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Julien Ricaud

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SYMMETRY BREAKING IN THE PERIODIC THOMAS–FERMI–DIRAC–VON WEIZSÄCKER MODEL

JULIEN RICAUD

ABSTRACT. We consider the Thomas–Fermi–Dirac–von Weizsäcker model for a system composed of infinitely many nuclei placed on a periodic lattice and electrons with a periodic density. We prove that if the Dirac constant is small enough, the electrons have the same periodicity as the nuclei. On the other hand if the Dirac constant is large enough, the 2-periodic electronic minimizer is not 1-periodic, hence symmetry breaking occurs. We analyze in detail the behavior of the electrons when the Dirac constant tends to infinity and show that the electrons all concentrate around exactly one of the 8 nuclei of the unit cell of size 2, which is the explanation of the breaking of symmetry. Zooming at this point, the electronic density solves an effective nonlinear Schrödinger equation in the whole space with nonlinearity $u^{7/3} - u^{4/3}$. Our results rely on the analysis of this nonlinear equation, in particular on the uniqueness and non-degeneracy of positive solutions.

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1. INTRODUCTION

Symmetry breaking is a fundamental question in Physics which is largely discussed in the literature. In this paper, we consider the particular case of electrons

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in a periodic arrangement of nuclei. We assume that we have classical nuclei located on a 3D periodic lattice and we ask whether the quantum electrons will have the symmetry of this lattice. We study this question for the Thomas–Fermi–Dirac–von Weizsäcker (TFDW) model which is the most famous non-convex model occurring in Orbital-free Density Functional Theory. In short, the energy of this model takes the form

$$\int_{\mathbb{K}} |\nabla \sqrt{\rho}|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{K}} \rho^{\frac{5}{3}} - \frac{3}{4} c \int_{\mathbb{K}} \rho^{\frac{4}{3}} + \frac{1}{2} \int_{\mathbb{K}} (G \star \rho) \rho - \int_{\mathbb{K}} G \rho, \quad (1.1)$$

where \mathbb{K} is the unit cell, ρ is the density of the electrons and G is the periodic Coulomb potential. The non-convexity is (only) due to the term $-\frac{3}{4}c \int \rho^{\frac{4}{3}}$. We refer to [18, 13, 5, 4, 57] for a derivation of models of this type in various settings.

We study the question of symmetry breaking with respect to the parameter $c > 0$. In this paper, we prove for $c > 0$ that:

- if c is small enough, then the density ρ of the electrons is unique and has the same periodicity as the nuclei, that is, there is no symmetry breaking;
- if c is large enough, then there exist 2-periodic arrangements of the electrons which have an energy that is lower than any 1-periodic arrangement, that is, there is symmetry breaking.

Our method for proving the above two results is perturbative and does not provide any quantitative bound on the value of c in the two regimes. For small c we perturb around $c = 0$ and use the uniqueness and non degeneracy of the TFW minimizer, which comes from the strict convexity of the associated functional. This is very similar in spirit to a result by Le Bris [27] in the whole space.

The main novelty of the paper, is the regime of large c . The $\rho^{\frac{4}{3}}$ term in (1.1) favours concentration and we will prove that the electronic density concentrates at some points in the unit cell \mathbb{K} in the limit $c \rightarrow \infty$ (it converges weakly to a sum of Dirac deltas). Zooming around one point of concentration at the scale $1/c$ we get a simple effective model posed on the whole space \mathbb{R}^3 where all the Coulomb terms have disappeared. The effective minimization problem is of NLS-type with two subcritical power nonlinearities:

$$J_{\mathbb{R}^3}(\lambda) = \inf_{\substack{v \in H^1(\mathbb{R}^3) \\ \|v\|_{L^2(\mathbb{R}^3)}^2 = \lambda}} \left\{ \int_{\mathbb{R}^3} |\nabla v|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{R}^3} |v|^{\frac{10}{3}} - \frac{3}{4} \int_{\mathbb{R}^3} |v|^{\frac{8}{3}} \right\}. \quad (1.2)$$

The main argument is that it is favourable to put all the mass of the unit cell at one concentration point, due to the strict binding inequality

$$J_{\mathbb{R}^3}(\lambda) < J_{\mathbb{R}^3}(\lambda') + J_{\mathbb{R}^3}(\lambda - \lambda')$$

that we prove in Section 3.1. Hence for the 2-periodic problem, when c is very large the 8 electrons of the double unit cell prefer to concentrate at only one point of mass 8, instead of 8 points of mass 1. This is the origin of the symmetry breaking for large c . Of course the exact same argument works for a union of n^3 unit cells.

Let us remark that the uniqueness of minimizers for the effective model $J_{\mathbb{R}^3}(\lambda)$ in (1.2) is an open problem that we discuss in Section 2.2. We can however prove that any non-negative solution of the corresponding nonlinear equation

$$-\Delta Q_\mu + c_{TF} Q_\mu^{\frac{7}{3}} - Q_\mu^{\frac{5}{3}} = -\mu Q_\mu$$

is unique and nondegenerate (up to translations). We conjecture (but are unable to prove) that the mass $\int Q_\mu^2$ is an increasing function of μ . This would imply uniqueness of minimizers and is strongly supported by numerical simulations. Under this conjecture we can prove that there are exactly 8 minimizers for c large enough, which are obtained one from each other by applying 1-translations.

The TFDW model studied in this paper is a very simple spinless empirical theory which approximates the true many-particle Schrödinger problem. The term $-\frac{3}{4}c \int \rho^{\frac{4}{3}}$ is an approximation to the *exchange-correlation energy* and c is only determined on empirical grounds. The exchange part was computed by Dirac [9] in 1930 using an infinite non-interacting Fermi gas leading to the value $c_D := \sqrt[3]{6q^{-1}\pi^{-1}}$, where q is the number of spin states. For the spinless model (i.e. $q = 1$) that we are studying, this gives $c_D \approx 1.24$, which corresponds to the constant 0.93 generally appearing in the literature, namely, $\frac{3}{4}c_D \approx 0.93$. It is natural to use a constant $c > c_D$ in order to account for correlation effects. On the other hand, the famous Lieb-Oxford inequality [35, 42, 26, 43] suggests to take $\frac{3}{4}c_D \leq 1.64$. It has been argued in [50, 52, 29] that for the classical interacting uniform electron gas one should use the value $\frac{3}{4}c \approx 1.44$ which is the energy of Jellium in the body-centered cubic (BCC) Wigner crystal and is implemented in the most famous Kohn-Sham functionals [51]. However, this has recently been questioned in [31] by Lewin and Lieb. In any case, all physically reasonable choices lead to c of the order of 1.

We have run some numerical simulations presented later in Section 2.3, using nuclei of (pseudo) charge $Z = 1$ on a BCC lattice of side-length 4\AA . We found that symmetry breaking occurs at about $c \approx 3.3$. More precisely, the 2-periodic ground state was found to be 1-periodic if $c \lesssim 3.30$ but really 2-periodic for $c \gtrsim 3.31$. The numerical value $c \approx 3.3$ (which corresponds to $\frac{3}{4}c \approx 2.48$) obtained as critical constant in our numerical simulations is above the usual values chosen in the literature. However, it is of the same order of magnitude and this critical constant could be closer to 1 for other periodic arrangements of nuclei.

There exist various works on the TFDW model for N electrons on the whole space \mathbb{R}^3 . For example, Le Bris proved in [27] that there exists $\varepsilon > 0$ such that minimizers exist for $N < Z + \varepsilon$, improving the result for $N \leq Z$ by Lions [46]. It is also proved in [27] that minimizers are unique for c small enough if $N \leq Z$. Non existence if N is large enough and Z small enough has been proved by Nam and Van Den Bosch in [48].

On the other hand, symmetry breaking has been studied in many situations. For discrete models on lattices, the instability of solutions having the same periodicity as the lattice is proved in [14, 49] while [22, 37, 23, 40, 39, 41, 12, 15] prove for different models (and different dimensions) that the solutions have a different periodicity than the lattice. On finite domains and at zero temperature, symmetry breaking is proved in [54] for a one dimensional gas on a circle of finite length and in [53] on toruses and spheres in dimension $d \leq 3$. On the whole space \mathbb{R}^3 , symmetry breaking is proved in [2], namely, the minimizers are not radial for N large enough.

The paper is organized as follows. We present our main results for the periodic TFDW model and for the effective model, together with our numerical simulations, in Section 2. In Section 3, we study the effective model $J_{\mathbb{R}^3}(\lambda)$ on the whole space. Then, in Section 4, we prove our results for the regime of small c . Finally, we prove the symmetry breaking in the regime of large c in Section 5.

2. MAIN RESULTS

For simplicity, we restrict ourselves to the case of a cubic lattice with one atom of charge $Z = 1$ at the center of each unit cell. We denote by $\mathcal{L}_{\mathbb{K}}$ our lattice which is based on the natural basis and its unit cell is the cube $\mathbb{K} := [-\frac{1}{2}; \frac{1}{2}]^3$, which contains one atom of charge $Z = 1$ at the position $R = 0$. The Thomas–Fermi–Dirac–von Weizsäcker model we are studying is then the functional energy

$$\mathcal{E}_{\mathbb{K},c}(w) = \int_{\mathbb{K}} |\nabla w|^2 + \frac{3}{5}c_{TF} \int_{\mathbb{K}} |w|^{\frac{10}{3}} - \frac{3}{4}c \int_{\mathbb{K}} |w|^{\frac{8}{3}} + \frac{1}{2}D_{\mathbb{K}}(|w|^2, |w|^2) - \int_{\mathbb{K}} G_{\mathbb{K}}|w|^2, \quad (2.1)$$

on the unit cell \mathbb{K} . Here

$$D_{\mathbb{K}}(f, g) = \int_{\mathbb{K}} \int_{\mathbb{K}} f(x) G_{\mathbb{K}}(x - y) g(y) \, dy \, dx,$$

where $G_{\mathbb{K}}$ is the \mathbb{K} -periodic Coulomb potential which satisfies

$$-\Delta G_{\mathbb{K}} = 4\pi \left(\sum_{k \in \mathcal{L}_{\mathbb{K}}} \delta_k - 1 \right) \quad (2.2)$$

and is uniquely defined up to a constant that we fix by imposing $\min_{x \in \mathbb{K}} G_{\mathbb{K}}(x) = 0$.

We are interested in the behavior when c varies of the minimization problem

$$E_{\mathbb{K}, \lambda}(c) = \inf_{\substack{w \in H_{\text{per}}^1(\mathbb{K}) \\ \|w\|_{L^2(\mathbb{K})}^2 = \lambda}} \mathcal{E}_{\mathbb{K}, c}(w), \quad (2.3)$$

where the subscript *per* stands for \mathbb{K} -periodic boundary conditions. We want to emphasize that even if the true \mathbb{K} -periodic TFDW model requires that $\lambda = Z$ (see [7]), we study it for any λ in this paper.

Finally, for any $N \in \mathbb{N} \setminus \{0\}$, we denote by $N \cdot \mathbb{K}$ the union of N^3 cubes \mathbb{K} forming the cube $N \cdot \mathbb{K} = \left[-\frac{N}{2}, \frac{N}{2}\right]^3$. The N^3 charges are then located at the positions

$$\{R_j\}_{1 \leq j \leq N^3} \subset \left\{ \left(n_1 - \frac{N+1}{2}, n_2 - \frac{N+1}{2}, n_3 - \frac{N+1}{2} \right) \mid n_i \in \mathbb{N} \cap [1; N] \right\}.$$

2.1. Symmetry breaking. The main results presented in this paper are the two following theorems.

Theorem 1 (Uniqueness for small c). *Let \mathbb{K} be the unit cube and c_{TF}, λ be two positive constants. There exists $\delta > 0$ such that for any $0 \leq c < \delta$, the following holds:*

- i. *The minimizer w_c of the periodic TFDW problem $E_{\mathbb{K}, \lambda}(c)$ in (2.3) is unique, up to a phase factor. It is non constant, strictly positive, in $H_{\text{per}}^2(\mathbb{K})$ and the unique ground-state eigenfunction of the \mathbb{K} -periodic self-adjoint operator*

$$H_c := -\Delta + c_{TF} |w_c|^{\frac{4}{3}} - c |w_c|^{\frac{2}{3}} - G_{\mathbb{K}} + (|w_c|^2 \star G_{\mathbb{K}}).$$

- ii. *This \mathbb{K} -periodic function w_c is the unique minimizer of all of the $(N \cdot \mathbb{K})$ -periodic TFDW problems $E_{N \cdot \mathbb{K}, N^3 \lambda}(c)$, for any integer $N \geq 1$.*

Theorem 2 (Symmetry breaking for large c). *Let \mathbb{K} be the unit cube, c_{TF}, λ be two positive constants, and $N \geq 2$ be an integer. For c large enough, symmetry breaking occurs:*

$$E_{N \cdot \mathbb{K}, N^3 \lambda}(c) < N^3 E_{\mathbb{K}, \lambda}(c).$$

Precisely, the periodic TFDW problem $E_{N \cdot \mathbb{K}, N^3 \lambda}(c)$ on $N \cdot \mathbb{K}$ admits (at least) N^3 distinct non-negative minimizers which are obtained one from each other by applying translations of the lattice $\mathcal{L}_{\mathbb{K}}$. Denoting w_c any one of these minimizers, there exists a subsequence $c_n \rightarrow \infty$ such that

$$c_n^{-\frac{3}{2}} w_n \left(R + \frac{\cdot}{c_n} \right) \xrightarrow[n \rightarrow \infty]{} Q, \quad (2.4)$$

strongly in $L_{\text{loc}}^p(\mathbb{R}^3)$ for $2 \leq p < +\infty$, with R the position of one of the N^3 charges in $N \cdot \mathbb{K}$. Here Q is a minimizer of the variational problem for the effective model

$$J_{\mathbb{R}^3}(N^3 \lambda) = \inf_{\substack{u \in H^1(\mathbb{R}^3) \\ \|u\|_{L^2(\mathbb{R}^3)}^2 = N^3 \lambda}} \left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{R}^3} |u|^{\frac{10}{3}} - \frac{3}{4} \int_{\mathbb{R}^3} |u|^{\frac{8}{3}} \right\}, \quad (2.5)$$

which must additionally minimize

$$S(N^3\lambda) = \inf_v \left\{ \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|v(x)|^2 |v(y)|^2}{|x-y|} dy dx - \int_{\mathbb{R}^3} \frac{|v(x)|^2}{|x|} dx \right\}, \quad (2.6)$$

where the minimization is performed among all possible minimizers of (2.5). Finally, when $c \rightarrow \infty$, $E_{N\cdot\mathbb{K}, N^3\lambda}(c)$ has the expansion

$$E_{N\cdot\mathbb{K}, N^3\lambda}(c) = c^2 J_{\mathbb{R}^3}(N^3\lambda) + cS(N^3\lambda) + o(c). \quad (2.7)$$

Theorem 1 will be proved in Section 4 while Section 5 will be dedicated to the proof of Theorem 2. A natural question that comes with Theorem 2 is to know if c needs to be really large for the symmetry breaking to happen. We present some numerical answers to this question later in Section 2.3. Notice that the inequality $E_{N\cdot\mathbb{K}, N^3\lambda}(c) < N^3 E_{\mathbb{K}, \lambda}(c)$ in Theorem 2 is an immediate consequence of the first order expansion in (2.7)

$$E_{N\cdot\mathbb{K}, N^3\lambda}(c) = c^2 J_{\mathbb{R}^3}(N^3\lambda) + o(c^2)$$

which is proved in Proposition 24, since one has $J_{\mathbb{R}^3}(N^3\lambda) < N^3 J_{\mathbb{R}^3}(\lambda)$ as it will be proved in Proposition 12 of Section 3.

Remark (Generalizations). For simplicity we have chosen to deal with a cubic lattice with one nucleus of charge 1 per unit cell, but the exact same results hold in a more general situation. We can take a charge Z larger than 1, several charges (of different values) per unit cell and a more general lattice than \mathbb{Z}^3 . More precisely, the \mathbb{K} -periodic Coulomb potential $G_{\mathbb{K}}$ appearing in (2.1), in both $D_{\mathbb{K}}$ and $\int G|w|^2$, should then verify

$$-\Delta G_{\mathbb{K}} = 4\pi \left(\sum_{k \in \mathcal{L}_{\mathbb{K}}} \delta_k - \frac{1}{|\mathbb{K}|} \right),$$

and the term $\int_{\mathbb{K}} G_{\mathbb{K}} |w|^2$ should be replaced by $\int_{\mathbb{K}} \sum_{i=1}^{N_q} z_i G_{\mathbb{K}}(\cdot - R_i) |w|^2$ where z_i and R_i are the charges and locations of the N_q nuclei in the unit cell \mathbb{K} .

Finally, in Theorem 2, denoting by $z_+ := \max_{1 \leq i \leq N_q} \{z_i\} > 0$ the largest charge inside \mathbb{K} and by $N_+ \geq 1$ the number of charges inside \mathbb{K} that are equal to z_+ , the location R would now be one of the $N_+ \mathbb{K}^3$ positions of charges z_+ — which means that the minimizer concentrate on one of the nuclei with largest charge — and S would be replaced by

$$S(\lambda) = \inf_v \left\{ \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|v(x)|^2 |v(y)|^2}{|x-y|} dy dx - z_+ \int_{\mathbb{R}^3} \frac{|v(x)|^2}{|x|} dx \right\}.$$

2.2. Study of the effective model in \mathbb{R}^3 . We present in this section the effective model in the whole space \mathbb{R}^3 . We want to already emphasize that the uniqueness of minimizers for this problem is an open difficult question as we will explain later in this section.

The functional to be considered is

$$u \mapsto \mathcal{J}_{\mathbb{R}^3}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{R}^3} |u|^{\frac{10}{3}} - \frac{3}{4} \int_{\mathbb{R}^3} |u|^{\frac{8}{3}} \quad (2.8)$$

and the minimization problem (2.5) is

$$J_{\mathbb{R}^3}(\lambda) = \inf_{\substack{u \in H^1(\mathbb{R}^3) \\ \|u\|_{L^2(\mathbb{R}^3)}^2 = \lambda}} \mathcal{J}_{\mathbb{R}^3}(u). \quad (2.9)$$

The first important result for this effective model is about the existence of minimizers and the fact that they are radial decreasing. We state those results in the following theorem, the proof of which is the subject of Section 3.1.

Theorem 3 (Existence of minimizers for the effective model in \mathbb{R}^3). *Let $c_{TF} > 0$ and $\lambda > 0$ be fixed constants.*

- i. *There exist minimizers for $J_{\mathbb{R}^3}(\lambda)$. Up to a phase factor and a space translation, any minimizer Q is a positive radial strictly decreasing $H^2(\mathbb{R}^3)$ -solution of*

$$-\Delta Q + c_{TF}|Q|^{\frac{4}{3}}Q - |Q|^{\frac{2}{3}}Q = -\mu Q. \quad (2.10)$$

Here $-\mu < 0$ is simple and is the smallest eigenvalue of the self-adjoint operator $H_Q := -\Delta + c_{TF}|Q|^{\frac{4}{3}} - |Q|^{\frac{2}{3}}$.

- ii. *We have the strictly binding inequality*

$$\forall 0 < \lambda' < \lambda, \quad J_{\mathbb{R}^3}(\lambda) < J_{\mathbb{R}^3}(\lambda') + J_{\mathbb{R}^3}(\lambda - \lambda'). \quad (2.11)$$

- iii. *For any minimizing sequence $(Q_n)_n$ of $J_{\mathbb{R}^3}(\lambda)$, there exists $\{x_n\} \subset \mathbb{R}^3$ such that $Q_n(\cdot - x_n)$ strongly converges in $H^1(\mathbb{R}^3)$ to a minimizer, up to the extraction of a subsequence.*

An important result about the effective model on \mathbb{R}^3 is the following result giving the uniqueness and the non-degeneracy of positive solutions Q to the Euler–Lagrange equation (2.10) for any admissible $\mu > 0$. The proof of this theorem is the subject of Section 3.2.

Theorem 4 (Uniqueness and non-degeneracy of positive solutions). *Let $c_{TF} > 0$. If $\frac{64}{15}c_{TF}\mu \geq 1$, then the Euler–Lagrange equation (2.10) has no non-trivial solution in $H^1(\mathbb{R}^3)$. For $0 < \frac{64}{15}c_{TF}\mu < 1$, the Euler–Lagrange equation (2.10) has, up to translations, a unique non-negative solution $Q_\mu \neq 0$ in $H^1(\mathbb{R}^3)$. This solution is radial decreasing and non-degenerate: the linearized operator*

$$L_\mu^+ = -\Delta + \frac{7}{3}c_{TF}|Q_\mu|^{\frac{4}{3}} - \frac{5}{3}|Q_\mu|^{\frac{2}{3}} + \mu \quad (2.12)$$

with domain $H^2(\mathbb{R}^3)$ and acting on $L^2(\mathbb{R}^3)$ has the kernel

$$\text{Ker } L_\mu^+ = \text{span} \{ \partial_{x_1} Q_\mu, \partial_{x_2} Q_\mu, \partial_{x_3} Q_\mu \}. \quad (2.13)$$

Note that the condition $\frac{64}{15}c_{TF}\mu \geq 1$ comes directly from Pohozaev’s identity, see e.g. [3].

Remark. *The linearized operator L_μ for the equation (2.10) at Q_μ is*

$$L_\mu h = -\Delta h + \left(c_{TF}|Q_\mu|^{\frac{4}{3}} - |Q_\mu|^{\frac{2}{3}} \right) h + \left(\frac{2}{3}c_{TF}|Q_\mu|^{\frac{4}{3}} - \frac{1}{3}|Q_\mu|^{\frac{2}{3}} \right) (h + \bar{h}) + \mu h.$$

Note that it is not \mathbb{C} -linear. Separating its real and imaginary parts, it is convenient to rewrite it as

$$L_\mu = \begin{pmatrix} L_\mu^+ & 0 \\ 0 & L_\mu^- \end{pmatrix},$$

where L_μ^+ is as in (2.12) while L_μ^- is the operator

$$L_\mu^- = -\Delta + c_{TF}|Q_\mu|^{\frac{4}{3}} - |Q_\mu|^{\frac{2}{3}} + \mu = H_{Q_\mu} + \mu. \quad (2.14)$$

The result about the lowest eigenvalue of the operator H_Q in Theorem 3 exactly gives that $\text{Ker } L_\mu^- = \text{span} \{ Q_\mu \}$. Hence, Theorem 4 implies that

$$\text{Ker } L_\mu = \text{span} \left\{ \begin{pmatrix} 0 \\ Q_\mu \end{pmatrix}, \begin{pmatrix} \partial_{x_1} Q_\mu \\ 0 \end{pmatrix}, \begin{pmatrix} \partial_{x_2} Q_\mu \\ 0 \end{pmatrix}, \begin{pmatrix} \partial_{x_3} Q_\mu \\ 0 \end{pmatrix} \right\}.$$

The natural step one would like to perform now is to deduce the uniqueness of minimizers from the uniqueness of Euler–Lagrange positive solutions as it has been done for many equations [34, 60, 28, 10, 11, 55]. An argument of this type relies on the fact that $\mu \mapsto M(\mu) := \|Q_\mu\|_{L^2(\mathbb{R}^3)}^2$ is a bijection, which is an easy result for models with trivial scalings like the nonlinear Schrödinger equation with only

one power nonlinearity. However, for the effective problem of this section, we are unable to prove that this mapping is a bijection.

In [24], Killip, Oh, Pocovnicu and Visan study extensively a similar problem with another non-linearity including two powers, namely the *cubic-quintic NLS on \mathbb{R}^3* which is associated with the energy

$$\int_{\mathbb{R}^3} \frac{1}{2} |\nabla u|^2 + \frac{1}{6} |u|^6 - \frac{1}{4} |u|^4. \quad (2.15)$$

They discussed at length the question of uniqueness of minimizers and could also not solve it for their model. An important difference between (2.15) and effective problem of this section is that the map $\mu \mapsto M(\mu)$ is for sure not a bijection in their case. But it is conjectured to be one if one only retains *stable* solutions [24, Conjecture 2.6].

If we cannot prove uniqueness of minimizers, we can nevertheless prove that for any mass $\lambda > 0$ there is a finite number of μ 's in $(0; \frac{15}{64c_{TF}})$ for which the unique positive solution to the associated Euler–Lagrange problem has a mass equal to λ and, consequently, that there is a finite number of minimizers of the TFDW problem for any given mass constraint.

Proposition 5. *Let $\lambda > 0$ and $c_{TF} > 0$. There exist finitely many μ 's for which the mass $M(\mu)$ of Q_μ is equal to λ .*

Proof of Proposition 5. By Theorem 3, we know that for any mass constraint $\lambda \in (0, +\infty)$, there exist at least one minimizer to the corresponding $J_{\mathbb{R}^3}(\lambda)$ minimization problem. Therefore, for any $\lambda \in (0, +\infty)$, there exists at least one μ such that the unique positive solution Q_μ to the associated Euler–Lagrange equation is a minimizer of $J_{\mathbb{R}^3}(\lambda)$ and thus is of mass $M(\mu) = \lambda$. We therefore obtain that $(0; \frac{15}{64c_{TF}}) \ni \mu \mapsto M(\mu) \in (0; +\infty)$ is onto. Moreover, this map is real-analytic since the non-degeneracy in Theorem 4 and the analytic implicit function theorem give that $\mu \mapsto Q_\mu$ is real analytic. The map M being onto and real-analytic, then for any $\lambda \in (0; +\infty)$ there exists a finite number of μ 's, which are all in $(0; \frac{15}{64c_{TF}})$, such that the mass $M(\mu)$ of the unique positive solution Q_μ is equal to λ . \square

We have performed some numerical computations of the solution Q_μ and the results strongly support the uniqueness of minimizers since M was found to be increasing, see Figure 1.

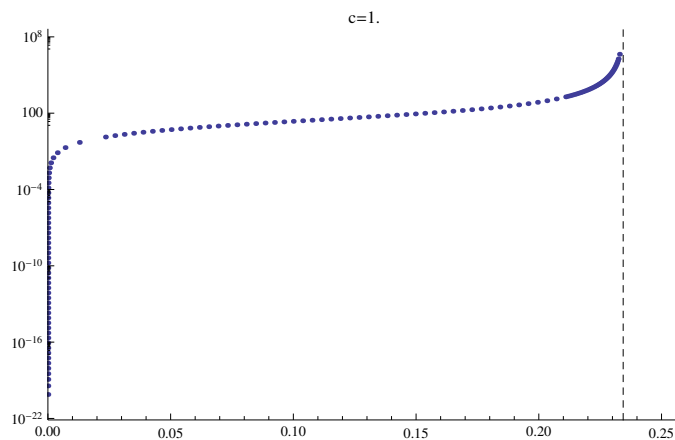


FIGURE 1. Plot of $\mu \mapsto \ln(M(\mu))$ on $(0; \frac{15}{64c_{TF}})$.

Conjecture 6. *The function*

$$\begin{aligned} \left(0; \frac{15}{64c_{TF}}\right) &\rightarrow (0; +\infty) \\ \mu &\mapsto M(\mu) \end{aligned} \quad (2.16)$$

is strictly increasing and one-to-one. Consequently, for any $0 < \mu < \frac{15}{64c_{TF}}$, there exists a unique minimizer Q_μ of $J_{\mathbb{R}^3}(\lambda)$, up to a phase and a space translation.

Remark. *Following the method of [24], one can prove there exist $C, C' > 0$ such that $M(\mu) = C\mu^{\frac{3}{2}} + o(\mu^{\frac{3}{2}})_{\mu \rightarrow 0^+}$ and $M(\mu) = C'(\mu - \mu_*)^{-3} + o((\mu - \mu_*)^{-3})_{\mu \rightarrow \mu_*^-}$ where $\mu_* = \frac{15}{64c_{TF}}$.*

This conjecture on M is related to the stability condition on $(L_\mu^+)^{-1}$ that appears in works like [61, 19]. Indeed, differentiating the Euler–Lagrange equation (2.10) with respect to μ , we obtain that $L_\mu^+(\frac{dQ_\mu}{d\mu}) = -Q_\mu$ which thus leads to

$$\frac{d}{d\mu} \int Q_\mu^2 = 2 \left\langle Q_\mu, \frac{dQ_\mu}{d\mu} \right\rangle = -2 \left\langle Q_\mu, (L_\mu^+)^{-1} Q_\mu \right\rangle.$$

Thus our conjecture is that $\langle Q_\mu, (L_\mu^+)^{-1} Q_\mu \rangle < 0$ for all $0 < \mu < \frac{15}{64c_{TF}}$ and this corresponds to the fact that all the solutions are local strict minimizers.

Theorem 7. *If Conjecture 6 holds then, for c large enough, there are exactly N^3 non-negative minimizers for the periodic TFDW problem $E_{N \cdot \mathbb{K}, N^3 \lambda}(c)$.*

The proof of Theorem 7 is the subject of Section 5.4.

2.3. Numerical simulations. The occurrence of symmetry breaking is an important question in practical calculations. Concerning the general behavior of DFT on this matter, we refer to the discussion in [59] and the references therein.

Our numerical simulations have been run using the software *PROFESS v.3.0* [8] which is based on pseudo-potentials (see Remark 8 below): we have used a (BCC) Lithium crystal of side-length 4Å (in order to be physically relevant as the two first alkali metals Lithium and Sodium organize themselves on BCC lattices with respective side length 3.51Å and 4.29Å) for which one electron is treated while the two others are included in the pseudo-potential, simulating therefore a lattice of pseudo-atoms with pseudo-charge $Z = \lambda = 1$. The relative gain of energy of 2-periodic minimizers compared to 1-periodic ones is plotted in Figure 2. Symmetry breaking occurs at about $c \approx 3.30$ which corresponds to $\frac{3}{4}c \approx 2.48$. More precisely, minimizing the $2 \cdot \mathbb{K}$ problem and the $1 \cdot \mathbb{K}$ problem result in the same minimum energy (up to a factor 8) if $c \lesssim 3.30$ while, for $c \gtrsim 3.31$, we have found (at least) one 2-periodic function for which the energy is lower than the minimal energy for the $1 \cdot \mathbb{K}$ problem.

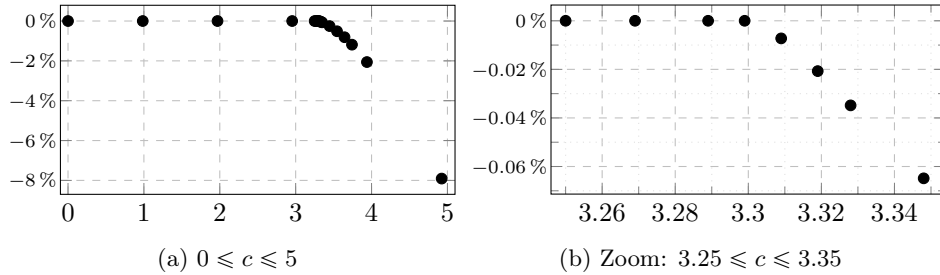


FIGURE 2. Relative gain of energy $\frac{8E_{\mathbb{K},\lambda}(c) - E_{2 \cdot \mathbb{K}, 8\lambda}(c)}{8E_{\mathbb{K},\lambda}(c)}$.

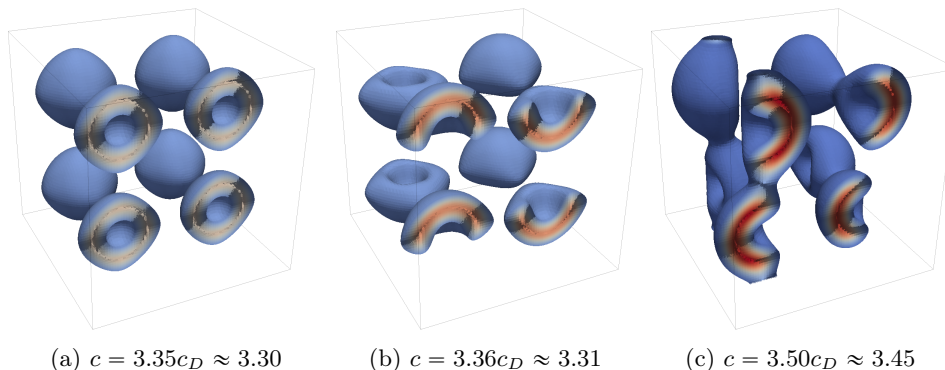


FIGURE 3. Electron density for $Z = 1$ and length side 4\AA . Same "dark-blue to white to dark-red" density scale for (a), (b) and (c).

- (a) The computed 2-periodic minimizer is still 1-periodic.
 (b-c) The computed 2-periodic minimizer is not 1-periodic.

The plots of the computed minimizers presented in Figure 3 visually confirm the symmetry breaking. They also suggest that the electronic density is very much concentrated. However, since the computation uses pseudo-potentials, only one outer shell electron is computed and the density is sharp on an annulus for these values of c .

The numerical value of the critical constant $\frac{3}{4}c \approx 2.48$ obtained in our numerical simulations is outside the usual values $\frac{3}{4}c \in [0.93; 1.64]$ chosen in the literature. However, it is of the same order of magnitude and one cannot exclude that symmetry breaking would happen inside this range for different systems, meaning for different values of Z and/or of the size of the lattice.

Remark 8 (Pseudo-potentials). *The software PROFESS v.3.0 that we used in our simulations is based on pseudo-potentials [21]. This means that only n outer shell electrons among the N electrons of the unit cell are considered. The $N - n$ other ones are described through a pseudo-potential, together with the nucleus. Mathematically, this means that we have $\lambda = n$ and that the nucleus-electron interaction $-N \int_{\mathbb{K}} G_{\mathbb{K}} |w|^2$ is replaced by $-\int_{\mathbb{K}} G_{ps} |w|^2$ where the \mathbb{K} -periodic function $G_{ps}(x)$ behaves like $n/|x|$ when $|x| \rightarrow 0$. All our results apply to this case as well. More precisely, we only need that $G_{ps}(x) - n/|x|$ is bounded on \mathbb{K} . We emphasize that the electron-electron interaction $D_{\mathbb{K}}$ is not changed by this generalization, and still involves the periodic Coulomb potential $G_{\mathbb{K}}$.*

3. THE EFFECTIVE MODEL IN \mathbb{R}^3

This section is dedicated to the proof of Theorem 3 and Theorem 4. We first give a lemma on the functional $\mathcal{J}_{\mathbb{R}^3}$, which has been defined in (2.8).

Lemma 9. *For $c_{TF}, \lambda > 0$ and $u \in H^1(\mathbb{R}^3)$ such that $\|u\|_2^2 = \lambda$, we have*

$$\mathcal{J}_{\mathbb{R}^3}(u) \geq \|\nabla u\|_{L^2(\mathbb{R}^3)}^2 - \frac{15}{64} \frac{\lambda}{c_{TF}}. \quad (3.1)$$

Proof of Lemma 9. By Hölder's inequality

$$\|u\|_{2\mu}^{2\mu(\delta-1)} \leq \lambda^{\delta-\mu} \|u\|_{2\delta}^{2\delta(\mu-1)}, \quad \forall 1 \leq \mu \leq \delta \leq 3,$$

where, for shortness, we write $\|\cdot\|_p$ instead of $\|\cdot\|_{L^p(\mathbb{R}^3)}$, we conclude that

$$\frac{3}{5} c_{TF} \|u\|_{\frac{10}{3}}^{\frac{10}{3}} - \frac{3}{4} \|u\|_{\frac{10}{3}}^{\frac{10}{3}} \geq \frac{3c_{TF}}{5\lambda} \left[\left(\|u\|_{\frac{10}{3}}^{\frac{10}{3}} - \frac{5\lambda}{8c_{TF}} \right)^2 - \frac{25\lambda^2}{64c_{TF}^2} \right] \geq -\frac{15\lambda}{64c_{TF}}.$$

□

We deduce from this some preliminary properties for the effective model in \mathbb{R}^3 .

Lemma 10 (A priori properties of $J_{\mathbb{R}^3}(\lambda)$). *Let c_{TF} and λ be positive constants. We have*

$$-\frac{15}{64} \frac{\lambda}{c_{TF}} < J_{\mathbb{R}^3}(\lambda) < 0. \quad (3.2)$$

The function, $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$ is continuous on $[0; +\infty)$.

Proof of Lemma 10. The negativity of $J_{\mathbb{R}^3}(\lambda)$ is obtained by taking ν large enough in the computation of $\mathcal{J}_{\mathbb{R}^3}(\nu^{-\frac{3}{2}}u(\nu^{-1}\cdot))$. Lemma 9 gives the lower bound in (3.2), which implies the continuity at $\lambda = 0$. Moreover, after scaling, we have

$$J_{\mathbb{R}^3}(\lambda) = \lambda \underbrace{\inf_{\substack{u \in H^1(\mathbb{R}^3) \\ \|u\|_{L^2(\mathbb{R}^3)}^2 = 1}} \left\{ \lambda^{-\frac{2}{3}} \|\nabla u\|_{L^2(\mathbb{R}^3)}^2 + \frac{3}{5} c_{TF} \|u\|_{L^{\frac{10}{3}}(\mathbb{R}^3)}^{\frac{10}{3}} - \frac{3}{4} \|u\|_{L^{\frac{8}{3}}(\mathbb{R}^3)}^{\frac{8}{3}} \right\} \\ =: F(\lambda^{-2/3})$$

where F is concave on $[0; +\infty)$ hence continuous on $(0; +\infty)$. This shows that $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$ is continuous as well. □

3.1. Proof of Theorem 3. We divide the proof into several steps for clarity.

Step 1: Large binding inequality.

Lemma 11. *Let $c_{TF} \geq 0$ be a constant. Then*

$$J_{\mathbb{R}^3}(\lambda) \leq J_{\mathbb{R}^3}(\lambda') + J_{\mathbb{R}^3}(\lambda - \lambda'), \quad \forall 0 \leq \lambda' \leq \lambda \quad (3.3)$$

Consequently, $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$ is strictly decreasing on $[0; +\infty)$.

Proof of Lemma 11. The inequality (3.3) is obtained by computing $\mathcal{J}_{\mathbb{R}^3}(\varphi + \chi)$ where φ and χ are two bubbles of disjoint compact supports and of respective masses λ' and $\lambda - \lambda'$. The strict monotonicity follows by Lemma 10. □

Remark. *The strict inequality in (3.3), which is important for applying Lions' concentration-compactness method, actually holds and is proved later in Proposition 12.*

Step 2: For any $\lambda > 0$, $J_{\mathbb{R}^3}(\lambda)$ has a minimizer. This is a classical result to which we will only give a sketch of proof (for a detailed proof, see [56]). First, by rearrangement inequalities, we have $\mathcal{J}_{\mathbb{R}^3}(v) \geq \mathcal{J}_{\mathbb{R}^3}(v^*)$ for every $v \in H^1(\mathbb{R}^3)$. Therefore, one can restrict the minimization to non-negative radial decreasing functions. By the compact embedding $H_{rad}^1(\mathbb{R}^3) \hookrightarrow L^p(\mathbb{R}^3)$, for $2 < p < 6$, we find

$$J_{\mathbb{R}^3}(\lambda') \leq \mathcal{J}_{\mathbb{R}^3}(Q) \leq \liminf \mathcal{J}_{\mathbb{R}^3}(Q_n) = J_{\mathbb{R}^3}(\lambda) \quad (3.4)$$

for a minimizing sequence $Q_n \rightharpoonup Q$ and where $\lambda' := \|Q\|_{L^2(\mathbb{R}^3)}^2 \leq \lambda$. Then, by Lemma 11, $\lambda' = \lambda$ and the limit is strong in $L^2(\mathbb{R}^3)$, hence in $H^1(\mathbb{R}^3)$ by classical arguments. This proves that the limit Q is a minimizer. The fact that the convergence is strong in $H^1(\mathbb{R}^3)$ is then a classical result.

Step 3: Any minimizer is in $H^2(\mathbb{R}^3)$ and solves the E-L equation (2.10). The proof that any minimizer solves the Euler–Lagrange equation is classical and implies, together with $u \in H^1(\mathbb{R}^3)$, that $u \in H^2(\mathbb{R}^3)$ by elliptic regularity. Moreover, we have

$$\mu = - \frac{\|\nabla Q\|_{L^2(\mathbb{R}^3)}^2 + c_{TF} \|Q\|_{L^{\frac{10}{3}}(\mathbb{R}^3)}^{\frac{10}{3}} - \|Q\|_{L^{\frac{8}{3}}(\mathbb{R}^3)}^{\frac{8}{3}}}{\lambda}. \quad (3.5)$$

Step 4: Strict binding inequality.

Proposition 12. *Let $c_{TF} > 0$ and $\lambda > 0$.*

$$\forall 0 < \lambda' < \lambda, J_{\mathbb{R}^3}(\lambda) < J_{\mathbb{R}^3}(\lambda') + J_{\mathbb{R}^3}(\lambda - \lambda'). \quad (2.11)$$

In particular, for any integer $N \geq 2$,

$$J_{\mathbb{R}^3}(N^3\lambda) < N^3 J_{\mathbb{R}^3}(\lambda) < 0. \quad (3.6)$$

Proof of Proposition 12. By the same scaling as in Lemma 10, we have

$$J_{\mathbb{R}^3}(\lambda) = \lambda \inf_{\substack{u \in H^1(\mathbb{R}^3) \\ \|u\|_{L^2(\mathbb{R}^3)}^2 = 1}} \underbrace{\left\{ \lambda^{-\frac{2}{3}} \|\nabla u\|_{L^2(\mathbb{R}^3)}^2 + \frac{3}{5} c_{TF} \|u\|_{L^{\frac{10}{3}}(\mathbb{R}^3)}^{\frac{10}{3}} - \frac{3}{4} \|u\|_{L^{\frac{8}{3}}(\mathbb{R}^3)}^{\frac{8}{3}} \right\}}_{=: \mathcal{F}_\lambda(u)}. \quad (3.7)$$

Let $\lambda > \lambda' > 0$. By Step 2, the minimization problem

$$\inf_{\substack{u \in H^1(\mathbb{R}^3) \\ \|u\|_{L^2(\mathbb{R}^3)}^2 = 1}} \left\{ \|\nabla u\|_{L^2(\mathbb{R}^3)}^2 + \frac{3}{5} c_{TF} \lambda'^{\frac{2}{3}} \|u\|_{L^{\frac{10}{3}}(\mathbb{R}^3)}^{\frac{10}{3}} - \frac{3}{4} \lambda'^{\frac{2}{3}} \|u\|_{L^{\frac{8}{3}}(\mathbb{R}^3)}^{\frac{8}{3}} \right\}$$

has a minimizer $Q_{\lambda'}$ which, by Step 3, is in $H^2(\mathbb{R}^3)$ thus continuous. In particular, $\|\nabla Q_{\lambda'}\|_{L^2(\mathbb{R}^3)} > 0$ thus $\mathcal{F}_{\lambda'}(Q_{\lambda'}) > \mathcal{F}_\lambda(Q_{\lambda'})$, where \mathcal{F}_λ is defined in (3.7). Therefore

$$J_{\mathbb{R}^3}(\lambda') = \lambda' \mathcal{F}_{\lambda'}(Q_{\lambda'}) > \lambda' \mathcal{F}_\lambda(Q_{\lambda'}) = \frac{\lambda'}{\lambda} \mathcal{J}_{\mathbb{R}^3}(Q_{\lambda'}(\lambda^{-1/3} \cdot)) \geq \frac{\lambda'}{\lambda} J_{\mathbb{R}^3}(\lambda),$$

and we finally obtain

$$J_{\mathbb{R}^3}(\lambda - \lambda') + J_{\mathbb{R}^3}(\lambda') > \frac{\lambda - \lambda'}{\lambda} J_{\mathbb{R}^3}(\lambda) + \frac{\lambda'}{\lambda} J_{\mathbb{R}^3}(\lambda) = J_{\mathbb{R}^3}(\lambda),$$

as we wanted. \square

Step 5: $-\mu < 0$. Let us choose v in the minimization domain of $J_{\mathbb{R}^3}(1)$. Then, defining the positive number

$$\alpha_0 = \frac{3}{8} \frac{\|v\|_{8/3}^{8/3} \lambda^{1/3}}{\|\nabla v\|_2^2 + \frac{3}{5} c_{TF} \|v\|_{10/3}^{10/3} \lambda^{2/3}},$$

we can obtain for any $\lambda > 0$ an upper bound on $J_{\mathbb{R}^3}(\lambda)$. Namely

$$J_{\mathbb{R}^3}(\lambda) \leq \mathcal{J}_{\mathbb{R}^3} \left(\sqrt{\lambda} \alpha_0^{3/2} v(\alpha_0 \cdot) \right) = -\frac{9}{64} \lambda^{5/3} \frac{\|v\|_{8/3}^{16/3}}{\|\nabla v\|_2^2 + \frac{3}{5} c_{TF} \|v\|_{10/3}^{10/3} \lambda^{2/3}}. \quad (3.8)$$

Moreover, for all ε and for Q a minimizer to $J_{\mathbb{R}^3, c}(\lambda)$, we have

$$\mathcal{J}_{\mathbb{R}^3}((1 - \varepsilon)Q) = \mathcal{J}_{\mathbb{R}^3}(Q) + 2\varepsilon\lambda\mu + O(\varepsilon^2),$$

which leads, together with (3.3) and the fact that Q is a minimizer of $J_{\mathbb{R}^3}(\lambda)$, to

$$2\varepsilon\lambda\mu + O(\varepsilon^2) \geq J_{\mathbb{R}^3}((1 - \varepsilon)^2\lambda) - J_{\mathbb{R}^3}(\lambda) \geq -J_{\mathbb{R}^3}(\varepsilon(2 - \varepsilon)\lambda),$$

for any $\varepsilon \in (0; 2)$. Using this last inequality together with the upper bound (3.8), we get for any $\varepsilon \in (0; 1)$ that

$$2\lambda\mu \geq \frac{9}{64} \varepsilon^{2/3} (2 - \varepsilon)^{5/3} \lambda^{5/3} \frac{\|v\|_{8/3}^{16/3}}{\|\nabla v\|_2^2 + \frac{3}{5} c_{TF} \|v\|_{10/3}^{10/3} \varepsilon^{2/3} (2 - \varepsilon)^{2/3} \lambda^{2/3}} + O(\varepsilon)$$

which leads to $\mu > 0$ by taking ε small enough.

Step 6: Positivity of non-negative minimizers. Let $Q \geq 0$ be a minimizer. By Step 3, $0 \neq Q \in H^2(\mathbb{R}^3) \subset C_0^0(\mathbb{R}^3)$ and $W := c_{TF}|Q|^{\frac{4}{3}} - |Q|^{\frac{2}{3}} + \mu$ is in $L^\infty(\mathbb{R}^3)$. Therefore, the Euler–Lagrange equation gives $Q > 0$ thanks to [38, Theorem 9.10].

Step 7: Non-negative minimizers are radial strictly decreasing up to translations. This step is a consequence of Step 6 and is the subject of the following proposition.

Proposition 13. *Let $\lambda > 0$. Any positive minimizer to $J_{\mathbb{R}^3}(\lambda)$ is radial strictly decreasing, up to a translation.*

Proof of Proposition 13. Let $0 \leq Q \in H^1(\mathbb{R}^3; \mathbb{R})$ be a minimizer of $J_{\mathbb{R}^3}(\lambda)$. We denote by Q^* its Schwarz rearrangement which is, as mentioned in first part of Step 2, also a minimizer and, consequently, $\int_{\mathbb{R}^3} |\nabla Q^*|^2 = \int_{\mathbb{R}^3} |\nabla Q|^2$. Moreover, by Step 3 and Step 6, $Q > 0$ and $Q^* > 0$ are in $H^2(\mathbb{R}^3; \mathbb{R})$ and solutions of the Euler–Lagrange equation (2.10). They are therefore real-analytic (see e.g. [47]) which implies that $|\{x|Q(x) = t\}| = |\{x|Q^*(x) = t\}| = 0$ for any t . In particular, the radial non-increasing function Q^* is in fact radial strictly decreasing. We then use [6, Theorem 1.1] to obtain $Q^* = Q$ a.e., up to a translation. Finally, Q and Q^* being continuous, the equality holds in fact everywhere. \square

Step 8: $-\mu$ is the lowest eigenvalue of H_Q , is simple, and $Q = z|Q|$. It is classical that the first eigenvalue of a Schrödinger operator $-\Delta + V$ is non-degenerate and that any non-negative eigenfunction must be the first, see e.g. [38, Chapter 11].

Step 9: Minimizing sequences are precompact up to a translations. Since the strict binding inequality (2.11) holds, this follows from a result of Lions in [45, Theorem I.2].

This concludes the proof of Theorem 3. \square

3.2. Proof of Theorem 4. The uniqueness of radial solutions has been proved by Serrin and Tang in [58]. However, we need the non-degeneracy of the solution. Both uniqueness and non-degeneracy can be proved following line by line the method in [32, Thm. 2] (the argument is detailed in [56]). One slight difference is the application of the moving plane method to prove that positive solutions are radial. Contrarily to [32] we cannot use [17, Thm. 2] because our function

$$F_\mu(y) = -c_{TF}y^{\frac{7}{3}} + y^{\frac{5}{3}} - \mu y \quad (3.9)$$

is not C^2 . However, given that non-negative solutions are positive, one can show that they are C^∞ and, therefore, we can apply [33, Thm. 1.1]. \square

4. REGIME OF SMALL c : UNIQUENESS OF THE MINIMIZER TO $E_{\mathbb{K},\lambda}(c)$

We first give some useful properties of $G_{\mathbb{K}}$ in the following lemma.

Lemma 14 (The periodic Coulomb potential $G_{\mathbb{K}}$). *The function $G_{\mathbb{K}} - |\cdot|^{-1}$ is bounded on \mathbb{K} . Thus, there exists C such that for any $x \in \mathbb{K} \setminus \{0\}$, we have*

$$0 \leq G_{\mathbb{K}}(x) \leq \frac{C}{|x|}. \quad (4.1)$$

In particular, $G_{\mathbb{K}} \in L^p(\mathbb{K})$ for $1 \leq p < 3$. The Fourier transform of $G_{\mathbb{K}}$ is

$$\hat{G}_{\mathbb{K}}(\xi) = 4\pi \sum_{k \in \mathcal{L}_{\mathbb{K}}^* \setminus \{0\}} \frac{\delta_k(\xi)}{|k|^2} + \delta_0(\xi) \int_{\mathbb{K}} G_{\mathbb{K}}(x) dx \quad (4.2)$$

where $\mathcal{L}_{\mathbb{K}}^*$ is the reciprocal lattice of $\mathcal{L}_{\mathbb{K}}$. Hence, for any $f \neq 0$ for which $D_{\mathbb{K}}(f, f)$ is defined, we have $D_{\mathbb{K}}(f, f) > 0$.

Proof of Lemma 14. The first part follows from the fact that

$$\lim_{x \rightarrow 0} G_{\mathbb{K}}(x) - |x|^{-1} = M \in \mathbb{R},$$

see [44, VI.2]. The expression of the Fourier transform is a direct computation. \square

4.1. Existence of minimizers to $E_{\mathbb{K},\lambda}(c)$. In order to prove Theorem 1, we need the existence of minimizers to $E_{\mathbb{K},\lambda}(c)$, for any $c \geq 0$, which is done in this section.

Proposition 15 (Existence of minimizers to $E_{\mathbb{K},\lambda}(c)$). *Let \mathbb{K} be the unit cube and, $c_{TF} > 0$, $\lambda > 0$ and $c \geq 0$ be real constants.*

- i. There exists a non-negative minimizer to $E_{\mathbb{K},\lambda}(c)$ and any minimizing sequence $(w_n)_n$ strongly converges in $H_{per}^1(\mathbb{K})$ to a minimizer, up to extraction of a sub-sequence.*
- ii. Any minimizer w_c is in $H_{per}^2(\mathbb{K})$, is non-constant and solves the Euler–Lagrange equation*

$$\left(-\Delta + c_{TF}|w_c|^{\frac{4}{3}} - c|w_c|^{\frac{2}{3}} - G_{\mathbb{K}} + (|w_c|^2 \star G_{\mathbb{K}}) \right) w_c = -\mu_{w_c} w_c, \quad (4.3)$$

with

$$\mu_{w_c} = -\frac{\|\nabla w_c\|_2^2 + c_{TF} \|w_c\|_{10/3}^{10/3} - c \|w_c\|_{8/3}^{8/3} + D_{\mathbb{K}}(|w_c|^2, |w_c|^2) - \langle G_{\mathbb{K}}, |w_c|^2 \rangle_{L^2(\mathbb{K})}}{\lambda}. \quad (4.4)$$

- iii. Up to a phase factor, a minimizer w_c is positive and the unique ground-state eigenfunction of the self-adjoint operator, with domain $H_{per}^2(\mathbb{K})$,*

$$H_{w_c} := -\Delta + c_{TF}|w_c|^{\frac{4}{3}} - c|w_c|^{\frac{2}{3}} - G_{\mathbb{K}} + (|w_c|^2 \star G_{\mathbb{K}}).$$

Since the problem is posed on a bounded domain, this is a classical result to which we only give a sketch of proof. For a detailed proof, see [56]. Note that for shortness, we have denoted $\|\cdot\|_p = \|\cdot\|_{L^p(\mathbb{K})}$.

Sketch of proof of Proposition 15. In order to prove *i.*, we need the following result that will be useful all along the paper, and is somewhat similar to Lemma 9.

Lemma 16. *For any $c \geq 0$, $c_{TF}, \lambda > 0$, there exist positive constants $a < 1$ and C such that, for any $u \in H_{per}^1(\mathbb{K})$ such that $\|u\|_2^2 = \lambda$, we have*

$$\mathcal{E}_{\mathbb{K},c}(u) \geq a \|\nabla u\|_{L^2(\mathbb{K})}^2 - \frac{15}{64} \frac{\lambda}{c_{TF}} c^2 - \lambda C. \quad (4.5)$$

Proof of Lemma 16. The same use of Hölder's inequality as in Lemma 9 (but on \mathbb{K}) gives us that

$$\frac{3}{5} c_{TF} \|u\|_{L^{\frac{10}{3}}(\mathbb{K})}^{\frac{10}{3}} - \frac{3}{4} c \|u\|_{L^{\frac{8}{3}}(\mathbb{K})}^{\frac{8}{3}} \geq -\frac{15}{64} \frac{\lambda}{c_{TF}} c^2.$$

Moreover, for any $\varepsilon > 0$, we have

$$\left| \int_{\mathbb{K}} G_{\mathbb{K}} |u|^2 \right| \leq \varepsilon \|u\|_{L^6(\mathbb{K})}^2 + \lambda C_{\varepsilon}.$$

Indeed $G_{\mathbb{K}} = \mathbf{1}_{\{|\cdot| < r\}} G_{\mathbb{K}} + \mathbf{1}_{\mathbb{K} \setminus \{|\cdot| < r\}} G_{\mathbb{K}} \in L^{\frac{3}{2}}(\mathbb{K}) + L^{\infty}(\mathbb{K})$, by (4.1), and r can be chosen such that $\|\mathbf{1}_{\{|\cdot| < r\}} G_{\mathbb{K}}\|_{L^{\frac{3}{2}}(\mathbb{K})} \leq \varepsilon$ to obtain the claimed inequality. The above

results, together with Sobolev embeddings and $D_{\mathbb{K}}(u^2, u^2) \geq 0$, gives

$$\begin{aligned} \mathcal{E}_{\mathbb{K},c}^{\varepsilon}(u) &= \|\nabla u\|_{L^2(\mathbb{K})}^2 + \frac{3}{5}c_{TF} \|u\|_{L^{\frac{10}{3}}(\mathbb{K})}^{\frac{10}{3}} - \frac{3}{4}c \|u\|_{L^{\frac{8}{3}}(\mathbb{K})}^{\frac{8}{3}} + \frac{1}{2}D_{\mathbb{K}}(u^2, u^2) - \int_{\mathbb{K}} G_{\mathbb{K}} u^2 \\ &\geq \|\nabla u\|_{L^2(\mathbb{K})}^2 - \frac{15}{64} \frac{\lambda}{c_{TF}} c^2 - \varepsilon \|u\|_{L^6(\mathbb{K})}^2 - \lambda C_{\varepsilon} \\ &\geq (1 - \varepsilon S) \|\nabla u\|_{L^2(\mathbb{K})}^2 - \frac{15}{64} \frac{\lambda}{c_{TF}} c^2 - \lambda(C_{\varepsilon} + \varepsilon S) \end{aligned}$$

for any $\varepsilon > 0$ and where S is the constant from the Sobolev embedding. Choosing ε such that $\varepsilon S < 1$ concludes the proof. \square

The above result together with the fact that $H^1(\mathbb{K})$ is compactly embedded in $L^p(\mathbb{K})$ for $1 \leq p < 6$ (since the cube \mathbb{K} is bounded) and with Fatou's Lemma implies the existence of a minimizer and the strong convergence in $H^1(\mathbb{K})$ of any minimizing sequence. Moreover, the convexity inequality for gradients (see [38, Theorem 7.8]) implies the existence of a non-negative minimizer and concludes the proof of *i*.

To prove that any minimizer w_c is in $H_{\text{per}}^2(\mathbb{K})$, we write

$$-\Delta w_c = -c_{TF}|w_c|^{\frac{4}{3}}w_c + c|w_c|^{\frac{2}{3}}w_c + G_{\mathbb{K}}w_c - (|w_c|^2 \star G_{\mathbb{K}})w_c - \mu_c w_c$$

and prove that the right hand side is in $L^2(\mathbb{K})$, which will give $w_c \in H_{\text{per}}^2(\mathbb{K})$ by elliptic regularity for the periodic Laplacian. We note that $|w_c|^{\frac{4}{3}}w_c$ and $|w_c|^{\frac{2}{3}}w_c$ are in $L^2(\mathbb{K})$, by Sobolev embeddings, since $w_c \in H_{\text{per}}^1(\mathbb{K})$ which also gives, together with $G_{\mathbb{K}} \in L^2(\mathbb{K})$ by Lemma 14, that $|w_c|^2 \star G_{\mathbb{K}} \in L^{\infty}(\mathbb{K})$. It remains to prove that $G_{\mathbb{K}}w_c \in L^2(\mathbb{K})$: equation (4.1) and the periodic Hardy inequality on \mathbb{K} give

$$\|G_{\mathbb{K}}w_c\|_{L^2(\mathbb{K})} \leq C \|\cdot\|^{-1}w_c\|_{L^2(\mathbb{K})} \leq C' \|w_c\|_{H_{\text{per}}^1(\mathbb{K})}.$$

Finally, since $G_{\mathbb{K}}$ is not constant, the constant functions are not solutions of the Euler–Lagrange equation hence are not minimizers. This concludes the proof of *ii*.

Let w_c be a non-negative minimizer, then $0 \neq w_c \geq 0$ is in $H^2(\mathbb{K}) \subset L^{\infty}(\mathbb{K})$ and is a solution of $(-\Delta + C)u = (f + G_{\mathbb{K}} + C)u$, with $G_{\mathbb{K}}$ bounded below and

$$f = -c_{TF}|w_c|^{\frac{4}{3}} + c|w_c|^{\frac{2}{3}} - (|w_c|^2 \star G_{\mathbb{K}}) - \mu_{w_c} \in L^{\infty}(\mathbb{K}),$$

thus $(-\Delta + C)w_c \geq 0$ for $C \gg 1$. Hence, $w_c > 0$ on \mathbb{K} since the periodic Laplacian is positive improving [38, Theorem 9.10]. Consequently, $w_c > 0$ verifies $H_{w_c}w_c = -\mu_{w_c}w_c$ and this implies that for any $u \in H_{\text{per}}^1(\mathbb{K})$ it holds

$$\langle u, (H_{w_c} + \mu_{w_c})u \rangle_{L^2(\mathbb{K})} = \langle w_c^2, |\nabla(uw_c^{-1})|^2 \rangle_{L^2(\mathbb{K})} \geq 0.$$

This vanishes only if there exists $\alpha \in \mathbb{C}$ such that $u = \alpha w_c$ a.e. It proves w_c is the unique ground state of H_{w_c} and concludes the proof of Proposition 15. \square

From this existence result, we deduce the following corollary.

Corollary 17. *On $[0, +\infty)$, $c \mapsto E_{\mathbb{K},\lambda}(c)$ is continuous and strictly decreasing.*

Proof of Corollary 17. Let $0 \leq c_1 < c_2$ and, let w_1 and w_2 be corresponding minimizers, which exist by Proposition 15. On one hand, we have

$$\begin{aligned} E_{\mathbb{K},\lambda}(c_2) &\leq \mathcal{E}_{\mathbb{K},c_2}^{\varepsilon}(w_1) = E_{\mathbb{K},\lambda}(c_1) - \frac{3}{4}(c_2 - c_1) \|w_1\|_{L^{\frac{8}{3}}(\mathbb{K})}^{\frac{8}{3}} \\ &< E_{\mathbb{K},\lambda}(c_1) \leq \mathcal{E}_{\mathbb{K},c_1}^{\varepsilon}(w_2) = E_{\mathbb{K},\lambda}(c_2) + \frac{3}{4}(c_2 - c_1) \|w_2\|_{L^{\frac{8}{3}}(\mathbb{K})}^{\frac{8}{3}}. \end{aligned}$$

This gives that $E_{\mathbb{K},\lambda}(c)$ is strictly decreasing on $[0, +\infty)$ but also the left-continuity for any $c_2 > 0$. Moreover, $c_2 \mapsto \|w_2\|_{H^1(\mathbb{K})}$ is uniformly bounded on any bounded

interval since

$$E_{\mathbb{K},\lambda}(0) \geq E_{\mathbb{K},\lambda}(c_2) = \mathcal{E}_{\mathbb{K},c_2}(w_2) \geq a \|\nabla w_2\|_{L^2(\mathbb{K})}^2 - \frac{15}{64} \frac{\lambda}{c_{TF}} c_2^2 - \lambda C \quad (4.6)$$

by Lemma 16. Hence, by the Sobolev embedding, we have

$$E_{\mathbb{K},\lambda}(c_2) < E_{\mathbb{K},\lambda}(c_1) \leq E_{\mathbb{K},\lambda}(c_2) + \frac{3}{4}(c_2 - c_1)C_1\lambda^{5/6} \|w_2\|_{H^1(\mathbb{K})},$$

which gives the right-continuity and concludes the proof of Corollary 17. \square

4.2. Limit case $c = 0$: the TFW model. In order to prove Theorem 1, we need some results on the TFW model which corresponds to the TFDW model for $c = 0$. For clarity, we denote

$$\mathcal{E}_{\mathbb{K}}^{TFW}(w) := \mathcal{E}_{\mathbb{K},0}(w) = \int_{\mathbb{K}} |\nabla w|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{K}} |w|^{\frac{10}{3}} + \frac{1}{2} D_{\mathbb{K}}(|w|^2, |w|^2) - \int_{\mathbb{K}} G_{\mathbb{K}} |w|^2, \quad (4.7)$$

and similarly $E_{\mathbb{K},\lambda}^{TFW} := E_{\mathbb{K},\lambda}(0)$.

By Proposition 15, there exist minimizers to $E_{\mathbb{K},\lambda}^{TFW}$, and we now prove the uniqueness of minimizer for the TFW model.

Proposition 18. *The minimization problem $E_{\mathbb{K},\lambda}^{TFW}$ admits, up to phase, a unique minimizer w_0 which is non constant and strictly positive. Moreover, w_0 is the unique ground-state eigenfunction of the self-adjoint operator*

$$H := -\Delta + c_{TF}|w_0|^{\frac{4}{3}} - G_{\mathbb{K}} + (|w_0|^2 \star G_{\mathbb{K}}),$$

with domain $H_{per}^2(\mathbb{K})$, acting on $L_{per}^2(\mathbb{K})$, and with ground-state eigenvalue

$$-\mu_0 = \frac{\|\nabla w_0\|_2^2 + c_{TF} \|w_0\|_{10/3}^{10/3} + D_{\mathbb{K}}(w_0^2, w_0^2) - \langle G_{\mathbb{K}}, w_0^2 \rangle_{L^2(\mathbb{K})}}{\lambda}. \quad (4.8)$$

Proof of Proposition 18. By Proposition 15, we only have to prove the uniqueness. It follows from the convexity of the $\rho \mapsto |\nabla \sqrt{\rho}|^2$ (see [36, Proposition 7.1]) and the strict convexity of $\rho \mapsto D_{\mathbb{K}}(\rho, \rho)$. \square

4.3. Proof of Theorem 1: uniqueness in the regime of small c . We first prove one convergence result and a uniqueness result under a condition on $\min_{\mathbb{K}} \rho$.

Lemma 19. *Let $\{c_n\}_n \subset \mathbb{R}_+$ be such that $c_n \rightarrow \bar{c}$. If $\{w_{c_n}\}_n$ is a sequence of respective positive minimizers to $E_{\mathbb{K},\lambda}(c_n)$ and $\{\mu_{w_{c_n}}\}_n$ the associated Euler–Lagrange multipliers, then there exists a subsequence c_{n_k} such that the convergence*

$$(w_{c_{n_k}}, \mu_{w_{c_{n_k}}}) \xrightarrow[k \rightarrow \infty]{} (\bar{w}, \mu_{\bar{w}})$$

holds strongly in $H_{per}^2(\mathbb{K}) \times \mathbb{R}$, where \bar{w} is a positive minimizer to $E_{\mathbb{K},\lambda}(\bar{c})$ and $\mu_{\bar{w}}$ is the associated multiplier.

Additionally, if $E_{\mathbb{K},\lambda}(\bar{c})$ has a unique positive minimizer \bar{w} then the result holds for the whole sequence $c_n \rightarrow \bar{c}$:

$$(w_{c_n}, \mu_{w_{c_n}}) \xrightarrow[n \rightarrow \infty]{} (\bar{w}, \mu_{\bar{c}}).$$

We will only use the case $\bar{c} = 0$, for which we have proved the uniqueness of the positive minimizer, but we state this lemma for any $\bar{c} \geq 0$.

Proof of Lemma 19. We first prove the convergence in $H_{per}^1(\mathbb{K}) \times \mathbb{R}$. By the continuity of $c \mapsto E_{\mathbb{K},\lambda}(c)$ proved in Corollary 17, $\{w_{c_n}\}_{n \rightarrow \infty}$ is a positive minimizing sequence of $E_{\mathbb{K},\lambda}(\bar{c})$. Thus, by Proposition 15, up to a subsequence (denoted the same for shortness), w_{c_n} converges strongly in $H_{per}^1(\mathbb{K})$ to a minimizer \bar{w} of $E_{\mathbb{K},\lambda}(\bar{c})$.

Moreover, for any c , (w_c, μ_{w_c}) is a solution of the Euler–Lagrange equation

$$\left(-\Delta + c_{TF} w_c^{\frac{4}{3}} - c w_c^{\frac{2}{3}} - G_{\mathbb{K}} + (w_c^2 \star G_{\mathbb{K}})\right) w_c = -\mu_{w_c} w_c.$$

Thus, as c_n goes to \bar{c} , $\mu_{w_{c_n}}$ converges to $\mu \in \bar{\mathbb{R}}$ satisfying

$$-\Delta \bar{w} + c_{TF} \bar{w}^{\frac{7}{3}} - \bar{c} \bar{w}^{\frac{5}{3}} - G_{\mathbb{K}} \bar{w} + (\bar{\rho} \star G_{\mathbb{K}}) \bar{w} = -\mu \bar{w}.$$

In particular, $\mu = \mu_{\bar{w}}$. At this point, we proved the convergence in $H_{\text{per}}^1(\mathbb{K}) \times \mathbb{R}$:

$$(w_{c_n}, \mu_{w_{c_n}}) \xrightarrow{n \rightarrow \infty} (\bar{w}, \mu_{\bar{w}}).$$

If, additionally, the positive minimizer \bar{w} of $E_{\mathbb{K}, \lambda}(\bar{c})$ is unique, then any positive minimizing sequence must converge in $H_{\text{per}}^1(\mathbb{K})$ to \bar{w} , so the whole sequence $\{w_{c_n}\}_{n \rightarrow \infty}$ in fact converges to the unique positive minimizer \bar{w} .

We turn to the proof of the convergence in $H_{\text{per}}^2(\mathbb{K})$. For any $c_n \geq 0$, by Proposition 15, w_{c_n} is in $H_{\text{per}}^2(\mathbb{K})$ thus we have

$$\begin{aligned} (-\Delta - G_{\mathbb{K}} + \beta)(w_{c_n} - \bar{w}) &= -c_{TF}(w_{c_n}^{\frac{7}{3}} - \bar{w}^{\frac{7}{3}}) + (c_n - \bar{c})w_{c_n}^{\frac{5}{3}} + \bar{c}(w_{c_n}^{\frac{5}{3}} - \bar{w}^{\frac{5}{3}}) \\ &\quad - ((w_{c_n}^2 - \bar{w}^2) \star G_{\mathbb{K}}) w_{c_n} - (\bar{w}^2 \star G_{\mathbb{K}})(w_{c_n} - \bar{w}) \\ &\quad - (\mu_{w_{c_n}} - \mu_{\bar{w}})w_{c_n} + (\beta - \mu_{\bar{w}})(w_{c_n} - \bar{w}) =: \varepsilon_n. \end{aligned}$$

The right side ε_n converges to 0 in $L_{\text{per}}^2(\mathbb{K})$. Moreover, by the Rellich-Kato theorem, the operator $-\Delta - G_{\mathbb{K}}$ is self-adjoint on $H_{\text{per}}^2(\mathbb{K})$ and bounded below, hence we conclude that

$$\begin{aligned} \|w_{c_n} - \bar{w}\|_{H^2(\mathbb{K})} &= \left\| (-\Delta - G_{\mathbb{K}} + \beta)^{-1} \varepsilon_n \right\|_{H^2(\mathbb{K})} \\ &\leq \left\| (-\Delta - G_{\mathbb{K}} + \beta)^{-1} \right\|_{L^2(\mathbb{K}) \rightarrow H_{\text{per}}^2(\mathbb{K})} \|\varepsilon_n\|_{L^2(\mathbb{K})} \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

This concludes the proof of Lemma 19. \square

Proposition 20 (Conditional uniqueness). *Let \mathbb{K} be the unit cube, $N \geq 1$ be an integer, $c_{TF} > 0$, $c \geq 0$ and $\mu \in \mathbb{R}$ be constants. Let $w > 0$ be such that $w \in H^1(N \cdot \mathbb{K})$ and w is a $N \cdot \mathbb{K}$ -periodic solution of*

$$\left(-\Delta + c_{TF} w^{\frac{4}{3}} - c w^{\frac{2}{3}} + (w^2 \star G_{\mathbb{K}}) - G_{\mathbb{K}}\right) w = -\mu w. \quad (4.9)$$

If $\min_{N \cdot \mathbb{K}} w > \left(\frac{c}{c_{TF}}\right)^{\frac{3}{2}}$, then w is the unique minimizer of $E_{N \cdot \mathbb{K}, \int_{N \cdot \mathbb{K}} |w|^2}(c)$.

Proof of Proposition 20. First, the hypothesis give $w \in H_{\text{per}}^2(N \cdot \mathbb{K})$, by the same proof as in Proposition 15. Moreover, we have the following lemma.

Lemma 21. *Let $\rho > 0$ and $\rho' \geq 0$ such that $\sqrt{\rho} \in H_{\text{per}}^2(\mathbb{K})$ and $\sqrt{\rho'} \in H_{\text{per}}^1(\mathbb{K})$. Then*

$$\int_{\mathbb{K}} \left| \nabla \sqrt{\rho'} \right|^2 - \int_{\mathbb{K}} \left| \nabla \sqrt{\rho} \right|^2 + \int_{\mathbb{K}} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}} (\rho' - \rho) \geq 0.$$

Proof of Lemma 21. Using the fact that

$$\sqrt{\rho} \Delta \sqrt{\rho} = \frac{\sqrt{\rho}}{2} \nabla [\sqrt{\rho} \nabla (\ln \rho)] = \frac{1}{2} \rho \Delta (\ln \rho) + \frac{1}{4} \rho |\nabla (\ln \rho)|^2$$

and defining $h = \rho' - \rho$, one obtains

$$\int_{N \cdot \mathbb{K}} \left| \nabla \sqrt{\rho + h} \right|^2 - \int_{N \cdot \mathbb{K}} \left| \nabla \sqrt{\rho} \right|^2 + \int_{N \cdot \mathbb{K}} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}} h = \frac{1}{4} \int_{N \cdot \mathbb{K}} \left| \frac{h \nabla \rho}{\rho \sqrt{\rho + h}} - \frac{\nabla h}{\sqrt{\rho + h}} \right|^2 \geq 0.$$

\square

Let w' be in $H_{\text{per}}^1(N \cdot \mathbb{K})$ such that $\int_{N \cdot \mathbb{K}} w^2 = \int_{N \cdot \mathbb{K}} |w'|^2$ and $|w'| \neq w$. Defining $\rho = w^2$ and $\rho' = |w'|^2$, this means that $\int_{N \cdot \mathbb{K}} h = 0$ where $h := \rho' - \rho \neq 0$. We have

$$\begin{aligned} & \mathcal{E}_{N \cdot \mathbb{K}, c}(|w'|) - \mathcal{E}_{N \cdot \mathbb{K}, c}(w) \\ &= \left\langle \left(-\Delta + c_{TF} w^{\frac{4}{3}} - c w^{\frac{2}{3}} + w^2 \star G_{N \cdot \mathbb{K}} - G_{N \cdot \mathbb{K}} + \mu \right) w, h w^{-1} \right\rangle_{L^2(N \cdot \mathbb{K})} \\ &+ \int_{N \cdot \mathbb{K}} |\nabla \sqrt{\rho + h}|^2 - \int_{N \cdot \mathbb{K}} |\nabla \sqrt{\rho}|^2 + \int_{N \cdot \mathbb{K}} \frac{\Delta \sqrt{\rho}}{\sqrt{\rho}} h + \frac{1}{2} D_{N \cdot \mathbb{K}}(h, h) \\ &+ \frac{3}{5} c_{TF} \left(\int_{N \cdot \mathbb{K}} (\rho + h)^{\frac{5}{3}} - \rho^{\frac{5}{3}} - \frac{5}{3} \rho^{\frac{2}{3}} h \right) - \frac{3}{4} c \left(\int_{N \cdot \mathbb{K}} (\rho + h)^{\frac{4}{3}} - \rho^{\frac{4}{3}} - \frac{4}{3} \rho^{\frac{1}{3}} h \right) \\ &> \int_{N \cdot \mathbb{K}} F(\rho') - F(\rho) - F'(\rho)(\rho' - \rho), \end{aligned}$$

with $F(X) = \frac{3}{5} c_{TF} X^{\frac{5}{3}} - \frac{3}{4} c X^{\frac{4}{3}}$. The above inequality comes from (4.9) together with Lemma 21 and with $D_{\mathbb{K}}(h, h) > 0$ for $h \neq 0$. Defining now

$$F_X(Y) = F(Y) - F(X) - F'(X)(Y - X),$$

one can check, as soon as $X \geq \sqrt[3]{\frac{c}{c_{TF}}}$, that $F'_X < 0$ on $(0, X)$ and $F'_X > 0$ on $(X, +\infty)$. Moreover, $F'_X(0) < 0$ if $X > \sqrt[3]{\frac{c}{c_{TF}}}$. Thus F_X has a global strict minimum on \mathbb{R}_+ at X and this minimum is zero. Consequently, if $\min_{N \cdot \mathbb{K}} w \geq \left(\frac{c}{c_{TF}}\right)^{3/2}$, then $\mathcal{E}_{\mathbb{K}, c}(w') \geq \mathcal{E}_{\mathbb{K}, c}(|w'|) > \mathcal{E}_{\mathbb{K}, c}(w)$ for any $w' \in H_{\text{per}}^1(N \cdot \mathbb{K})$ such that $|w'| \neq w$ and $\int_{N \cdot \mathbb{K}} |w'|^2 = \int_{N \cdot \mathbb{K}} w^2$. This ends the proof of Proposition 20. \square

We have now all the tools to prove the uniqueness of minimizers for c small.

Proof of Theorem 1. We have already proved all the results of *i.* of Theorem 1 in Proposition 15 except for the uniqueness that we prove now. Let $(w_c)_{c \rightarrow 0^+}$ be a sequence of respective positive minimizers to $E_{\mathbb{K}, \lambda}(c)$. By Proposition 18, $E_{\mathbb{K}, \lambda}(0)$ has a unique minimizer thus, by Proposition 19, w_c converges strongly in $H^2(\mathbb{K})$ hence in $L^\infty(\mathbb{K})$ to the unique positive minimizer w_0 to $E_{\mathbb{K}, \lambda}(0)$. Therefore, for c small enough we have

$$\min_{\mathbb{K}} w_c \geq \frac{1}{2} \min_{\mathbb{K}} w_0 > \left(\frac{c}{c_{TF}}\right)^{\frac{3}{2}}$$

and we can apply Proposition 20 (with $N = 1$) to the minimizer $w_c > 0$ to conclude that it is the unique minimizer of $E_{\mathbb{K}, \lambda}(c)$.

We now prove *ii.* of Theorem 1. We fix c small enough such that $E_{\mathbb{K}, \lambda}(c)$ has an unique minimizer w_c . Then w_c being \mathbb{K} -periodic, it is $N \cdot \mathbb{K}$ -periodic for any integer $N \geq 1$ and verifies all the hypothesis of Proposition 20 hence it is also the unique minimizer of $E_{N \cdot \mathbb{K}, \int_{N \cdot \mathbb{K}} |w_c|^2}(c) = E_{N \cdot \mathbb{K}, N^3 \lambda}(c)$. \square

5. REGIME OF LARGE c : SYMMETRY BREAKING

This section is dedicated to the proof of the main result of the paper, namely Theorem 2. We introduce for clarity some notations for the rest of the paper. We will denote the minimization problem for the effective model on the unit cell \mathbb{K} by

$$J_{\mathbb{K}, \lambda}(c) = \inf_{\substack{v \in H_{\text{per}}^1(\mathbb{K}) \\ \|v\|_{L^2(\mathbb{K})}^2 = \lambda}} \mathcal{J}_{\mathbb{K}, c}(v), \quad (5.1)$$

where

$$\mathcal{J}_{\mathbb{K}, c}(v) = \int_{\mathbb{K}} |\nabla v|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{K}} |v|^{\frac{10}{3}} - \frac{3}{4} c \int_{\mathbb{K}} |v|^{\frac{8}{3}}. \quad (5.2)$$

The first but important result is that we have for $J_{\mathbb{K},\lambda}$ the existence result equivalent to the existence result of Proposition 15 for $E_{\mathbb{K},\lambda}$.

The minima of the effective model and of the TFDW model also verify the following a priori estimates which will be useful all along this section.

Lemma 22 (A priori estimates on minimal energy). *Let \mathbb{K} be the unit cube and c_{TF} and c be two positive constant. We have*

$$-\lambda C - \frac{15}{64} \frac{\lambda}{c_{TF}} c^2 \leq E_{\mathbb{K},\lambda}(c), \quad (5.3)$$

for some constant $C > 0$, and

$$-\frac{15}{64} \frac{\lambda}{c_{TF}} c^2 \leq J_{\mathbb{K},\lambda}(c) \leq -\frac{3}{4} \frac{\lambda^{\frac{4}{3}}}{|\mathbb{K}|^{\frac{1}{3}}} c + \frac{3}{5} c_{TF} \frac{\lambda^{\frac{5}{3}}}{|\mathbb{K}|^{\frac{2}{3}}}. \quad (5.4)$$

Moreover, for all K such that $0 < K < -J_{\mathbb{R}^3,\lambda}$, there exists $c_* > 0$ such that for all $c \geq c_*$ we have

$$-\frac{15}{64} \frac{\lambda}{c_{TF}} c^2 \leq J_{\mathbb{K},\lambda}(c) \leq -c^2 K < 0. \quad (5.5)$$

Proof of Lemma 22. The inequality (5.3) has been proved in Lemma 16, the proof of which also leads to the inequality

$$\mathcal{J}_{\mathbb{K},c}(v) \geq \|\nabla v\|_{L^2(\mathbb{K})}^2 - \frac{15}{64} \frac{\lambda}{c_{TF}} c^2, \quad (5.6)$$

hence the lower bound in (5.4). The upper bound in (5.4) is a simple computation of $\mathcal{J}_{\mathbb{K},c}(\bar{v})$ for the constant function $\bar{v} = \sqrt{\frac{\lambda}{|\mathbb{K}|}}$, defined on \mathbb{K} , which belongs to the minimizing domain.

To prove (5.5), let K be such that $0 < K < -J_{\mathbb{R}^3,\lambda}$. Fix $f \in C_c^\infty(\mathbb{R}^3)$ such that $K = -\mathcal{J}_{\mathbb{R}^3}(f) > 0$. Such a f exists since $J_{\mathbb{R}^3,\lambda} < 0$ and $C_c^\infty(\mathbb{R}^3)$ is dense in $H^1(\mathbb{R}^3)$. Thus, there exists $c_* > 0$ such that for any $c \geq c_*$, the support of $f_c := c^{3/2} f(c \cdot)$ is strictly included in \mathbb{K} . This implies, for any $c \geq c_*$, that

$$J_{\mathbb{K},\lambda}(c) \leq \mathcal{J}_{\mathbb{K},c}(f_c) = \int_{\mathbb{R}^3} |\nabla f_c|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{R}^3} |f_c|^{\frac{10}{3}} - \frac{3}{4} c \int_{\mathbb{R}^3} |f_c|^{\frac{8}{3}} = c^2 \mathcal{J}_{\mathbb{R}^3}(f),$$

and this concludes the proof of Lemma 22. \square

We introduce the notation \mathbb{K}_c which will be the dilation of \mathbb{K} by a factor $c > 0$. Namely, if \mathbb{K} is the unit cube, then

$$\mathbb{K}_c := c \cdot \mathbb{K} := \left[-\frac{c}{2}; \frac{c}{2} \right]^3. \quad (5.7)$$

Moreover, we use the notation \check{v} to denote the dilation of v : for any v defined on \mathbb{K} , \check{v} is defined on \mathbb{K}_c by $\check{v}(x) := c^{-3/2} v(c^{-1}x)$.

A direct computation gives $\mathcal{J}_{\mathbb{K},c}(v) = c^2 \mathcal{J}_{\mathbb{K}_c,1}(\check{v})$, for any $v \in H_{\text{per}}^1(\mathbb{K})$. Consequently, $J_{\mathbb{K},\lambda}(c) = c^2 J_{\mathbb{K}_c,\lambda}(1)$ and v is a minimizer of $J_{\mathbb{K},\lambda}(c)$ if and only if \check{v} is a minimizer of $J_{\mathbb{K}_c,\lambda}(1)$. Finally, when v is a minimizer of $J_{\mathbb{K},\lambda}(c)$, we have some a priori bounds on several norms of \check{v} which are given in the following corollary of Lemma 22.

Corollary 23 (Uniform norm bounds on minimizers of $J_{\mathbb{K}_c,\lambda}(1)$). *Let \mathbb{K} be the unit cube and λ be positive. Then there exist $C > 0$ and $c_* > 0$ such that for any $c \geq c_*$, a minimizer \check{v}_c of $J_{\mathbb{K}_c,\lambda}(1)$ verifies*

$$\frac{1}{C} \leq \|\nabla \check{v}_c\|_{L^2(\mathbb{K}_c)}, \|\check{v}_c\|_{L^{10/3}(\mathbb{K}_c)}, \|\check{v}_c\|_{L^{8/3}(\mathbb{K}_c)} \leq C.$$

Proof of Corollary 23. By (5.4) and (5.6), we obtain for c large enough that any any minimizer v_c of $J_{\mathbb{K},\lambda}(c)$ verifies

$$\|\nabla \check{v}_c\|_{L^2(\mathbb{K}_c)}^2 = c^{-2} \|\nabla v_c\|_{L^2(\mathbb{K})}^2 \leq \frac{15}{64} \frac{\lambda}{c_{TF}}.$$

Applying, on \mathbb{K} , Hölder's inequality and Sobolev embeddings to v_c , we obtain that there exists C such that

$$\forall c \geq c_*, \quad \|\nabla \check{v}_c\|_{L^2(\mathbb{K}_c)}, \|\check{v}_c\|_{L^{10/3}(\mathbb{K}_c)}, \|\check{v}_c\|_{L^{8/3}(\mathbb{K}_c)} \leq C.$$

By (5.5), for any K such that $0 < K < -J_{\mathbb{R}^3,\lambda}$, there exists $c_* > 0$ such that

$$\forall c \geq c_*, \quad 0 < \frac{4}{3}K \leq -\frac{4}{3}J_{\mathbb{K}_c,\lambda}(1) \leq \|\check{v}_c\|_{L^{8/3}(\mathbb{K}_c)}^{8/3}$$

and, consequently, such that

$$\forall c \geq c_*, \quad \|\check{v}_c\|_{L^{10/3}(\mathbb{K}_c)}^{10/3} \geq \frac{1}{\lambda} \left(\|\check{v}_c\|_{L^{8/3}(\mathbb{K}_c)}^{8/3} \right)^2 > \frac{16}{9} \frac{K^2}{\lambda} > 0.$$

We then obtain the lower bound for the gradient by the Sobolev embeddings. This concludes the proof of Corollary 23. \square

5.1. Concentration-compactness. To prove the symmetry breaking stated in Theorem 2, we prove the following result using the concentration-compactness method as a key ingredient.

Proposition 24. *Let \mathbb{K} be the unit cube and λ be positive. Then*

$$\lim_{c \rightarrow \infty} c^{-2} E_{\mathbb{K},\lambda}(c) = J_{\mathbb{R}^3,\lambda} = \lim_{c \rightarrow \infty} c^{-2} J_{\mathbb{K},\lambda}(c).$$

Moreover, for any sequence w_c of minimizers to $E_{\mathbb{K},\lambda}(c)$, there exists a subsequence $c_n \rightarrow \infty$ and a sequence translations $\{x_n\} \subset \mathbb{R}^3$ such that the sequence of dilated functions $\check{w}_n := c_n^{-3/2} w_{c_n}(c_n^{-1} \cdot)$ verifies

- i. $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_n(\cdot + x_n)$ converges to a minimizer u of $J_{\mathbb{R}^3,\lambda}$ strongly in $L^p(\mathbb{R}^3)$ for $2 \leq p < 6$, as n goes to infinity;
- ii. $\mathbb{1}_{\mathbb{K}_{c_n}} \nabla \check{w}_n(\cdot + x_n) \rightarrow \nabla u$ strongly in $L^2(\mathbb{R}^3)$.

The same holds for any sequence v_c of minimizers of $J_{\mathbb{K},\lambda}(c)$.

Before proving Proposition 24, we give and prove several intermediate results, the first of which is the following proposition which will allow us to deduce the results for $E_{\mathbb{K},\lambda}$ from those for $J_{\mathbb{K},\lambda}$.

Lemma 25. *Let $\lambda > 0$. Then*

$$\frac{E_{\mathbb{K},\lambda}(c)}{J_{\mathbb{K},\lambda}(c)} \xrightarrow{c \rightarrow \infty} 1.$$

Proof of Lemma 25. Let w_c and v_c be minimizers of $E_{\mathbb{K},\lambda}(c)$ and $J_{\mathbb{K},\lambda}(c)$ respectively which exist by Proposition 15 and the equivalent result for $J_{\mathbb{K},\lambda}(c)$. Thus

$$\frac{1}{2} D_{\mathbb{K}}(w_c^2, w_c^2) - \int_{\mathbb{K}} G_{\mathbb{K}} w_c^2 \leq E_{\mathbb{K},\lambda}(c) - J_{\mathbb{K},\lambda}(c) \leq \frac{1}{2} D_{\mathbb{K}}(v_c^2, v_c^2) - \int_{\mathbb{K}} G_{\mathbb{K}} v_c^2.$$

By the Hardy inequality on \mathbb{K} and (4.1), we have

$$\left| \int_{\mathbb{K}} G_{\mathbb{K}} v_c^2 \right| \leq \lambda \|G_{\mathbb{K}} v_c\|_{L^2(\mathbb{K})} \leq C \lambda \|v_c\|_{H^1(\mathbb{K})}$$

and similarly $|\int_{\mathbb{K}} G_{\mathbb{K}} w_c^2| \lesssim \|w_c\|_{H^1(\mathbb{K})}$. Moreover, we claim that

$$D_{\mathbb{K}}(v_c^2, v_c^2) \lesssim \|v_c\|_{H^1(\mathbb{K})}. \quad (5.8)$$

To prove (5.8) we define, for each spatial direction $i \in \{1, 2, 3\}$ of the lattice, the intervals $I_i^{(-1)} := [-1; -1/2)$, $I_i^{(0)} := [-1/2; 1/2)$ and $I_i^{(+1)} := [1/2; 1)$, and the

parallelepipeds $\mathbb{K}^{(\sigma_1, \sigma_2, \sigma_3)} = I_1^{(\sigma_1)} \times I_2^{(\sigma_2)} \times I_3^{(\sigma_3)}$ which let us rewrite $\mathbb{K} = \mathbb{K}^{(0,0,0)}$ and $\mathbb{K}_2 = 2 \cdot \mathbb{K} := [-1; 1]^3$ as the union of the 27 sets

$$\mathbb{K}_2 = \bigcup_{\sigma \in \{-1; 0; +1\}^3} \mathbb{K}^\sigma.$$

We thus have by (4.1) and the Hardy-Littlewood-Sobolev inequality that

$$\iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in \mathbb{K}^\sigma}} v_c^2(x) G_{\mathbb{K}}(x-y) v_c^2(y) dx dy \lesssim \iint_{\mathbb{K} \times \mathbb{K}} \frac{v_c^2(x) v_c^2(y)}{|x-y-\sigma|} dy dx \lesssim \|v_c\|_{L^{\frac{12}{5}}(\mathbb{K})}^4.$$

Consequently, by Hölder's inequality and Sobolev embeddings, we have

$$\begin{aligned} |D_{\mathbb{K}}(v_c^2, v_c^2)| &= \left| \sum_{\sigma \in \{-1; 0; +1\}^3} \iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in \mathbb{K}^\sigma}} v_c^2(x) G_{\mathbb{K}}(x-y) v_c^2(y) dx dy \right| \\ &\lesssim \|v_c\|_{L^{\frac{12}{5}}(\mathbb{K})}^4 \lesssim \|v_c\|_{H^1(\mathbb{K})} \|v_c\|_{L^2(\mathbb{K})}^3. \end{aligned} \quad (5.9)$$

This proves (5.8) which also holds for w_c .

Then, on one hand, by (4.6) applied to $c_1 = 0 \leq c_2 = c$, there exist positive constants $a < 1$ and C such that for any $c > 0$ we have

$$a \|\nabla w_c\|_{L^2(\mathbb{K})}^2 \leq \frac{15}{64} \frac{\lambda}{c_{TF}} c^2 + E_{\mathbb{K}, \lambda}(0) + \lambda C.$$

On the other hand, the upper bound in (5.5) together with the (5.6) applied to v_c , give that there exists $c_* > 0$ such that

$$\exists K > 0, \forall c \geq c_*, \quad \|\nabla v_c\|_{L^2(\mathbb{K})}^2 \leq \left(\frac{15}{64} \frac{\lambda}{c_{TF}} - K \right) c^2. \quad (5.10)$$

Consequently, for c large enough, we have

$$|J_{\mathbb{K}, \lambda}(c) - E_{\mathbb{K}, \lambda}(c)| \lesssim c$$

hence, using (5.5), we finally obtain

$$\left| \frac{E_{\mathbb{K}, \lambda}(c)}{J_{\mathbb{K}, \lambda}(c)} - 1 \right| \lesssim c^{-1}.$$

This concludes the proof of Lemma 25. \square

We now prove that the periodic effective model converges,

$$\lim_{c \rightarrow \infty} c^{-2} J_{\mathbb{K}, \lambda}(c) = J_{\mathbb{R}^3, \lambda},$$

by proving the two associated inequalities. We first prove the upper bound then use the concentration-compactness method to prove the converse inequality. The strong convergence of minimizers stated in Proposition 24 will be a by-product of the method.

Lemma 26 (Upper bound). *Let \mathbb{K} be the unit cube and λ be positive. Then there exists $\beta > 0$ such that*

$$J_{\mathbb{K}, \lambda}(c) \leq c^2 J_{\mathbb{R}^3, \lambda} + o(e^{-\beta c}).$$

Proof of Lemma 26. This result is obtained by computing $\mathcal{J}_{\mathbb{K}_c, 1}(Q_c)$ where

$$Q_c = \frac{\sqrt{\lambda} \chi_c Q}{\|\chi_c Q\|_{L^2(\mathbb{R}^3)}},$$

for $Q \in H^1(\mathbb{R}^3)$ a minimizer of $J_{\mathbb{R}^3, \lambda}$, with $\chi_c \in C_c^\infty(\mathbb{R}^3)$, $0 \leq \chi_c \leq 1$, $\chi_c \equiv 0$ on $\mathbb{R}^3 \setminus \mathbb{K}_{c+1}$, $\chi_c \equiv 1$ on \mathbb{K}_c and $\|\nabla \chi_c\|_{L^\infty(\mathbb{R}^3)}$ bounded. Indeed, by the well-known exponential decay of continuous positive solution to the Euler-Lagrange equations

with strictly negative Lagrange multiplier, one obtains the exponential decay when r goes to infinity of the norm $\|\nabla Q\|_{L^2(\mathbb{C}_B(0,r))}$ and the norms $\|Q\|_{L^p(\mathbb{C}_B(0,r))}$ for $p > 0$, and consequently the claimed upper bound. \square

Lemma 27 (Lower bound). *Let \mathbb{K} be the unit cube and λ be positive. Then*

$$\liminf_{c \rightarrow \infty} c^{-2} J_{\mathbb{K},\lambda}(c) \geq J_{\mathbb{R}^3,\lambda}.$$

See [56] for a detailed proof.

Sketch of proof of Lemma 27. This result relies on Lions' concentration-compactness method and on the following result. Since this lemma is well-known, we omit its proof. Similar statements can be found for example in [16, 1, 20, 25, 30, 56].

Lemma 28 (Splitting in localized bubbles). *Let \mathbb{K} be the unit cube, $\{\varphi_c\}_{c \geq 1}$ be a sequence of functions such that $\varphi_c \in H_{per}^1(\mathbb{K}_c)$ for all c , with $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ uniformly bounded. Then there exists a sequence of functions $\{\varphi^{(1)}, \varphi^{(2)}, \dots\}$ in $H^1(\mathbb{R}^3)$ such that the following holds. For any $\varepsilon > 0$ and any fixed sequence $0 \leq R_k \rightarrow \infty$, there exist: $J \geq 0$, a subsequence $\{\varphi_{c_k}\}$, sequences $\{\xi_k^{(1)}, \dots, \xi_k^{(J)}\}$, $\{\psi_k\}$ in $H_{per}^1(\mathbb{K}_{c_k})$ and sequences of space translations $\{x_k^{(1)}, \dots, x_k^{(J)}\}$ in \mathbb{R}^3 such that*

$$\lim_{k \rightarrow \infty} \left\| \varphi_{c_k} - \sum_{j=1}^J \xi_k^{(j)}(\cdot - x_k^{(j)}) - \psi_k \right\|_{H^1(\mathbb{K}_{c_k})} = 0,$$

where

- $\{\xi_k^{(1)}, \dots, \xi_k^{(J)}\}, \{\psi_k\}$ have uniformly bounded $H^1(\mathbb{K}_{c_k})$ -norms,
- $\mathbb{1}_{\mathbb{K}_{c_k}} \xi_k^{(j)} \rightharpoonup \varphi^{(j)}$ weakly in $H^1(\mathbb{R}^3)$ and strongly in $L^p(\mathbb{R}^3)$ for $2 \leq p < 6$,
- $\text{supp}(\mathbb{1}_{\mathbb{K}_{c_k}} \xi_k^{(j)}) \subset B(0, R_k)$ for all $j = 1, \dots, J$ and all k ,
- $\text{supp}(\mathbb{1}_{\mathbb{K}_{c_k}} \psi_k) \subset \mathbb{K}_{c_k} \setminus \bigcup_{j=1}^J B(x_k^{(j)}, 2R_k)$ for all k ,
- $|x_k^{(i)} - x_k^{(j)}| \geq 5R_k$ for all $i \neq j$ and all k ,
- $\int_{\mathbb{K}_{c_k}} |\psi_k|^{\frac{8}{3}} \leq \varepsilon$.

Remark. *In the proof of Lemma 27, we really need to use all the bubbles because we do not know well enough the energy of ψ_k . In similar proofs, it is often possible to conclude after extracting few bubbles, using that $\mathcal{J}(\psi_k) \geq J(\int |\psi_k|^2)$ which allows to conclude. However, in our case, $J_{\mathbb{K}_c}(\int |\psi_k|^2)$ depends on c hence the same inequality of course holds but does not allow us to conclude. We therefore need to extract all the bubbles (up to ε).*

We apply Lemma 28 to the sequence $(\check{v}_c)_{c \geq 1}$ of minimizers to $J_{\mathbb{K}_c,\lambda}(1)$ which verifies the hypothesis by the upper bound proved in Corollary 23. The lower bound in that corollary excludes the case $J = 0$. Indeed, in that case we would have $\lim_{k \rightarrow \infty} \|\varphi_{c_k} - \psi_k\|_{H^1(\mathbb{K}_{c_k})} = 0$ and $\int_{\mathbb{K}_{c_k}} |\psi_k|^{\frac{8}{3}} \leq \varepsilon$ hence $\int_{\mathbb{K}_{c_k}} |\varphi_k|^{\frac{8}{3}} \leq 2\varepsilon$, for k large enough, contradicting the mentioned lower bound. Consequently, there exists $J \geq 1$ such that

$$\check{v}_{c_k} = \psi_k + \varepsilon_k + \sum_{j=1}^J \check{v}_k^{(j)}(\cdot - x_k^{(j)})$$

where $\|\varepsilon_k\|_{H^1(\mathbb{K}_{c_k})} \rightarrow 0$ and, for a each k , the supports of the $\check{v}_k^{(j)}(\cdot - x_k^{(j)})$'s and ψ_k are pairwise disjoint. The support properties, the Minkowski inequality, Sobolev

embeddings and the fact that $\text{supp}(\mathbf{1}_{\mathbb{K}_{c_k}} \check{v}_k^{(j)}) \subset B(0, R_k) \subset \mathbb{K}_{c_k}$, give that

$$\begin{aligned} J_{\mathbb{K}_{c_k}}(\lambda) &= \mathcal{J}_{\mathbb{K}_{c_k}}(\check{v}_{c_k}) = \mathcal{J}_{\mathbb{K}_{c_k}}(\psi_k) + \sum_{j=1}^J \mathcal{J}_{\mathbb{R}^3}(\mathbf{1}_{\mathbb{K}_{c_k}} \check{v}_k^{(j)}) + o(1)_{c_k \rightarrow \infty} \\ &\geq -\frac{3}{4}\varepsilon + \sum_{j=1}^J \mathcal{J}_{\mathbb{R}^3}(\mathbf{1}_{\mathbb{K}_{c_k}} \check{v}_k^{(j)}) + o(1)_{c_k \rightarrow \infty}. \end{aligned}$$

Moreover, the strong convergence of $\mathbf{1}_{\mathbb{K}_{c_k}} \check{v}_k^{(j)}$ in L^2 and the continuity of $\lambda \mapsto J_{\mathbb{R}^3, \lambda}$, proved in Lemma 10, imply, for all $j = 1, \dots, J$, that

$$\mathcal{J}_{\mathbb{R}^3}(\mathbf{1}_{\mathbb{K}_{c_k}} \check{v}_k^{(j)}) \geq J_{\mathbb{R}^3}(\|\check{v}_k^{(j)}\|_{L^2(\mathbb{K}_{c_k})}^2) \xrightarrow{k \rightarrow \infty} J_{\mathbb{R}^3}(\lambda^{(j)}),$$

where, for any j , $\lambda^{(j)} := \|\check{v}^{(j)}\|_{L^2(\mathbb{R}^3)}$ is the mass of the limit of $\mathbf{1}_{\mathbb{K}_{c_k}} \check{v}_k^{(j)}$. We also have denoted $J_{\mathbb{R}^3}(\lambda) := J_{\mathbb{R}^3, \lambda}$ to simplify notations here. Those inequalities together with the strict binding proved in Proposition 12 lead to

$$\frac{3}{4}\varepsilon + \liminf_{k \rightarrow \infty} J_{\mathbb{K}_{c_k}}(\lambda) \geq \sum_{j=1}^J J_{\mathbb{R}^3}(\lambda^{(j)}) > J_{\mathbb{R}^3}(\lambda) - J_{\mathbb{R}^3}\left(\lambda - \sum_{j=1}^J \lambda^{(j)}\right) \geq J_{\mathbb{R}^3}(\lambda).$$

The last inequality comes from the fact that $0 \leq \|\psi_k\|_{L^2(\mathbb{K}_{c_k})}^2 = \lambda - \sum_{j=1}^J \lambda^{(j)} + o(1)$

thus $\lambda - \sum_{j=1}^J \lambda^{(j)} \geq 0$ and this implies that $J_{\mathbb{R}^3}\left(\lambda - \sum_{j=1}^J \lambda^{(j)}\right) \leq 0$. This concludes the proof of Lemma 27. \square

We can now compute the main term of $E_{\mathbb{K}, \lambda}(c)$ stated in Proposition 24.

Proof of Proposition 24. Propositions 26 and 27 give, for $\lambda > 0$, the limit

$$\lim_{c \rightarrow \infty} c^{-2} J_{\mathbb{K}, \lambda}(c) = J_{\mathbb{R}^3, \lambda}$$

and Lemma 25 gives then the same limit for $E_{\mathbb{K}, \lambda}(c)$. Proposition 27 also gives that $(\check{v}_c)_{c \geq 1}$ has at least a first extracted bubble $0 \neq \check{v} \in H^1(\mathbb{R}^3)$ to which $\mathbf{1}_{\mathbb{K}_{c_k}} \check{v}_{c_k}(\cdot + x_k)$ converges weakly in $L^2(\mathbb{R}^3)$. This leads to

$$J_{\mathbb{K}_{c_k}, \lambda}(1) = \mathcal{J}_{\mathbb{K}_{c_k}, 1}(\check{v}_{c_k}(\cdot + x_k)) = \mathcal{J}_{\mathbb{R}^3}(\check{v}) + \mathcal{J}_{\mathbb{K}_{c_k}, 1}(\check{v}_{c_k}(\cdot + x_k) - \check{v}) + o(1) \quad (5.11)$$

by the following lemma.

Lemma 29. *Let \mathbb{K} be the unit cube and $\{\varphi_c\}_{c \geq 1}$ be a sequence of functions on \mathbb{R}^3 with $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ uniformly bounded such that $\mathbf{1}_{\mathbb{K}_c} \varphi_c \xrightarrow{c \rightarrow \infty} \varphi$ weakly in $L^2(\mathbb{R}^3)$. Then $\varphi \in H^1(\mathbb{R}^3)$ and, up to the extraction of a subsequence, we have*

- (1) $\mathbf{1}_{\mathbb{K}_c} \nabla \varphi_c \rightharpoonup \nabla \varphi$ weakly in $L^2(\mathbb{R}^3)$,
- (2) $\|\nabla(\varphi_c - \varphi)\|_{L^2(\mathbb{K}_c)}^2 = \|\nabla \varphi_c\|_{L^2(\mathbb{K}_c)}^2 - \|\nabla \varphi\|_{L^2(\mathbb{R}^3)}^2 + o_{c \rightarrow \infty}(1)$,
- (3) $\|\varphi_c - \varphi\|_{L^p(\mathbb{K}_c)}^p = \|\varphi_c\|_{L^p(\mathbb{K}_c)}^p - \|\varphi\|_{L^p(\mathbb{R}^3)}^p + o_{c \rightarrow \infty}(1)$, for $p \in \{\frac{8}{3}, \frac{10}{3}\}$.

Proof of Lemma 29. By the mean of a regularization function (as in the proof of Lemma 26) together with the uniform boundedness of φ_c in $H^1(\mathbb{K}_c)$ and the uniqueness of the limit, one obtains that the limit φ is in $H^1(\mathbb{R}^3)$. Since (1) is a classical result and (2) a direct consequence of it, we only prove here (3).

By means of a regularization function, the Rellich-Kondrachov theorem together with the weak convergence in $L^2(\mathbb{R}^3)$ of $\mathbf{1}_{\mathbb{K}_c} \varphi_c$ and of $\mathbf{1}_{\mathbb{K}_c} \nabla \varphi_c$, one obtains that

$|\varphi_c - \varphi| \rightharpoonup 0$ weakly in $L^p(\mathbb{R}^3)$ for $2 \leq p \leq 6$. Using now, for all $p > 2$, the bound

$$\left| |\varphi_c(x) - \varphi(x)|^p - |\varphi_c(x)|^p + |\varphi(x)|^p \right| \leq \sum_{k=1}^{\lfloor p \rfloor} \binom{p}{k} |\varphi(x)|^{p-k} |\varphi_c(x) - \varphi(x)|^k,$$

which comes from direct computations, one obtains (3) from the weak convergence of $|\varphi - \varphi_c| \rightharpoonup 0$ in $L^2(\mathbb{R}^3)$. \square

To obtain for $E_{\mathbb{K},\lambda}(c)$ an expansion similar to (5.11), we proceed the same way. We first show that the sequence of minimizers \check{w}_c is uniformly bounded in $H_{\text{per}}^1(\mathbb{K}_c)$ using the upper bound in the following lemma, which is equivalent to Corollary 23 for \check{v}_c .

Lemma 30 (Uniform norm bounds on minimizers of $E_{\mathbb{K},\lambda}(c)$). *Let \mathbb{K} be the unit cube, λ, c_{TF} and c be positive. Then there exist $C > 0$ and $c_* > 0$ such that for any $c \geq c_*$, the dilation $\check{w}_c(x) := c^{-3/2}w_c(c^{-1}x)$ of a minimizer w_c to $E_{\mathbb{K},\lambda}(c)$ verifies*

$$\frac{1}{C} \leq \|\nabla \check{w}_c\|_{L^2(\mathbb{K}_c)}, \|\check{w}_c\|_{L^{10/3}(\mathbb{K}_c)}, \|\check{w}_c\|_{L^{8/3}(\mathbb{K}_c)} \leq C.$$

Proof of Lemma 30. As seen in the proof of Lemma 25, $\|\nabla w_c\|_{L^2(\mathbb{K})} = O(c)$ hence

$$\|\nabla \check{w}_c\|_{L^2(\mathbb{K}_c)}^2 = c^{-2} \|\nabla w_c\|_{L^2(\mathbb{K})}^2 = O(1)$$

and, using Sobolev embeddings for the two other norms, we have

$$\forall c \geq c_*, \quad \|\nabla \check{w}_c\|_{L^2(\mathbb{K}_c)}, \|\check{w}_c\|_{L^{10/3}(\mathbb{K}_c)}, \|\check{w}_c\|_{L^{8/3}(\mathbb{K}_c)} \leq C'.$$

Let K be such that $0 < K < -J_{\mathbb{R}^3,\lambda}$ and $\varepsilon > 0$, then by (5.5) and Lemma 25, there exists $C > 0$ such that

$$c^2 K - \varepsilon \leq -J_{\mathbb{K},\lambda}(c) - \varepsilon \leq -E_{\mathbb{K},\lambda}(c) \leq c \left(C + \frac{3}{4} \|w_c\|_{L^{8/3}(\mathbb{K})}^{\frac{8}{3}} \right)$$

for c 's large enough and, consequently that

$$K - \frac{C + \varepsilon}{c^2} \leq \frac{3}{4} \|\check{w}_c\|_{L^{8/3}(\mathbb{K}_c)}^{8/3}.$$

We conclude this proof of Lemma 30 as we did in the proof of Corollary 23. \square

We now come back to the proof of Proposition 24. We apply Lemma 28 to $\{\check{w}_c\}$ and, as for \check{v}_c , the lower bound in Lemma 30 implies that $J \geq 1$, namely that there exist at least a first extracted bubble $0 \neq \check{w} \in H^1(\mathbb{R}^3)$ such that $\mathbf{1}_{\mathbb{K}_{c_k}} \check{w}_{c_k}(\cdot + y_k) \rightharpoonup \check{w}$ weakly in $L^2(\mathbb{R}^3)$. Lemma 29 then leads to

$$\begin{aligned} c_k^{-2} E_{\mathbb{K},\lambda}(c_k) &= \mathcal{J}_{\mathbb{K}_{c_k},1}(\check{w}_{c_k}(\cdot + y_k)) + O(c_k^{-1}) \\ &= \mathcal{J}_{\mathbb{R}^3}(\check{w}) + \mathcal{J}_{\mathbb{K}_{c_k},1}(\check{w}_{c_k}(\cdot + y_k) - \check{w}) + o(1), \end{aligned}$$

where the term $O(c^{-1})$ comes from $D_{\mathbb{K}}(w_c^2, w_c^2) = O(c)$ and $\int_{\mathbb{K}} G_{\mathbb{K}} w_c^2 = O(c)$ obtained in the proof of Lemma 25.

Since in both cases J and E , the left hand side converges to $J_{\mathbb{R}^3}(\lambda)$, the end of the argument will be the same and we will therefore only write it in the case of E . Defining $\lambda_1 := \|\check{w}\|_{L^2(\mathbb{R}^3)}^2$, which is strictly positive since $\check{w} \neq 0$, we thus have

$$c_k^{-2} E_{\mathbb{K},\lambda}(c_k) \geq J_{\mathbb{R}^3}(\lambda_1) + J_{\mathbb{K}_{c_k}}(\|\check{w}_{c_k}(\cdot + y_k) - \check{w}\|_{L^2(\mathbb{K}_{c_k})}^2) + o(1).$$

Since $\|\check{w}_{c_k}(\cdot + y_k) - \check{w}\|_{L^2(\mathbb{K}_{c_k})}^2 = \lambda - \lambda_1 + o(1)$, then for any $\varepsilon > 0$, we have

$$c_k^{-2} E_{\mathbb{K},\lambda}(c_k) \geq J_{\mathbb{R}^3}(\lambda_1) + J_{\mathbb{K}_{c_k}}(\lambda - \lambda_1 + \varepsilon) + o(1),$$

By the convergence of $c^{-2} E_{\mathbb{K},\lambda}(c)$ for any $\lambda > 0$, this leads to

$$J_{\mathbb{R}^3}(\lambda) \geq J_{\mathbb{R}^3}(\lambda_1) + J_{\mathbb{R}^3}(\lambda - \lambda_1 + \varepsilon)$$

and, sending ε to 0, the continuity of $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$, proved in Lemma 10, gives

$$J_{\mathbb{R}^3}(\lambda) \geq J_{\mathbb{R}^3}(\lambda_1) + J_{\mathbb{R}^3}(\lambda - \lambda_1).$$

We recall that $\lambda_1 > 0$ hence, if $\lambda_1 < \lambda$ then the above large inequality would contradict the strict binding proved in Proposition 12, hence $\lambda_1 = \lambda$. This convergence of the norms combined with the original weak convergence in $L^2(\mathbb{R}^3)$ gives the strong convergence in $L^2(\mathbb{R}^3)$ of $\mathbf{1}_{\mathbb{K}_c} \check{w}_c(\cdot + y_k)$ to \check{w} hence in $L^p(\mathbb{R}^3)$ for $2 \leq p < 6$ by Hölder's inequality, Sobolev embeddings and the facts that \check{w}_c is uniformly bounded in $H_{\text{per}}^1(\mathbb{K}_c)$ and that $\check{w} \in H^1(\mathbb{R}^3)$. The strong convergence holds in particular in $L^{\frac{8}{3}}(\mathbb{R}^3)$ thus we have proved that \check{w} is the first and only bubble.

Finally, for any $\varepsilon > 0$, we now have, for k large enough, that

$$\begin{aligned} c_k^{-2} E_{\mathbb{K}, \lambda}(c_k) &= \mathcal{J}_{\mathbb{R}^3}(\check{w}) + \mathcal{J}_{\mathbb{K}_{c_k}, 1}(\check{w}_{c_k}(\cdot + y_k) - \check{w}) + o(1) \\ &\geq \mathcal{J}_{\mathbb{R}^3}(\check{w}) + J_{\mathbb{K}_{c_k}}(\varepsilon) + o(1). \end{aligned}$$

This leads to $J_{\mathbb{R}^3}(\lambda) \geq \mathcal{J}_{\mathbb{R}^3}(\check{w}) + J_{\mathbb{R}^3}(\varepsilon)$, then to $J_{\mathbb{R}^3}(\lambda) \geq \mathcal{J}_{\mathbb{R}^3}(\check{w})$ by the continuity of $J_{\mathbb{R}^3}(\lambda)$ proved in Lemma 10. Since $\|\check{w}\|_{L^2(\mathbb{R}^3)}^2 = \lambda$, this concludes the proof of Proposition 24 up to the convergence of $\mathbf{1}_{\mathbb{K}_{c_n}} \nabla \check{w}_n(\cdot + x_n)$ and $\mathbf{1}_{\mathbb{K}_{c_n}} \nabla \check{v}_n(\cdot + x_n)$ that we deduce now from the above results. Indeed, by the convergence in $L^p(\mathbb{R}^3)$ of $\check{w}_n(\cdot + x_n)$ and since $|\int_{\mathbb{K}} G_{\mathbb{K}} w_n^2| + |D_{\mathbb{K}}(w_n^2, w_n^2)| = O(c_n)$, we know, except for the gradient term, that all terms of $c_n^{-2} E_{\mathbb{K}, \lambda}(c_n)$ (resp. $c_n^{-2} J_{\mathbb{K}, \lambda}(c_n)$) converge thus the gradient term too. Then we apply Lemma 29 to obtain the strong convergence in $L^2(\mathbb{R}^3)$ from this convergence in norm just obtained. \square

Let us emphasize that all the results stated in this section still hold true in the case of several charges per cell (for example for the union $N \cdot \mathbb{K}$) with same proofs. The modifications only come from the factor $\int_{\mathbb{K}} G_{\mathbb{K}} w_c^2$ being replaced by $\int_{\mathbb{K}} \sum_{i=1}^{N_q} G_{\mathbb{K}}(\cdot - R_i) |w_c|^2$ — see (5.12) — therefore only the proofs of Proposition 24, Lemma 25 and Lemma 30 are slightly changed by a factor N_q in the bounds of the modified term, but their statement is unchanged. Consequently, as mentioned in Section 2.1, the results

$$\lim_{c \rightarrow \infty} c^{-2} E_{N \cdot \mathbb{K}, N^3 \lambda}(c) = J_{\mathbb{R}^3, N^3 \lambda} \quad \text{and} \quad \lim_{c \rightarrow \infty} c^{-2} E_{\mathbb{K}, \lambda}(c) = J_{\mathbb{R}^3, \lambda}$$

from Proposition 24 and the result

$$J_{\mathbb{R}^3}(N^3 \lambda) < N^3 J_{\mathbb{R}^3}(\lambda)$$

from Proposition 12 imply together the symmetry breaking

$$E_{N \cdot \mathbb{K}, N^3 \lambda}(c) < N^3 E_{\mathbb{K}, \lambda}(c).$$

We now give two corollaries of Proposition 24. We state and prove them in the case of one charge per unit cell but they hold, with similar proof, for several charges.

Corollary 31 (Convergence of Euler–Lagrange multiplier). *Let $\{w_c\}$ be a sequence of minimizers to $E_{\mathbb{K}, \lambda}(c)$ and $\{\mu_c\}$ the sequence of associated Euler–Lagrange multipliers, as in Proposition 15. Then there exists a subsequence $c_n \rightarrow \infty$ such that*

$$c_n^{-2} \mu_{c_n} \xrightarrow[n \rightarrow \infty]{} \mu_{\mathbb{R}^3, \{w_{c_n}\}}$$

with $\mu_{\mathbb{R}^3, \{w_{c_n}\}}$ the Euler–Lagrange multiplier associated with the minimizer to $J_{\mathbb{R}^3}(\lambda)$ to which the subsequence of dilated functions $\mathbf{1}_{\mathbb{K}_{c_n}} \check{w}_{c_n}(\cdot + x_n)$ converges strongly.

The same holds for sequences $\{v_c\}$ of Euler–Lagrange multipliers associated with minimizers to $J_{\mathbb{K}, \lambda}(c)$.

Proof of Corollary 31. Let u be the minimizer of $J_{\mathbb{R}^3}(\lambda)$ to which $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_{c_n}(\cdot + x_n)$ converges strongly in $L^p(\mathbb{R}^3)$ for $2 \leq p < 6$, by Proposition 24 which also gives that $\mathbb{1}_{\mathbb{K}_{c_n}} \nabla \check{w}_{c_n}(\cdot + x_n) \rightarrow \nabla u$ strongly in $L^2(\mathbb{R}^3)$, and $\mu_{\mathbb{R}^3, u}$ the Euler–Lagrange multiplier associated with this u by Theorem 3.

By Lemma 30 and the formula (4.4) giving an expression of μ_c , we then obtain

$$-c_n^{-2} \mu_{c_n} \lambda \rightarrow \|\nabla u\|_{L^2(\mathbb{R}^3)}^2 + c_{TF} \|u\|_{L^{10/3}(\mathbb{R}^3)}^{10/3} - \|u\|_{L^{8/3}(\mathbb{R}^3)}^{8/3}.$$

Therefore, by (3.5) which gives an expression of the Euler–Lagrange parameter $\mu_{\mathbb{R}^3, u}$ associated with this u , we have

$$c_n^{-2} \mu_{c_n} \xrightarrow{c \rightarrow \infty} \mu_{\mathbb{R}^3, u}.$$

Since u depends on $\{w_{c_n}\}$, we can of course rename $\mu_{\mathbb{R}^3, \{w_{c_n}\}} := \mu_{\mathbb{R}^3, u}$. The result for $J_{\mathbb{K}, \lambda}(c)$ is proved the same way. \square

Lemma 32 (L^∞ -convergence). *Let $\{w_c\}_c$ be a sequence of minimizers to $E_{\mathbb{K}, \lambda}(c)$ and u be the minimizer to $J_{\mathbb{R}^3}(\lambda)$ to which the subsequence of rescaled functions $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_{c_n}(\cdot + x_n)$ converges. Then*

$$\|\check{w}_{c_n}(\cdot + x_n) - u\|_{H^2(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow +\infty} 0 \quad \text{and} \quad \|\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_{c_n}(\cdot + x_n) - u\|_{L^\infty(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow +\infty} 0.$$

The same result holds for a sequence $\{v_c\}_c$ of minimizers to $J_{\mathbb{K}, \lambda}(c)$.

Proof of Lemma 32. For shortness, we omit the spatial translations $\{x_n\}$ in this proof. We define $u_c = \zeta_c u$ where ζ_c is a smooth function such that $0 \leq \zeta_c \leq 1$, $\zeta_c \equiv 0$ on $\mathbb{R}^3 \setminus \mathbb{K}_c$ and $\zeta_c \equiv 1$ on \mathbb{K}_{c-1} . Since $u \in H^2(\mathbb{R}^3)$ by Theorem 3 and $\|\zeta_c\|_\infty + \|\nabla \zeta_c\|_\infty + \|\Delta \zeta_c\|_\infty < \infty$, we have to prove $\|\check{w}_{c_n} - u_{c_n}\|_{H^2(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow +\infty} 0$. Moreover, by the Rellich-Kato theorem, the operator $-\Delta_{\text{per}} - c^{-2} G_{\mathbb{K}}(c^{-1} \cdot)$ is self-adjoint of domain $H_{\text{per}}^2(\mathbb{K}_c)$ and bounded below. Therefore, there exists $0 < C < 1$ such that, for any β large enough and any $c \geq 1$, we have

$$\|\check{w}_c - u_c\|_{H_{\text{per}}^2(\mathbb{K}_c)} \leq C \|(-\Delta_{\text{per}} - c^{-2} G_{\mathbb{K}}(c^{-1} \cdot) + \beta)(\check{w}_c - u_c)\|_{L_{\text{per}}^2(\mathbb{K}_c)}.$$

Thus, denoting $\mathcal{C}_c^- := \mathbb{K}_c \setminus \mathbb{K}_{c-1}$ and $\mu_{\mathbb{R}^3}$ the Euler–Lagrange parameter associated with u , we have by the Euler–Lagrange equations (2.10) and (4.3) that

$$\begin{aligned} & \|\check{w}_c - u_c\|_{H_{\text{per}}^2(\mathbb{K}_c)} \\ & \leq C c_{TF} \left\| \zeta_c^{\frac{3}{7}} u - \check{w}_c \right\|_{L^4(\mathbb{K}_c)} \left\| \zeta_c^{\frac{4}{7}} |u|^{\frac{4}{3}} + |\check{w}_c|^{\frac{4}{3}} \right\|_{L^4(\mathbb{K}_c)} + \|u\|_{L^2(\mathcal{C}_c^-)} \|\Delta \zeta_c\|_{L^\infty(\mathbb{K}_c)} \\ & + C \left\| \zeta_c^{\frac{3}{5}} u - \check{w}_c \right\|_{L^4(\mathbb{K}_c)} \left\| \zeta_c^{\frac{2}{5}} |u|^{\frac{2}{3}} + |\check{w}_c|^{\frac{2}{3}} \right\|_{L^4(\mathbb{K}_c)} + 2 \|\nabla \zeta_c\|_{L^\infty(\mathbb{K}_c)} \|\nabla u\|_{L^2(\mathcal{C}_c^-)} \\ & + C |\mu_{\mathbb{R}^3} - c^{-2} \mu_c| \|\check{w}_c\|_{L^2(\mathbb{K}_c)} + C (\mu_{\mathbb{R}^3} + \beta) \|\zeta_c u - \check{w}_c\|_{L^2(\mathbb{K}_c)} \\ & + C c^{-2} \|G_{\mathbb{K}}(c^{-1} \cdot)\|_{L^{5/2}(\mathbb{K}_c)} \|u_c\|_{L^{10}(\mathbb{K}_c)} + C c^{-2} \| |u_c|^2 \star G_{\mathbb{K}} \|_{L^\infty(\mathbb{K})} \|\check{w}_c\|_{L^2(\mathbb{K}_c)}, \end{aligned}$$

for any $c > 0$. Therefore, combining that the $L^\infty(\mathbb{K}_c)$ norms of ζ_c and of its derivatives are finite, that $\|\nabla u\|_{L^2(\mathcal{C}_c^-)} + \|u\|_{L^2(\mathcal{C}_c^-)} \rightarrow 0$, that $c^{-2} \|G_{\mathbb{K}}(c^{-1} \cdot)\|_{L^{5/2}(\mathbb{K}_c)} = c^{-\frac{4}{5}} \|G_{\mathbb{K}}\|_{L^{5/2}(\mathbb{K})} \rightarrow 0$ and that, for any $\alpha > 0$ and $2 \leq p \leq 6$, we have

$$\|\zeta_{c_n}^\alpha u - \check{w}_{c_n}\|_{L^p(\mathbb{K}_{c_n})} = \|(1 - \zeta_{c_n}^\alpha)u\|_{L^p(\mathbb{K}_{c_n})} + \|u - \check{w}_{c_n}\|_{L^p(\mathbb{K}_{c_n})} \rightarrow 0,$$

all together with Corollary 31, we conclude that

$$\|\check{w}_{c_n} - u_{c_n}\|_{H_{\text{per}}^2(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow +\infty} 0.$$

The proof for v_c is similar but easier and shorter, we thus omit it.

We then conclude the proof of Lemma 32 using that for any $c^* > 0$, there exists C such that for any $c \in [c^*, \infty)$ and $f \in H^2(\mathbb{K}_c)$, we have $\|f\|_{L^\infty(\mathbb{K}_c)} \leq C \|f\|_{H^2(\mathbb{K}_c)}$ which can be proved by means of Fourier series. \square

5.2. Location of the concentration points. In this section we consider the union of N^3 cubes \mathbb{K} , each containing one charge $q = 1$ — that we can assume to be at the center of the cube \mathbb{K} — forming together the cube $\mathbb{K}_N := N \cdot \mathbb{K}$. The energy of the unit cell \mathbb{K}_N is then

$$\mathcal{E}_{\mathbb{K}_N, c}(w) = \mathcal{J}_{\mathbb{K}_N, c}(w) + \frac{1}{2} D_{\mathbb{K}_N}(|w|^2, |w|^2) - \int_{\mathbb{K}_N} \sum_{i=1}^{N^3} G_{\mathbb{K}_N}(\cdot - R_i) |w|^2, \quad (5.12)$$

where $\{R_i\}_{1 \leq i \leq N^3}$ denote the positions of the N^3 charges.

In this section, we prove a localization type result (Proposition 33) — that any minimizer concentrates around the position of a charge of the lattice — and a lower bound on the number of distinct minimizers (Proposition 35).

Proposition 33 (Minimizers' concentration point). *Let $\{R_j\}_{1 \leq j \leq N^3}$ be the respective positions of the N^3 charges inside \mathbb{K}_N . Then the sequence $\{x_n\} \subset c_n \cdot \mathbb{K}_N$ of translations associated with the subsequence $\{w_{c_n}\}$ of minimizers to $E_{\mathbb{K}_N, N^3 \lambda}(c_n)$ such that the rescaled sequence $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_{c_n}(\cdot + x_n)$ converges to Q , a the minimizer to $J_{\mathbb{R}^3, N^3 \lambda}$, verifies*

$$x_n = c_n R_i + o(1)$$

as $n \rightarrow \infty$, for one i . Consequently, for $2 \leq p < +\infty$,

$$\|\check{w}_{c_n}(\cdot + c_n R_i) - Q\|_{L^p(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow +\infty} 0.$$

Proof of Proposition 33. Since the w_{c_n} 's are minimizers, we have for any R_j that

$$\mathcal{E}_{\mathbb{K}_N, c_n}(w_{c_n}) \leq \mathcal{E}_{\mathbb{K}_N, c_n}\left(w_{c_n}\left(\cdot + \frac{x_n}{c_n} - R_j\right)\right)$$

which leads to

$$\begin{aligned} & - \sum_{i=1}^{N^3} \int_{\mathbb{K}_N c_n} G_{\mathbb{K}_N}\left(\frac{x}{c_n} + \frac{x_n}{c_n} - R_i\right) \left| \check{w}_{c_n}\left(x + \frac{x_n}{c_n}\right) \right|^2 dx \\ & \leq - \sum_{i=1}^{N^3} \int_{\mathbb{K}_N c_n} G_{\mathbb{K}_N}\left(\frac{x}{c_n} + R_j - R_i\right) \left| \check{w}_{c_n}\left(x + \frac{x_n}{c_n}\right) \right|^2 dx \end{aligned}$$

since the four first terms of $\mathcal{E}_{\mathbb{K}_N, c}$ are invariant under spatial translations. Lemma 34 below then gives, on one hand, that the right hand side of this inequality is equal to $-c_n \int_{\mathbb{R}^3} \frac{Q^2(x)}{|x|} dx + o(c_n)$ because $c_n |R_j - R_i| \rightarrow \infty$ for $i \neq j$ and, on the other hand, that $|x_n - c_n R_i|$ must be bounded for one i , that we denote i_0 , because otherwise the left hand side would be equal to $o(c_n)$. Therefore, still by Lemma 34, the term for i_0 in the left hand side is equal to $-c_n \int_{\mathbb{R}^3} \frac{Q^2(x)}{|x-\eta|} dx + o(c_n)$ for a given $\eta \in \mathbb{R}^3$ (and up to a subsequence) and the other terms of the sum to $o(c_n)$. However,

$$\int_{\mathbb{R}^3} \frac{Q^2(x)}{|x|} dx > \int_{\mathbb{R}^3} \frac{Q^2(x)}{|x-\eta|} dx$$

if $\eta \neq 0$, implying that the w_{c_n} are not minimizers for n large enough. Hence $\eta = 0$, which means by Lemma 34 that $x_n = c_n R_{i_0} + o(1)$ as $n \rightarrow \infty$.

The last result of Proposition 33 is a direct consequence of the convergence of the $L^p(\mathbb{K}_{c_n})$ -norms proved in Proposition 24 and Lemma 32 together with the fact that $x_n - c_n R_{i_0} = o(1)$.

Lemma 34. *Let $\{y_n\}_n \subset \mathbb{K}$, $\{f_c\}_c \subset L^2_{per}(\mathbb{K}_c)$ and $\{g_c\}_c \subset L^2_{per}(\mathbb{K}_c)$ be two sequences such that $\|f_c\|_{H^1_{per}(\mathbb{K}_c)} + \|g_c\|_{H^1_{per}(\mathbb{K}_c)}$ is uniformly bounded. We assume that there exist f and g in $H^1(\mathbb{R}^3)$ and a subsequence c_n such that $\|f_{c_n} - f\|_{L^2(K_{c_n})} \xrightarrow{n \rightarrow \infty} 0$ and $\mathbb{1}_{\mathbb{K}_{c_n}} g_{c_n} \xrightarrow{n \rightarrow \infty} g$ weakly in $L^2(\mathbb{R}^3)$. Then,*

- i. if $c_n|y_n| \rightarrow +\infty$, then $c_n^{-1} \int_{\mathbb{K}_{c_n}} G_{\mathbb{K}}(c_n^{-1} \cdot -y_n) f_{c_n} g_{c_n} \xrightarrow{n \rightarrow \infty} 0$,
- ii. if $c_n|y_n| \rightarrow 0$, then $c_n^{-1} \int_{\mathbb{K}_{c_n}} G_{\mathbb{K}}(c_n^{-1} \cdot -y_n) f_{c_n} g_{c_n} \xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^3} \frac{f(x)g(x)}{|x|} dx$,
- iii. otherwise, there exist $\eta \in \mathbb{R}^3 \setminus \{0\}$ and a subsequence n_k such that

$$c_{n_k}^{-1} \int_{\mathbb{K}_{c_{n_k}}} G_{\mathbb{K}}(c_{n_k}^{-1} \cdot -y_{n_k}) f_{c_{n_k}} g_{c_{n_k}} \xrightarrow{k \rightarrow \infty} \int_{\mathbb{R}^3} \frac{f(x)g(x)}{|x - \eta|} dx.$$

Moreover, replacing $\|f_{c_n} - f\|_{L^2(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow \infty} 0$ by $\|f_{c_n} - f\|_{H^1(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow \infty} 0$, the uniform bound on $\|g_c\|_{H^1_{\text{per}}(\mathbb{K}_c)}$ by an uniform bound on $\|g_c\|_{L^2_{\text{per}}(\mathbb{K}_c)}$ and $g \in H^1(\mathbb{R}^3)$ by $g \in L^2(\mathbb{R}^3)$, then i. still holds true and, in the special case $y_n = 0$, ii. too.

Remark. We state the lemma in a more general settings than needed for Proposition 33 in order for it to be also useful for the proof of Lemma 42.

Proof of Lemma 34. Using the same notation \mathbb{K}^σ as in the proof of Lemma 25, we notice that $\mathbb{K} - \tau := \{x \in \mathbb{R}^3 | x - \tau \in \mathbb{K}\} \subset \mathbb{K}_2 = \mathbb{K} \cup \bigcup_{(0,0,0) \neq \sigma \in \{0; \pm 1\}^3} \mathbb{K}^\sigma$, for any $\tau \in \mathbb{K}$. Therefore, by Lemma 14, there exists $C > 0$ such that for any $\varphi_c \in L^2(\mathbb{K}_c)$, $\psi_c \in H^1(\mathbb{K}_c)$, $y \in \mathbb{K}$ and $c > 0$,

$$c^{-1} \left| \int_{\mathbb{K}_c} G_{\mathbb{K}}(c^{-1} \cdot -y) \varphi_c \psi_c \right| \leq C \sum_{\sigma \in \{-1; 0; +1\}^3} \left\| \frac{\varphi_c \psi_c}{|\cdot - c(y + \sigma)|} \right\|_{L^1(\mathbb{K}_c)}.$$

Then, by the Hardy inequality on \mathbb{K}_c , which is uniform on $[c_*, \infty)$ for any $c_* > 0$, there exists C' such that for any $y \in \mathbb{K}$ and any $c \geq 1$, we obtain

$$c^{-1} \left| \int_{\mathbb{K}_c} G_{\mathbb{K}}(c^{-1} \cdot -y) \varphi_c \psi_c \right| \leq 27C' \|\varphi_c\|_{L^2(\mathbb{K}_c)} \|\psi_c\|_{H^1(\mathbb{K}_c)}.$$

Therefore, the weak convergence of g_{c_n} and the Hardy inequality to f on \mathbb{R}^3 give

$$\begin{aligned} & c_n^{-1} \left| \int_{\mathbb{K}_{c_n}} G_{\mathbb{K}}(c_n^{-1} \cdot -y_n) (f_{c_n} g_{c_n} - fg) \right| \\ & \leq 27 \left(C' \|f_{c_n} - f\|_{L^2(\mathbb{K}_{c_n})} \|g_{c_n}\|_{H^1(\mathbb{K}_{c_n})} + 2C \left\| \frac{f(g_{c_n} - g)}{|\cdot - c(y + \sigma)|} \right\|_{L^1(\mathbb{K}_{c_n})} \right) \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

Replacing $\|f_{c_n} - f\|_{L^2(\mathbb{K}_{c_n})} \|g_{c_n}\|_{H^1(\mathbb{K}_{c_n})}$ by $\|f_{c_n} - f\|_{H^1(\mathbb{K}_{c_n})} \|g_{c_n}\|_{L^2(\mathbb{K}_{c_n})}$ gives this same convergence to 0 under the second set of conditions.

We are therefore left with the study of $c_n^{-1} \int_{\mathbb{K}_{c_n}} G_{\mathbb{K}}(c_n^{-1} \cdot -y_n) fg$ as $n \rightarrow \infty$ and we start with the case $c_n|y_n| \rightarrow +\infty$. For $c > 0$, $y \in \mathbb{K}$ and $\sigma \in \{-1; 0; +1\}^3$, we have

$$\begin{aligned} & c^{-1} \int_{\mathbb{K}_c} \mathbf{1}_{\mathbb{K}^\sigma}(c^{-1} \cdot -y) G_{\mathbb{K}}(c^{-1} \cdot -y) |fg| \\ & \lesssim \int_{\mathbb{R}^3} \frac{\mathbf{1}_{B(0, \frac{c}{2}|y + \sigma|)}}{|\cdot - c(y + \sigma)|} |fg| + \int_{\mathbb{R}^3} \frac{\mathbf{1}_{B(c(y + \sigma), R)}}{|\cdot - c(y + \sigma)|} |fg| + \int_{cB(0, \frac{c}{2}|y + \sigma|)} \frac{\mathbf{1}_{cB(c(y + \sigma), R)}}{|\cdot - c(y + \sigma)|} |fg| \\ & \lesssim \frac{2}{c|y + \sigma|} \|fg\|_{L^1(\mathbb{R}^3)} + \|f\|_{H^1(\mathbb{R}^3)} \|g\|_{L^2(B(c(y + \sigma), R))} + \frac{1}{R} \|fg\|_{L^1(cB(0, \frac{c}{2}|y + \sigma|))}, \end{aligned}$$

for any $R > 0$. Since f is in $H^1(\mathbb{R}^3)$ and g at least in $L^2(\mathbb{R}^3)$, the last two terms tends to 0 and $\|fg\|_{L^1(\mathbb{R}^3)}$ is bounded hence, on one hand we obtain, for $\sigma = (0, 0, 0)$, the convergence to 0 (for the subsequence c_n) from $c_n|y_n| \rightarrow +\infty$ and, on the other hand, there exists $R' > 0$ such that $|y + \sigma| > R'$ for any $\{-1; 0; +1\}^3 \ni \sigma \neq (0, 0, 0)$ and any $y \in \mathbb{K}$, ending the proof that the above tends to 0. We finally obtain that

$$\frac{1}{c_n} \int_{\mathbb{K}_{c_n}} G_{\mathbb{K}}(c_n^{-1} \cdot -y_n) |fg| = \sum_{\sigma \in \{0; \pm 1\}^3} \frac{1}{c_n} \int_{\mathbb{K}_{c_n}} [\mathbf{1}_{\mathbb{K}^\sigma} G_{\mathbb{K}}](c_n^{-1} \cdot -y_n) |fg| \xrightarrow{n \rightarrow \infty} 0,$$

concluding the proof of *i.* under the two sets of hypothesis.

We now suppose that $c_n|y_n|$ does not diverge hence it is bounded up to a subsequence n_k and, consequently, $y_{n_k} \rightarrow 0$. However, by Lemma 14, there exists $M' > 0$ such that $|\cdot|^{-1} - G_{\mathbb{K}}| \leq M'$ on \mathbb{K} , thus there exists $M > 0$ such that

$$\begin{aligned} \left| G_{\mathbb{K}} - \frac{1}{|\cdot|} \right| \mathbf{1}_{\mathbb{K}-\tau} &\leq \left(M' \mathbf{1}_{\mathbb{K}} + \frac{\mathbf{1}_{c_{\mathbb{K}}}}{|\cdot|} + C \sum_{(0,0,0) \neq \sigma \in \{0; \pm 1\}^3} \frac{\mathbf{1}_{\mathbb{K}\sigma}}{|\cdot + \tau - \sigma| - |\tau|} \right) \mathbf{1}_{\mathbb{K}-\tau} \\ &\leq (M' + R^{-1} + 52CR^{-1}) \mathbf{1}_{\mathbb{K}-\tau} \leq M \mathbf{1}_{\mathbb{K}-\tau}. \end{aligned}$$

for $\tau \in B(0, R/2)$ and where $R := \min_{x \in \partial \mathbb{K}} |x| > 0$ therefore $B(0, R) \subset \mathbb{K}$. Hence

$$\left| \int_{\mathbb{K}_{c_{n_k}}} \left(\frac{1}{c_{n_k}} G_{\mathbb{K}} \left(\frac{\cdot}{c_{n_k}} - y_{n_k} \right) - |\cdot - c_{n_k} y_{c_{n_k}}|^{-1} \right) fg \right| \leq \frac{M}{c_{n_k}} \|fg\|_{L^1(\mathbb{R}^3)} = O\left(\frac{1}{c_{n_k}}\right).$$

Moreover,

$$\left| \int_{\mathbb{R}^3} (1 - \mathbf{1}_{\mathbb{K}_{c_{n_k}}}(x)) \frac{f(x)g(x)}{|x - c_{n_k} y_{c_{n_k}}|} dx \right| \lesssim \|f\|_{L^2(c_{\mathbb{K}_{c_{n_k}}})} \|g\|_{H^1(\mathbb{R}^3)} \rightarrow 0$$

and we are left with the study of

$$\left| \int_{\mathbb{R}^3} \frac{f(x)g(x)}{|x - c_{n_k} y_{c_{n_k}}|} - \frac{f(x)g(x)}{|x - \eta|} dx \right| \leq 4|\eta - c_{n_k} y_{c_{n_k}}| \|f\|_{H^1(\mathbb{R}^3)} \|g\|_{H^1(\mathbb{R}^3)}$$

which tends to 0 if we choose η as the limit (up to another subsequence) of the bounded sequence $c_{n_k} y_{n_k}$. Finally, if we have in fact $c_n y_n \rightarrow 0$ then $\eta = 0$, otherwise, we can find a subsequence such that $c_{n_k} y_{n_k} \rightarrow \eta \neq 0$.

Under the second set of conditions and if $y_n = 0$, we have

$$\left| \int_{\mathbb{K}_{c_n}} (c_n^{-1} G_{\mathbb{K}}(c_n^{-1} x) - |x|^{-1}) f(x)g(x) dx \right| \leq \frac{M'}{c_n} \|fg\|_{L^1(\mathbb{R}^3)} = O(c_n^{-1}).$$

This concludes the proof of Lemma 34. \square

This concludes the proof of Proposition 33. \square

We now prove that $E_{\mathbb{K}_N, N^3 \lambda}(c)$ admits at least N^3 distinct minimizers.

Proposition 35. *For c_n large enough, there exist at least N^3 non-negative minimizers to the minimization problem $E_{\mathbb{K}_N, N^3 \lambda}(c_n)$ which are translations one of each other by vectors $R_j - R_k$, $1 \leq j \neq k \leq N^3$, where $\{R_i\}_{1 \leq i \leq N^3}$ are the respective positions of the N^3 charges inside \mathbb{K}_N .*

Proof of Proposition 35. First, in Proposition 33, we have seen that for any sequence $\{w_c\}_{c \rightarrow +\infty}$ of minimizers of $E_{\mathbb{K}_N, N^3 \lambda}(c)$ must concentrate, up to a subsequence, at the position of one nucleus of the unit cell, denoted R_{j_0} . Then, given that the four first terms of $\mathcal{E}_{\mathbb{K}_N, c}$ are invariant under any translations and $\int G_{\mathbb{K}} |w_c|^2$ is invariant under $R_j - R_k$ translations, we have that each $w_c(\cdot + R_i - R_{j_0})$, for $1 \leq i \leq N^3$, is also a minimizer of $E_{\mathbb{K}_N, N^3 \lambda}(c)$. Since, the N^3 sequences of minimizers $\{w_{c_n}(\cdot + R_i - R_{j_0})\}_i$ have distinct limits as $n \rightarrow \infty$, there are at least N^3 distinct minimizers for n large enough. \square

5.3. Second order expansion of $E_{\mathbb{K}, \lambda}(c)$ and number of minimizers. The goal of this subsection is to prove the expansion (2.7). To do so, we improve the convergence rate of the first order expansion of $J_{\mathbb{K}, \lambda}(c)$ proved in Proposition 24. Namely, we prove that there exists $\beta > 0$ such that

$$J_{\mathbb{K}, \lambda}(c) = c^2 J_{\mathbb{R}^3}(\lambda) + o(e^{-\beta c}). \quad (5.13)$$

We recall that we have proved in Lemma 26 that there exists $\beta > 0$ such that

$$J_{\mathbb{K}, \lambda}(c) \leq c^2 J_{\mathbb{R}^3}(\lambda) + o(e^{-\beta c})$$

and we now turn to the proof of the converse inequality.

Lemma 36. *There exists $\beta > 0$ such that*

$$J_{\mathbb{K},\lambda}(c) \geq c^2 J_{\mathbb{R}^3,\lambda} + o(e^{-\beta c}).$$

Our proof relies on the exponential decay with c of the minimizers to $J_{\mathbb{K}_c,\lambda}(1)$ close to the border of the cube \mathbb{K}_c , proved in Lemma 37.

Proof of Lemma 36. As the problems $J_{\mathbb{K},\lambda}(c)$ are invariant by spatial translations, we can suppose that $x_n = 0$ in the convergences of the subsequence of rescaled functions $\mathbf{1}_{\mathbb{K}_{c_n}} \check{v}_{c_n}(\cdot + x_n)$.

Lemma 37 (Exponential decrease of minimizers to $J_{\mathbb{K}_c,\lambda}(1)$). *Let $\{v_c\}_c$ be a sequence of non-negative minimizers to $J_{\mathbb{K},\lambda}(c)$ such that a subsequence of rescaled functions $\mathbf{1}_{\mathbb{K}_{c_n}} \check{v}_{c_n}$ converges weakly to a minimizer of $J_{\mathbb{R}^3}(\lambda)$. Then there exist $C, \gamma > 0$ such that for c large enough, we have $0 \leq \check{v}_{c_n}(x) < Ce^{-\gamma c}$ for $x \in \mathbb{K}_c \setminus \mathbb{K}_{c-1}$.*

Proof of Lemma 37. We denote by u the minimizer of $J_{\mathbb{R}^3}(\lambda)$ to which $\mathbf{1}_{\mathbb{K}_{c_n}} \check{v}_{c_n}$ converges strongly and by $\mu_{\mathbb{R}^3}$ the Euler–Lagrange parameter (2.10) associated with this specific u . The Euler–Lagrange equation associated with $J_{\mathbb{K}_{c_n},\lambda}(1)$ — solved by \check{v}_{c_n} — gives

$$\left(-\Delta + \frac{\mu_{\mathbb{R}^3}}{4}\right) \check{v}_{c_n} \leq \left(|\check{v}_{c_n}|^{\frac{2}{3}} + \frac{\mu_{\mathbb{R}^3}}{4} - c_n^{-2} \mu_{c_n}\right) \check{v}_{c_n}.$$

We now define $\Omega_{c_n} = (1 + \varepsilon)\mathbb{K}_{c_n} \setminus B(0, \alpha)$ where α is such that $|u|^{\frac{2}{3}} \leq \min\{\frac{1}{2}, \frac{\mu_{\mathbb{R}^3}}{4}\}$ on $\mathbb{R}^3 \setminus B(0, \alpha)$. Such α exists by the exponential decay of u at infinity. Therefore, by Lemma 32, for any c_n large enough, we have $|\check{v}_{c_n}|^{2/3} \leq \min\{1, \frac{\mu_{\mathbb{R}^3}}{2}\}$ on $\mathbb{K}_{c_n} \setminus B(0, \alpha)$ but also on Ω_{c_n} by periodicity of \check{v}_{c_n} and for any c_n large enough (depending on ε) in order to have

$$(1 + \varepsilon)\mathbb{K}_{c_n} \cap \bigcup_{k \in \mathcal{Z}_{\mathbb{K}} \setminus \{0\}} B(c_n k, \alpha) = \emptyset.$$

Together with Corollary 31, it gives on Ω_{c_n} , for c_n large enough, that

$$\left(-\Delta + \frac{\mu_{\mathbb{R}^3}}{4}\right) \check{v}_{c_n} \leq 0 \quad \text{and} \quad |\check{v}_{c_n}| \leq 1.$$

We now define on $\mathbb{R}^3 \setminus B(0, \nu)$, for any $\nu > 0$, the positive function

$$f_\nu(x) = \nu |x|^{-1} e^{\frac{\sqrt{\mu_{\mathbb{R}^3}}}{2}(\nu - |x|)}$$

which solves

$$-\Delta f_\nu + \frac{\mu_{\mathbb{R}^3}}{4} f_\nu = 0$$

on $\mathbb{R}^3 \setminus B(0, \nu)$ and verifies $f_\nu = 1$ on the boundary $\partial B(0, \nu)$. On each $(1 + \varepsilon)\mathbb{K}_{c_n}$, we define the positive function

$$f_0(x) = \sum_{j=1}^3 \frac{\cosh\left(\frac{\sqrt{\mu_{\mathbb{R}^3}}}{2} x_j\right)}{\cosh\left(\frac{\sqrt{\mu_{\mathbb{R}^3}}}{4} (1 + \varepsilon) c_n\right)}$$

which solves

$$-\Delta f_0 + \frac{\mu_{\mathbb{R}^3}}{4} f_0 = 0$$

on $(1 + \varepsilon)\mathbb{K}_{c_n}$ and verifies $1 \leq f_0 \leq 3$ on the boundary $\partial((1 + \varepsilon)\mathbb{K}_c)$. Denoting by g the function $g := f_0 + f_\alpha$, we have for c_n large enough that

$$\left(-\Delta + \frac{\mu_{\mathbb{R}^3}}{4}\right) (\check{v}_{c_n} - g) \leq 0, \quad \text{on } \Omega_{c_n} \quad \text{and} \quad \check{v}_{c_n} - g \leq 0, \quad \text{on } \partial\Omega_{c_n},$$

hence the maximum principle implies that $\check{v}_{c_n} \leq g$ on Ω_{c_n} .

On one hand, since the function f_0 is even along each spatial direction of the cube and increasing on $[0; (1 + \varepsilon)\frac{c_n}{2})$ in those directions, we have that for any $x \in \mathbb{K}_{c_n}$, so in particular on $\mathbb{K}_{c_n} \setminus \mathbb{K}_{c_n-1}$, that

$$0 < f_0(x) \leq f_0\left(\frac{c_n}{2}(1, 1, 1)\right) \leq 2 \sum_{j=1}^3 e^{-\varepsilon \frac{\sqrt{\mu_{\mathbb{R}^3}}}{4} c_n}.$$

On the other hand, $|x| \geq (c_n - 1)m > 0$ for $x \in \mathbb{K}_{c_n} \setminus \mathbb{K}_{c_n-1}$, with $m := \min_{\partial \mathbb{K}} |x|$, thus

$$0 < f_\alpha(x) \leq \alpha e^{\frac{\sqrt{\mu_{\mathbb{R}^3}}}{2}(\alpha+m)} m^{-1} (c_n - 1)^{-1} e^{-\frac{\sqrt{\mu_{\mathbb{R}^3}}}{2} m c_n}$$

on $\mathbb{K}_{c_n} \setminus \mathbb{K}_{c_n-1}$. Hence there exist $C > 0$ and $\gamma := \frac{\sqrt{\mu_{\mathbb{R}^3}}}{2} \min\{\frac{\varepsilon}{2}; m\} > 0$ such that for c_n large enough and any $x \in \mathbb{K}_{c_n} \setminus \mathbb{K}_{c_n-1}$, we conclude that

$$0 \leq \check{v}_{c_n}(x) \leq g(x) < C e^{-\gamma c}. \quad \square$$

We now conclude the proof of Lemma 36. We define $\chi_c \in C_c^\infty(\mathbb{R}^3)$, $0 \leq \chi_c \leq 1$, $\chi_c \equiv 0$ on $\mathbb{R}^3 \setminus \mathbb{K}_c$ and $\chi_c \equiv 1$ on \mathbb{K}_{c-1} . Since $|\mathbb{K}_c \setminus \mathbb{K}_{c-1}| \leq |\mathbb{K}_c| = c^3 |\mathbb{K}|$ for any $c > 1$ and by Lemma 37, we have that there exist $0 < \alpha < \gamma$ such that

$$\begin{aligned} 0 \leq \|\check{v}_{c_n}\|_{L^p(\mathbb{K}_{c_n})}^p - \|\chi_{c_n} \check{v}_{c_n}\|_{L^p(\mathbb{R}^3)}^p &= \int_{\mathbb{K}_{c_n} \setminus \mathbb{K}_{c_n-1}} (1 - \chi_{c_n}^p) |\check{v}_{c_n}|^p \\ &\leq C^p e^{-p\gamma c_n} |\mathbb{K}_{c_n} \setminus \mathbb{K}_{c_n-1}| = o(e^{-p\alpha c_n}), \end{aligned}$$

for any $p \in [2; 6]$. Moreover, for any $c > 1$, we have

$$\left| \int_{\mathbb{R}^3} \chi_c \check{v}_c \nabla \chi_c \cdot \nabla \check{v}_c \right| = \frac{1}{2} \left| \int_{\mathbb{R}^3} |\check{v}_c|^2 \nabla(\chi_c \nabla \chi_c) \right| \leq \frac{1}{2} \int_{\mathbb{K}_c \setminus \mathbb{K}_{c-1}} |\check{v}_c|^2 (\chi_c |\Delta \chi_c| + |\nabla \chi_c|^2)$$

hence

$$\|\nabla(\chi_{c_n} \check{v}_{c_n})\|_{L^2(\mathbb{R}^3)}^2 = \|\chi_{c_n} \nabla \check{v}_{c_n}\|_{L^2(\mathbb{K}_{c_n})}^2 + o(e^{-2\alpha c_n}) \leq \|\nabla \check{v}_{c_n}\|_{L^2(\mathbb{K}_{c_n})}^2 + o(e^{-2\alpha c_n}).$$

Consequently, there exists $\beta > 0$ such that

$$J_{\mathbb{R}^3}(\lambda) \leq \mathcal{J}_{\mathbb{R}^3} \left(\frac{\sqrt{\lambda} \chi_{c_n} u}{\|\chi_{c_n} u\|_{L^2(\mathbb{R}^3)}} \right) \leq \mathcal{J}_{\mathbb{K}_{c_n}}(\check{v}_{c_n}) + o(e^{-\beta c_n}) = J_{\mathbb{K}_{c_n}}(\lambda) + o(e^{-\beta c_n}).$$

This concludes the proof of Lemma 36. \square

We can now turn to the proof of the second-order expansion of the energy.

Proposition 38 (Second order expansion of the energy). *We have the expansion*

$$\begin{aligned} E_{\mathbb{K}_N, N^3 \lambda}(c) &= c^2 J_{\mathbb{R}^3, N^3 \lambda} \\ &+ c \inf_u \left\{ \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u(x)|^2 |u(y)|^2}{|x-y|} dy dx - \int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|} dx \right\} + o(c), \end{aligned} \quad (5.14)$$

where the infimum is taken over all the minimizers of $J_{\mathbb{R}^3, N^3 \lambda}$.

Proof of Proposition 38. In order to deal with the term $D_{\mathbb{K}}$, we first prove a convergence result similar to what we did in Lemma 34 for term $\int G|w|^2$.

Lemma 39. *Let v_c be such that the rescaled function $\check{v}_c = c^{-3/2} v_c(c^{-1}x)$ verifies*

$$\mathbf{1}_{\mathbb{K}_c} \check{v}_c \xrightarrow{c \rightarrow \infty} v$$

strongly in $L^2(\mathbb{R}^3) \cap L^{\frac{12}{5}}(\mathbb{R}^3)$, then

$$c^{-1} D_{\mathbb{K}}(v_c^2, v_c^2) \rightarrow \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{v^2(x) v^2(y)}{|x-y|} dy dx =: D_{\mathbb{R}^3}(v^2, v^2).$$

Proof of Lemma 39. We have

$$\begin{aligned} D_{\mathbb{R}^3}(v^2, v^2) - c^{-1}D_{\mathbb{K}}(v_c^2, v_c^2) \\ = D_{\mathbb{R}^3}(v^2, v^2 - \mathbf{1}_{\mathbb{K}_c}\check{v}_c^2) + D_{\mathbb{R}^3}(v^2 - \mathbf{1}_{\mathbb{K}_c}\check{v}_c^2, \mathbf{1}_{\mathbb{K}_c}\check{v}_c^2) \\ + c^{-1} \int_{\mathbb{K}} \int_{\mathbb{K}} v_c^2(x) (|x-y|^{-1} - G_{\mathbb{K}}(x-y)) v_c^2(y) dy dx. \end{aligned}$$

By the Hardy-Littlewood-Sobolev inequality and the strong convergence of $\mathbf{1}_{\mathbb{K}_c}\check{v}_c$ in $L^{12/5}(\mathbb{R}^3)$, the two first terms of the right hand side vanish.

To prove that the last term vanishes too, we split the double integral over $\mathbb{K} \times \mathbb{K}$ into several parts depending on the location of $x - y$.

We start by proving the convergence for $x - y \in \mathbb{K}$. By Lemma 14,

$$\begin{aligned} c^{-1} \iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in \mathbb{K}}} v_c^2(x) |x-y|^{-1} - G_{\mathbb{K}}(x-y) v_c^2(y) dy dx \\ \leq \frac{M}{c} \iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in \mathbb{K}}} v_c^2(x) v_c^2(y) dx dy \leq \frac{M}{c} \|v_c\|_{L^2(\mathbb{K})}^4 = \frac{M}{c} \|\check{v}_c\|_{L^2(\mathbb{K}_c)}^4 \xrightarrow{c \rightarrow \infty} 0. \end{aligned}$$

When $x - y \notin \mathbb{K}$, we treat first the term due to $|\cdot|^{-1}$. We have

$$c^{-1} \iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in 2\mathbb{K} \setminus \mathbb{K}}} \frac{v_c^2(x) v_c^2(y)}{|x-y|} dy dx \leq 2c^{-1} \|v_c\|_{L^2(\mathbb{K})}^4 \xrightarrow{c \rightarrow \infty} 0.$$

To deal with the remaining terms due to $G_{\mathbb{K}}$ when $x - y \notin \mathbb{K}$, we will use the same notation \mathbb{K}^σ as in the proof of Lemma 25. By (4.1), we therefore have to prove, for $\sigma \in \{-1, 0, +1\}^3 \setminus (0, 0, 0)$, the vanishing of

$$\left| c^{-1} \iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in \mathbb{K}^\sigma}} v_c^2(x) G_{\mathbb{K}}(x-y) v_c^2(y) dy dx \right| \lesssim \iint_{\substack{\mathbb{K}_c \times \mathbb{K}_c \\ x-y \in c \cdot \mathbb{K}^\sigma}} \frac{\check{v}_c^2(x) \check{v}_c^2(y)}{|x-y - c\sigma|} dy dx.$$

Let $0 < \nu < \frac{1}{4}$. Given that $\sigma \neq (0, 0, 0)$, we have

$$\{(x, y) \in \mathbb{K}_c \times \mathbb{K}_c \mid x - y \in c \cdot \mathbb{K}^\sigma\} \cap B(0, c\nu) \times B(0, c\nu) = \emptyset.$$

Hence, using the Hardy-Littlewood-Sobolev inequality, we obtain

$$\left| \frac{1}{c} \iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in \mathbb{K}^\sigma}} v_c^2(x) G_{\mathbb{K}}(x-y) v_c^2(y) dy dx \right| \lesssim 2 \|\check{v}_c\|_{L^{12/5}(\mathbb{K}_c \setminus B(0, c\nu))}^2 \|\check{v}_c\|_{L^{12/5}(\mathbb{K}_c)}^2$$

and the right hand side vanishes when $c \rightarrow 0$ since $\|\check{v}_c\|_{L^{12/5}(\mathbb{K}_c \setminus B(0, c\nu))}^2$ vanishes and $\|\check{v}_c\|_{L^{12/5}(\mathbb{K}_c)}^2$ is bounded, both by the $L^{12/5}(\mathbb{R}^3)$ -convergence of $\mathbf{1}_{\mathbb{K}_c}\check{v}_c$. This concludes the proof of Lemma 39. \square

Let w_c be a sequence of minimizers to $E_{\mathbb{K}_N, N^3\lambda}(c)$. By Propositions 24 and 33, the convergence rate (5.13), and Lemmas 36 and 39, we obtain

$$E_{\mathbb{K}_N, N^3\lambda}(c) = c^2 J_{\mathbb{R}^3, N^3\lambda} + c \left(\frac{1}{2} D_{\mathbb{R}^3}(|Q|^2, |Q|^2) - \int_{\mathbb{R}^3} \frac{|Q(x)|^2}{|x|} dx \right) + o(c),$$

where Q is the minimizer of $J_{\mathbb{R}^3, N^3\lambda}$ to which $\mathbf{1}_{c_n \cdot \mathbb{K}_N} \check{w}_{c_n}(\cdot + x_n)$ converges strongly.

Let us now prove that Q must also minimize the term of order c . We suppose that there exists a minimizer u of $J_{\mathbb{R}^3, N^3\lambda}$ such that $\mathcal{S}(u) < \mathcal{S}(Q)$, where

$$\mathcal{S}(f) := \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|f(x)|^2 |f(y)|^2}{|x-y|} dy dx - \int_{\mathbb{R}^3} \frac{|f(x)|^2}{|x|} dx.$$

By arguing as in Propositions 26 and 36, and defining, for a fixed small $\eta \in (0; 1)$, the smooth function $\chi \in C_0^\infty(\mathbb{K}_N)$ verifying $0 \leq \chi \leq 1$, $\chi|_{(1-\eta)\cdot\mathbb{K}_N} \equiv 1$, $\chi|_{\mathbb{R}^3 \setminus \mathbb{K}_N} \equiv 0$, we can prove that there exists $\nu > 0$ such that

$$\mathcal{J}_{\mathbb{K}_N, c} \left(\sqrt{N^3\lambda} \frac{u(c)\chi}{\|u(c)\chi\|_{L^2(\mathbb{K}_N)}} \right) = c^2 J_{\mathbb{R}^3, N^3\lambda} + o(e^{-\nu c})_{c \rightarrow \infty}.$$

On the other hand, since $\frac{\sqrt{N^3\lambda}\chi(c^{-1}\cdot)}{\|c^{3/2}u(c)\chi\|_{L^2(\mathbb{K}_N)}} \mathbf{1}_{c\cdot\mathbb{K}_N} u \rightarrow u$ strongly in $L^2(\mathbb{R}^3) \cap L^4(\mathbb{R}^3)$, we apply Lemmas 34 and 39 to it and finally obtain

$$\begin{aligned} \mathcal{E}_{\mathbb{K}_N, c} \left(\sqrt{N^3\lambda} \frac{[u(c)\chi](\cdot - R_{j_0})}{\|u(c)\chi\|_{L^2(\mathbb{K}_N)}} \right) &= c^2 J_{\mathbb{R}^3, N^3\lambda} + c\mathcal{S}(u) + o(c) \\ &< c^2 J_{\mathbb{R}^3, N^3\lambda} + c\mathcal{S}(Q) + o(c) = E_{\mathbb{K}_N, N^3\lambda}(c), \end{aligned}$$

leading to a contradiction which finally proves that Q minimizes \mathcal{S} and thus concludes the proof of Proposition 38. \square

Theorem 2 is therefore proved combining the results of Proposition 24, Proposition 33, Proposition 35 and Proposition 38.

5.4. Proof of Theorem 7 on the number of minimizers. The arguments developed in this section do not rely on what we have done in Section 5.3.

We can expand the functional $\mathcal{E}_{\mathbb{K}, c}^\circ$ around a minimizer w_c as

$$\begin{aligned} \mathcal{E}_{\mathbb{K}, c}^\circ(w_c + f) &= E_{\mathbb{K}, \lambda}(c) + \langle \mathring{L}_c^+ f_1, f_1 \rangle_{L^2(\mathbb{K})} + \langle \mathring{L}_c^- f_2, f_2 \rangle_{L^2(\mathbb{K})} - 2\mu_c \langle w_c, f_1 \rangle_{L^2(\mathbb{K})} \\ &\quad - \mu_c \|f\|_{L^2(\mathbb{K})}^2 + 2D_{\mathbb{K}}(\Re(w_c \bar{f}), \Re(w_c \bar{f})) + o(\|f\|_{H^1(\mathbb{K})}^2), \end{aligned} \quad (5.15)$$

for $f \in H_{\text{per}}^1(\mathbb{K}, \mathbb{C})$, with $f_1 := \Re(f)$, $f_2 := \Im(f)$ and where

$$\mathring{L}_c^- := -\Delta + c_{TF}|w_c|^{\frac{4}{3}} - c|w_c|^{\frac{2}{3}} + \mu_c - \mathcal{G} + |w_c|^2 \star G_{\mathbb{K}} \quad (5.16)$$

and

$$\mathring{L}_c^+ = -\Delta + \frac{7}{3}c_{TF}|w_c|^{\frac{4}{3}} - \frac{5}{3}c|w_c|^{\frac{2}{3}} + \mu_c - \mathcal{G} + |w_c|^2 \star G_{\mathbb{K}}, \quad (5.17)$$

where \mathcal{G} is defined by

$$\mathcal{G} := \sum_{i=1}^{N^3} G_{\mathbb{K}_N}(\cdot - R_i).$$

We have used here that

$$\begin{aligned} \int |w+h|^p - \int |w|^p - p \int |w|^{p-2} \Re(w\bar{h}) \\ - \frac{p(p-2)}{2} \int_{w(\cdot) \neq 0} |w|^{p-4} |\Re(w\bar{h})|^2 - \frac{p}{2} \int |w|^{p-2} |h|^2 = o(\|h\|_{H^1}^2). \end{aligned} \quad (5.18)$$

for any complex-valued $w, h \in H^1$ and $2 \leq p < 4$.

Let us suppose that Conjecture 6 holds and that there exist two sequences w_c and ω_c of non-negative minimizers to $E_{\mathbb{K}_N, N^3\lambda}(c)$ concentrating around the same nucleus at position $R \in \mathbb{K}$. Then, by Proposition 33, we have for $2 \leq p < +\infty$ that

$$\|\check{w}_{c_n}(\cdot + c_n R) - Q\|_{L^p(\mathbb{K}_{c_n})} + \|\check{\omega}_{c_n}(\cdot + c_n R) - Q\|_{L^p(\mathbb{K}_{c_n})} \xrightarrow{n \rightarrow +\infty} 0$$

for a subsequence c_n . We define the real-valued $f_n := w_{c_n} - \omega_{c_n}$, which verifies that $\|\check{f}_n\|_{H^2_{\text{per}}(\mathbb{K}_{c_n})}$ uniformly bounded and, for $c_n > 0$, the orthogonality properties

$$\langle w_{c_n} + \omega_{c_n}, f_n \rangle_{L^2_{\text{per}}(\mathbb{K})} = \langle \check{w}_{c_n} + \check{\omega}_{c_n}, \check{f}_n \rangle_{L^2_{\text{per}}(\mathbb{K}_{c_n})} = 0 \quad (5.19)$$

and

$$\langle \mathcal{G}(c_n^{-1}\cdot), \nabla((\check{w}_{c_n} + \check{\omega}_{c_n})\check{f}_n) \rangle_{L^2_{\text{per}}(\mathbb{K}_{c_n})} = 0 \quad (5.20)$$

Indeed, the fact that ω_c and w_c are real-valued gives the orthogonality (5.19). Moreover, the orthogonality property stated in the following lemma leads to (5.20).

Lemma 40. *If w_c is a real-valued minimizer to $E_{\mathbb{K},\lambda}(c)$, then w_c is orthogonal to $\mathcal{G}\nabla w_c$.*

Proof of Lemma 40. As mentioned in Proposition 35, the four first terms of $\mathcal{E}_{\mathbb{K},c}$ are invariant under any space translations thus we have

$$\mathcal{E}_{\mathbb{K},c}(w_c(\cdot + \tau)) = E_{\mathbb{K},\lambda}(c) - 2\tau \cdot \int_{\mathbb{K}} \mathcal{G}\Re(w_c \nabla \bar{w}_c) + O(|\tau|^2).$$

Hence $\langle \mathcal{G}, \Re(w_c \nabla \bar{w}_c) \rangle_{L^2(\mathbb{K})} = 0$ for any minimizer w_c . Since \mathcal{G} is real-valued, then $\langle w_c, \mathcal{G}\nabla w_c \rangle_{L^2(\mathbb{K})} = 0$ if w_c is a real-valued minimizer. \square

By property (5.20) together with $D_{\mathbb{K}}(h, h) \geq 0$ (Lemma 14) and

$$2\langle \check{w}_n, \check{f}_n \rangle_{L^2(\mathbb{K}_{c_n})} + \|\check{f}_n\|_{L^2(\mathbb{K}_{c_n})}^2 = \langle \check{w}_n + \check{\omega}_n, \check{f}_n \rangle_{L^2(\mathbb{K}_{c_n})} = 0,$$

we obtain from (5.15) that

$$E_{\mathbb{K},\lambda}(c_n) = \mathcal{E}_{\mathbb{K},c_n}(w_{c_n}) \geq E_{\mathbb{K},\lambda}(c_n) + c_n^2 \langle L_n^+ \check{f}_n, \check{f}_n \rangle_{\mathbb{K}_{c_n}} + o(\|f_n\|_{H^1(\mathbb{K})}^2)$$

where the operator L_n^+ on is defined on $L^2(\mathbb{K}_{c_n})$ by

$$L_n^+ = -\Delta + \frac{7}{3}c_{TF}|\check{w}_c|^{\frac{4}{3}} - \frac{5}{3}|\check{w}_c|^{\frac{2}{3}} + \frac{\mu_{c_n}}{c_n^2} + c_n^{-2}[-\mathcal{G} + |w_{c_n}|^2 \star G_{\mathbb{K}}](c_n^{-1}\cdot). \quad (5.21)$$

Therefore, by the ellipticity result $\langle L_n^+ \check{f}_n, \check{f}_n \rangle_{L^2(\mathbb{K}_{c_n})} \geq C\|\check{f}_n\|_{H^1(\mathbb{K}_{c_n})}^2 \geq 0$ of the next proposition, which rely on Conjecture 6, we obtain (for c_n large enough) that

$$0 \geq Cc_n^2 \|\check{f}_n\|_{H^1(\mathbb{K}_{c_n})}^2 + o(\|f_n\|_{H^1(\mathbb{K})}^2) = Cc_n^2 \|\check{f}_n\|_{H^1(\mathbb{K}_{c_n})}^2 + o(c_n^2 \|\check{f}_n\|_{H^1(\mathbb{K}_{c_n})}^2)$$

hence that $f_n \equiv 0$ for c large enough, i.e. $w_{c_n} \equiv \omega_{c_n}$. This mean that if Conjecture 6 holds then there cannot be more than N^3 non-negative minimizers for c large enough and, together with Proposition 35, this concludes the proof of Theorem 7. We are thus left with the proof of the following non-degeneracy result.

Proposition 41. *Let $(w_c)_c$ be a sequence of minimizer to $E_{\mathbb{K},\lambda}(c)$ and L_n^+ the associated operator as in (5.21). Then there exists $C, c_* > 0$ such that for any $c > c_*$ and any $f_n \in H^1(\mathbb{K}_c, \mathbb{C})$ verifying the two orthogonality properties (5.19) and (5.20), we have*

$$\langle L_n^+ f_n, f_n \rangle_{L^2(\mathbb{K}_{c_n})} \geq C \|f_n\|_{H^1(\mathbb{K}_{c_n})}^2. \quad (5.22)$$

Proof of Proposition 41. Following ideas in [61], we define

$$\alpha_n := \inf_{\substack{f \in H^1(\mathbb{K}_c) \\ \langle \check{w}_n + \check{\omega}_n, f \rangle_{L^2(\mathbb{K}_{c_n})} = 0 \\ \langle \mathcal{G}(c_n^{-1}\cdot), \nabla((\check{w}_{c_n} + \check{\omega}_{c_n})f) \rangle_{L^2(\mathbb{K}_{c_n})} = 0}} \frac{\langle L_n^+ f, f \rangle_{L^2(\mathbb{K}_{c_n})}}{\|f\|_{H^1(\mathbb{K}_{c_n})}^2}$$

and we will show that $\alpha_n > 0$ for c large enough.

Lemma 42. *Let $(w_c)_c$ be a sequence of minimizer to $E_{\mathbb{K},\lambda}(c)$ and Q the positive minimizer of $J_{\mathbb{R}^3,\lambda}$ associated with the converging subsequence $\mathbb{1}_{\mathbb{K}_{c_n}}\check{w}_{c_n}(\cdot + c_n R)$. Define as in (2.12) the operator L_μ^+ associated with Q and, as in (5.21), L_n^+ associated with w_{c_n} . Let f_n is a uniformly bounded sequence $H_{\text{per}}^1(\mathbb{K}_{c_n})$ then*

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \leq \liminf_{n \rightarrow \infty} \langle L_n^+ f_n, f_n \rangle_{L^2(\mathbb{K}_{c_n})},$$

with f such that $\mathbb{1}_{\mathbb{K}_{c_n}} f_n(\cdot + c_n R) \rightharpoonup f$ weakly converges in $L^2(\mathbb{R}^3)$.

Proof of Lemma 42. Up to the extraction of a subsequence (that we will omit in the notation), there exists f such that $\mathbb{1}_{\mathbb{K}_{c_n}} f_n(\cdot + c_n R) \rightharpoonup f$ weakly in $L^2(\mathbb{R}^3)$ because $f_n(\cdot + c_n R)$ is uniformly bounded in $H^1(\mathbb{K}_{c_n})$. Thus, by Lemma 29,

$$\liminf_{c \rightarrow \infty} \|\nabla f_n\|_{L^2(\mathbb{K}_{c_n})} = \liminf_{c \rightarrow \infty} \|\nabla f_n(\cdot + c_n R)\|_{L^2(\mathbb{K}_{c_n})} \geq \|\nabla f\|_{L^2(\mathbb{R}^3)}.$$

Moreover, $\|f_n\|_{H^1(\mathbb{K}_{c_n})}$ is uniformly bounded by hypothesis thus

$$c_n^{-2} \langle \mathcal{G}(c_n^{-1} \cdot) f_n, f_n \rangle \leq c_n^{-\frac{1}{2}} \|\mathcal{G}\|_{L^2(\mathbb{K})} \|f_n\|_{L^4(\mathbb{K}_{c_n})}^2 \xrightarrow{c \rightarrow +\infty} 0$$

and, by the same argument as the one to obtain (5.9), we have

$$c_n^{-2} \langle |w_{c_n}|^2 \star G_{\mathbb{K}}(c_n^{-1} \cdot) f_n, f_n \rangle \lesssim c_n^{-1} \|\check{w}_{c_n}\|_{L^{\frac{12}{5}}(\mathbb{K}_{c_n})}^2 \|f_n\|_{L^{\frac{12}{5}}(\mathbb{K}_{c_n})}^2 \xrightarrow{c \rightarrow +\infty} 0.$$

Moreover, by Proposition 24, $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_n(\cdot + c_n R)$ strongly converges in $L^q(\mathbb{R}^3)$ for $2 \leq q < 6$ hence for $p = \frac{2}{3}$ and $p = \frac{4}{3}$ we have

$$\langle |\check{w}_{c_n}|^p, |f_n|^2 \rangle_{L^2(\mathbb{K}_{c_n})} = \langle |\check{w}_{c_n}(\cdot + c_n R)|^p, |f_n(\cdot + c_n R)|^2 \rangle_{L^2(\mathbb{K}_{c_n})} \rightarrow \langle |Q|^p, |f|^2 \rangle_{L^2(\mathbb{R}^3)}.$$

Finally, by Corollary 31 and weak convergence in $L^2(\mathbb{R}^3)$ of $\mathbb{1}_{\mathbb{K}_{c_n}} f_n(\cdot + c_n R)$,

$$\liminf_{n \rightarrow \infty} \frac{\mu_{c_n}}{c_n^2} \|f_n\|_{L^2(\mathbb{K}_{c_n})}^2 = \liminf_{n \rightarrow \infty} \frac{\mu_{c_n}}{c_n^2} \|f_n(\cdot + c_n R)\|_{L^2(\mathbb{K}_{c_n})}^2 \geq \mu \|f\|_{L^2(\mathbb{R}^3)}^2.$$

This concludes the proof of Lemma 42. \square

We now prove that α_n cannot tend to zero. Let suppose it does, then there exists a sequence of $f_n \in H^1(\mathbb{K}_{c_n})$ such that $\|f_n\|_{H^1(\mathbb{K}_{c_n})} = 1$, $\langle \check{w}_{c_n} + \check{\omega}_{c_n}, f_n \rangle_{L_{\text{per}}^2(\mathbb{K}_{c_n})} = 0$ and $\langle \mathcal{G}(c_n^{-1} \cdot), \nabla((\check{w}_{c_n} + \check{\omega}_{c_n}) \check{f}_n) \rangle_{L_{\text{per}}^2(\mathbb{K}_{c_n})} = 0$, with $\langle L_n^+ f_n, f_n \rangle_{L^2(\mathbb{K}_{c_n})} \rightarrow 0$.

Thus, by the uniform boundedness of $\|f_n\|_{H^1(\mathbb{K}_{c_n})}$, $\mathbb{1}_{\mathbb{K}_{c_n}} f_n$ converges weakly in $L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$ to a f which verifies $\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \leq 0$, by Lemma 42, and $\|f\|_{H^1(\mathbb{K}_{c_n})} \leq 1$. We claim that f also solves the orthogonality properties

$$\langle f, Q \rangle_{L^2(\mathbb{R}^3)} = 0 \quad \text{and} \quad \langle f, Q \nabla |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = 0.$$

Indeed, on one hand we deduce from the uniqueness of $Q \geq 0$ (given by the conjecture), that $\mathbb{1}_{\mathbb{K}_{c_n}}(\check{w}_{c_n}(\cdot + c_n R) + \check{\omega}_{c_n}(\cdot + c_n R)) \rightarrow 2Q$ in $L^2(\mathbb{R}^3) \cap L^{6^-}(\mathbb{R}^3)$. This, together with (5.19) and the weak convergence of the f_n 's leads to $\langle f, Q \rangle_{L^2(\mathbb{R}^3)} = 0$. On another hand, the uniqueness of Q gives also the $L^2(\mathbb{R}^3)$ strong convergence

$$\mathbb{1}_{\mathbb{K}_{c_n}} \nabla(\check{w}_{c_n}(\cdot + c_n R) + \check{\omega}_{c_n}(\cdot + c_n R)) \rightarrow 2\nabla Q \in H^1(\mathbb{R}^3).$$

Thus, applying Lemma 34 on one hand to it and $\mathbb{1}_{\mathbb{K}_{c_n}} f_n(\cdot + c_n R) \rightharpoonup f \in H^1(\mathbb{R}^3)$ with the first set of conditions in Lemma 34 and, on the other hand, to $\mathbb{1}_{\mathbb{K}_{c_n}}(\check{w}_{c_n}(\cdot + c_n R) + \check{\omega}_{c_n}(\cdot + c_n R)) \rightarrow 2Q$ and $\mathbb{1}_{\mathbb{K}_{c_n}} \nabla f_n(\cdot + c_n R) \rightharpoonup \nabla f \in L^2(\mathbb{R}^3)$ — which comes from Lemma 29 — with the second set of conditions, we obtain

$$\langle \mathcal{G}(c_n^{-1} \cdot + R), \nabla[(\check{w}_{c_n}(\cdot + c_n R) + \check{\omega}_{c_n}(\cdot + c_n R)) \check{f}_n(\cdot + c_n R)] \rangle_{L_{\text{per}}^2(\mathbb{K}_{c_n})} \rightarrow 2 \int_{\mathbb{R}^3} \frac{\nabla(fQ)}{|\cdot|}.$$

Finally, (5.20) implies that $\langle f, Q \nabla |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = -\langle \nabla(fQ), |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = 0$ and our claim is proved.

As we will prove in Proposition 43, if Conjecture 6 holds then these two orthogonality properties imply that there exists $\alpha > 0$ such that

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \geq \alpha \|f\|_{H^1(\mathbb{R}^3)}^2$$

hence $f \equiv 0$ due to $\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \leq 0$ obtained previously. Since the terms involving a power of $|w_{c_n}|$ converge and $f \equiv 0$, we have

$$o(1) = \langle L_n^+ f_n, f_n \rangle_{L^2(\mathbb{K}_{c_n})} = \|\nabla f_n\|_{L^2(\mathbb{K}_{c_n})}^2 + \mu \|f_n\|_{L^2(\mathbb{K}_{c_n})}^2 + o(1)$$

hence both norms vanish, since $\mu > 0$, which means that $\|f_n\|_{H^1(\mathbb{K}_{c_n})} \rightarrow 0$. This contradicts $\|f_n\|_{H^1(\mathbb{K}_{c_n})} = 1$ and concludes the proof that α_n cannot vanish, hence that of Proposition 41. \square

We are left with the proof of Proposition 43.

Proposition 43. *If Conjecture 6 holds then there exists $\alpha > 0$ such that*

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \geq \alpha \|f\|_{H^1(\mathbb{R}^3)}^2, \quad (5.23)$$

for all $f \in H^1(\mathbb{R}^3)$ such that $\langle f, Q \rangle_{L^2(\mathbb{R}^3)} = 0$ and $\langle f, Q \nabla |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = 0$.

The proof of this proposition uses the celebrated method of Weinstein [61] and Grillakis–Shatah–Strauss [19]. The idea is the following. Using a Perron-Frobenius argument in each spherical harmonics sector as in [61, 28, 32], one obtains that the linearized operator L_μ^+ has only one negative eigenvalue with (unknown) eigenfunction φ_0 in the sector of angular momentum $\ell = 0$, and has 0 as eigenvalue of multiplicity three with corresponding eigenfunctions $\partial_{x_i} Q$. On the orthogonal of these four functions, L_μ^+ is positive definite. In our setting, we have to study L_μ^+ on the orthogonal of Q and the three functions $x_i |x|^{-3} Q(x)$ which are different from the mentioned eigenfunctions. Arguing as in [61], we show below that the restriction of L_μ^+ to the angular momentum sector $\ell = 1$ is positive definite on the orthogonal of the functions $x_i |x|^{-3} Q(x)$. The argument is general and actually works for functions of the form $\partial_{x_i}(\eta(|x|))Q(x) = x_i |x|^{-1} \eta'(|x|)Q(x)$ where η is any non constant monotonic function on \mathbb{R} . On the other hand, the argument is more subtle for Q in the angular momentum sector $\ell = 0$ and this is where we need Conjecture 6.

Proof of Proposition 43. First we note that it is obviously enough to prove it for f real valued but also that it is enough to prove

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \geq \alpha \|f\|_{L^2(\mathbb{R}^3)}^2 \quad (5.24)$$

with $\alpha > 0$. Indeed, if f verifies (5.24) then, for any $\varepsilon > 0$, we have

$$\langle L_\mu^+ f, f \rangle_{L^2} \geq \left((1 - \varepsilon)\alpha + \varepsilon \left(\mu - \frac{7}{3} c_{TF} \|Q\|_{L^\infty}^{\frac{4}{3}} - \frac{5}{3} \|Q\|_{L^\infty}^{\frac{2}{3}} \right) \right) \|f\|_{L^2}^2 + \varepsilon \|\nabla f\|_{L^2}^2,$$

hence f verifies (5.23) too (for a smaller $\alpha > 0$).

Since Q is a radial function, the operator L_μ^+ commutes with rotations in \mathbb{R}^3 and we will therefore decompose $L^2(\mathbb{R}^3)$ using spherical harmonics: for any $f \in L^2(\mathbb{R}^3)$,

$$f(x) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} f_\ell^m(r) Y_\ell^m(\Omega),$$

where $x = r\Omega$ with $r = |x|$ and $\Omega \in \mathbb{S}^2$. This yields the direct decomposition

$$L^2(\mathbb{R}^3) = \bigoplus_{\ell=0}^{\infty} \mathcal{H}_{(\ell)}$$

and L_μ^+ maps into itself each

$$\mathcal{H}_{(\ell)} := L^2(\mathbb{R}_+, r^2 dr) \otimes \text{span}\{Y_\ell^m\}_{m=-\ell}^\ell.$$

Using the well-known expression of $-\Delta$ on $\mathcal{H}_{(\ell)}$, we obtain that

$$L_\mu^+ = \bigoplus_{\ell=0}^{\infty} L_{\mu,\ell}^+$$

where the $L_{\mu,\ell}^+$'s are operators acting on $L^2(\mathbb{R}_+, r^2 dr)$ given by

$$L_{\mu,\ell}^+ = -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{\ell(\ell+1)}{r^2} + \frac{7}{3} c_{TF} |Q_\mu|^{\frac{4}{3}} - \frac{5}{3} |Q_\mu|^{\frac{2}{3}} + \mu.$$

We thus prove inequality (5.24) by showing that there exists $\alpha > 0$ such that for each ℓ the inequality holds for any $f \in \mathcal{H}_{(\ell)} \cap H^1(\mathbb{R}^3)$ verifying $\langle f, Q \rangle = 0$ and $\langle f, Q \nabla |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = 0$.

Arguing as in [28], we have first the following result.

Lemma 44 (Perron–Frobenius property of the $L_{\mu,\ell}^+$). *Each $L_{\mu,\ell}^+$ has the Perron–Frobenius property: its lowest eigenvalue $e_{\mu,\ell}$ is simple and the corresponding eigenfunction $\varphi_\ell(r)$ is strictly positive.*

Proof for the sector $\ell = 1$. We start with the case $\ell = 1$ and prove that

$$\alpha_1 := \inf_{\substack{f \in \mathcal{H}_{(1)} \cap H^1(\mathbb{R}^3) \\ \langle f, Q \nabla |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = 0}} \frac{\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)}}{\|f\|_{L^2(\mathbb{R}^3)}^2} > 0. \quad (5.25)$$

Since Q is radial, we have for $i = 1, 2, 3$, that

$$\partial_{x_i} Q(x) = Q'(r) \frac{x_i}{r} \in \mathcal{H}_{(1)}.$$

Moreover, by the non-degeneracy result of Theorem 4, we know that $\partial_{x_i} Q$ is an eigenfunction of L_μ^+ associated with the eigenvalue 0 hence $Q'(r)$ is an eigenfunction of $L_{(1)}^+$ associated with the eigenvalue $e_{\mu,1} = 0$. Therefore, the fact that $Q'(r) < 0$ (as proved in Theorem 3) implies, using the Perron-Frobenius property verified by $L_{(1)}^+$, that $e_{\mu,1} = 0$ is the lowest eigenvalue of $L_{(1)}^+$ and is simple with $-Q' > 0$ the associated eigenfunction. Consequently, we have for any $f \in \mathcal{H}_{(1)}$ that

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} = \sum_{m=-1}^1 \langle L_{(1)}^+ f^m(r), f^m(r) \rangle_{L^2(\mathbb{R}_+, r^2 dr)} \geq 0$$

and in particular that $\alpha_1 \geq 0$.

We thus suppose that $\alpha_1 = 0$ and prove it is impossible. Let f_n be a minimizing sequence to (5.25) with $\|f_n\|_{L^2(\mathbb{R}^3)} = 1$. One has

$$\|\nabla f_n\|_{L^2(\mathbb{R}^3)}^2 \leq \langle L_\mu^+ f_n, f_n \rangle_{L^2(\mathbb{R}^3)} + \frac{5}{3} \|Q\|_{L^\infty(\mathbb{R}^3)}^{\frac{2}{3}}$$

and consequently the sequence f_n is bounded in $H^1(\mathbb{R}^3)$. We denote by f its weak limit in $H^1(\mathbb{R}^3)$, up to an extraction of a subsequence, which is in $\mathcal{H}_{(1)}$. We have

$$0 \leq \langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \leq \liminf \langle L_\mu^+ f_n, f_n \rangle_{L^2(\mathbb{R}^3)} = \alpha_1 = 0,$$

where the second inequality is due to

$$\liminf \|\nabla f_n\|_{L^2(\mathbb{R}^3)}^2 \geq \|\nabla f\|_{L^2(\mathbb{R}^3)}^2, \quad \liminf \|f_n\|_{L^2(\mathbb{R}^3)}^2 \geq \|f\|_{L^2(\mathbb{R}^3)}^2,$$

$\mu > 0$ and to $\langle |Q|^p f_n, f_n \rangle_{L^2(\mathbb{R}^3)} \rightarrow \langle |Q|^p f, f \rangle_{L^2(\mathbb{R}^3)}$, for $p = \frac{2}{3}$ and $p = \frac{4}{3}$, obtained by a similar argument to the one in proof of Lemma 42. It implies that

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} = 0$$

hence, $f = \sum_{i=1}^3 c_i \partial_{x_i} Q$ by the Perron-Frobenius property and since $\{\frac{x_1}{r}, \frac{x_2}{r}, \frac{x_3}{r}\}$ is an orthogonal basis of $\text{span}\{Y_1^{-1}, Y_1^0, Y_1^1\}$. However, for any $i = 1, 2, 3$, we have after passing to the weak limit that

$$\int_{\mathbb{R}^3} \frac{x_i}{|x|^3} f(x) Q(x) dx = 0.$$

We then remark that, since Q is radial, we have

$$\int_{\mathbb{R}^3} \frac{x_i}{|x|^3} Q(x) \partial_{x_j} Q(x) dx = \int_{\mathbb{R}^3} \frac{x_j x_i}{|x|^4} Q(x) Q'(x) dx = 0, \quad \forall i \neq j.$$

This gives, for $i = 1, 2, 3$, that

$$0 = \int_{\mathbb{R}^3} \frac{x_i}{|x|^3} f(x) Q(x) dx = c_i \int_{\mathbb{R}^3} \frac{x_i^2}{|x|^4} Q(x) Q'(x) dx$$

but $Q > 0$ and $Q' < 0$, hence $c_i = 0$ thus $f \equiv 0$. We thus have obtained, if $\alpha_1 = 0$, that any minimizing sequence f_n to (5.25) converges weakly to 0 in $H^1(\mathbb{R}^3)$. This gives $\langle |Q|^p f_n, f_n \rangle_{L^2(\mathbb{R}^3)} \rightarrow 0$ and

$$\|\nabla f_n\|_{L^2(\mathbb{R}^3)}^2 + \mu \|f_n\|_{L^2(\mathbb{R}^3)}^2 = \langle L_\mu^+ f_n, f_n \rangle_{L^2(\mathbb{R}^3)} + o(1) \rightarrow \alpha_1 = 0$$

therefore $f_n \rightarrow 0$ strongly in $H^1(\mathbb{R}^3)$, because $\mu > 0$, which contradicts the fact that $\|f_n\|_{L^2(\mathbb{R}^3)} = 1$. We have thus proved that $\alpha_1 > 0$.

Proof for the sector $\ell \geq 2$. We now deal with the cases $\ell \geq 2$ and prove that there exists $\alpha > 0$ such that

$$\langle L_{\mu, \ell}^+ \varphi, \varphi \rangle_{L^2(\mathbb{R}_+, r^2 dr)} \geq \alpha \|\varphi\|_{L^2(\mathbb{R}_+, r^2 dr)}^2 \quad (5.26)$$

for any $\varphi \in L^2(\mathbb{R}_+, r^2 dr)$. Since for such φ we have

$$\langle L_{\mu, \ell}^+ \varphi, \varphi \rangle_{L^2(\mathbb{R}_+, r^2 dr)} = \langle L_{(\ell-1)}^+ \varphi, \varphi \rangle_{L^2(\mathbb{R}_+, r^2 dr)} + 2(\ell-1) \|\varphi/r\|_{L^2(\mathbb{R}_+, r^2 dr)}^2, \quad (5.27)$$

it is then sufficient to prove (5.26) in the case $\ell = 2$ in order to prove it for all $\ell \geq 2$.

For $\ell = 2$, we can assume that $\inf \sigma(L_{(2)}^+)$ is attained because, otherwise,

$$V := \frac{7}{3} c_{TF} |Q_\mu|^{4/3} - \frac{5}{3} |Q_\mu|^{2/3}$$

being bounded and vanishing as $r \rightarrow \infty$, it is well-known that $\sigma_{\text{ess}}(L_{(2)}^+) = [\mu; +\infty)$ and (5.26) follows. We thus have, by (5.27) and $L_{(1)}^+ \geq 0$, that the eigenvalue $e_{\mu, 2} = \inf \sigma(L_{(2)}^+)$ and its associated eigenfunction $\varphi_2 \neq 0$ verify that

$$e_{\mu, 2} = \inf \sigma(L_{(2)}^+) \geq 2 \frac{\|\varphi_2/r\|_{L^2(\mathbb{R}_+, r^2 dr)}^2}{\|\varphi_2\|_{L^2(\mathbb{R}_+, r^2 dr)}^2} > 0$$

and (5.26) is therefore proved. It concludes the case $\ell \geq 2$.

Proof for the sector $\ell = 0$. We conclude with the case $\ell = 0$ and prove that for any $f \in \mathcal{H}_{(0)}$, we have

$$\alpha_0 := \inf_{\substack{f \in \mathcal{H}_{(0)} \cap H^1(\mathbb{R}^3) \\ \langle f, Q \rangle_{L^2(\mathbb{R}^3)} = 0}} \frac{\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)}}{\|f\|_{L^2(\mathbb{R}^3)}^2} > 0. \quad (5.28)$$

We already know that $\alpha_0 \geq 0$ because Q is a minimizer. Indeed, for $f \in H^1(\mathbb{R}^3)$ such that $\langle f, Q \rangle_{L^2(\mathbb{R}^3)} = 0$, through a computation similar to (5.15) and using (2.10),

(3.5), (5.18) and that Q is a minimizer of $J_{\mathbb{R}^3}(\lambda)$, we obtain

$$\begin{aligned} \mathcal{J}_{\mathbb{R}^3}(Q) &\leq \mathcal{J}_{\mathbb{R}^3}\left(\frac{Q + \varepsilon f}{\|Q + \varepsilon f\|_2} \|Q\|_2\right) \\ &= \mathcal{J}_{\mathbb{R}^3}(Q) + \varepsilon^2(\langle L_\mu^+ \mathfrak{R}f, \mathfrak{R}f \rangle_{L^2(\mathbb{R}^3)} + \langle L_\mu^- \mathfrak{S}f, \mathfrak{S}f \rangle_{L^2(\mathbb{R}^3)}) + o(\varepsilon^2) \end{aligned}$$

which implies in particular that $\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \geq 0$ for as soon as $\langle f, Q \rangle_{L^2(\mathbb{R}^3)} = 0$.

We thus suppose $\alpha_0 = 0$ and prove it is impossible. Let f_n be a minimizing sequence to (5.28) with $\|f_n\|_{L^2(\mathbb{R}^3)} = 1$. As in the proof of case $\ell = 1$ above, f_n is in fact bounded in $H^1(\mathbb{R}^3)$ and denoting by $f \in \mathcal{H}_{(0)}$ its weak limit in $H^1(\mathbb{R}^3)$, up to a subsequence, we have $\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} = 0$. This leads, to $L_\mu^+ f = \beta Q$ thus, using that L_μ^+ is inversible, to $f = \beta(L_\mu^+)^{-1}Q$. Consequently,

$$0 = \langle f, Q \rangle_{L^2(\mathbb{R}^3)} = \beta \langle Q, (L_\mu^+)^{-1}Q \rangle_{L^2(\mathbb{R}^3)}$$

hence $\beta = 0$ since $\langle Q, (L_\mu^+)^{-1}Q \rangle_{L^2(\mathbb{R}^3)} < 0$ by Conjecture 6. We have obtained $f \equiv 0$ which is absurd as before. \square

This concludes the proof of Theorem 7. \square

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CNRS, UNIVERSITÉ DE CERGY-PONTOISE, DÉPARTEMENT DE MATHÉMATIQUES, 95000 CERGY-PONTOISE, FRANCE

CNRS, CEREMADE, UNIVERSITÉ PARIS-DAUPHINE, PSL RESEARCH UNIVERSITY, 75016 PARIS, FRANCE

E-mail address: julien.ricaud@u-cergy.fr