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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 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 nonnegative 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 $\frac{3}{4}c_D \approx 0.93$, which is the constant generally appearing in the literature. 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 $\frac{3}{4}c$ 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 $\frac{3}{4}c \approx 2.48$. More precisely, the 2-periodic ground state was found to be 1-periodic if $\frac{3}{4}c \lesssim 2.474$ but really 2-periodic for $\frac{3}{4}c \gtrsim 2.482$. The numerical value $\frac{3}{4}c \approx 2.48$ 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 $\mathbb{K} := \left[-\frac{1}{2}; \frac{1}{2}\right)^3$, 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, 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. The $N\mathbb{K}$ -periodic extension of the \mathbb{K} -periodic minimizer w_c is the unique minimizer of all the $N\mathbb{K}$ -periodic TFDW problems $E_{N \cdot \mathbb{K}, N^3 \lambda}(c)$, for any integer $N \geq 1$. Moreover*

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

Theorem 2 (Asymptotics for large c). *Let \mathbb{K} be the unit cube, c_{TF}, λ be two positive constants, and $N \geq 1$ be an integer. For c large enough, the periodic TFDW problem $E_{N \cdot \mathbb{K}, N^3 \lambda}(c)$ on $N \cdot \mathbb{K}$ admits (at least) N^3 distinct nonnegative 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*

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

strongly in $L^p_{loc}(\mathbb{R}^3)$ 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. The leading order in (2.7)

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

together with the strict binding inequality $J_{\mathbb{R}^3}(N^3\lambda) < N^3 J_{\mathbb{R}^3}(\lambda)$ for $N \geq 2$, proved later in Proposition 13 of Section 3, imply immediately that symmetry breaking occurs.

Corollary 3 (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:*

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

Although the leading order is sufficient to prove the occurrence of symmetry breaking, Theorem 2 gives a precise description of the behavior of the electrons, which all concentrate at one of the N^3 nuclei of the cell $N \cdot \mathbb{K}$. 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.

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

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

Remark (Model on \mathbb{R}^3). *In this paper, we study the TFDW model for a periodic system, because such orbital-free theories are often used in practice for infinite systems. However, Theorem 2 can be adapted to the TFDW model in the whole space \mathbb{R}^3 , with finitely many nuclei of charges z_1, \dots, z_n and $\lambda \leq \sum_i z_i$ electrons, using similar proofs. In the limit $c \rightarrow \infty$, the λ electrons all concentrate at one of the nuclei with the largest charge $z_+ := \max\{z_i\}$ and solve the same effective problem. Therefore, uniqueness does not hold if there are several such nuclei of charge z_+ .*

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 4 (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 5 (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 nonnegative 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 4 exactly gives that $\text{Ker } L_\mu^- = \text{span}\{Q_\mu\}$. Hence, Theorem 5 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, proving the injection property being the issue.

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 6. *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 6. By Theorem 4, 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 5 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 $\left(0; \frac{15}{64c_{TF}}\right)$, 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.

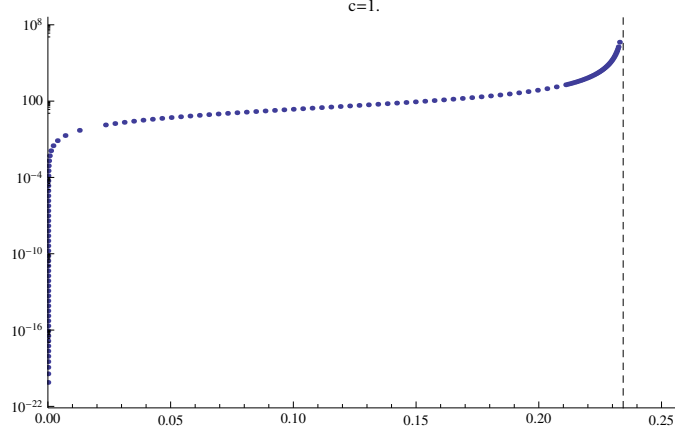


FIGURE 1. Plot of $\mu \mapsto \ln(M(\mu))$ on $\left(0; \frac{15}{64c_{TF}}\right)$.

Conjecture 7. *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. *It should be possible to show that the energy $\mu \mapsto \mathcal{J}_{\mathbb{R}^3}(Q_\mu)$ is strictly decreasing close to $\mu = 0$ and $\mu = \mu_*$, and real-analytic on $(0, \mu_*)$. Using the concavity of $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$ (see Lemma 11) one should be able to prove that the function $\lambda \mapsto \mu(\lambda)$ is increasing and continuous, except at a countable set of points where it can jump. From the analyticity there must be a finite number of jumps and we conclude that $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$ has a unique minimizer for all λ except at these finitely many points.*

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

The proof of Theorem 8 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 with a constant $c_W = 0.186$ in front of the gradient term (see [36] for the choice of this value) and using the software *PROFESS v.3.0* [8] which is based on pseudo-potentials (see Remark 9 below): we have used a (BCC) Lithium crystal of side-length 4\AA (in order to be physically relevant as the two first alkali metals Lithium and Sodium organize themselves on BCC lattices with respective side length 3.51\AA and 4.29\AA) 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 $\frac{3}{4}c \approx 2.48$. More precisely, minimizing the $2 \cdot \mathbb{K}$

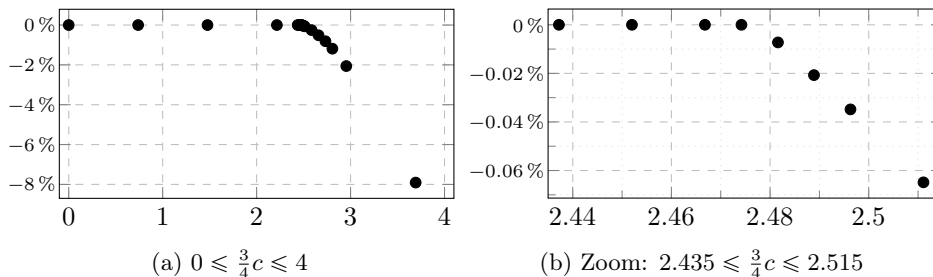


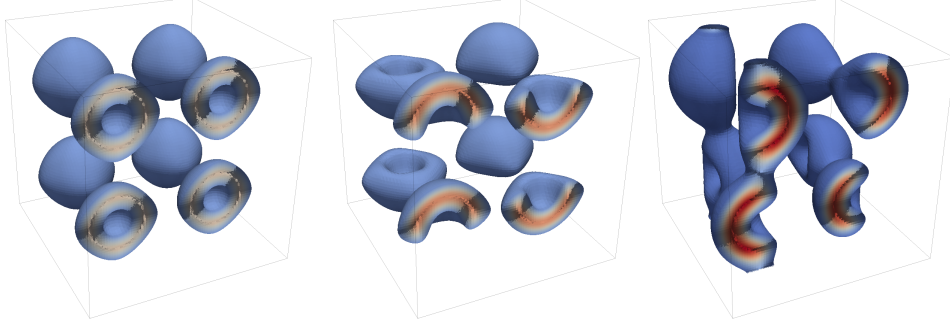
FIGURE 2. Relative gain of energy $\frac{8E_{\mathbb{K}, \lambda}(c) - E_{2 \cdot \mathbb{K}, 8\lambda}(c)}{8E_{\mathbb{K}, \lambda}(c)}$.

problem and the $1 \cdot \mathbb{K}$ problem result in the same minimum energy (up to a factor 8) if $\frac{3}{4}c \lesssim 2.474$ while, for $\frac{3}{4}c \gtrsim 2.482$, 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. Note that changing c_W would affect the critical value of the Dirac constant at which symmetry breaking occurs but the value of c_W does not affect the mathematical proofs (which are presented with $c_W = 1$ for convenience).

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 9 (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*



(a) $\frac{3}{4}c = \frac{3}{4}3.35\sqrt{\frac{3}{\pi}} \approx 2.474$ (b) $\frac{3}{4}c = \frac{3}{4}3.36\sqrt{\frac{3}{\pi}} \approx 2.482$ (c) $\frac{3}{4}c = \frac{3}{4}3.50\sqrt{\frac{3}{\pi}} \approx 2.585$

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.

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 4 and Theorem 5. We first give a lemma on the functional $\mathcal{J}_{\mathbb{R}^3}$, which has been defined in (2.8).

Lemma 10. 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 10. It follows from

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

□

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

Lemma 11 (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 $[0; +\infty)$ and negative, concave and strictly decreasing on $(0; +\infty)$.

Proof of Lemma 11. The negativity of $J_{\mathbb{R}^3}(\lambda)$ is obtained by taking ν large enough in the computation of $\mathcal{J}_{\mathbb{R}^3}(\nu^{-\frac{2}{3}}u(\nu^{-1}\cdot))$. Lemma 10 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 $t \mapsto F(t)$ is concave on $[0; +\infty)$, since $a \mapsto \inf_u (af(u) + g(u))$ is concave for all f, g , hence continuous on $(0; +\infty)$ on which it is also negative (because $J_{\mathbb{R}^3}$ is negative) and non-decreasing. The continuity of F gives that $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$ is continuous as well. Moreover, if f is a concave non-decreasing negative function, then $\lambda \mapsto \lambda f(\lambda^{-2/3})$ is concave strictly decreasing on $(0, \infty)$, which proves that our energy J is concave. To prove that, one can regularize f by means of a convolution and then compute its first two derivatives. \square

3.1. Proof of Theorem 4. We divide the proof into several steps for clarity.

Step 1: Large binding inequality.

Lemma 12. *Let $c_{TF} \geq 0$ be a constant. Then*

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

Proof of Lemma 12. 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 $\lambda - \lambda'$. \square

Remark. *The strict inequality in (3.3), which is important for applying Lions' concentration-compactness method, actually holds and is proved later in Proposition 13.*

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 nonnegative 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, $J_{\mathbb{R}^3}$ being strictly decreasing 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.

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

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

Step 4: Strict binding inequality.

Proposition 13. *Let $c_{TF} > 0$ and $\lambda > 0$.*

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

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 13. By the same scaling as in Lemma 11, 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

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

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 nonnegative minimizers. Let $Q \geq 0$ be a minimizer. By Step 3, $0 \neq Q \in H^2(\mathbb{R}^3) \subset C(\mathbb{R}^3)$ 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: nonnegative 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 14. *Let $\lambda > 0$. Any positive minimizer to $J_{\mathbb{R}^3}(\lambda)$ is radial strictly decreasing, up to a translation.*

Proof of Proposition 14. 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 nonnegative 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 4. \square

3.2. Proof of Theorem 5. 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 nonnegative 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 15 (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 15. 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 16 (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 nonnegative 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 16. In order to prove i., we need the following result that will be useful all along the paper, and is somewhat similar to Lemma 10.

Lemma 17. *There exist positive constants $a < 1$ and C such that for any $c \geq 0$, $c_{TF}, \lambda > 0$ and any $u \in H_{per}^1(\mathbb{K})$ with $\|u\|_2^2 = \lambda$, 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 17. As in Lemma 10 (but on \mathbb{K}) we have

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

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

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

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 nonnegative minimizer and concludes the proof of *i*.

To prove that any minimizer w_c is in $H^2_{\text{per}}(\mathbb{K})$, 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 $w_c \in H^2_{\text{per}}(\mathbb{K})$ 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 $w_c \in H^1_{\text{per}}(\mathbb{K})$ which also gives, together with $G_{\mathbb{K}} \in L^2(\mathbb{K})$ by Lemma 15, 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

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

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 nonnegative 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 $u \in H^1_{\text{per}}(\mathbb{K})$ 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 $u = \alpha w_c$ ae. It proves w_c is the unique ground state of H_{w_c} and concludes the proof of Proposition 16. \square

From this existence result, we deduce the following corollary.

Corollary 18. *On $[0, +\infty)$, $c \mapsto E_{\mathbb{K},\lambda}(c)$ is continuous and strictly decreasing.*

Proof of Corollary 18. Let $0 \leq c_1 < c_2$ and, let w_1 and w_2 be corresponding minimizers, which exist by Proposition 16. On one hand, we have

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

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 17. 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 18. \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 16, there exist minimizers to $E_{\mathbb{K},\lambda}^{TFW}$, and we now prove the uniqueness of minimizer for the TFW model.

Proposition 19. *The minimization problem $E_{\mathbb{K},\lambda}^{TFW}$ admits, up to phase, a unique minimizer w_0 which is non constant and 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 19. By Proposition 16, 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 20. *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 20. 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 18, $\{w_{c_n}\}_{n \rightarrow \infty}$ is a positive minimizing sequence of $E_{\mathbb{K},\lambda}(\bar{c})$. Thus, by Proposition 16, 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 $\mu \in \overline{\mathbb{R}}$ 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 $H_{per}^1(\mathbb{K}) \times \mathbb{R}$:

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

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 16, 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 20. \square

Proposition 21 (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*

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

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 21. First, the hypothesis give $w \in H_{\text{per}}^2(N \cdot \mathbb{K})$, by the same proof as in Proposition 16. Moreover, we have the following lemma.

Lemma 22. *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*

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

Proof of Lemma 22. 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

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

\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 22 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 21. \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 16 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 19, $E_{\mathbb{K}, \lambda}(0)$ has a unique minimizer thus, by Proposition 20, 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 21 (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 21 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

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

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 16 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 23 (A priori estimates on minimal energy). *Let \mathbb{K} be the unit cube and $c_{TF} > 0$ be a constant. There exists $C > 0$ such that for any $c > 0$ we have*

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

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 23. The inequality (5.3) has been proved in Lemma 17, 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 23. \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

$$\mathcal{J}_{\mathbb{K},c}(v) = c^2 \mathcal{J}_{\mathbb{K}_c,1}(\check{v}), \quad (5.8)$$

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 23.

Corollary 24 (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 24. 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

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

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 24. \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 25. *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 25, 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 26. *Let $\lambda > 0$. Then*

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

Proof of Lemma 26. 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 16 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

$$D_{\mathbb{K}}(v_c^2, v_c^2) \lesssim \|v_c\|_{H^1(\mathbb{K})}. \quad (5.9)$$

To prove (5.9) 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

$$\begin{aligned} |D_{\mathbb{K}}(v_c^2, v_c^2)| &= \left| \sum_{\sigma \in \{-1; 0; +1\}^3} \iint_{\substack{\mathbb{K} \times \mathbb{K} \\ x-y \in \mathbb{K}^\sigma}} v_c^2(x) G_{\mathbb{K}}(x-y) v_c^2(y) dx dy \right| \\ &\lesssim \|v_c\|_{L^{\frac{12}{5}}(\mathbb{K})}^4 \lesssim \|v_c\|_{H^1(\mathbb{K})} \|v_c\|_{L^2(\mathbb{K})}^3. \end{aligned} \quad (5.10)$$

This proves (5.9) 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

$$\exists K > 0, \forall c \geq c_*, \quad \|\nabla v_c\|_{L^2(\mathbb{K})}^2 \leq \left(\frac{15}{64} \frac{\lambda}{c_{TF}} - K \right) c^2. \quad (5.11)$$

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 26. \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 25 will be a by-product of the method.

Lemma 27 (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 27. Using the scaling equality (5.8), 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 28 (Lower bound). *Let \mathbb{K} be the unit cube and λ be positive. Then*

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

Sketch of proof of Lemma 28. See [56] for a detailed proof. 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 29 (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. *The proof of Lemma 28 relies on the concentration-compactness method. Extracting only one bubble ($J = 1$) by a localization method would not allow us to conclude since we have little information on the energy of the remainder ψ_k . In similar proofs in the literature, it is often possible to conclude after extracting few bubbles, using that $\mathcal{J}(\psi_k) \geq J(\int |\psi_k|^2)$. 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 as many bubbles as necessary such as to sufficiently decrease the energy of ψ_k .*

We apply Lemma 29 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 24. 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 11, imply, for all $j = 1, \dots, J$, that

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

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 13 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 28. \square

We can now compute the main term of $E_{\mathbb{K}, \lambda}(c)$ stated in Proposition 25.

Proof of Proposition 25. Propositions 27 and 28 give, for $\lambda > 0$, the limit

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

and Lemma 26 gives then the same limit for $E_{\mathbb{K}, \lambda}(c)$. Proposition 28 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

$$J_{\mathbb{K}_{c_k}, \lambda}(1) = \mathcal{J}_{\mathbb{K}_{c_k}, 1}(\check{v}_{c_k}(\cdot + x_k)) = \mathcal{J}_{\mathbb{R}^3}(\check{v}) + \mathcal{J}_{\mathbb{K}_{c_k}, 1}(\check{v}_{c_k}(\cdot + x_k) - \check{v}) + o(1) \quad (5.12)$$

by the following lemma.

Lemma 30. *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*

- i. $\mathbf{1}_{\mathbb{K}_c} \nabla \varphi_c \rightharpoonup \nabla \varphi$ weakly in $L^2(\mathbb{R}^3)$,
- ii. $\|\nabla(\varphi_c - \varphi)\|_{L^2(\mathbb{K}_c)}^2 = \|\nabla \varphi_c\|_{L^2(\mathbb{K}_c)}^2 - \|\nabla \varphi\|_{L^2(\mathbb{R}^3)}^2 + o_{c \rightarrow \infty}(1)$,
- iii. $\|\varphi_c - \varphi\|_{L^p(\mathbb{K}_c)}^p = \|\varphi_c\|_{L^p(\mathbb{K}_c)}^p - \|\varphi\|_{L^p(\mathbb{R}^3)}^p + o_{c \rightarrow \infty}(1)$, for $2 \leq p \leq 6$.

Proof of Lemma 30. By the mean of a regularization function (as in the proof of Lemma 27) 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 *i.* is a classical result and *ii.* a direct consequence of it, we only prove here *iii.*

The weak convergence in $L^2(\mathbb{R}^3)$ of $\mathbf{1}_{\mathbb{K}_c} \nabla \varphi_c$ gives the convergence a.e. of φ_c to φ , up to a subsequence, by [38, Corollary 8.7]. Since $|\varphi_c - \varphi|$ is uniformly bounded in $L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$, this implies *iii.* by the *Missing term in Fatou's lemma* Theorem (see [38, Theorem 1.9]). \square

To obtain for $E_{\mathbb{K},\lambda}(c)$ an expansion similar to (5.12), we proceed the same way. We first show that the sequence of minimizers \check{w}_c is uniformly bounded in $H^1_{\text{per}}(\mathbb{K}_c)$ using the upper bound in the following lemma, which is equivalent to Corollary 24 for \check{v}_c .

Lemma 31 (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 31. As seen in the proof of Lemma 26, $\|\nabla w_c\|_{L^2(\mathbb{K})} = O(c)$ 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 26, there exists $C > 0$ such that

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

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 31 as we did in the proof of Corollary 24. \square

We now come back to the proof of Proposition 25. We apply Lemma 29 to $\{\check{w}_c\}$ and, as for \check{v}_c , the lower bound in Lemma 31 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 30 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 26.

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 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 $\|\check{w}_{c_k}(\cdot + y_k) - \check{w}\|_{L^2(\mathbb{K}_c)}^2 = \lambda - \lambda_1 + o(1)$, 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 11, 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 13, 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 11. Since $\|\check{w}\|_{L^2(\mathbb{R}^3)}^2 = \lambda$, this concludes the proof of Proposition 25 up to the convergence of $\mathbb{1}_{\mathbb{K}_{c_n}} \nabla \check{w}_n(\cdot + x_n)$ and $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_n(\cdot + x_n)$ 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 30 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 (5.13) — therefore only the proofs of Proposition 25, Lemma 26 and Lemma 31 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 25 and the result

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

from Proposition 13 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 25. We state and prove them in the case of one charge per unit cell but they hold, with similar proof, for several charges.

Corollary 32 (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 16. 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 $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_{c_n}(\cdot + x_n)$ 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 32. 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 25 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 4.

By Lemma 31 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 33 (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 33. 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 4 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

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

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 32, 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 33 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

$$\mathcal{E}_{\mathbb{K}_N, c}(w) = \mathcal{J}_{\mathbb{K}_N, c}(w) + \frac{1}{2} D_{\mathbb{K}_N}(|w|^2, |w|^2) - \int_{\mathbb{K}_N} \sum_{i=1}^{N^3} G_{\mathbb{K}_N}(\cdot - R_i) |w|^2, \quad (5.13)$$

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 34) — that any minimizer concentrates around the position of a charge of the lattice — and a lower bound on the number of distinct minimizers (Proposition 36).

Proposition 34 (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 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 34. 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

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

since the first four terms of $\mathcal{E}_{\mathbb{K}_N, c}$ are invariant under spatial translations. Lemma 35 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 35, 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 35 that $x_n = c_n R_{i_0} + o(1)$ as $n \rightarrow \infty$.

The last result of Proposition 34 is a direct consequence of the convergence of the $L^p(\mathbb{K}_{c_n})$ -norms proved in Proposition 25 and Lemma 33 together with the fact that $x_n - c_n R_{i_0} = o(1)$.

Lemma 35. *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 $\|g_c\|_{H^1_{per}(\mathbb{K}_c)}$ by an uniform bound on $\|g_c\|_{L^2_{per}(\mathbb{K}_c)}$ 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 setting than needed for Proposition 34 in order for it to be also useful for the proof of Lemma 43.

Proof of Lemma 35. Using the same notation \mathbb{K}^σ as in the proof of Lemma 26, 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 15, 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 15, there exists $M' > 0$ such that $\left| |\cdot|^{-1} - G_{\mathbb{K}} \right| \leq M'$ 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 35. \square

This concludes the proof of Proposition 34. \square

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

Proposition 36. *For c_n large enough, there exist at least N^3 nonnegative 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 36. First, in Proposition 34, we have seen that 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 $E_{\mathbb{K}, \lambda}(c)$. 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 25. Namely, we prove that there exists $\beta > 0$ such that

$$J_{\mathbb{K}, \lambda}(c) = c^2 J_{\mathbb{R}^3}(\lambda) + o(e^{-\beta c}). \quad (5.14)$$

We recall that we have proved in Lemma 27 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 37. *There exists $\beta > 0$ such that*

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

Proof of Lemma 37. 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 $\mathbb{1}_{\mathbb{K}_{c_n}} \check{v}_{c_n}(\cdot + x_n)$. Our proof relies on the exponential decay with c of the minimizers to $J_{\mathbb{K},\lambda}(1)$ close to the border of the cube \mathbb{K}_c .

Lemma 38 (Exponential decrease of minimizers to $J_{\mathbb{K},\lambda}(1)$). *Let $\{v_c\}_c$ be a sequence of nonnegative minimizers to $J_{\mathbb{K},\lambda}(c)$ such that a subsequence of rescaled functions $\mathbb{1}_{\mathbb{K}_{c_n}} \check{v}_{c_n}$ 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 38. We denote by u the minimizer of $J_{\mathbb{R}^3}(\lambda)$ to which $\mathbb{1}_{\mathbb{K}_{c_n}} \check{v}_{c_n}$ 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 33, 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

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

Together with Corollary 32, 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 37. 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 38, 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 37. \square

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

Proposition 39 (Second order expansion of the energy). *We have the expansion*

$$\begin{aligned} E_{\mathbb{K}_N, N^3 \lambda}(c) &= c^2 J_{\mathbb{R}^3, N^3 \lambda} \\ &+ c \inf_u \left\{ \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|u(x)|^2 |u(y)|^2}{|x-y|} dy dx - \int_{\mathbb{R}^3} \frac{|u(x)|^2}{|x|} dx \right\} + o(c), \end{aligned} \quad (5.15)$$

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

Proof of Proposition 39. In order to deal with the term $D_{\mathbb{K}}$, we first prove a convergence result similar to what we did in Lemma 35 for term $\int G|w|^2$.

Lemma 40. *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 40. 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 15,

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

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 26. 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 40. \square

Let w_c be a sequence of minimizers to $E_{\mathbb{K}_N, N^3\lambda}(c)$. By Propositions 25 and 34, the convergence rate (5.14), and Lemmas 37 and 40, 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 27 and 37, 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 35 and 40 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 39. \square

Theorem 2 is therefore proved combining the results of Proposition 25, Proposition 34, Proposition 36 and Proposition 39.

5.4. Proof of Theorem 8 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

$$\begin{aligned} \mathcal{E}_{\mathbb{K}, c}^\circ(w_c + f) &= E_{\mathbb{K}, \lambda}(c) + \langle \mathring{L}_c^+ f_1, f_1 \rangle_{L^2(\mathbb{K})} + \langle \mathring{L}_c^- f_2, f_2 \rangle_{L^2(\mathbb{K})} - 2\mu_c \langle w_c, f_1 \rangle_{L^2(\mathbb{K})} \\ &\quad - \mu_c \|f\|_{L^2(\mathbb{K})}^2 + 2D_{\mathbb{K}}(\Re(w_c \bar{f}), \Re(w_c \bar{f})) + o(\|f\|_{H^1(\mathbb{K})}^2), \end{aligned} \quad (5.16)$$

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

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

and

$$\mathring{L}_c^+ = -\Delta + \frac{7}{3}c_{TF}|w_c|^{\frac{4}{3}} - \frac{5}{3}c|w_c|^{\frac{2}{3}} + \mu_c - \mathcal{G} + |w_c|^2 \star G_{\mathbb{K}}, \quad (5.18)$$

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

$$\begin{aligned} &\int |w+h|^p - \int |w|^p - p \int |w|^{p-2} \Re(w\bar{h}) \\ &\quad - \frac{p(p-2)}{2} \int_{w(\cdot) \neq 0} |w|^{p-4} |\Re(w\bar{h})|^2 - \frac{p}{2} \int |w|^{p-2} |h|^2 = o(\|h\|_{H^1}^2). \end{aligned} \quad (5.19)$$

for any complex-valued $w, h \in H^1$ and $2 \leq p < 4$ (see [56] for details).

Let us suppose that Conjecture 7 holds and that there exist two sequences w_c and ν_c of nonnegative minimizers to $E_{\mathbb{K}_N, N^3\lambda}(c)$ concentrating around the same nucleus at position $R \in \mathbb{K}$. Then, by Proposition 34, we have for $2 \leq p < +\infty$ that

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

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

$$\langle w_{c_n} + \nu_{c_n}, f_n \rangle_{L^2_{\text{per}}(\mathbb{K})} = \langle \check{w}_{c_n} + \check{\nu}_{c_n}, \check{f}_n \rangle_{L^2_{\text{per}}(\mathbb{K}_{c_n})} = 0 \quad (5.20)$$

and

$$\langle \mathcal{G}(c_n^{-1}\cdot), \nabla((\check{w}_{c_n} + \check{\nu}_{c_n})\check{f}_n) \rangle_{L^2_{\text{per}}(\mathbb{K}_{c_n})} = 0 \quad (5.21)$$

Indeed, the fact that ν_c and w_c are real-valued gives the orthogonality (5.20). Moreover, the orthogonality property stated in the following lemma leads to (5.21).

Lemma 41. *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 41. As mentioned in Proposition 36, 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 (5.21) together with $D_{\mathbb{K}}(h, h) \geq 0$ (Lemma 15) and

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

we obtain from (5.16) that

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

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

$$L_n^+ = -\Delta + \frac{7}{3}c_{TF}|\check{w}_c|^{\frac{4}{3}} - \frac{5}{3}|\check{w}_c|^{\frac{2}{3}} + \frac{\mu_{c_n}}{c_n^2} + c_n^{-2}[-\mathcal{G} + |w_{c_n}|^2 \star G_{\mathbb{K}}](c_n^{-1}\cdot). \quad (5.22)$$

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 7, 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. $w_{c_n} \equiv \nu_{c_n}$. This means that if Conjecture 7 holds then there cannot be more than N^3 nonnegative minimizers for c large enough and, together with Proposition 36, this concludes the proof of Theorem 8. We are thus left with the proof of the following non-degeneracy result.

Proposition 42. *Let $(w_c)_c$ be a sequence of minimizer to $E_{\mathbb{K},\lambda}(c)$ and L_n^+ the associated operator as in (5.22). 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 (5.20) and (5.21), we have*

$$\langle L_n^+ f_n, f_n \rangle_{L^2(\mathbb{K}_{c_n})} \geq C \|f_n\|_{H^1(\mathbb{K}_{c_n})}^2. \quad (5.23)$$

Proof of Proposition 42. Following ideas in [61], we define

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

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

Lemma 43. *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 (5.22), L_n^+ associated with w_{c_n} . Let $(f_n)_n$ be a uniformly bounded sequence of $H_{\text{per}}^1(\mathbb{K}_{c_n})$ 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 43. 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 30,

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

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 (5.10), 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 25, $\mathbb{1}_{\mathbb{K}_{c_n}} \check{w}_n(\cdot + c_n R)$ 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 32 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 43. \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 $\|f_n\|_{H^1(\mathbb{K}_{c_n})} = 1$, $\langle \check{w}_{c_n} + \check{v}_{c_n}, f_n \rangle_{L_{\text{per}}^2(\mathbb{K}_{c_n})} = 0$ and $\langle \mathcal{G}(c_n^{-1} \cdot), \nabla((\check{w}_{c_n} + \check{v}_{c_n}) \check{f}_n) \rangle_{L_{\text{per}}^2(\mathbb{K}_{c_n})} = 0$, 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 43, 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 $\mathbb{1}_{\mathbb{K}_{c_n}} (\check{w}_{c_n}(\cdot + c_n R) + \check{v}_{c_n}(\cdot + c_n R)) \rightarrow 2Q$ in $L^2(\mathbb{R}^3) \cap L^{6^-}(\mathbb{R}^3)$. This, together with (5.20) 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

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

Thus, applying Lemma 35 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 35 and, on the other hand, to $\mathbb{1}_{\mathbb{K}_{c_n}} (\check{w}_{c_n}(\cdot + c_n R) + \check{v}_{c_n}(\cdot + c_n R)) \rightarrow 2Q$ 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 30 — with the second set of conditions, we obtain

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

Finally, (5.21) 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 44, if Conjecture 7 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 42. \square

We are left with the proof of Proposition 44.

Proposition 44. *If Conjecture 7 holds then there exists $\alpha > 0$ such that*

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \geq \alpha \|f\|_{H^1(\mathbb{R}^3)}^2, \quad (5.24)$$

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 7.

Proof of Proposition 44. First we note that it is obviously enough to prove it for f real valued but also that it is enough to prove

$$\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)} \geq \alpha \|f\|_{L^2(\mathbb{R}^3)}^2 \quad (5.25)$$

with $\alpha > 0$. Indeed, if f verifies (5.25) 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 (5.24) 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 (5.25) 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 45 (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 positive.*

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

$$\alpha_1 := \inf_{\substack{f \in \mathcal{H}_{(1)} \cap H^1(\mathbb{R}^3) \\ \langle f, Q \nabla |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = 0}} \frac{\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)}}{\|f\|_{L^2(\mathbb{R}^3)}^2} > 0. \quad (5.26)$$

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

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

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 (5.26) 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 a 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 43. 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, since $\langle f_n, Q \nabla |\cdot|^{-1} \rangle_{L^2(\mathbb{R}^3)} = 0$, we have for any $i = 1, 2, 3$ 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 (5.26) 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 $\alpha > 0$, independent of ℓ , such that

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

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

$$\langle L_{\mu, \ell}^+ \varphi, \varphi \rangle_{L^2(\mathbb{R}_+, r^2 dr)} = \langle L_{\mu, \ell-1}^+ \varphi, \varphi \rangle_{L^2(\mathbb{R}_+, r^2 dr)} + 2\ell \|\varphi/r\|_{L^2(\mathbb{R}_+, r^2 dr)}^2, \quad (5.28)$$

it is then sufficient to prove (5.27) in the case $\ell = 2$ in order to prove it for all $\ell \geq 2$.

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

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

being bounded and vanishing as $r \rightarrow \infty$, it is well-known that $\sigma(L_{\mu, 2}^+) = \sigma_{\text{ess}}(L_{\mu, 2}^+) = [\mu; +\infty)$ and (5.27) follows. We thus have, by (5.28) and $L_{\mu, 1}^+ \geq 0$, that the eigenvalue $e_{\mu, 2} = \inf \sigma(L_{\mu, 2}^+)$ and its associated eigenfunction $\varphi_2 \not\equiv 0$ verify that

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

and (5.27) 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

$$\alpha_0 := \inf_{\substack{f \in \mathcal{H}_{(0)} \cap H^1(\mathbb{R}^3) \\ \langle f, Q \rangle_{L^2(\mathbb{R}^3)} = 0}} \frac{\langle L_\mu^+ f, f \rangle_{L^2(\mathbb{R}^3)}}{\|f\|_{L^2(\mathbb{R}^3)}^2} > 0. \quad (5.29)$$

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 (5.16) and using (2.10),

(3.5), (5.19) and that Q is a minimizer of $J_{\mathbb{R}^3}(\lambda)$, we obtain

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

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 (5.29) 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 invertible, 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 7. We have obtained $f \equiv 0$ which is absurd as before. \square

This concludes the proof of Theorem 8. \square

REFERENCES

- [1] H. BAHOURI AND P. GÉRARD, *High frequency approximation of solutions to critical nonlinear wave equations*, Amer. J. Math., 121 (1999), pp. 131–175.
- [2] J. BELLAZZINI AND M. GHIMENTI, *Symmetry breaking for Schrödinger-Poisson-Slater energy*, ArXiv:1601.05626, (2016).
- [3] H. BERESTYCKI AND P.-L. LIONS, *Nonlinear scalar field equations. I. Existence of a ground state*, Arch. Rational Mech. Anal., 82 (1983), pp. 313–345.
- [4] O. BOKANOWSKI, B. GREBERT, AND N. J. MAUSER, *Local density approximations for the energy of a periodic Coulomb model*, Math. Models Methods Appl. Sci., 13 (2003), pp. 1185–1217.
- [5] O. BOKANOWSKI AND N. J. MAUSER, *Local approximation for the Hartree–Fock exchange potential: a deformation approach*, Math. Models Methods Appl. Sci., 9 (1999), pp. 941–961.
- [6] J. E. BROTHERS AND W. P. ZIEMER, *Minimal rearrangements of Sobolev functions*, J. Reine Angew. Math., 384 (1988), pp. 153–179.
- [7] I. CATTO, C. LE BRIS, AND P.-L. LIONS, *The mathematical theory of thermodynamic limits: Thomas–Fermi type models*, Oxford Mathematical Monographs, The Clarendon Press, Oxford University Press, New York, 1998.
- [8] M. CHEN, J. XIA, C. HUANG, J. M. DIETERICH, L. HUNG, I. SHIN, AND E. A. CARTER, *Introducing PROFESS 3.0: An advanced program for orbital-free density functional theory molecular dynamics simulations*, Comput. Phys. Commun., 190 (2015), pp. 228 – 230.
- [9] P. A. DIRAC, *Note on exchange phenomena in the Thomas atom*, Proc. Camb. Philos. Soc., 26 (1930), pp. 376–385.
- [10] R. L. FRANK AND E. LENZMANN, *Uniqueness of non-linear ground states for fractional Laplacians in \mathbb{R}* , Acta Math., 210 (2013), pp. 261–318.
- [11] R. L. FRANK, E. LENZMANN, AND L. SILVESTRE, *Uniqueness of radial solutions for the fractional Laplacian*, Comm. Pure Appl. Math., 69 (2016), pp. 1671–1726.
- [12] R. L. FRANK AND E. H. LIEB, *Possible lattice distortions in the Hubbard model for graphene*, Phys. Rev. Lett., 107 (2011), p. 066801.
- [13] G. FRIESECKE, *Pair correlations and exchange phenomena in the free electron gas*, Comm. Math. Phys., 184 (1997), pp. 143–171.
- [14] H. FRÖHLICH, *On the theory of superconductivity: the one-dimensional case*, Proc. R. Soc. Lond. A, 223 (1954), pp. 296–305.
- [15] M. GARCIA ARROYO AND E. SÉRÉ, *Existence of kink solutions in a discrete model of the polyacetylene molecule*. working paper or preprint, Dec. 2012.
- [16] P. GÉRARD, *Description du défaut de compacité de l’injection de Sobolev*, ESAIM Control Optim. Calc. Var., 3 (1998), pp. 213–233.
- [17] B. GIDAS, W. M. NI, AND L. NIRENBERG, *Symmetry of positive solutions of nonlinear elliptic equations in \mathbb{R}^N* , Adv. Math. Suppl. Stud. A, 7 (1981), pp. 369–402.
- [18] G. M. GRAF AND J. P. SOLOVEJ, *A correlation estimate with applications to quantum systems with Coulomb interactions*, Rev. Math. Phys., 6 (1994), pp. 977–997. Special issue dedicated to Elliott H. Lieb.

- [19] M. GRILLAKIS, J. SHATAH, AND W. STRAUSS, *Stability theory of solitary waves in the presence of symmetry. I*, J. Funct. Anal., 74 (1987), pp. 160–197.
- [20] T. HMIDI AND S. KERAANI, *Blowup theory for the critical nonlinear Schrödinger equations revisited*, Int. Math. Res. Not., (2005), pp. 2815–2828.
- [21] R. A. JOHNSON, *Empirical potentials and their use in the calculation of energies of point defects in metals*, J. Phys. F: Met. Phys., 3 (1973), p. 295.
- [22] T. KENNEDY AND E. H. LIEB, *An itinerant electron model with crystalline or magnetic long range order*, Phys. A, 138 (1986), pp. 320–358.
- [23] ———, *Proof of the Peierls instability in one dimension*, Phys. Rev. Lett., 59 (1987), pp. 1309–1312.
- [24] R. KILLIP, T. OH, O. POCOVNICU, AND M. VIŞAN, *Solitons and scattering for the cubic-quintic nonlinear Schrödinger equation on \mathbb{R}^3* , Arch. Rational Mech. Anal., 225 (2017), pp. 469–548.
- [25] R. KILLIP AND M. VIŞAN, *Nonlinear schrödinger equations at critical regularity*. Lecture notes for the summer school of Clay Mathematics Institute, 2008.
- [26] G. KIN-LIC CHAN AND N. C. HANDY, *Optimized Lieb–Oxford bound for the exchange-correlation energy*, Phys. Rev. A, 59 (1999), pp. 3075–3077.
- [27] C. LE BRIS, *Quelques problèmes mathématiques en chimie quantique moléculaire*, PhD thesis, École Polytechnique, 1993.
- [28] E. LENZMANN, *Uniqueness of ground states for pseudorelativistic Hartree equations*, Anal. PDE, 2 (2009), pp. 1–27.
- [29] M. LEVY AND J. P. PERDEW, *Tight bound and convexity constraint on the exchange-correlation-energy functional in the low-density limit, and other formal tests of generalized-gradient approximations*, Phys. Rev. B, 48 (1993), pp. 11638–11645.
- [30] M. LEWIN, *Variational Methods in Quantum Mechanics*. Unpublished lecture notes (University of Cergy-Pontoise), 2010.
- [31] M. LEWIN AND E. H. LIEB, *Improved Lieb–Oxford exchange-correlation inequality with a gradient correction*, Phys. Rev. A, 91 (2015), p. 022507.
- [32] M. LEWIN AND S. ROTA NODARI, *Uniqueness and non-degeneracy for a nuclear nonlinear Schrödinger equation*, Nonlinear Differ. Equat. Appl., 22 (2015), pp. 673–698.
- [33] C. LI, *Monotonicity and symmetry of solutions of fully nonlinear elliptic equations on unbounded domains*, Comm. Partial Differential Equations, 16 (1991), pp. 585–615.
- [34] E. H. LIEB, *Existence and uniqueness of the minimizing solution of Choquard’s nonlinear equation*, Studies in Appl. Math., 57 (1976/1977), pp. 93–105.
- [35] ———, *A lower bound for Coulomb energies*, Phys. Lett. A, 70 (1979), pp. 444–446.
- [36] ———, *Thomas–Fermi and related theories of atoms and molecules*, Rev. Modern Phys., 53 (1981), pp. 603–641.
- [37] ———, *A model for crystallization: a variation on the Hubbard model*, Phys. A, 140 (1986), pp. 240–250. Statphys 16 (Boston, Mass., 1986).
- [38] E. H. LIEB AND M. LOSS, *Analysis*, vol. 14 of Graduate Studies in Mathematics, American Mathematical Society, Providence, RI, second ed., 2001.
- [39] E. H. LIEB AND B. NACHTERGAELE, *Dimerization in ring-shaped molecules: the stability of the Peierls instability*, in XIth International Congress of Mathematical Physics (Paris, 1994), Int. Press, Cambridge, MA, 1995, pp. 423–431.
- [40] ———, *Stability of the Peierls instability for ring-shaped molecules*, Phys. Rev. B, 51 (1995), p. 4777.
- [41] ———, *Bond alternation in ring-shaped molecules: The stability of the Peierls instability*, Int. J. Quantum Chemistry, 58 (1996), pp. 699–706.
- [42] E. H. LIEB AND S. OXFORD, *Improved lower bound on the indirect Coulomb energy*, Int. J. Quantum Chem., 19 (1980), pp. 427–439.
- [43] E. H. LIEB AND R. SEIRINGER, *The stability of matter in quantum mechanics*, Cambridge University Press, Cambridge, 2010.
- [44] E. H. LIEB AND B. SIMON, *The Thomas–Fermi theory of atoms, molecules and solids*, Advances in Math., 23 (1977), pp. 22–116.
- [45] P.-L. LIONS, *The concentration-compactness principle in the calculus of variations. The locally compact case. II*, Ann. Inst. H. Poincaré Anal. Non Linéaire, 1 (1984), pp. 223–283.
- [46] ———, *Solutions of Hartree–Fock equations for Coulomb systems*, Comm. Math. Phys., 109 (1987), pp. 33–97.
- [47] C. B. MORREY, JR., *On the analyticity of the solutions of analytic non-linear elliptic systems of partial differential equations. I. Analyticity in the interior*, Amer. J. Math., 80 (1958), pp. 198–218.
- [48] P. T. NAM AND H. VAN DEN BOSCH, *Nonexistence in Thomas–Fermi–Dirac–von Weizsäcker Theory with Small Nuclear Charges*, Math. Phys. Anal. Geom., 20 (2017), p. 20:6.

- [49] R. E. PEIERLS, *Quantum Theory of Solids*, Clarendon Press, 1955.
- [50] J. P. PERDEW, *Unified Theory of Exchange and Correlation Beyond the Local Density Approximation*, in *Electronic Structure of Solids '91*, P. Ziesche and H. Eschrig, eds., Akademie Verlag, Berlin, 1991, pp. 11–20.
- [51] J. P. PERDEW, K. BURKE, AND M. ERNZERHOF, *Generalized gradient approximation made simple*, *Phys. Rev. Lett.*, 77 (1996), pp. 3865–3868.
- [52] J. P. PERDEW AND Y. WANG, *Accurate and simple analytic representation of the electron-gas correlation energy*, *Phys. Rev. B*, 45 (1992), pp. 13244–13249.
- [53] E. PRODAN, *Symmetry breaking in the self-consistent Kohn–Sham equations*, *J. Phys. A*, 38 (2005), pp. 5647–5657.
- [54] E. PRODAN AND P. NORDLANDER, *Hartree approximation. III. Symmetry breaking*, *J. Math. Phys.*, 42 (2001), pp. 3424–3438.
- [55] J. RICAUD, *On uniqueness and non-degeneracy of anisotropic polarons*, *Nonlinearity*, 29 (2016), pp. 1507–1536.
- [56] ———, *Symétrie et brisure de symétrie pour certains problèmes non linéaires*, PhD thesis, Université de Cergy-Pontoise, June 2017.
- [57] R. SEIRINGER, *A correlation estimate for quantum many-body systems at positive temperature*, *Rev. Math. Phys.*, 18 (2006), pp. 233–253.
- [58] J. SERRIN AND M. TANG, *Uniqueness of ground states for quasilinear elliptic equations*, *Indiana Univ. Math. J.*, 49 (2000), pp. 897–923.
- [59] C. D. SHERRILL, M. S. LEE, AND M. HEAD-GORDON, *On the performance of density functional theory for symmetry-breaking problems.*, *Chem. Phys. Lett.*, 302 (1999), pp. 425–430.
- [60] P. TOD AND I. M. MOROZ, *An analytical approach to the Schrödinger–Newton equations*, *Nonlinearity*, 12 (1999), pp. 201–216.
- [61] M. I. WEINSTEIN, *Modulational stability of ground states of nonlinear Schrödinger equations*, *SIAM J. Math. Anal.*, 16 (1985), pp. 472–491.

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