla\sqrt{\rho}\right|^2 + \varepsilon^2 \rho^{\frac{5}{3}} + \rho \cdot G_\varepsilon \star \left(\frac{1}{2}\rho - m\right) + \varepsilon E x_3 \rho, \tag{2.3}$$

which is strictly convex on the convex set K_λ defined for $\lambda > 0$ by

$$K_\lambda = \left\{\rho \geq 0, \quad \sqrt{\rho} \in H^1(\Gamma_\varepsilon), \quad |x_3|\rho \in L^1(\Gamma_\varepsilon), \qquad \frac{1}{\varepsilon^2}\int_{\Gamma_\varepsilon} \rho = \lambda > 0\right\}.$$

The energy $\mathcal{E}_\varepsilon$ is called the thin film Thomas-Fermi-von Weizsäcker (TFW) energy (see [7]).

2.2 Mathematical results

The above model (2.3) was derived in [7] in the particular case of a neutral isolated system, i.e when $E = 0$. Hence the first step of our work is to study it when $E \neq 0$:

Theorem 2.1 (Crystal Ionized by the Electric Field)
Assume that $0 \leq E < \frac{1}{\varepsilon}$. *Then, setting*

$$\lambda_c = (1 - \varepsilon E)\left(\frac{1}{\varepsilon^2}\int_{\Gamma_\varepsilon} m\right),$$

we have:

(i) If $\lambda > \lambda_c$, $\inf_{K_\lambda} \mathcal{E}_\varepsilon = -\infty$.

(ii) If $0 \leq \lambda \leq \lambda_c$, $\inf_{K_\lambda} \mathcal{E}_\varepsilon > -\infty$, *and this energy admits a unique minimizer* $\rho_\lambda \in K_\lambda$. *This solution satisfies in particular the following Euler-Lagrange equations on* Γ_ε *with* $u_\lambda = \sqrt{\rho_\lambda}$*:*

$$\begin{cases} -\varepsilon^4 \Delta u_\lambda + \frac{5}{3}\varepsilon^2 u_\lambda^{\frac{7}{3}} = \phi_\lambda u_\lambda, \\ \\ \phi_\lambda = G_\varepsilon \star \left(m - u_\lambda^2\right) - \varepsilon E x_3 - \theta_\lambda, \end{cases} \tag{2.4}$$

where θ_λ *is a constant which is the Lagrange multiplier for the constraint* $\frac{1}{\varepsilon^2}\int_{\Gamma_\varepsilon} \rho = \lambda$.

As in the one-dimensional model this result states that only ionized solutions exist in a constant exterior electric field.

Let us recall the

Theorem 2.2 (I. Catto, Cl. Le Bris, P.-L. Lions [9]; Existence and Uniqueness of a Periodic Solution)
For $m_{per}(x) = \sum_{k \in \mathbf{Z}^3} \delta(x-k)$, *there exists one and only one solution* $(u_{per}, \phi_{per}) \in L^\infty\left(\mathbf{R}^3\right) \times L^1_{unif}\left(\mathbf{R}^3\right)$ *to the following system (obtained from (2.4) for* $\varepsilon = 1$, $N = +\infty$ *and* $E = 0$*)*

$$\begin{cases} -\Delta u_{per} + \frac{5}{3} u_{per}^{\frac{7}{3}} = \phi_{per} u_{per}, \\ -\Delta \phi_{per} = m_{per} - u_{per}^2. \\ u_{per} \geq 0 \end{cases} \tag{2.5}$$

In particular this solution is $\mathbf{Z}^3$-periodic. We recall that

$$L^1_{unif}\left(\mathbf{R}^3\right) = \left\{\phi \in L^1_{loc}(\mathbf{R}^3),\ \sup_{x\in\mathbf{R}^3} |\phi|_{L^1(B_1(x))} < +\infty\right\}$$

In the following, we will consider the solution ρ_λ given by theorem 2.1 for $\lambda = \lambda_c$ and we denote it by ρ. For this solution we prove the

Theorem 2.3 (Exponential Decay of the Electric Field Inside the Crystal)
Let $0 \le E < \frac{1}{\varepsilon}$ and $\lambda = \lambda_c$. Then there exist two positive constants C_1, C_2 (which only depend on a bound on E and not on ε) such that the minimizing density ρ and the total electric field E_{tot} (given by equation (2.2)) satisfy with $\rho_{per}(x) = u^2_{per}(x)$:

$$\left.\begin{array}{l} \left|\rho(x) - \rho_{per}\left(\frac{x}{\varepsilon}\right)\right| \\ \left|E_{tot}(x) + \left(\nabla\phi_{per}\right)\left(\frac{x}{\varepsilon}\right)\right| \end{array}\right\} \quad \le \quad C_1 e^{-C_2\frac{d(x)}{\varepsilon}},$$

where $d(x) = d\left(x_3, [-1,1]^c\right)$ is the distance of a point x in the crystal to the boundary of the crystal.

Here again, as in the one-dimensional version (section 1.1), this result states that in the limit $\varepsilon \to 0$, the electric field has no effect inside the crystal, giving an estimate of the penetration length with respect to ε.

2.3 Relation with the physical model before renormalization

In this section we recall the physical model. We will denote with a tilde some physical quantities to avoid every ambiguity with the corresponding renormalized quantities.

We consider a crystal which is a collection of nuclei on a lattice

$$\mu\tilde{\varepsilon}\mathbf{Z}^3 \cap \left(\mathbf{R}^2 \times [-\tilde{L}, \tilde{L}]\right),$$

where $2\tilde{L}$ is the thickness of the crystal and $2\pi\tilde{\varepsilon}$ is Bohr's radius:

$$\tilde{\varepsilon} = \frac{\left(\dfrac{\hbar^2}{2m_e}\right)}{\left(\dfrac{e^2}{\varepsilon_0}\right)}.$$

The parameter μ is adimensional and is only useful to fix the size of the lattice cell. The lattice cell is denoted by

$$\tilde{\Gamma} = \left[-\frac{\mu\tilde{\varepsilon}}{2}, \frac{\mu\tilde{\varepsilon}}{2}\right)^2 \times \mathbf{R}.$$

Each nucleus is assumed to carry a charge $\tilde{z}e$ where e is the electron charge and $\tilde{z}$ is an integer. On a cell, the physical charge density of the nuclei is

$$\tilde{m}(\tilde{x}) = \sum_{k\in[-N,N]} \tilde{z}e\delta(\tilde{x} - k\mu\tilde{\varepsilon}e_3),$$

where $2N+1$ is the total number of nuclei in each cell $\tilde{\Gamma}$, and the integer N is defined by $N+\frac{1}{2} = \frac{\tilde{L}}{\mu\tilde{\varepsilon}}$.

If we denote by $\tilde{\rho}$ the electronic density, we get for a neutral crystal $\int_{\tilde{\Gamma}} \tilde{\rho} = (2N+1)\tilde{z}$ and for a ionized crystal we have

$$\int_{\tilde{\Gamma}} \tilde{\rho} = (2N+1)\tilde{z} - I,$$

where I is the positive ionization.

Then the Thomas-Fermi-von Weizsäcker energy is

$$\tilde{\mathcal{E}}(\tilde\rho) = \int_{\tilde\Gamma} \frac{\hbar^2}{2m_e}\left|\nabla\sqrt{\tilde\rho}\right|^2 + C_{TF}\frac{\hbar^2}{2m_e}\tilde\rho^{\frac{5}{3}} + e\tilde\rho\cdot\tilde G\star\left(\frac{1}{2}e\tilde\rho-\tilde m\right) + e\tilde E\tilde x_3\tilde\rho,$$

where $\tilde E$ is the exterior electric field, C_{TF} is an adimensional constant, and the convolution is defined by $\tilde G\star\tilde\sigma(\tilde x) = \int_{\tilde\Gamma} d\tilde y \quad \tilde G(\tilde x-\tilde y)\tilde\sigma(\tilde y)$, and

$$\varepsilon_0\tilde G(\tilde x) = -\frac{1}{2(\mu\tilde\varepsilon)^2}|\tilde x_3| + \frac{1}{4\pi}\sum_{\tilde k\in\mu\tilde\varepsilon\mathbf{Z}^2\times\{0\}}\left(\frac{1}{|\tilde x-\tilde k|} - \frac{1}{(\mu\tilde\varepsilon)^2}\int_{[-\frac{\mu\tilde\varepsilon}{2},\frac{\mu\tilde\varepsilon}{2}[\times\{0\}}\frac{d\tilde y}{|\tilde x-\tilde y-\tilde k|}\right) + \frac{M}{\mu\tilde\varepsilon},$$

where M is the adimensional constant previously introduced in (2.1).

Now, if we set

$$x = \frac{\tilde x}{\tilde L} \qquad \text{and} \qquad \varepsilon = \frac{\tilde\varepsilon}{\tilde L}(C_{TF})^{\frac{3}{2}},$$

we get a model similar to our renormalized model but with nuclei on a lattice $\nu\varepsilon\mathbf{Z}^3$ with a modified charge z, where these quantities are given by

$$z = (C_{TF})^{\frac{3}{2}}\tilde z \qquad \text{and} \qquad \nu = \frac{\mu}{(C_{TF})^{\frac{3}{2}}}.$$

In our model, to simplify the presentation, we make the following assumptions

$$z = 1 \qquad \text{and} \qquad \nu = 1.$$

As a consequence, on the renormalized cell $\Gamma_\varepsilon = \left[-\frac{\varepsilon}{2},\frac{\varepsilon}{2}\right)^2\times\mathbf{R}$, we define the renormalized densities by

$$\rho(x) = \varepsilon^3\tilde L^3(C_{TF})^{\frac{3}{2}}\tilde\rho(\tilde x) \quad \text{and} \quad m(x) = \varepsilon^3\tilde L^3(C_{TF})^{\frac{3}{2}}\tilde m(\tilde x)$$

and the renormalized energy $\mathcal{E}_\varepsilon$ and the exterior electric field E are chosen proportional to the corresponding physical quantities $\tilde{\mathcal{E}}$ and $\tilde E$. We then get exactly the model presented in subsection 2.1 with the renormalized energy (2.3).

3 Proof of Theorem 2.1

3.1 Preliminaries

Before proving Theorem 2.1 let us present the following straightforward but useful lemma:

Lemma 3.1 *Let*

$$\mathcal{E}_\varepsilon(\rho,m,E) = \int_{\Gamma_\varepsilon}\varepsilon^4\left|\nabla\sqrt{\rho}\right|^2 + \varepsilon^2\rho^{\frac{5}{3}} + \rho\cdot G_\varepsilon\star\left(\frac{1}{2}\rho-m\right) + \varepsilon E x_3\rho$$

and

$$K_\lambda^\varepsilon = \left\{\rho\geq 0, \quad \sqrt{\rho}\in H^1(\Gamma_\varepsilon), \quad |x_3|\rho\in L^1(\Gamma_\varepsilon), \qquad \frac{1}{\varepsilon^2}\int_{\Gamma_\varepsilon}\rho = \lambda > 0\right\}.$$

Let us define

$$\overline{x} = \frac{x}{\varepsilon}$$

and $\overline{\rho}(\overline{x}) = \rho(x)$,$\overline{m}(\overline{x}) = m(x)$. *Then*

$$\left(\rho(x) \quad \textit{minimizes} \quad \mathcal{E}_\varepsilon(\rho,m,E) \quad \textit{on} \quad K_\lambda^\varepsilon\right) \Longleftrightarrow \left(\overline{\rho}(\overline{x}) \quad \textit{minimizes} \quad \mathcal{E}_1(\overline{\rho},\overline{m},E) \quad \textit{on} \quad K^1_{\frac{\lambda}{\varepsilon}}\right)$$

Notations
When $\varepsilon = 1$, we simply drop the index ε and use the notations:

$$\mathcal{E}(\rho) = \int_\Gamma |\nabla\sqrt{\rho}|^2 + \rho^{\frac{5}{3}} + \rho \cdot G \star \left(\frac{1}{2}\rho - m\right) + Ex_3\rho$$

with

$$\Gamma = \left[-\frac{1}{2}, \frac{1}{2}\right)^2 \times \mathbf{R}$$

$$G = G_1$$

$$m(x) = \sum_{k=-N}^{N} \delta(x - ke_3) \quad \text{on} \quad \Gamma$$

and

$$K_\lambda = \left\{\rho \geq 0, \quad \sqrt{\rho} \in H^1(\Gamma), \quad |x_3|\rho \in L^1(\Gamma), \qquad \int_\Gamma \rho = \lambda > 0\right\}.$$

Here $\lambda_c = \left(1 - E\right)\left(\int_\Gamma m\right)$ and $\int_\Gamma m = 2N + 1$.

3.2 Main proof

Let us first say that the proof of theorem 2.1 is essentially an adaptation of the original proof of R. Benguria, H. Brézis, E. H. Lieb [5]. From Lemma 3.1, this proof reduces to the case $\varepsilon = 1$.

Step 1 : $\mathcal{E}$ is well defined on K_λ

We will check that the energy $\mathcal{E}$ is well defined on K_λ. To do this we need to rewrite the Green function G as

Lemma 3.2

$$G = -\frac{1}{2}|x_3| + \frac{\zeta(x)}{|x|} + \tilde{G}(x)$$

where $\zeta \in C_0^\infty(\Gamma)$ satisfies $\frac{1}{4\pi} \geq \zeta \geq 0$ and for $\delta > 0$ small enough

$$\zeta = \begin{cases} \frac{1}{4\pi} & on \quad B_\delta(0) \\ 0 & on \quad (B_{2\delta}(0))^c \end{cases}$$

Here $\tilde{G}$ satisfies

$$\begin{cases} \tilde{G}(x) \longrightarrow 0 \quad as \quad x \longrightarrow 0 \\ \tilde{G}(x) - \frac{1}{2}|x_3| \in C^\infty(\Gamma) \\ \tilde{G}(x) = 0\left(|x_3|^{-\alpha}\right) \quad as \quad x \longrightarrow +\infty \\ \nabla\tilde{G}(x) = 0\left(|x_3|^{-(1+\alpha)}\right) \quad as \quad x \longrightarrow +\infty \end{cases}$$

for every $0 < \alpha < 1$.

Proof: See [7] Proposition 3.2, Lemma 3.1. $\Diamond$

We now remark that the only possible singular terms in the energy are

$$\begin{aligned} &I_1 = \textstyle\int_\Gamma \rho^{\frac{5}{3}} \\ &I_2 = \textstyle\int_\Gamma \rho G = \int_\Gamma \rho\left(\tilde{G} - \frac{1}{2}|x_3|\right) + I_2' \quad \text{with} \quad I_2' = \int_\Gamma \rho\frac{\zeta}{|x|} \\ &I_3 = \textstyle\int_\Gamma \rho\left(G \star \rho\right) = I_3' + I_3'' + I_3''' \end{aligned}$$

with

$$\begin{aligned} &I_3' = \textstyle\int_\Gamma \rho\left(\tilde{G} \star \rho\right) \\ &I_3'' = -\frac{1}{2}\textstyle\int\int \rho(x)|x_3 - y_3|\rho(y) \\ &I_3''' = \textstyle\int\int \rho(x)\frac{\zeta(x-y)}{|x-y|}\rho(y) \end{aligned}$$

Considering

$$\tilde{\rho}(x) = \eta(x_1, x_2)\rho(x)$$

where $\eta \in C_0^\infty(\mathbf{R}^2)$ and

$$\begin{cases} \eta = 1 & \text{on} \quad \left[-\frac{1}{2}, \frac{1}{2}\right)^2 \\ \eta \geq 0 \end{cases}$$

Using as in [5] the Sobolev injection

$$\exists C > 0, \forall u \in H^1(\mathbf{R}^3), |u|_{L^6(\mathbf{R}^3)} \leq C|\nabla u|_{L^2(\mathbf{R}^3)}$$

we deduce that $\tilde{\rho} \in L^3(\mathbf{R}^3)$. Because $\rho \in L^1(\Gamma)$ we deduce by Hölder inequality that

$$I_1 < +\infty$$

Using again $\tilde{\rho}$ in place of ρ we bound I_2' by Hölder inequality because $\frac{\zeta(x)}{|x|} \in L^{\frac{5}{2}}(\Gamma)$, and we bound I_3''' using the fact that $\frac{\zeta(x)}{|x|} \star \tilde{\rho} \in L^\infty(\Gamma)$ by Young inequality. To finish, I_3' is bounded because $\tilde{G} \in L^\infty(\Gamma)$ and $|I_3''| < +\infty$ is a consequence of $|x_3 - y_3| \leq |x_3| + |y_3|$ and $|x_3|\rho \in L^1(\Gamma)$.

Step 2 : Proof of i)

As one may expect, the energy reaches $-\infty$ when some of the electrons are driven away by the electric field. In order to mathematically account for that, we introduce a non-negative function $\chi \in C_0^\infty(\Gamma)$ such that $\int_\Gamma \chi = 1$, and define

$$\rho_n(x) = \frac{\lambda + \lambda_c}{2}\chi + \frac{\lambda - \lambda_c}{2}\chi(x + ne_3),$$

ρ_n being periodically repeated along $\mathbf{Z}^2 \times \{0\}$. Here $\lambda_c = 2N + 1 - 2E = (1 - \varepsilon E)\int m$ with $\varepsilon = \frac{1}{N+\frac{1}{2}}$. If n is large enough to ensure that $\mathrm{supp}(\chi) \cap \mathrm{supp}(\chi(\cdot + ne_3)) = \emptyset$, then $\int_\Gamma \rho_n = \lambda$ and ρ_n is a test-function for the energy. We compute:

$$\begin{aligned} \mathcal{E}(\rho_n) \quad = \quad & \mathcal{E}\left(\frac{\lambda + \lambda_c}{2}\chi\right) + \frac{\lambda - \lambda_c}{2}\int_\Gamma |\nabla\sqrt{\chi}|^2 + \left(\frac{\lambda - \lambda_c}{2}\right)^{5/3}\int_\Gamma \chi^{5/3} \\ & + \frac{(\lambda - \lambda_c)^2}{8}\int_{\Gamma\times\Gamma} \chi(x)G(x-y)\chi(y)dxdy \\ & + \frac{\lambda - \lambda_c}{2}\int_\Gamma \chi(x + ne_3)V(x)dx. \end{aligned}$$

where $V(x) = \frac{\lambda+\lambda_c}{2}\chi \star G - \sum_{|j|\leq N} G(x - je_3) + Ex_3$, (with the convolution taken over Γ).

Since only the last term in the energy depends on n, and since by lemma 3.2 we have

$$V(x) = -\frac{(\lambda - \lambda_c)}{4}|x_3| + 2Ex_3^+ + r(x)$$

where $r \in L^\infty(\Gamma)$, we deduce when $\lambda > \lambda_c$ that

$$\lim_{n\to+\infty} \mathcal{E}(\rho_n) = -\infty$$

Step 3 : Convexity of the energy $\mathcal{E}$ on K_λ

For $\rho \in K_\lambda$, we can rewrite the energy as

$$\mathcal{E}(\rho) = \int_\Gamma |\nabla\sqrt{\rho}|^2 + \rho^{\frac{5}{3}} + v\rho + w\rho + \frac{1}{2}D_G(\rho - \lambda\chi, \rho - \lambda\chi) - C_\lambda \tag{3.1}$$

where $v \in L^{\frac{5}{2}}(\Gamma)$, $w \in L^\infty_{loc}(\Gamma)$ with $C(1+|x_3|) \geq w \geq 1$, D_G is a positive symmetric bilinear form on $K_\lambda - \lambda\chi$ and C_λ is a constant. More precisely we have

$$v(x) = -\sum_{|j|\leq N} \frac{\zeta(x-je_3)}{|x-je_3|}$$

$$w(x) = A(x) + 2Ex_3^+ + \frac{(\lambda-\lambda_c)}{2}|x_3| \tag{3.2}$$

where

$$A(x) = -\sum_{|j|\leq N}\left(\tilde{G}(x-je_3) - \frac{1}{2}\left(|x_3-j| - |x_3|\right)\right) - \lambda\left(G\star\chi - \frac{1}{2}|x_3|\right) + A_0$$

where A_0 is constant such that $A \geq 1$. And the constant C_λ is then given by

$$C_\lambda = A_0 - \frac{\lambda^2}{2}\int_\Gamma \chi(G\star\chi)$$

Moreover the bilinear form D_G is given by the following property

Lemma 3.3 *The following symmetric bilinear form*

$$D_G(f,g) := \int_{\Gamma\times\Gamma} f(x)G(x-y)g(y)$$

is continuous on the Banach space $Y = \left\{f \in L^1(\Gamma)\cap L^{\frac{5}{3}}(\Gamma), |x_3|f \in L^1(\Gamma)\right\}$. *Moreover for*

$$Y_0 = \left\{f \in Y, \quad \int_\Gamma f = 0\right\}$$

we have

$$\forall f \in Y_0, \quad \nabla(G\star f) \in L^2(\Gamma) \tag{3.3}$$

and

$$\forall f,g \in Y_0, \quad D_G(f,g) = \int_\Gamma \nabla(G\star f)\cdot\nabla(G\star g)$$

In particular D_G is positive on Y_0.

Remark 3.4 *Let us point out that the convexity of the bilinear form D_G is subjected to the constraint $f \in Y_0$. In other words, $\mathcal{E}$ is strictly convex on the hyperplanes $\{\int_\Gamma \rho = \lambda\}$, for each λ, but not on the whole space. This accounts for the existence of λ_c, which would not possibly exist if $\mathcal{E}$ was convex on the whole space.*

The first two terms of the energy are strictly convex with respect to ρ (see [5]). Because every positive quadratic form is convex, the map $f \longmapsto D_G(f,f)$ is convex on $Y_0 \supset (K_\lambda - \lambda\chi)$, and we deduce in particular that $\mathcal{E}$ is strictly convex on K_λ.

From the expression (3.1), we see that $\mathcal{E}$ is naturally defined and strictly convex on

$$K'_\lambda = \left\{\rho \geq 0, \quad \sqrt{\rho} \in H^1(\Gamma)\cap L^2(w), \quad \nabla(G\star(\rho-\lambda_c\chi)) \in L^2(\Gamma)\right\} \supset K_\lambda \quad \text{for} \quad 0 \leq \lambda \leq \lambda_c$$

where w is defined in (3.2) and

$$L^2(w) = \left\{u \in L^2(\Gamma), \quad \int_\Gamma u^2 w < +\infty\right\}$$

with the norm $|u|_{L^2(w)} = \left(\int_\Gamma u^2 w\right)^{\frac{1}{2}}$. The fact that $K'_{\lambda_c} \supset K_{\lambda_c}$ and $K'_\lambda = K_\lambda$ for $\lambda < \lambda_c$, is a consequence of (3.3) and the fact that

$$\forall \lambda \in [0,\lambda_c], \quad (\rho \in K'_\lambda) \Longrightarrow \left(\int_\Gamma \rho = \lambda\right)$$

This is proved by the lemma

Lemma 3.5 *If $f \in L^1(\Gamma)$, then $\nabla(G \star f)$ is defined in $\mathcal{D}'(\Gamma)$. Moreover*

$$\left(\nabla(G \star f) \in L^2(\Gamma)\right) \Longrightarrow \left(\int_\Gamma f = 0\right)$$

Step 4 : Minimizing sequences on K'_λ
We first remark that for $\lambda \le \lambda_c$ and $\rho \in K'_\lambda$, we have (following the bounds on I'_2):

$$\mathcal{E}(\rho) \ge -C + |\rho|_{\frac{5}{3}}^{\frac{5}{3}} - C\,|\rho|_{\frac{5}{3}} \tag{3.4}$$

We then consider a minimizing sequence $(\rho_n)_n$ in K'_λ. From (3.4) and the expression of the energy (3.1) we deduce

$$\left\{\begin{array}{lcl} |\sqrt{\rho_n}|_{H^1} & \le & C \\ |\rho_n|_{L^{\frac{5}{3}}} & \le & C \\ |\sqrt{\rho_n}|_{L^2(w)} & \le & C \\ |\nabla(G \star (\rho_n - \lambda\chi)|_{L^2} & \le & C \end{array}\right.$$

Up to extracting a subsequence we have $\sqrt{\rho_n} \to \sqrt{\rho_\infty}$ in L^2_{loc}, i.e.

$$\rho_n \to \rho_\infty \quad \text{in} \quad L^1_{loc}$$

Moreover

$$\left\{\begin{array}{lcll} \sqrt{\rho_n} & \rightharpoonup & \sqrt{\rho_\infty} & \text{in} \;\; H^1_{weak} \\ \rho_n & \rightharpoonup & \rho_\infty & \text{in} \;\; L^{\frac{5}{3}}_{weak} \\ \sqrt{\rho_n} & \rightharpoonup & \sqrt{\rho_\infty} & \text{in} \;\; L^2(w)_{weak} \\ \nabla(G \star (\rho_n - \lambda\chi) & \rightharpoonup & F_\infty & \text{in} \;\; L^2_{weak} \end{array}\right.$$

where the limits are identified using the convergence in the sense of distributions. Moreover we have the

Lemma 3.6 $F_\infty = \nabla(G \star (\rho_\infty - \lambda\chi)$

By continuity of each convex term Φ of the energy on each corresponding reflexive Banach space, we get

$$\Phi(\rho_\infty) \le \liminf_{n\to+\infty} \Phi(\rho_n)$$

and then

$$\mathcal{E}(\rho_\infty) \le \liminf_{n\to+\infty} \mathcal{E}(\rho_n) = \inf_{K'_\lambda} \mathcal{E}$$

In particular, by construction we get $\rho_\infty \in K'_\lambda$. The uniqueness of the solution in K'_λ (and then in K_λ) is a consequence of the strict convexity of the energy on K'_λ.

Step 5 : Euler-Lagrange equation and $\rho_\infty \in K_\lambda$

Let

$$D_\lambda = \left\{\zeta \in H^1(\Gamma), \zeta^2 \in K'_\lambda\right\}$$

Using the fact that for $\rho = \zeta^2$ (note that we do not assume $\zeta \ge 0$):

$$\nabla\sqrt{\rho} = \nabla\zeta\,(sgn(\zeta))$$

we see that

$$\mathcal{E}(\rho) = \Phi(|\zeta|) = \Phi(\zeta)$$

where

$$\Phi(\zeta) := \int_\Gamma |\nabla\zeta|^2 + |\zeta|^{\frac{10}{3}} + \zeta^2 \cdot G \star \left(\frac{1}{2}\zeta^2 - m\right) + Ex_3\zeta^2$$

Because $\inf_{K'_\lambda} \mathcal{E} = \inf_{D_\lambda} \Phi = \Phi(\sqrt{\rho_\infty})$, we then write down the Euler-Lagrange equation satisfied by $u = \sqrt{\rho_\infty}$,

$$-\Delta u + \frac{5}{3}u^{7/3} = \phi u \tag{3.5}$$

with

$$\phi = G \star \left(m - u^2\right) - Ex_3 - \theta$$

where θ is the Lagrange multiplier associated with the mass constraint $\int_\Gamma u^2 = \lambda$. This implies in particular that

$$-\Delta\phi = m - u^2 \tag{3.6}$$

We then use the following lemma which is proved in the following section:

Lemma 3.7 *If $(u, \phi) \in$ is solution of (3.5)-(3.6) with $u \geq 0$, then there exists a constant $C > 0$ such that*

$$u(x) \leq \frac{C}{1 + |x_3|^{\frac{3}{2}}}$$

For $\lambda < \lambda_c$, we have $K'_\lambda = K_\lambda$, but for $\lambda = \lambda_c$ we only know that $\rho_\infty \in K'_{\lambda_c} \supset K_{\lambda_c}$. Then lemma 3.7 implies that $\rho_\infty = u^2$ satisfies $x_3\rho_\infty \in L^1(\Gamma)$, which implies $\rho_\infty \in K_\lambda$ for every $\lambda \in [0, \lambda_c]$. This ends the proof of theorem 2.1.$\Diamond$

3.3 Proofs of the lemmata

Proof of lemma 3.3: Following the proof of the bounds on the term I_3, we get for $f, g \in Y$

$$|D_G(f,g)| \leq C|f|_Y|g|_Y$$

where

$$|f|_Y = |(1 + |x_3|)f|_{L^1} + |f|_{L^{\frac{5}{3}}}$$

which proves the continuity of D_G on Y.
For $f \in Y$, we have

$$-\Delta(G \star f) = f \tag{3.7}$$

Then by elliptic estimates and Sobolev injections, we have $G \star f \in C^0(\Gamma)$ and

$$G \star f = -\frac{1}{2}\left(\int_\Gamma f\right)|x_3| + \frac{1}{2}sgn(x_3)\left(\int_\Gamma x_3 f\right) + o(1) \quad \text{as} \quad |x_3| \to +\infty \tag{3.8}$$

Now for $f \in Y_0 \cap C_0^\infty(\Gamma)$, multiplying equation (3.7) by $G \star f$ and integrating by part, we get

$$\int_\Gamma |\nabla (G \star f)|^2 = \int_\Gamma f\,(G \star f)$$

Using the density of $Y_0 \cap C_0^\infty(\Gamma)$ in Y_0, we get for all $f \in Y_0$:

$$\begin{array}{rcl} D_G(f,f) & = & \lim\limits_{f_n \to f, f_n \in Y_0 \cap C_0^\infty(\Gamma)} \int_\Gamma |\nabla (G \star f_n)|^2 \\ & \geq & \int_\Gamma \left| \lim\limits_n (\nabla (G \star f_n)) \right|^2 \\ & = & \int_\Gamma |\nabla (G \star f)|^2 \end{array}$$

which implies in particular (3.3). Here we have used the

Lemma 3.8 *If $f_n \to f$ in Y, then $\nabla (G \star f_n) \to \nabla (G \star f)$ in $\mathcal{D}'(\Gamma)$.*

Now the bilinear form defined by

$$B(f,g) = \int_\Gamma \nabla (G \star f) \cdot \nabla (G \star g)$$

is well defined on Y_0 and and satisfies the Cauchy-Schwarz inequality

$$|B(f,g)| \leq (B(f,f))^{\frac{1}{2}} (B(g,g))^{\frac{1}{2}}$$

which proves that B is continuous on Y_0. Because B is equal to D_G on $Y_0 \cap C_0^\infty(\Gamma)$ which dense in Y_0, we deduce that $D_G = B$ on Y_0. This ends the proof of the lemma.

Proof of lemma 3.8

Let us consider $\phi = (\phi_1, \phi_2, \phi_3) \in (C_0^\infty(\Gamma))^3$ and $f \in Y$. Then we can write

$$< \nabla (G \star f), \phi >= \int_\Gamma \tilde{v} f + \tilde{w} f - \tilde{C} f \tag{3.9}$$

where $\tilde{v} \in L^{\frac{5}{2}}(\Gamma) = \left(L^{\frac{5}{3}}(\Gamma)\right)'$, $\tilde{w} \in L^\infty(\Gamma)$ and satisfies $\tilde{w} \geq 0$, and $\tilde{C}$ is a constant only dependent on ϕ. We take $-\tilde{v} = -G \star (\nabla \cdot \phi) + \frac{1}{2} \left(\int_\Gamma \phi_3\right) sgn(x_3)$, $\tilde{w} = \frac{1}{2} \left(\int_\Gamma \phi_3\right) \left(sgn(x_3) + sgn\left(\int_\Gamma \phi_3\right)\right)$, and $\tilde{C} = -\frac{1}{2} \left|\int_\Gamma \phi_3\right|$. The fact that the second member of (3.9) is continuous on Y proves the lemma.

Proof of lemma 3.5

Let us remark that $< \nabla (G \star f), \phi >$ is defined by the second member of (3.9) for $\phi \in (C_0^\infty(\Gamma))^3$ and $f \in L^1(\Gamma)$. Now we remark that for $s = sgn\left(\int_\Gamma \phi_3\right)$, we have

$$\lim_{n \to +\infty} < \nabla (G \star f), \phi(\cdot + sn) >= \lim_{n \to +\infty} \int_\Gamma \left(\tilde{v}(\cdot + sn) + \tilde{w}(\cdot + sn) + \tilde{C}\right) f = \frac{1}{2} \left|\int_\Gamma \phi_3\right| \left(\int_\Gamma f\right)$$

Now if $\nabla (G \star f) \in L^2(\Gamma)$ we deduce that $\int_\Gamma f = 0$. This ends the proof of the lemma.

Proof of lemma 3.6.

Let $f \in L^1(\Gamma) \cap L^{\frac{5}{3}}(\Gamma)$. Let us recall that for $\phi = (\phi_1, \phi_2, \phi_3) \in (C_0^\infty(\Gamma))^3$ such that $\int_\Gamma \phi_3 = 0$, (3.9) implies:

$$< \nabla (G \star f), \phi >= \int_\Gamma \tilde{v} f$$

where $\tilde{v} \in L^{\frac{5}{2}}(\Gamma) = \left(L^{\frac{5}{3}}(\Gamma)\right)'$. Because $\rho_n \rightharpoonup \rho_\infty$ in $L^{\frac{5}{3}}_{weak}$, we deduce that for $f_n = \rho_n - \lambda\chi$:

$$\lim_{n \to +\infty} < \nabla (G \star f_n), \phi >=< \nabla (G \star f_\infty), \phi >$$

with $f_\infty = \rho_\infty - \lambda\chi$. Because $\nabla (G \star f_n) \rightharpoonup F_\infty$ in L^2_{weak} we deduce that

$$\forall \phi \in C_0^\infty(\Gamma) \quad \text{with} \quad \int_\Gamma \phi = 0, \quad < \nabla (G \star f_\infty), \phi >=< F_\infty, \phi >$$

which implies

$$F_\infty = \nabla\left(G \star f_\infty\right) + Ce_3$$

where C is constant and $f_\infty \in L^1(\Gamma) \cap L^{\frac{5}{3}}(\Gamma)$. Using the same argument as in the proof of lemma 3.5 we see in $\pm\infty$ that

$$\frac{1}{2}\int_\Gamma f_\infty \pm C = 0$$

which implies $C = \int_\Gamma f_\infty = 0$. This ends the proof of the lemma.

4 A priori bounds

4.1 First a priori bounds

We are going to need the following bounds:

Proposition 4.1 *Let (u, ϕ) be a solution of*

$$\begin{cases} -\varepsilon^2 \Delta u + \frac{5}{3} u^{\frac{7}{3}} = u\phi \\ \phi = \varepsilon \sum_{|j| \le N_\varepsilon} G_\varepsilon\left(x - j\varepsilon e_3\right) - \frac{1}{\varepsilon^2} u^2 \star_{\Gamma_\varepsilon} G_\varepsilon - \varepsilon E x_3 - \theta_\varepsilon\big) \end{cases} \tag{4.1}$$

where θ_ε is the associated Lagrange multiplier. Then we have, for some constants C independent of ε:

(i) $\theta_\varepsilon \ge 0$,

(ii) $\phi(x) \le \frac{C}{|x_3|^2}$ *on* $\{|x_3| > 1\}$,

(iii) $u(x) \le \frac{C}{|x_3|^{3/2}}$ *on* $\{|x_3| > 1\}$,

(iv) $u(x) \le C$ *on* $\mathbf{R}^3$,

(v) For all $p < 3$, and for any open bounded set ω of $\mathbf{R}^2$, $\|\phi^+\|_{L^p(\omega\times\mathbf{R})} \le C|\omega|$,

(vi) $\phi^- \le C + 2\varepsilon E x_3^+$.

Proof: The proofs of (ii) and (iii) are adaptations of those of [7], which we reproduce here. We introduce the function $e_R(x) = \frac{\sin(\pi|x|/R)}{|x|\sqrt{2\pi R}}$, that is, the ground state of the Laplacian on B_R with homogeneous Dirichlet boundary conditions, and define $g_R = e_R^2$. (Note that $\int_{B_R} g_R = 1$ and $\int |\nabla e_R|^2 = \frac{\pi^2}{R^2}$.) We prolong g_R outside B_R by 0. Then, we have Lemma 2.1 of [7] (see also [6] or [15]), namely:

Lemma 4.2 (Benguria, Lieb, [6]) *Let $\rho = u^2$ be the solution of (4.1), and ϕ defined by (4.1). Then, for any $R > 0$, we have:*

$$g_R \star \phi \le \frac{5}{3} g_R \star u^{4/3} + \frac{\varepsilon^2\pi^2}{R^2}.$$

And if $|x_3| - R > 1$, $\phi \le \phi \star g_R$.

The first inequality is due to the fact that u is th ground state of the operator $-\varepsilon^2\Delta + \frac{5}{3}u^{4/3} - \phi$, so that $\varepsilon^2 \int |\nabla e_R(\cdot - y)|^2 + \int (\frac{5}{3}u^{4/3} - \phi) g_R \ge 0$. The second one comes from the fact that on $B_R + x$, ϕ is subharmonic and thus satisfies the mean-value inequality.

Next, denoting by $\tilde\phi$ the function $\phi \star g_R - \frac{\varepsilon^2\pi^2}{R^2}$, we have, using Jensen's inequality,

$$\tilde\phi \le \frac{5}{3} g_R \star u^{4/3} \le \frac{5}{3}(g_R \star u^2)^{2/3}.$$

Noticing that $-\varepsilon^2\Delta(g_R \star \phi) = 4\pi(m_\varepsilon \star g_R - u^2 \star g_R)$, we infer that

$$-\varepsilon^2\Delta\tilde{\phi} + \frac{5}{3}(\tilde{\phi})_+^{3/2} \leq 4\pi m_\varepsilon \star g_R.$$

In particular, for $R \geq 1$, $-\varepsilon^2\Delta\tilde{\phi} + \frac{5}{3}(\tilde{\phi})_+^{3/2}$ is bounded from above, since m_ε is a bounded measure. Following the ideas of [8], we infer that $\tilde{\phi}$ is bounded independently of ε, since $C + \frac{\alpha R'^4}{(R'^2 - |x|^2)^4}$ is a supersolution of the above equation as soon as $\alpha \geq 60^2\varepsilon^4$. Next, we introduce the function $U(x) = \frac{a}{(|x_3|^2 - R^2)^2} + \frac{bR'^4}{(R'^2 - |x_3|^2)^4}$, with $R' > R + 1 > 2$ This is a supersolution in the set $\{|x_3| > R + 1\} \cap B_{R'}$ as soon as $a \geq \left(\frac{27\varepsilon^2 R^2}{5(2R+1)}\right)^2$ and $a \geq \frac{\|\tilde{\phi}\|_\infty}{(2R+1)^2}$. This implies in particular that $\tilde{\phi} \leq U$ on $\{|x_3| > R + 1\} \cap B_{R'}$. Letting then R' go to infinity, we find that there is a constant independent of R and ε such that

$$\tilde{\phi} \leq \frac{CR^2}{(|x_3|^2 - R^2)^2}$$

on the set $\{|x_3| \geq R + 1\}$. This means in particular, using the second point of Lemma 4.2, that $\phi \leq \frac{CR^2}{(|x_3|^2 - R^2)^2} + \frac{\varepsilon^2\pi^2}{R^2}$ if $|x_3| - R \geq 1$. Hence, for any $|x_3| > 2$, taking $R = \frac{|x_3|}{2}$, we have $\phi \leq \frac{C}{|x_3|^2}$. We then conclude that (ii) holds by pointing out that $\tilde{\phi}$ is also bounded, so that if $1 < |x_3| < 2$, taking $R = \frac{1+|x_3|}{2}$ implies $\phi \leq \tilde{\phi} + \frac{4\varepsilon^2\pi^2}{(1+|x_3|)^2} \leq C$. Next, we insert (ii) into (4.1), getting

$$-\varepsilon^2\Delta u + \frac{4}{3}u^{7/3} \leq \frac{C}{|x_3|^{7/2}},$$

for some constant C. Hence, using exactly the same technics, but with the supersolution $V(x) = \frac{a}{(|x_3|^2 - R^2)^{3/2}} + \frac{bR'^{3/2}}{(R'^2 - |x|^2)^{3/2}}$, we show (iii). Then, with (4.1) and the fact that $G_\varepsilon(x) = \frac{1}{|x|} - \frac{2\pi|x_3|}{\varepsilon^2} + \tilde{G}_\varepsilon(x)$ on Γ_ε, where $\tilde{G}_\varepsilon$ is smooth and goes to 0 as $|x_3| \to \infty$ (see [7]), it is not difficult to show that $\lim_{x_3 \to -\infty} \phi = -\theta_\varepsilon$, so that with (ii), this implies (i).

In order to show (v), we use again that

$$\phi \star g_R \leq C,$$

with C independent of ε. Taking $R = \frac{\varepsilon}{4}$, we infer using the second part of Lemma 4.2 that $\phi(x) \leq C + \frac{\varepsilon^2\pi^2}{R^2} = C + 16\pi^2$ on the set $\mathbf{R}^3 \setminus \bigcup_{i \in \varepsilon\mathbf{Z}^3 \cap \{|x_3|<1\}} B_{\frac{\varepsilon}{4}}(i)$. On the other hand, in each ball $B_{\frac{\varepsilon}{4}}(i)$, ϕ satisfies $-\varepsilon^2\Delta\phi \leq 4\pi\varepsilon^3\delta_i$. Since the function $C + 16\pi^2 + \frac{\varepsilon}{|x-i|}$ is a supersolution of this equation and is greater than ϕ on the boundary of the ball, we deduce that $\phi \leq C + 16\pi^2 + \frac{\varepsilon}{|x-i|}$ in $B_{\frac{\varepsilon}{4}}(i)$. As a consequence, we have

$$\int_{B_{\frac{\varepsilon}{4}}(i)} (\phi_+)^p \leq \varepsilon^3 C + \varepsilon^p \int_{B_{\frac{\varepsilon}{4}}(0)} \frac{dx}{|x|^p} \leq C\varepsilon^3,$$

for any $p < 3$. This implies that for any bounded set Ω, we have $\|\phi^+\|_{L^p(\Omega)} \leq C|\Omega|$. Hence, with the help of (ii), we deduce (v). The last step of the proof is to show the following:

$$u^{4/3} \leq \phi + C - \frac{2\varepsilon^3 E}{2\pi} f_0 \star_{\Gamma_0} (G_\varepsilon - \frac{2\pi}{\varepsilon^2}x_3), \tag{4.2}$$

for some constant C and some smooth function f_0 having compact support with respect to x_3, and such that $\int_{\Gamma_\varepsilon} f_0 = 1$ (C depends on f_0 in fact.) This inequality will allow to conclude that (iv) and (vi) hold. In order to show (4.2), we introduce the function $w = u^{4/3} - (\phi + \theta_\varepsilon) + \frac{\varepsilon^3 E}{2\pi} f_0 \star (G_\varepsilon - \frac{2\pi}{\varepsilon^2}x_3) - C_0 - (C_0 - \theta_\varepsilon)^+$, where $C = 2C_0$ will be chosen later on. One easily computes:

$$\varepsilon^2\Delta w \geq \frac{4}{3}u^{4/3}(\frac{5}{3}u^{4/3} - \phi - 3\pi u^{2/3}),$$

on any set containing no nuclei. Hence, if $S = \{w > 0\}$, which clearly contains no nuclei, we have on S $-\phi \geq \theta_\varepsilon - u^{4/3} + (C_0 - \theta_\varepsilon)^+ + C_0 - \frac{2\varepsilon^3 E}{2\pi} f_0 \star (G_\varepsilon - \frac{2\pi}{\varepsilon^2} x_3)$, which implies $\varepsilon^2 \Delta w \geq \frac{4}{3} u^{4/3} (\frac{2}{3} u^{4/3} - 3\pi u^{2/3} + C_0)$, whenever C_0 is chosen large enough to have $C_0 - \frac{2\varepsilon^3 E}{2\pi} f_0 \star (G_\varepsilon - \frac{2\pi}{\varepsilon^2} x_3) \geq 0$, which is always possible according to the definition of G_ε, and may be done so that C_0 does not depend on ε. Moreover, if we have in addition $C_0 \geq \frac{27\pi^2}{8}$, then the polynomial $\frac{2}{3} t^2 - 3\pi t + C_0$ is non-negative, so that $\varepsilon^2 \Delta w \geq 0$. It is easily seen, using (iii) and the definitions of λ_c and ϕ (4.1), together with the fact that $G_\varepsilon = -\frac{2\pi}{\varepsilon^2} |x_3| + o(1)$ as $|x_3| \to \infty$, that we have:

$$\phi(x) = -\varepsilon E(x_3 + |x_3|) - \theta_\varepsilon + o(1) \quad \text{as} \quad |x_3| \to \infty,$$

with $o(1)$ possibly depending on ε. Hence, since in addition $\frac{2\varepsilon^3 E}{2\pi} f_0 \star (G_\varepsilon - \frac{2\pi}{\varepsilon^2} x_3) = -2\varepsilon E x_3^+ + o(1)$, $w(x) = -(C_0 - \theta_\varepsilon)^+ - C_0 + o(1)$. Thus, w goes to some negative constant as $|x_3| \to \infty$, so that S is bounded with respect to $|x_3|$. This implies that on ∂S, $w = 0$, so that $w \leq 0$ on S, thanks to the periodicity with respect to x_1 and x_2. Hence, $S = \emptyset$, which implies (4.2). This shows in particular that u is bounded on the set $\{|x_3| < 1\} \setminus \bigcup_{i \in \varepsilon \mathbf{Z}^3} B_{\frac{\varepsilon}{4}}(i)$. Inside the balls, we use here again supersolution methods, since we have $-\varepsilon^2 \Delta u + \frac{2}{3} u^{7/3} \leq C + C \frac{\varepsilon^{7/4}}{|x-i|^{7/4}}$ on each ball $B_{\frac{\varepsilon}{4}}(i)$, according to the bound $\phi \leq C + \frac{C\varepsilon}{|x-i|}$ on each ball. One easily shows that the function $A + B \frac{|x-i|^{1/4}}{\varepsilon^{1/4}}$ is a supersolution of this problem as soon as A and B are chosen properly, and that they may be chosen independently of ε, so that $u \leq C + C \frac{|x|^{1/4}}{\varepsilon^{1/4}} \leq C$ on $B_{\frac{\varepsilon}{4}}(i)$. This completes the proof of (iv). The proof of (vi) then only amounts, with the help of (4.2), to point out that $\frac{2\varepsilon^3 E}{2\pi} f_0 \star (G_\varepsilon - \frac{2\pi}{\varepsilon^2} x_3) \geq -C - 2\varepsilon E x_3^+$, which follows from the definition of f_0 and the fact that $G_\varepsilon(x) \geq -\frac{2\pi}{\varepsilon^2} |x_3| - C$. $\diamond$

We next point out that, integrating the equation $-\Delta v + \frac{5}{3} v^{7/3} - \psi v = 0$ against $v \xi^2$, where $\xi \in \mathcal{D}(\mathbf{R}^3)$ and satisfies $\xi = 1$ in the unit cube Q, $\xi = 0$ in $\mathbf{R}^3 \setminus 2Q$ and $0 \leq \xi \leq 1$, together with $|\nabla \xi| \leq 2$, using the fact that $\int -\Delta v v \xi^2 = \int |\nabla(\xi v)|^2 - \int v^2 |\nabla \xi|^2$,

$$\int_Q |\nabla v|^2 \leq 4 \int_{2Q} v^2 + \int_{2Q} \psi^+ v^2 \leq C + C \int_{2Q} \psi^+ \leq C,$$

where we have used (iv) and (v) of Proposition 4.1. As a consequence, since the same argument is valid with $\xi(\cdot + x_0)$ instead of ξ, v is bounded in H^1_{loc}. Hence, ψ being bounded in $L^p_{unif}(\mathbf{R}^3)$, we may extract from (v, ψ) a subsequence such that v converges strongly in $L^2_{loc}(\mathbf{R}^3)$ and ψ converges weakly in $L^p_{loc}(\mathbf{R}^3)$, for $p < 3$. Moreover, using (v) and (vi) of Proposition 4.1, ψ is bounded in $L^1_{unif}(\{|x_3| < \frac{1}{\varepsilon}\})$, so that its limit is in $L^1_{unif}(\mathbf{R}^3)$. Hence, the limit of (v, ψ), which satisfy (5.4), must be (u_{per}, ϕ_{per}). We now need the following Lemma, which is an adapted version of Theorem 5.9 of [9].

Lemma 4.3 *Let (v_n, ψ_n) be a solution of*

$$\begin{cases} -\Delta v + \frac{5}{3} v^{7/3} - \psi v = 0, \\ -\Delta \psi = \sum_{k \in \mathbf{Z}^3 \cap \{|k_3| < n\}} \delta_k - v^2, \\ v \geq 0, \end{cases}$$

such that $\|v_n\|_{L^\infty(\{|x_3|<n\})} + \|\psi_n\|_{L^1_{unif}(\{|x_3|<n\})}$ is bounded independently of n. Then for any sequence R_n such that $R_n \leq n$, $\frac{R_n}{n} \longrightarrow 1$ and $n - R_n \longrightarrow \infty$ as $n \to \infty$. Then we have:

$$\|u_{per} - v_n\|_{L^\infty(\{|x_3|<R_n\})} \longrightarrow 0 \quad \text{as} \quad n \to \infty, \tag{4.3}$$

$$\|\phi_{per} - \psi_n\|_{L^\infty(\{|x_3|<R_n\})} \longrightarrow 0 \quad \text{as} \quad n \to \infty, \tag{4.4}$$

where (u_{per}, ϕ_{per}) is the unique solution of (5.4).

Proof: We refer the reader to [9] (proof of Theorem 5.9), since this proof may be readily adapted to our case. Note that the norm $\|\phi_{per} - \psi_n\|_{L^\infty(\{|x_3|<R_n\})}$ does make sense since ϕ_{per} and ψ_n have exactly the same singularities (the nuclei), which cancel. $\diamondsuit$

Remark 4.4 *The above Lemma states, roughly speaking, that, no matter what happens outside the crystal, in the limit $\frac{1}{n} = \varepsilon \to 0$, the electronic density inside the crystal (the term "inside" meaning the hypothesis we made on R_n) converges towards the density of the true crystal u_{per}.*

Looking closely at Lemma 4.3, one easily deduce that following corollary:

Corollary 4.5 *Let $\rho = u^2$ be the solution of (4.1), with $\lambda = \lambda_c$, and let ϕ be defined by (4.1). Then, for any sequence η such that $\eta \leq 1$, $\eta \to 1$, $\frac{\eta}{\varepsilon} \to \infty$, we have:*

$$\|u - u_{per}(\frac{x}{\varepsilon})\|_{L^\infty(\{|x_3|<1-\eta\})} \longrightarrow 0,$$

$$\|\phi - \phi_{per}(\frac{x}{\varepsilon})\|_{L^\infty(\{|x_3|<1-\eta\})} \longrightarrow 0$$

as $\varepsilon \to 0$. Here u_{per} and ϕ_{per} are the solutions of the system (5.4).

4.2 Exponential decay estimates

We prove the following theorem which, with the a priori bounds given in section 3 for $\varepsilon = 1$, implies theorem 2.3.

Theorem 4.6 *Let (u, ϕ) a solution on Γ of*

$$\begin{cases} -\Delta u + \frac{5}{3}u^{\frac{7}{3}} = \phi u \\ -\Delta\phi = m - u^2 \\ u > 0 \end{cases} \tag{4.5}$$

with $m(x) = \sum_{|k|\leq N} \delta(x - ke_3)$. We assume that there exists a constant $C_0 > 0$ such that such that

$$|u(x) - u_p(x)| + |\phi(x) - \phi_p(x)| \leq C_0 \quad on \quad \{-N \leq x_3 \leq N\}$$

where (u_p, ϕ_p) is the periodic solution. Then there exists two constants $C_1, C_2 > 0$ (which only depend on C_0 and not on N) such that

$$|u(x) - u_p(x)| + |\phi(x) - \phi_p(x)| \leq C_1 e^{-C_2 d(x)} \quad on \quad \{-N \leq x_3 \leq N\}$$

where $d(x) = d(x_3, [-N, N]^c)$.

The exponential decay far away from the boundary of the crystal presented in theorem 4.6 is physically significant and seems a new result according to our knowledge. This exponential decay is an illustration of the "strong uniqueness" of the solutions for this model and is a kind of Harnack effect but for a system. The explanation of the "strong uniqueness" is simply contained in the fact that the functional $\mathcal{E}$ is strictly convex which implies good properties of the following system (and also of its linearization):

$$\begin{cases} -\frac{\Delta u}{u} + \frac{5}{3}u^{\frac{4}{3}} = \phi \\ -\Delta\phi = m - u^2 \\ u > 0 \end{cases} \tag{4.6}$$

These properties are illustrated by the following result:

Lemma 4.7 *Let $(u,\phi),(v,\psi) \in L^\infty(\Gamma)\times L^1_{unif}(\Gamma)$ be two solutions of (4.6) with the same bounded measure m on Γ. Then, for any $\eta \in C_0^\infty(\Gamma)$ (i.e. having compact support with respect to x_3), we have with $u_1 = v-u$, $\phi_1 = \psi - \phi$:*

$$Q(u,v) + \frac{1}{2}\int_\Gamma |\nabla(\eta\phi_1)|^2 = \int_\Gamma \left(u_1^2 + \frac{1}{2}\phi_1^2\right)|\nabla\eta|^2 + A((u,\phi),(v,\psi)) \tag{4.7}$$

where Q is the sum of two positive terms

$$Q(u,v) = \int_\Gamma u^2 \left|\nabla\left(\frac{\eta u_1}{u}\right)\right|^2 + \eta^2(u+u_1)u_1\frac{5}{3}\left((u+u_1)^{4/3} - u^{4/3}\right)$$

and A is antisymmetric in $(u,\phi),(v,\psi)$:

$$A((u,\phi),(v,\psi)) = \frac{1}{2}\int_\Gamma \eta^2\phi_1 u_1^2$$

Proof: The equations satisfied by u,v,ϕ,ψ read:

$$\begin{cases} -\frac{\Delta u}{u} + \frac{5}{3}u^{4/3} - \phi = 0, \\ -\frac{\Delta v}{v} + \frac{5}{3}v^{4/3} - \psi = 0, \\ -\Delta(\psi-\phi) = u^2 - v^2. \end{cases} \tag{4.8}$$

Multiplying the last equation by $\phi_1\eta^2$ and integrating, we have:

$$\int_\Gamma -\eta^2\phi_1\Delta\phi_1 = -\int_\Gamma u_1(2u+u_1)\phi_1\eta^2,$$

so that, using the fact that $\int_\Gamma -\eta^2\xi\Delta\xi = \int_\Gamma |\nabla(\eta\xi)|^2 - \int_\Gamma \xi^2|\nabla\eta|^2$ for any $\eta \in C_0^\infty(\Gamma)$ and any sufficiently regular ξ, we deduce that

$$\frac{1}{2}\int_\Gamma |\nabla(\eta\phi_1)|^2 \quad = \quad \frac{1}{2}\int_\Gamma \phi_1^2|\nabla\eta|^2 - \frac{1}{2}\int_\Gamma u_1(2u+u_1)\phi_1\eta^2 \tag{4.9}$$

Next, we substract the first two equations of (4.8), multiply the difference by $\eta^2(u+u_1)u_1$ and get:

$$\int_\Gamma \left(\frac{\Delta u}{u} - \frac{\Delta v}{v}\right)(u+u_1)u_1\eta^2 + \int_\Gamma \frac{5}{3}\eta^2(u+u_1)u_1((u+u_1)^{4/3} - u^{4/3}) - \int_\Gamma \phi_1(u+u_1)u_1\eta^2 = 0.$$

Integrating by parts, one easily computes:

$$\int_\Gamma \left(\frac{\Delta u}{u} - \frac{\Delta v}{v}\right)(u+u_1)u_1\eta^2 = \int_\Gamma u^2\left|\nabla\left(\frac{\eta u_1}{u}\right)\right|^2 - \int_\Gamma u_1^2|\nabla\eta|^2.$$

As a consequence, we have

$$\int_\Gamma u^2\left|\nabla\left(\frac{\eta u_1}{u}\right)\right|^2 + \frac{5}{3}\eta^2(u+u_1)u_1(v^{4/3} - u^{4/3}) - \phi_1(u+u_1)u_1\eta^2 = \int_{\Gamma_1} u_1^2|\nabla\eta|^2. \tag{4.10}$$

Adding (4.9) and (4.10), we get (4.7). $\Diamond$

Proof of theorem 4.6

Let us define

$$M(d) = \sup_{d(x_3,[-N,N]^c)\geq d} |u(x) - u_p(x), \phi(x) - \phi_p(x)|$$

It is sufficient to prove that

$$\exists L > 0, \quad \exists \gamma \in (0,1), \quad \forall N > 0, \quad \forall d \leq N, \quad M(d+L) \leq \gamma M(d) \quad \text{if} \quad d + L < N$$

We argue by contradiction, assuming that

$$\forall L > 0, \quad \forall \gamma \in (0,1), \quad \exists N > 0, \quad \exists d \leq N, \quad M(d+L) > \gamma M(d) \quad \text{with} \quad d+L < N$$

Let us take sequence

$$\begin{cases} L_n \to +\infty \quad \text{as} \quad n \to +\infty \\ \gamma_n \to 1 \quad \text{as} \quad n \to +\infty \\ d_n + L_n \leq N_n \\ M(d_n + L_n) > \gamma_n M(d_n) \quad \text{for} \quad (u^n, \phi^n) \end{cases}$$

From the standard elliptic estimates, we get by compactness (up to extraction of a subsequence) that

$$(u^n, \phi^n) \to (u^\infty, \phi^\infty)$$

where (u^∞, ϕ^∞) is solution of (4.5) on Γ with $m(x) = \sum_{k \in \mathbf{Z}} \delta(x - ke_3)$. From theorem 2.2 we have

$$(u^\infty, \phi^\infty) = (u_p, \phi_p)$$

where we denote here the periodic solution by (u_p, ϕ_p). As a consequence

$$M(d_n + L_n) \to 0$$

We then consider the renormalized sequence

$$\left(\overline{u}_1^n, \overline{\phi}_1^n\right)(x) = \frac{(u^n - u_p, \phi - \phi_p)}{M(d_n + L_n)}(x + x^n)$$

where x^n is a point such that $d(x_3^n, [-N, N]^c) \geq d_n + L_n$ and

$$\frac{|u^n(x^n) - u_p(x^n)| + |\phi(x^n) - \phi_p(x^n)|}{M(d_n + L_n)} \longrightarrow 1$$

Up to extraction of a subsequence we get

$$\left(\overline{u}_1^n, \overline{\phi}_1^n\right) \to \left(\overline{u}_1^\infty, \overline{\phi}_1^\infty\right)$$

which satisfies

$$\sup_\Gamma |\overline{u}_1^\infty(x)| + |\overline{\phi}_1^\infty(x)| \leq 1 = |\overline{u}_1^\infty(0)| + |\overline{\phi}_1^\infty(0)| \tag{4.11}$$

Taking the limit in (4.7) we get (up to translate (u_p, ϕ_p)):

$$\int_\Gamma u_p^2 \left|\nabla\left(\frac{\eta \overline{u}_1^\infty}{u_p}\right)\right|^2 + \frac{20}{9}\eta^2 u_p^{\frac{4}{3}} + \frac{1}{2}\left|\nabla\left(\eta \overline{\phi}_1^\infty\right)\right|^2 = \int_\Gamma \left((\overline{u}_1^\infty)^2 + \frac{1}{2}(\overline{\phi}_1^\infty)^2\right)|\nabla \eta|^2$$

Then taking $\eta(x) = \eta_1(\lambda x_3)$ with $\lambda \to 0$ and

$$\eta_1 \in C_0^\infty(\Gamma)$$

with $\eta = 1$ for $x_3 \in [-1, 1]$, we get at the limit $\lambda = 0$:

$$\overline{u}_1^\infty = 0, \quad \nabla \overline{\phi}_1^\infty = 0$$

To conclude that $\overline{\phi}_1^\infty = 0$ we remark that the equations imply

$$\phi^n - \phi_p = -\frac{1}{u^n u_p}\nabla\left(u_p^2 \nabla\left(\frac{u^n - u_p}{u_p}\right)\right) + \frac{5}{3}\left((u^n)^{\frac{4}{3}} - u_p^{\frac{4}{3}}\right)$$

This gives at the limit

$$\overline{\phi}_1^\infty = -\frac{1}{u_p^2}\nabla\left(u_p^2 \nabla\left(\frac{\overline{u}_1^\infty}{u_p}\right)\right) + \frac{20}{9}u_p^{\frac{1}{3}}\overline{u}_1^\infty = 0$$

Finally $\overline{u}_1^\infty = \overline{\phi}_1^\infty = 0$ gives a contradiction with (4.11). This ends the proof of the theorem.

5 Appendix: An homogenization approach

We present in this Section an alternative approach using the two-scale convergence [1, 13]. In order to do so, we first re-write the system of PDE satisfied by u and ϕ:

$$\begin{cases} -\varepsilon^2 \Delta u + \frac{5}{3} u^{7/3} - \phi u = 0, \\ -\varepsilon^2 \Delta \phi = m - u^2. \end{cases} \tag{5.1}$$

5.1 Two-scale convergence

The key to the convergence problem is to postulate the following ansatz for the functions (u, ϕ):

$$\begin{cases} u = u_0(x, \frac{x}{\varepsilon}) + \varepsilon u_1(x, \frac{x}{\varepsilon}) + \varepsilon^2 u_2(x, \frac{x}{\varepsilon}) + \dots, \\ \phi = \phi_0(x, \frac{x}{\varepsilon}) + \varepsilon \phi_1(x, \frac{x}{\varepsilon}) + \varepsilon^2 \phi_2(x, \frac{x}{\varepsilon}) + \dots, \end{cases} \tag{5.2}$$

where the functions $u_i(x,y)$ and $\phi_i(x,y)$ are periodic in the second variable. Inserting this ansatz into (5.1), and noticing that $-\Delta u_i(x, \frac{x}{\varepsilon}) = -\Delta_x u_i(x, \frac{x}{\varepsilon}) - \frac{2}{\varepsilon} \nabla_x \cdot \nabla_y u_i(x, \frac{x}{\varepsilon}) - \frac{1}{\varepsilon^2} \Delta_y u_i(x, \frac{x}{\varepsilon})$, we have, isolating the term of order 0, and admitting that the two variables x and $y = \frac{x}{\varepsilon}$ decouple:

$$\begin{cases} -\Delta_y u_0 + \frac{5}{3} u_0^{7/3} - \phi_0 u_0 = 0, \\ -\Delta_y \phi_0 = m_0 - u_0^2, \end{cases} \tag{5.3}$$

where we have implicitly assumed that the nonlinear terms pass to the limit in the same fashion as the linear ones, and where $m_0(x,y) = 1_{\{|x_3|<1\}}(x) \sum_{k \in \mathbf{Z}^3} \delta_k(y)$ is the limit in the sense of two-scale convergence (see below) of m_ε. The above ansatz is justified by the notion of two-scale convergence, that we rapidly introduce, referring to [1, 13] for details.

Definition 5.1 *Let Ω be an open subset of $\mathbf{R}^n$, and Q the unit cube of $\mathbf{R}^n$. Let v_n be a sequence in $L^2(\Omega)$. We say that v_n two-scale converges to $v_\infty \in L^2(\Omega \times Q)$ if, for any function $\psi \in \mathcal{D}(\Omega; C^\infty_{per}(Q))$, we have*

$$\lim_{n \to \infty} \int_\Omega v_n(x) \psi(x, \frac{x}{\varepsilon}) dx = \int_{\Omega \times Q} v_\infty(x,y) \psi(x,y) dx dy.$$

Note that in practice, the sequence v_n will be indexed by a continuous variable ε, which will be supposed to go to 0. This of course makes no difference in the above definition. The following theorems are borrowed from [13] and [1], and are a way of making rigorous the above formal results.

Theorem 5.1 (Nguetseng, [13]) *From each bounded sequence v_ε in $L^2(\Omega)$, we can extract a subsequence that two-scale converge to some limit $v_0 \in L^2(\Omega \times Q)$.*

Of course, this is only a weak convergence result, and in order to pass to the limit in the nonlinear terms of (5.1), the following will be useful:

Theorem 5.2 (Allaire, [1]) *Let v_ε be a sequence of functions in $L^2(\Omega)$ which two-scale converges to $v_0 \in L^2(\Omega \times Q)$. Then*

$$\liminf_{\varepsilon \to 0} \|v_\varepsilon\|_{L^2(\Omega)} \geq \|v_0\|_{L^2(\Omega \times Q)},$$

and if equality is achieved, then

$$\lim_{\varepsilon \to 0} \|v_\varepsilon - v_0(x, \frac{x}{\varepsilon})\|_{L^2(\Omega)} = 0,$$

and, for any sequence w_ε of $L^2(\Omega)$ which two-scale converges to $w_0 \in L^2(\Omega \times Q)$, the sequence $v_\varepsilon w_\varepsilon$ two-scale converges to $v_0 w_0$.

5.2 Convergence at order 0

Setting $L^1_{unif}(\mathbf{R}^3) = \{f \in L^1_{loc}(\mathbf{R}^3), \quad \sup_{x\in\mathbf{R}^3} \|f\|_{L^1(B+x)} < \infty\}$, B being the unit ball of $\mathbf{R}^3$, we are now in position to prove the following:

Theorem 5.3 *Let $\rho = u^2$ be the solution of (4.1), and let ϕ be defined by (4.1). Then, up to extracting a subsequence, (u,ϕ) two-scale converges to $(u_0,\phi_0) \in L^2(\Gamma_1\times Q)$, which are solutions of (5.3), that is*

$$\left\{\begin{array}{l} -\Delta_y u_0 + \frac{5}{3}u_0^{7/3} - \phi_0 u_0 = 0, \\ -\Delta_y \phi_0 = m_0 - u_0^2, \end{array}\right.$$

with $m_0(x,y) = 1_{\{|x_3|<1\}}(x)\sum_{k\in\mathbf{Z}^3}\delta_k(y)$. In addition, denoting by (u_{per},ϕ_{per}) the unique solution (given by theorem 2.2) in $L^\infty(\mathbf{R}^3)\times L^1_{unif}(\mathbf{R}^3)$ of the problem

$$\left\{\begin{array}{l} -\Delta u_{per} + \frac{5}{3}u_{per}^{7/3} - \phi_{per}u_{per} = 0, \\ -\Delta\phi_{per} = \sum_{k\in\mathbf{Z}^3}\delta_k - u_{per}^2, \\ u \geq 0, \end{array}\right. \tag{5.4}$$

we have:

$$\left\{\begin{array}{l} u_0(x,y) = 1_{\{|x_3|<1\}}(x)u_{per}(y), \\ \phi_0(x,y) = \phi_{per}(y) \quad \textit{if} \quad |x_3| < 1 \end{array}\right. \tag{5.5}$$

Proof: The first point is that (5.4) has indeed a unique solution. This is insured by Theorem 6.5 of [9]. Thus, the definition of (u_{per},ϕ_{per}) is clear. using the bounds we have shown in Proposition 4.1, one easily shows that (u,ϕ) two-scale converges to some limit (u_0,ϕ_0). We are now going to show that this limit is indeed equal to $(u_{per}(y),\phi_{per}(y))$ if $|x_3| < 1$. In order to prove this claim, we introduce the following rescaled functions:

$$v(x) = u(\varepsilon x), \quad \psi(x) = \phi(\varepsilon x).$$

These functions satisfy the following system:

$$\left\{\begin{array}{l} -\Delta v + \frac{5}{3}v^{7/3} - \psi v = 0, \\ -\Delta\psi = \sum_{k\in\mathbf{Z}^3\cap\{|x_3|<\frac{1}{\varepsilon}\}}\delta_k - v^2. \end{array}\right.$$

Applying Lemma 4.3 to our sequence (v,ψ), one easily shows that if $R = \frac{1}{\varepsilon} - \frac{1}{\sqrt{\varepsilon}}$, then $\|u_{per} - v\|_{L^\infty(\{|x_3|<R)} \longrightarrow 0$ as $\varepsilon\to 0$. Now, denoting by $f(x,y)$ smooth function which is Q-periodic in y and has compact support in x, this support being included in $\{|x_3|<1\}$. Then, on the one hand,

$$\lim_{\varepsilon\to 0}\int u(x)f(x,\frac{x}{\varepsilon}) = \int_{\mathbf{R}^3}\int_Q u_0(x,y)f(x,y)dydx, \tag{5.6}$$

and on the other hand, we have, setting $\Omega = \cup_{y\in Q}\mathrm{supp}(f(\cdot,y))$.:

$$\begin{aligned} \int u(x)f(x,\frac{x}{\varepsilon})dx &= \varepsilon^3\int_{\frac{1}{\varepsilon}\Omega} v(y)f(\varepsilon y,y)dy \\ &= \int_{\frac{1}{\varepsilon}\Omega} u_{per}(y)f(\varepsilon y,y)dy + \varepsilon^3\int_{\frac{1}{\varepsilon}\Omega}(u_{per}(y)-v(y))f(\varepsilon y,y). \end{aligned}$$

Using the periodicity of u_{per} and of $f(x,\cdot)$, one easily sees that the first term converges towards $\int_{\mathbf{R}^3}\int_Q u_{per}(y)f(x,y)dydx$. The second one is dealt with using (4.3):

$$\begin{aligned}\left|\varepsilon^3\int_{\frac{1}{\varepsilon}\Omega}(u_{per}(y)-v(y))f(\varepsilon y,y)\right| &\leq \|u_{per}-v\|_{L^\infty(\{|x_3|<\frac{1}{\varepsilon}\})}\int|f(x,\frac{x}{\varepsilon})|dx\\ &\leq (\|u_{per}-v\|_{L^\infty(\{|x_3|<\frac{1}{\varepsilon}-\frac{1}{\sqrt{\varepsilon}}\})})\|f(\cdot,\frac{\cdot}{\varepsilon})\|_{L^1(\mathbf{R}^3)}\\ &\quad+\varepsilon^3(\|u_{per}\|_{L^\infty(Q)}+\|v\|_{L^\infty})\|f\|_{L^\infty}\left|\frac{1}{\varepsilon}\Omega\setminus(\frac{1}{\varepsilon}-\frac{1}{\sqrt{\varepsilon}})\Omega\right|\\ &\leq C\|u_{per}-v\|_{L^\infty(\{|x_3|<\frac{1}{\varepsilon}-\frac{1}{\sqrt{\varepsilon}}\})}+C\varepsilon^3(\frac{1}{\varepsilon^3}-(\frac{1}{\varepsilon}-\frac{1}{\sqrt{\varepsilon}})^3).\end{aligned}$$

These two terms converging to 0 as $\varepsilon\to\infty$, we deduce, using (5.6):

$$u_0(x,y)=u_{per}(y),\quad \forall|x_3|<1.$$

This implies in particular that $\|u_0\|_{L^2(Q\times\Gamma_1)}\geq 2\|u_{per}\|_{L^2(Q)}=2$. Since $\|u\|_{L^2(\Gamma_1)}=\frac{\lambda_\varepsilon}{\varepsilon^2}=2-\frac{\varepsilon^3E}{2\pi}\longrightarrow 2$ as $\varepsilon\to 0$, one easily sees that

$$\lim_{\varepsilon\to 0}\|u\|_{L^2(\Gamma_1)}=\|u_0\|_{L^2(Q\times\Gamma_1)}. \tag{5.7}$$

Using Proposition 5.2, this implies that

$$\|u_0(x,\frac{x}{\varepsilon})-u\|_{L^2(\Gamma_1)}\longrightarrow 0$$

as $\varepsilon\to 0$, so that the nonlinear terms pass to the limit in (4.1), showing (5.3), up to the fact that $-\varepsilon^2\Delta u$ two-scale converges to $-\Delta_y u_0$, which is shown by the following integrations by parts:

$$\begin{aligned}\int -\varepsilon^2\Delta u(x)f(x,\frac{x}{\varepsilon})dx &= \int u(x)(-\Delta_y f(x,\frac{x}{\varepsilon}))dx+2\varepsilon\int u(x)\nabla_x\cdot\nabla_y f(x,\frac{x}{\varepsilon})dx\\ &\quad+\varepsilon^2\int u(x)(-\Delta_x f(x,\frac{x}{\varepsilon}))dx.\end{aligned}$$

Equation (5.7) also shows that $\|u\|_{L^2(\Gamma_1\cap\{|x_3|>1\})}\longrightarrow 0$, so that we have $u_0(x,y)=0$ if $|x_3|>1$. This shows the first line of (5.5). In order to show the second one, we first point out that according to the uniqueness of the solution of (5.4) and to the bounds we have on ϕ, $\phi_0(x,y)=\phi_{per}(y)$ as soon as $|x_3|<1$, concluding our proof. $\Diamond$

Acknowledgments The authors are very grateful to Claude Le Bris for discussions and suggestions in the preparation of this work.

References

[1] G. Allaire, *Homogenization and two-scale convergence*, SIAM J. Math. Anal. **23**(6) (1992), 1482-1518.

[2] J.E. Avron and L.W. Herbst, *Spectral and scattering theory of Schrdinger operators related to the Stark effect*, Comm. Math. Phys. **52** (1977), 239.

[3] L.C. Balbás, M. Barranco, F. Garcias, A. Mañanes, J. Navarro, A. Rubio, L. Serra, *The static polarisability of metal clusters and spheres in an improved Thomas-Fermi approximation*, J. Phys.: Condens. Matter **1** (1989), 10391-10405.

[4] D. Bauer, F. Cornolti, A. Macchi, D. Pitrelli, *Ionization of the Thomas-Fermi atom in intense laser fields: the static limit revisited*, J. Phys. B **33** (2000), 829-842.

[5] R. Benguria, H. Brézis, E. H. Lieb, *The Thomas-Fermi-von Weizsäcker theory of atoms and molecules*, Comm. Math. Phys., **79** (1981), 167-180.

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

[7] X. Blanc and C. Le Bris, *Thomas-Fermi type models for polymers and thin films*, Adv. Diff. Equ. **5**(7-9) (2000), 977-1032.

[8] H. Brézis, *Semilinear Equations in* $\mathbf{R}^N$ *Without Conditions at Infinity*, Appl. Math. Optim. **12** (1984), 271-282.

[9] I. Catto, C. Le Bris, P.-L. Lions, Mathematical theory of thermodynamics limits, Thomas-Fermi type models, Oxford Mathematical Monographs, 1998.

[10] I. Catto, C. Le Bris, P.-L. Lions, *Limite thermodynamique pour les modles de type Thomas-Fermi [Thermodynamic limit for Thomas-Fermi type models]*, C. R. Acad. Sci. Paris, t. **322**, Série I, (1996) 357-364.

[11] E.H. Lieb, H. Narnhofer, *The thermodynamic limit for Jellium*, J. Stat. Phys. **12** (1975), 291-310.

[12] C. B. Morrey, Multiple Integrals in the Calculus of Variations, Springer-Verlag, 1966.

[13] G. Nguetseng, *A general convergence result for a functional related to the theory of homogenization*, SIAM J. Math. Anal. **20**(3) (1989), 608-623.

[14] R.G. Parr, W. Yang, Density-Functional Theory of Atoms and Molecules, Oxford University Press, 1989.

[15] J.P. Solovej, *Universality in the Thomas-Fermi-von Weizsäcker model of atoms and molecules*, Comm. Math. Phys. **129** (1990), 561-598.