Symétrie et brisure de symétrie pour certains problèmes non linéaires

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Thèse de Doctorat en Mathématiques

présentée par

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Résumé

Cette thèse est consacrée à l'étude mathématique de deux systèmes quantiques décrits par des modèles non linéaires : le polaron anisotrope et les électrons d'un cristal périodique. Après avoir prouvé l'existence de minimiseurs, nous nous intéressons à la question de l'unicité pour chacun des deux modèles. Dans une première partie, nous montrons l'unicité du minimiseur et sa non-dégénérescence pour le polaron décrit par l'équation de Choquard–Pekar anisotrope, sous la condition que la matrice diélectrique du milieu est presque isotrope. Dans le cas d'une forte anisotropie, nous laissons la question de l'unicité en suspens mais caractérisons précisément les symétries pouvant être dégénérées. Dans une seconde partie, nous étudions les électrons d'un cristal dans le modèle de Thomas–Fermi–Dirac–Von Weizsäcker périodique, en faisant varier le paramètre devant le terme de Dirac. Nous montrons l'unicité et la non-dégénérescence du minimiseur lorsque ce paramètre est suffisamment petit et mettons en évidence une brisure de symétrie lorsque celui-ci est grand.

Abstract

This thesis is devoted to the mathematical study of two quantum systems described by nonlinear models: the anisotropic polaron and the electrons in a periodic crystal. We first prove the existence of minimizers, and then discuss the question of uniqueness for both problems. In the first part, we show the uniqueness and nondegeneracy of the minimizer for the polaron, described by the Choquard–Pekar anisotropic equation, assuming that the dielectric matrix of the medium is almost isotropic. In the strong anisotropic setting, we leave the question of uniqueness open but identify the symmetry that can possibly be degenerate. In the second part, we study the electrons of a crystal in the periodic Thomas–Fermi–Dirac–Von Weizsäcker model, varying the parameter in front of the Dirac term. We show uniqueness and nondegeneracy of the minimizer when this parameter is small enough et prove the occurrence of symmetry breaking when it is large.

Contents

Introduction

Les modèles non linéaires tiennent une place importante dans la description et l'étude des systèmes quantiques. En effet, les modèles exacts, qui décrivent le comportement individuel de chacune des particules du système, sont le plus souvent linéaires. Cependant, ils sont inaccessibles numériquement si l'on veut obtenir des prédictions suffisamment précises, dès que le nombre de particule dépasse l'ordre d'une dizaine. Ceci est dû au fait que ces modèles exacts sont posés en très grande dimension (qui diverge exponentiellement avec le nombre de particules du système), ce qui induit une complexité de calcul inabordable. C'est afin de palier à cette difficulté que sont introduits des modèles simplifiés qui sont presque tous non-linéaires mais néanmoins posés en bien plus basse dimension.

Dans certains régimes, il est possible de montrer que les modèles exacts sont, au premier ordre, correctement approchés par des modèles non-linéaires simples. Ces derniers peuvent à leur tour servir de base pour des modèles non-linéaires empiriques utilisés en dehors du régime d'origine. L'exemple le plus célèbre de cette approche est la Théorie de la Fonctionnelle de la Densité (DFT) qui utilise des modèles non-linéaires empiriques dépendant uniquement de la densité ρ du système, voir par exemple [**PY94**] et ses références. Cette approche connaît un succès inégalé en chimie quantique, dans la théorie de la matière condensée, jusqu'au applications industrielles.

Comparés aux problèmes linéaires, les modèles non-linéaires apportent de nouvelles difficultés mathématiques qui à leur tour influencent leur caractère prédictif. Pour les problèmes linéaires, grâce au théorème de diagonalisation simultanée, nous savons qu'il existe toujours des vecteurs propres respectant les symétries du problème. En dehors du cas convexe, cet argument ne s'applique pas aux problèmes non-linéaires. Il devient alors important de savoir si les états d'équilibre du système respectent ou non les symétries. Une brisure de symétrie n'est pas nécessairement un inconvénient et peu même être nécessaire à l'obtention de meilleure prédiction. Sur ces questions dans le cas de la DFT, nous renvoyons par exemple à [**SLHG99**] et à [**PSB95**].

Mentionnons également que même dans le cas linéaire des brisures de symétrie peuvent être obtenues dans une limite où le nombre de particules tend vers l'infini. Auquel cas, les avantages mathématiques du caractère linéaire tendent à disparaître. Ces brisures de symétrie se manifestent par exemple dans les transitions de phases étudiées en physique statistique [**Rue99**]. Un solide est l'exemple typique d'une brisure de la symétrie de translation [**BL15**].

Des phénomènes de brisure de symétrie ont été mis en évidence mathématiquement dans de nombreux modèles. Dans le cadre de modèles discrets sur des réseaux, l'instabilité des solutions ayant la même périodicité que le réseau a été démontrée dans [**Frö54, Pei55**] pour les modèles qu'ils y considèrent, tandis que [**KL86, Lie86, KL87, LN95b, LN95a, LN96, FL11, GAS12**] ont prouvé, pour différents modèles (et differentes dimensions), que les solutions ont une périodicité distincte de celle du réseau. Concernant des modèles à température finie et sur des domaines finis, une brisure de symétrie est mise en évidence dans [**PN01**] pour un gaz unidimensionnel sur un cercle et dans [**Pro05**] sur des tores et des sphères en dimension $d \leqslant 3$. Enfin, sur tout l'espace $\mathbb{R}^3$, une brisure de symétrie est prouvée dans [**BG16**] pour le modèle considéré : les minimiseurs ne sont pas radiaux lorsque le nombre d'électrons est assez grands.

Cette thèse s'intéresse à deux modèles non-linéaires : le modèle de Choquard–Pekar anisotrope et le modèle de Thomas–Fermi–Dirac–von Weizsäcker (TFDW) périodique décrivant des électrons dans un cristal, que nous décrivons plus précisément ci-après et pour lesquels nous nous sommes intéressés à l'existence, l'unicité et la non-dégénérescence des minimiseurs ainsi qu'aux questions de symétrie et de brisure de symétrie.

1. Présentation des travaux sur le polaron anisotrope

Un polaron est un électron interagissant avec un cristal polarisable et capable de former un état lié via la déformation du cristal que sa propre charge induit.

Nous nous intéressons dans le premier chapitre de cette thèse au modèle de Pekar du polaron, dans lequel le cristal est remplacé par un milieu polarisable continu. Ce modèle décrit bien le système lorsque le polaron s'étend sur une région très grande comparée à la taille caractéristique du cristal. Dans ce modèle, l'interaction entre l'électron et le milieu est alors un champ coulombien attractif effectif.

Dans le cas d'un milieu polarisable isotrope, caractérisé par sa *constante diélectrique* $\varepsilon_M \geqslant 1$ (un réel), ce modèle de Pekar du polaron a été étudié par Lieb [**Lie77**]. D'une part il a montré l'existence de minimiseurs à valeurs complexes, sous contrainte de masse, pour la fonctionnelle

$$\frac{1}{2}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \,\mathrm{d}x - \frac{1-{\varepsilon_M}^{-1}}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|\psi(y)|^2|\psi(x)|^2}{|x-y|}\,\mathrm{d}y\,\mathrm{d}x \tag{0.1}$$

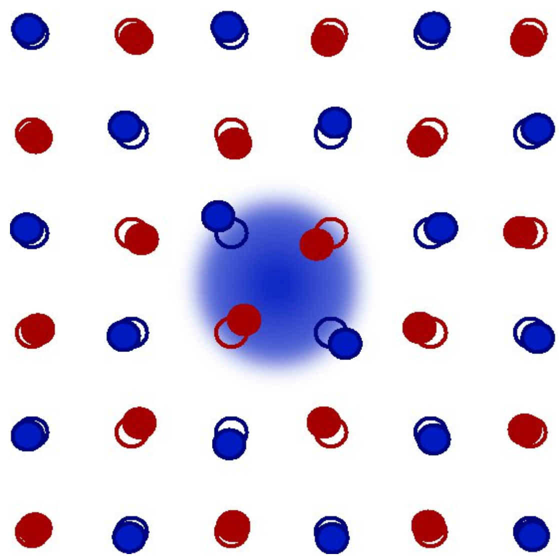


FIGURE 1. Représentation de la déformation du cristal due à la présence d'un l'électron (tache bleue diffuse) qui attire les charges positives (disques rouges) et repousse les charges négatives (disques bleus). Les anneaux représentent les positions des charges du cristal au repos.
Source : Image transmise par Lewin, Mathieu.

associée à l'équation non linéaire de *Choquard–Pekar*

$$\Big(-\frac{\Delta}{2} - (1 - {\varepsilon_M}^{-1})|\cdot|^{-1} \star |\psi|^2 \Big)\psi = -\mu\psi, \tag{0.2}$$

également appelée équation de *Schrodinger–Newton* ou équation de *Choquard.* D'autre part, il a prouvé l'unicité à translation spatiale et phase près, du minimiseur sous contrainte de masse. Ce minimiseur est strictement positif, radial, indéfiniment différentiable, (radialement) strictement décroissant avec une décroissance exponentielle à l'infini.

Notons que les équations ci-dessus sont données dans le système d'unités dans lequel la masse de l'électron, la constante de Planck réduite et la permittivité diélectrique du vide vérifient $m = 1$, $\hbar = 1$ et $4\pi\varepsilon_0 = 1$. Dans ce système d'unités, une constante diélectrique $\varepsilon_M = 1$ correspond au cas du vide.

Ensuite, Lenzmann a prouvé dans [**Len09**] que l'unique minimiseur positif Q est non dégénéré. C'est-à-dire que la linéarisation

$$\mathfrak{L}_Q\xi = -\frac{1}{2}\Delta\xi + \mu\xi - \left(V \star |Q|^2\right)\xi - 2Q\left(V \star (Q\xi)\right) \tag{0.3}$$

de l'équation de Choquard–Pekar (0.2), où $V(x) = (1-{\varepsilon_M}^{-1})|x|^{-1}$, a pour noyau

$$\ker_{|L^2(\mathbb{R}^3)} \mathfrak{L}_Q = \operatorname{span}\{\partial_{x_1}Q, \partial_{x_2}Q, \partial_{x_3}Q\}.$$

Cette non-dégénérescence est une propriété importante qui est utile dans des arguments de type *fonctions implicites.*

Le polaron anisotrope. Le premier chapitre de cette thèse se propose d'étendre l'étude du modèle du Polaron de Pekar au cas d'un milieu anisotrope. Un milieu anisotrope n'a plus un réel ε_M pour *constante diélectrique* mais une matrice symétrique réelle $M^{-1} \geqslant 1$, rendant ainsi compte du fait que le comportement du milieu n'est pas le même selon toutes les directions de l'espace. Ainsi, dans la fonctionnelle (0.1) et dans l'équation de Choquard–Pekar (0.2), le potentiel $(1-{\varepsilon_M}^{-1})|x|^{-1}$ doit être remplacé par le potentiel

$$\boxed{V_M(x) = \frac{1}{|x|} - \frac{1}{|M^{-1}x|},} \tag{0.4}$$

où l'on peut supposer, sans perte de généralité puisque M^{-1} est symétrique réelle, que M vérifie $M < 1$ et est diagonale avec des valeurs propres vérifiant $m_2 < 1$ et $0 < m_3 \leqslant m_2 \leqslant m_1 \leqslant 1$. La fonctionnelle anisotrope est alors

$$\boxed{\mathscr{E}^{V_M}(\psi) := \frac{1}{2}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \,\mathrm{d}x - \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |\psi(y)|^2 V_M(x-y)|\psi(x)|^2 \,\mathrm{d}y\,\mathrm{d}x,}$$

le problème de minimisation, pour une masse $\lambda > 0$ donnée, est

$$I_M(\lambda) := \min_{\substack{\psi\in H^1(\mathbb{R}^3)\\ \|\psi\|_2^2=\lambda}} \mathscr{E}^{V_M}(\psi) \tag{0.5}$$

et l'équation non linéaire associée est

$$\Big(-\frac{\Delta}{2} - V_M \star |\psi|^2\Big)\psi = -\mu\psi. \tag{0.6}$$

Le premier chapitre de cette thèse se propose donc de voir quels résultats obtenus dans le cadre isotrope s'étendent au modèle anisotrope.

Dérivation du modèle. L'équation de Choquard–Pekar isotrope (0.2) a été obtenue par Donsker–Varadhan [**DV83**] puis par Lieb–Thomas [**LT97**] à partir du modèle *linéaire* de Fröhlich dans une limite de couplage fort. Ce modèle décrit un électron en interaction avec un champ de phonons second quantifié, supposé homogène et isotrope. Dans ce modèle, la structure du cristal sous-jacent est donc absente. Le Hamiltonien du système prend la forme

$$H = -\Delta + \int_{\mathbb{R}^3} a_{\boldsymbol{k}}^\dagger a_{\boldsymbol{k}} \,\mathrm{d}\boldsymbol{k} - \frac{\sqrt{\alpha}}{\pi\sqrt{2}}\int_{\mathbb{R}^3}\left(\frac{a_{\boldsymbol{k}}}{|\boldsymbol{k}|}e^{\mathrm{i}\boldsymbol{k}\cdot x} + \frac{a_{\boldsymbol{k}}^\dagger}{|\boldsymbol{k}|}e^{-\mathrm{i}\boldsymbol{k}\cdot x}\right)\mathrm{d}\boldsymbol{k},$$

où les $\boldsymbol{k}$ sont les vecteurs d'ondes des phonons, $a_{\boldsymbol{k}}^{\dagger}$ et $a_{\boldsymbol{k}}$ les opérateurs de création et d'annihilation. Le modèle de Choquard–Pekar s'obtient lorsque la constante de couplage α tend vers l'infini, un régime qui est similaire à une limite semi-classique pour le champ des phonons. À la limite, les phonons sont au premier ordre décrits par un état cohérent, c'est-à-dire un champ classique. Pour des travaux similaires dans le cas de N électrons, voir [**MS07, FLST10, FLST11, FLS12, FLS13, BFL15, AH16**]. Le cas dynamique a été récemment étudié dans [**FS14, FZ17, Gri16, GSS16**]. De plus, le cas avec champ magnétique a été considéré dans [**AG14, GHW12, GW13**]. Remarquons que même si la dérivation de l'équation de Choquard–Pekar anisotrope à partir du Hamiltonien anisotrope de Fröhlich n'a jamais été réalisée à notre connaissance, on peut penser que les mêmes arguments s'appliquent.

Dans [**LR13a, LR13b**], Lewin et Rougerie ont adopté un point de vue différent. Ils ont dérivé le modèle de Choquard–Pekar à partir du modèle microscopique Hartree–Fock réduit du cristal dans une limite multi-échelle. Le caractère isotrope ou anisotrope de l'équation finale dépend alors du cristal considéré.

Résultats obtenus. Les résultats que nous avons obtenus pour ce modèle ont été publiés dans [**Ric16**]. La première partie de la thèse en donne une version plus détaillée. Le résultat d'existence de minimiseurs s'étend au cas anisotrope bien que la méthode preuve soit différente de celle donnée par Lieb dans le cas isotrope. En effet, la démonstration faite par Lieb repose sur l'isotropie puisqu'elle est basée sur le fait que $x \mapsto |x|^{-1}$ est radiale décroissante et utilise le réarrangement symétrique. Cette preuve ne fonctionnant plus dans le cas anisotrope, nous prouvons le résultat via la méthode de concentration-compacité de Lions [**Lio84a, Lio84b**].

THÉORÈME (Existence de minimiseurs). *Soient $\lambda > 0$ et V_M défini par* (0.4)*. Alors, $I_M(\lambda)$ a un minimiseur et toute suite minimisante converge fortement dans $H^1(\mathbb{R}^3)$ vers un minimiseur, à extraction d'un sous-suite près et à une translation spatiale près.*

De plus tout minimiseur ψ vérifie

(1) ψ est une $H^2(\mathbb{R}^3)$-solution de l'équation de Choquard–Pekar (0.6) *où $-\mu = \frac{d}{d\lambda}I(\lambda) < 0$ est la plus petite valeur propre de l'opérateur auto-adjoint $H_\psi := -\Delta/2 - |\psi|^2 \star V$, laquelle est simple ;*

(2) $\mu\lambda = -\lambda \dfrac{d}{d\lambda} I(\lambda) = -3\lambda^3 I(1) = \dfrac{3}{2}\|\nabla\psi\|_2^2 = \dfrac{3}{4}\left\langle V \star |\psi|^2, |\psi|^2 \right\rangle ;$

(3) $|\psi|$ est un minimiseur et $|\psi| > 0$;

(4) $\psi = z|\psi|$ pour un z donné tel que $|z| = 1$.

De plus, les résultats d'unicité et de non-dégénérescence du minimiseur sont étendus dans cette thèse au cas que nous appelons de *faible anisotropie* et qui correspond au cas où la matrice M est proche d'une homothétie. Nous prouvons ce résultat, donné dans le théorème ci-dessous, via un théorème de *fonctions implicites* dans le cadre d'un argument perturbatif autour du cas isotrope. Le résultat de non-dégénérescence du cas isotrope, prouvé dans **[Len09]**, est un ingrédient clé de notre démonstration.

THÉORÈME (Unicité et non-dégénérescence). *Soient $\lambda > 0$ et $0 < s < 1$. Il existe $\varepsilon > 0$ tel que, pour toute matrice 3×3 symétrique réelle $0 < M < 1$ vérifiant $\|M - s \cdot \mathrm{Id}\| < \varepsilon$, le minimiseur ψ du problème de minimisation $I_M(\lambda)$ défini par (0.5) est unique à phase et translation près. De plus, le minimiseur est pair selon chacun des vecteurs propres de M et*

$$\ker \mathfrak{L}_\psi = \mathrm{span}\,\{\partial_x \psi, \partial_y \psi, \partial_z \psi\}\,,$$

où $\mathfrak{L}_\psi$ est l'opérateur linéarisé défini par (0.3).

Nous développons également dans ce premier chapitre un travail sur les propriétés de symétrie des minimiseurs, en fonction de critères sur la matrice M. Nous prouvons que les minimiseurs sont toujours symétriques et strictement décroissants le long du demi-axe positif défini par le vecteur propre associé à la plus petite valeur propre de la constante (matricielle) diélécrique et donnons, pour chacune des deux autres directions principales du milieu, une condition suffisante assurant que les minimiseurs soient symétriques et strictement décroissants le long de chacun des demi-axes positifs définis par ces autres directions.

THÉORÈME (Symétrie des minimiseurs). *Soient $\lambda > 0$, V_M définie par (0.4), $0 < m_3 \leqslant m_2 \leqslant m_1 < 1$ les trois valeurs propres de M et e_1, e_2 et e_3 des vecteurs propres associés. Si $\psi_M \geqslant 0$ est un minimiseur de $I_M(\lambda)$ alors, à translation spatiale près, ψ_M est symétrique dans la direction de e_1 et strictement décroissante selon le demi-axe positif de cette direction. De plus, si $m_1^3 \leqslant m_2^2$, alors ψ_M est également symétrique et strictement décroissante selon e_2. Enfin, si $m_1^3 \leqslant m_3^2$, alors ψ_M est également symétrique et strictement décroissante selon e_3.*

Enfin, nous étudions dans la dernière partie du premier chapitre l'opérateur linéarisé, sous les conditions suffisantes mises en évidence précédemment. L'objectif serait de prouver la non-dégénérescence

$$\ker \mathfrak{L}_\psi = \mathrm{span}\,\{\partial_x \psi, \partial_y \psi, \partial_z \psi\}$$

au-delà du cas de *faible anisotropie*. Les travaux de cette thèse n'ont pas permis d'aboutir à ce résultat mais ont cependant conduit à un résultat partiel dans lequel nous n'avons pu exclure que des fonctions paires (à translation près) par rapport à chacune des directions principales du milieu ne puissent être dans le noyau. Précisément, nous démontrons le résultat suivant.

THÉORÈME. *Supposons que la matrice M décrivant le milieu polarisable vérifie $0 < m_3 \leqslant m_2 \leqslant m_1 < 1$ et $m_2 < 1$, ainsi que $m_1^3 \leqslant m_2^2$ et $m_1^3 \leqslant m_3^2$. Si ψ est une solution strictement positive et symétrique strictement décroissante (par rapport à chacune des directions principales du milieu) de l'équation de Choquard–Pekar* (0.6)*, alors*

$$\ker \mathfrak{L}_\psi = \operatorname{span}\{\partial_x\psi, \partial_y\psi, \partial_z\psi\} \bigoplus \ker(\mathfrak{L}_\psi)_{|L^2_{+,+,+}},$$

où $L^2_{+,+,+}$ est le sous-espace de $L^2(\mathbb{R}^3)$ des fonctions paires par rapport à chacune des directions principales. En particulier, ψ peut être un minimiseur de $I_M(\lambda)$.

Questions ouvertes. Cette thèse laisse ouverte la question de l'unicité du minimiseur en dehors du cas d'un milieu faiblement anisotrope. Nous conjecturons qu'il y a unicité (à translation près) au moins sur tout le domaine défini par $0 < m_3 \leqslant m_2 \leqslant m_1 < 1$, $m_1^3 \leqslant m_2^2$ et $m_1^3 \leqslant m_3^2$, c'est-à-dire là où les minimiseurs sont symétriques. Au delà de ce domaine, nous ne saurions nous prononcer.

2. Présentation des travaux sur le modèle TFDW périodique

Dans cette seconde partie, nous étudions le modèle TFDW périodique dans lequel des électrons sont placés dans un arrangement périodique de noyaux que nous supposons être classiques et être disposés selon un réseau périodique 3D. La question posée dans cette partie est si les électrons s'organisent selon la même symétrie que le réseau.

Nous étudions cette question pour le modèle TFDW sans spin, qui est une approximation simple du véritable problème de Schrödinger à N corps, et dont la fonctionnelle d'énergie prend la forme

$$\int_{\mathbb{K}} |\nabla\sqrt{\rho}|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{K}} \rho^{\frac{5}{3}} - \frac{3}{4}c\int_{\mathbb{K}} \rho^{\frac{4}{3}} + \frac{1}{2}\int_{\mathbb{K}} (G_{\mathbb{K}} \star \rho)\rho - \int_{\mathbb{K}} G_{\mathbb{K}}\rho, \tag{0.7}$$

où $\mathbb{K}$ est la cellule unité, ρ est la densité des électrons et $G_{\mathbb{K}}$ est le potential de Coulomb périodique sur $\mathbb{K}$. Notons que la non-convexité de ce modèle est due (uniquement) à la présence du terme $-\frac{3}{4}c\int\rho^{\frac{4}{3}}$ qui est une approximation de l'énergie d'*échange-correlation*, où la valeur de c n'est en pratique déterminée qu'empiriquement.

Nous menons notre étude sur l'éventuelle brisure de symétrie, en fonction du paramètre $c > 0$ et nous démontrons que

- pour c suffisamment petit, la densité ρ des électrons solution au problème est unique et présente la même périodicité que les noyaux ;
- pour c suffisamment grand, il existe (au moins) une organisation 2-périodique des électrons dont l'énergie est plus basse que n'importe quelle organisation 1-périodique : il y a une brisure de symétrie.

Le modèle. L'énergie associée à une fonction d'onde w, dans le modèle TFWD périodique, est

$$\boxed{\begin{aligned}\mathscr{E}_{\mathbb{K},c}(w) = \int_{\mathbb{K}} |\nabla w|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{K}} |w|^{\frac{10}{3}} - \frac{3}{4}c\int_{\mathbb{K}} |w|^{\frac{8}{3}} \\ + \frac{1}{2}\int_{\mathbb{K}}\int_{\mathbb{K}} |w(x)|^2 G_{\mathbb{K}}(x-y)|w(y)|^2 \,\mathrm{d}y\,\mathrm{d}x - \int_{\mathbb{K}} G_{\mathbb{K}}|w|^2,\end{aligned}} \tag{0.8}$$

et nous nous intéressons au problème de minimisation

$$E_{\mathbb{K},\lambda}(c) = \inf_{\substack{w\in H^1_{\mathrm{per}}(\mathbb{K}) \\ \|w\|^2_{L^2(\mathbb{K})}=\lambda}} \mathscr{E}_{\mathbb{K},c}(w).$$

Dérivation du modèle. Il n'existe pas, à notre connaissance, de dérivation du modèle TFWD périodique que nous étudions. En revanche, plusieurs dérivations de modèles de type Thomas–Fermi peuvent être trouvées dans la littérature. Le cas le plus célèbre est celui des atomes neutres pour lequel $N = Z$ tend vers l'infini. C'est un système où les N électrons se concentrent dans un voisinage de la position de l'unique noyau, ils sont donc très concentrés en espace. La première preuve de la validé du modèle de Thomas–Fermi [**Tho27, Fer27**] dans ce régime est due à Lieb–Simon [**LS73, LS77a, LS77b**]. Une autre limite du même type pour les systèmes gravitationnels a été considérée par Lieb, Thirring et Yau dans [**LT84, LY87**]. Ces deux résultats ont récemment généralisés à des potentiels quelconques par Fournais–Lewin–Solovej dans [**FLS15**].

Plus proche de notre situation, Graf et Solovej ont étudié dans [**GS94**] la limite de haute densité pour un système périodique infini (décrit par le problème de Schrödinger exact) dans lequel les noyaux ponctuels sont remplacés par une distribution de charge positive uniforme dans tout l'espace. Dans ce modèle système appelé *Jellium*, seuls les termes en $\rho^{\frac{5}{3}}$ et $\rho^{\frac{4}{3}}$ subsistent. Pour des travaux du même type, voir [**Fri97, Sei06**]. Pour d'autres résultats dans le cas périodique, voir [**BM99, BGM03**].

Résultats. Les résultats que nous avons obtenus pour ce modèle ont été soumis pour publication (voir [**Ric17**]). La seconde partie de la thèse en donne une version plus détaillée. Les résultats principaux sont les deux théorèmes suivants.

THÉORÈME (Unicité pour c petit). *Soit* $\mathbb{K}$ *la cellule unité et* c_{TF}, λ *deux constantes strictement positives. Il existe* $\delta > 0$ *tel que pour tout* $0 \leqslant c < \delta$, *les assertions suivantes soient vraies :*

i. Le minimiseur w_c *du problème TFDW périodique* $E_{\mathbb{K},\lambda}(c)$ *est* unique, *à phase près. Il est non-constant, strictement positif, dans* $H^2_{per}(\mathbb{K})$ *et est l'unique fonction propre de l'état fondamental de l'opérateur auto-adjoint* $\mathbb{K}$*-périodique*

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

ii. Cette fonction $\mathbb{K}$*-périodique* w_c *est l'*unique minimiseur *de tous les problèmes TFDW* $(N \cdot \mathbb{K})$*-périodiques* $E_{N\cdot\mathbb{K},N^3\lambda}(c)$, *pour tout entier* $N \geqslant 1$.

Pour démontrer ce résultat, nous suivons l'esprit de la preuve de Le Bris [**Le 93**] dans le cas de l'espace $\mathbb{R}^3$ tout entier. Nous utilisons un argument perturbatif autour de $c = 0$ — modèle de Thomas–Fermi–von Weizsäcker (TFW) périodique — et utilisons l'unicité et la non-dégénérescence des minimiseurs du modèle TFW, laquelle découle de la stricte convexité de la fonctionnelle associée.

THÉORÈME (Brisure de symétrie pour c grand). *Soit* $\mathbb{K}$ *la cellule unité,* c_{TF}, λ *deux constantes strictement positives et* $N \geqslant 2$ *un entier. Il y a brisure de symétrie dans le modèle TFWD périodique pour* c *assez grand :*

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

Plus précisément, le problème TFDW périodique sur $N \cdot \mathbb{K}$, $E_{N\cdot\mathbb{K},N^3\lambda}(c)$, *admet (au moins)* N^3 *minimiseurs positifs distincts qui sont des translations les uns des autres par les vecteurs du réseau. Si l'on dénote par* w_c *l'un de ces minimiseurs, il existe alors a sous-suite* $c_n \to \infty$ *telle que*

$$\boxed{{c_n}^{-\frac{3}{2}} w_{c_n}\left(R + \frac{\cdot}{c_n}\right) \underset{n\to\infty}{\longrightarrow} Q,}$$

fortement dans $L^p_{loc}(\mathbb{R}^3)$ *pour* $2 \leqslant p < +\infty$, *où* R *est la position de l'une des* N^3 *charges dans* $N \cdot \mathbb{K}$. *Ici,* Q *est un minimiseur du problème effectif*

$$J_{\mathbb{R}^3}(N^3\lambda) = \inf_{\substack{u\in H^1(\mathbb{R}^3)\\ \|u\|^2_{L^2(\mathbb{R}^3)}=N^3\lambda}} \left\{ \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{R}^3} |u|^{\frac{10}{3}} - \frac{3}{4} \int_{\mathbb{R}^3} |u|^{\frac{8}{3}} \right\}, \qquad (0.9)$$

qui de plus minimise

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

où la minimisation est faite sur tous les minimiseurs de (0.9)*. Enfin, lorsque* $c \to \infty$*,* $E_{N\cdot\mathbb{K},N^3\lambda}(c)$ *a pour développement*

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

Ce second théorème est la principale nouveauté apportée par cette partie de la thèse. Le terme de Dirac $-\frac{3}{4}c\int_{\mathbb{K}}|w|^{\frac{8}{3}}$ dans (0.7) tend à regrouper les électrons et ce théorème dit que, dans la limite $c \to \infty$, la densité électronique se concentre en certains point de la cellule unité $\mathbb{K}$. Il précise également que si l'on fait un zoom d'échelle $1/c$ sur l'un des points où se concentre la densité électronique, nous obtenons un modèle effectif simple dans tout $\mathbb{R}^3$, modèle dans lequel les termes de Coulomb ont disparu. L'argument derrière ce résultat est qu'il est favorable de concentrer la masse électronique présente dans la cellule unité en un point du fait de fait de l'inégalité stricte *de liaison* :

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

De ce fait, les N^3 électrons de la cellule unité du problème N-périodique se concentreront en un point de masse N^3 lorsque c est très grand, plutôt que de se concentrer en N^3 points de masse 1.

Cette seconde partie de la thèse s'intéresse également en détails au problème effectif limite (0.9). Ce problème effectif de minimisation est un problème NLS avec deux non-linéarités à puissance sous-critique : $|v|^{\frac{10}{3}} - |v|^{\frac{8}{3}}$. L'unicité de ses minimiseurs est un problème ouvert. Si cette thèse ne répond pas à ce problème, elle démontre néanmoins que toute solution positive de l'équation non-linéaire d'Euler–Lagrange associée

$$-\Delta Q_\mu + c_{TF}|Q_\mu|^{\frac{4}{3}}Q_\mu - |Q_\mu|^{\frac{2}{3}}Q_\mu = -\mu Q_\mu \tag{0.10}$$

est unique et non-dégénérée (à translations spatiales près).

Théorème (Unicité et non-dégénérescence des solutions positives à l'équation d'E–L associée au problème effectif sur $\mathbb{R}^3$). *Soit* $c_{TF} > 0$*. Si* $\frac{64}{15}c_{TF}\mu \geqslant 1$*, alors l'équation d'Euler–Lagrange* (0.10) *n'a pas de solution non triviale dans* $H^1(\mathbb{R}^3)$*. Si* $0 < \frac{64}{15}c_{TF}\mu < 1$*, l'équation d'Euler–Lagrange* (0.10) *a, à translations près, une unique solution positive* $Q_\mu \not\equiv 0$ *dans* $H^1(\mathbb{R}^3)$*. Cette solution est radialement décroissante et non-dégénérée : l'opérateur linéarisé*

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

de domaine $H^2(\mathbb{R}^3)$ *et agissant sur* $L^2(\mathbb{R}^3)$ *a pour noyau*

$$\operatorname{Ker} L_\mu^+ = \operatorname{span}\{\partial_{x_1}Q_\mu, \partial_{x_2}Q_\mu, \partial_{x_3}Q_\mu\}.$$

Enfin, cette seconde partie de la thèse formule la conjecture que $\int {Q_\mu}^2$ est une fonction strictement croissante en la variable μ, ce qui est fortement corroboré par les simulations numériques que nous avons menées et qui sont également présentées dans cette thèse. En supposant cette conjecture vraie, nous prouvons que le problème N-périodique a exactement N^3 minimiseurs distincts pour c assez grand.

Les simulations numériques présentées dans cette thèse ont été menées avec le programme *PROFESS v.3.0* [**CXH+15**] et nous avons ajouté à son code notre fonctionnelle d'énergie. Nos simulations ont été effectuées sur un cristal cubique centré de Lithium de côté de longueur 4Å pour lequel un électron est traité tandis que les deux autres sont inclus dans un pseudo-potentiel, simulant ainsi un réseau de pseudo-atomes de pseudo-charges $Z = \lambda = 1$. Nos résultats numériques, présentés en Figure 2, montrent une brisure de symétrie vers $c \approx 3,30$. En effet,

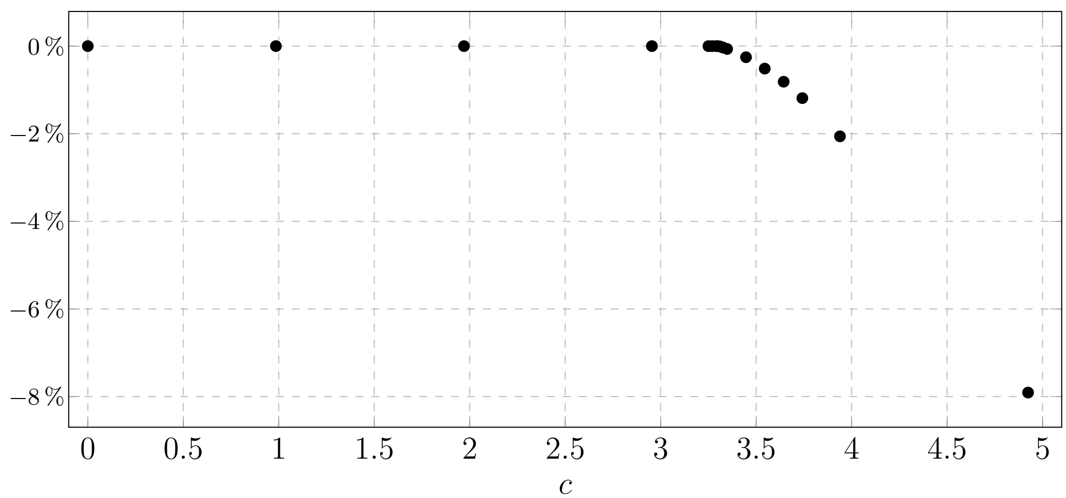
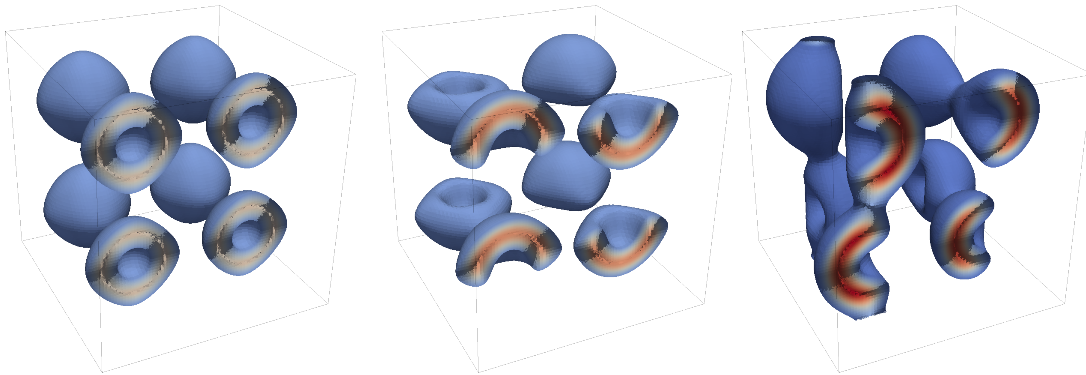


FIGURE 2. Estimation du gain relatif d'énergie $\frac{8E_{\mathbb{K},\lambda}(c)-E_{2\cdot\mathbb{K},8\lambda}(c)}{8E_{\mathbb{K},\lambda}(c)}$.

pour $c \lesssim 3,30$, les minimisations des problèmes sur $2\cdot\mathbb{K}$ (contenant 8 atomes) et sur $\mathbb{K}$ (contenant 1 atome) donnent la même énergie minimale à un facteur 8 près tandis que, pour $c \gtrsim 3,31$, nous trouvons une fonction 2-périodique pour laquelle l'énergie du problème sur $2\cdot\mathbb{K}$ est inférieure à (8 fois) l'énergie minimale pour le problème sur $\mathbb{K}$. De plus, la brisure de symétrie est confirmée visuellement par la représentation, pour trois valeurs de c, de la densité de probabilité du minimiseur 2-périodique simulé (Figure 3) : pour $c \approx 3,30$, le miniminiseur 2-périodique obtenu est en fait 1-périodique tandis que, pour $c \gtrsim 3,31$, le miniminiseur 2-périodique obtenu n'est plus 1-périodique.



(a) $c \approx 3,30$ (b) $c \approx 3,31$ (c) $c \approx 3,45$

FIGURE 3. Densité de probabilité, pour trois valeurs de c, du minimiseur 2-périodique simulé.

Questions ouvertes. Le premier problème concernant ce modèle laissé ouvert par cette thèse est évidemment la question de l'unicité des minimiseurs du problème limite que nous conjecturons. D'autre part, un travail intéressant serait d'étudier les questions développées dans cette thèse pour le modèle de Kohn–Sham qui est celui utilisé dans la pratique.

PARTIE 1

Study of the anisotropic polarons

Ce chapitre est une version plus détaillée de l'article publié

Julien Ricaud, *On uniqueness and non-degeneracy of anisotropic polarons*, Nonlinearity **29** (2016), no. 5, 1507–1536.

Abstract

We study the anisotropic Choquard–Pekar equation which describes a polaron in an anisotropic medium. We prove the uniqueness and non-degeneracy of minimizers in a weakly anisotropic medium. In addition, for a wide range of anisotropic media, we derive the symmetry properties of minimizers and prove that the kernel of the associated linearized operator is reduced, apart from three functions coming from the translation invariance, to the kernel on the subspace of functions that are even in each of the three principal directions of the medium.

Contents

1. Introduction

A *polaron* describes a quantum electron in a polar crystal. The atoms of the crystal are displaced due to the electrostatic force induced by the charge of the electron, and the resulting deformation is then felt by the electron itself. This coupled system (the electron and its polarization cloud) is a quasi-particle, called a polaron.

When the polaron extends over a domain much larger than the characteristic length of the underlying lattice, the crystal can be approximated by a continuous polarizable medium, leading to the so-called Pekar nonlinear model [**Pek54, Pek63**]. In this theory, the energy functional is

$$\mathscr{E}^V(\psi) = \frac{1}{2}\int_{\mathbb{R}^3} |\nabla\psi(x)|^2 \,\mathrm{d}x - \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} |\psi(y)|^2|\psi(x)|^2 V(x-y)\,\mathrm{d}y\,\mathrm{d}x, \tag{1.1}$$

where ψ is the wave function of the electron, in units such that the vacuum permittivity, the mass, and the charge of the electron are all normalized to one: $4\pi\varepsilon_0 = m_{e^-} = e = 1$. While, on the other hand,

$$-V \star |\psi|^2(x) = -\int_{\mathbb{R}^3} |\psi(y)|^2 V(x-y)\,\mathrm{d}y$$

is the mean-field self-trapping potential felt by the electron.

For an isotropic and homogeneous medium, characterized by its *relative permittivity* (or *relative dielectric constant*) $\varepsilon_M \geqslant 1$, the effective interaction potential is

$$V(x) = \frac{1-\varepsilon_M^{-1}}{|x|}. \tag{1.2}$$

For $\varepsilon_M > 1$ (equality corresponds to the medium being the vacuum), the so-called *Choquard–Pekar* or *Schrödinger–Newton* equation

$$\Big(-\frac{\Delta}{2} - V \star |\psi|^2\Big)\psi = -\mu\psi \tag{1.3}$$

is obtained by minimizing the energy $\mathscr{E}^V$ in (1.1) under the constraint $\int_{\mathbb{R}^3} |\psi|^2 = 1$, with associated Lagrange multiplier $\mu > 0$. Lieb proved in [**Lie77**] the uniqueness of minimizers, up to space translations and multiplication by a phase factor. This ground state Q is positive, smooth, radial decreasing, and has an exponential decay at infinity. That Q is also the unique positive solution to (1.3) was proved in [**MZ10**].

In [**Len09**], Lenzmann proved that Q is nondegenerate (this was also proved independently by Wei and Winter in [**WW09**]). Namely, the linearization

$$\mathfrak{L}_Q\xi = -\frac{1}{2}\Delta\xi + \mu\xi - \left(V \star |Q|^2\right)\xi - 2Q\left(V \star (Q\xi)\right) \tag{1.4}$$

of (1.3) has the trivial kernel

$$\ker_{|L^2(\mathbb{R}^3)} \mathfrak{L}_Q = \operatorname{span}\{\partial_{x_1}Q, \partial_{x_2}Q, \partial_{x_3}Q\} \tag{1.5}$$

which stems from the translation invariance. This nondegeneracy result is an important property which is useful in implicit function type arguments. Uniqueness and nondegeneracy were originally used in [**Len09**] to study a pseudo-relativistic model, and then in [**KMR09, Liu09, RN10, Stu10, FLS13, Sok14, Xia16**] for other models.

The purpose of this paper is to study the case of *anisotropic* media, for which the corresponding potential is

$$V(x) = \frac{1}{|x|} - \frac{1}{\sqrt{\det(M^{-1})}|M^{1/2}x|}, \qquad 0 < M \leqslant 1, \tag{1.6}$$

where $M^{-1} \geqslant 1$ is the (real and symmetric) static dielectric matrix of the medium. The mathematical expression is simpler in the Fourier domain:

$$\boxed{\widehat{V}(k) = 4\pi\left(\frac{1}{|k|^2} - \frac{1}{k^T M^{-1} k}\right).}$$

The form of the potential V in the anisotropic case is well-known in the physics literature and it has recently been derived by Lewin and Rougerie from a microscopic model of quantum crystals in [**LR13a**].

From a technical point of view, the fact that V in (1.6) is a difference of two Coulomb type potentials complicates the analysis. For this reason, we will also consider a simplified anisotropic model where V is replaced by

$$\boxed{V(x) = \frac{1}{|(1-S)^{-1}x|}, \qquad 0 \leqslant S < 1,} \tag{1.7}$$

and S is also a real and symmetric matrix. This simplified potential can be seen as an approximation of the potential (1.6) in the weakly anisotropic regime, that is, when M is close to an homothecy.

In this paper, we derive several properties of minimizers of $\mathscr{E}^V$ and of positive solutions to the nonlinear equation (1.3), when V is given by formulas (1.6) and (1.7). After some preparations in Section 2, we discuss the existence of minimizers and the compactness of minimizing sequences in Section 3. Then, based on the fundamental non degeneracy result [**Len09**], we prove in Section 4 the uniqueness and non-degeneracy of minimizers in a weakly anisotropic material. In Section 5, considering back general anisotropic materials, we investigate the symmetry properties of minimizers using rearrangement inequalities. Finally we discuss the linearized operator in Section 6. By using Perron–Frobenius type arguments, we are able to prove that for ψ a positive solution of the so-called *Choquard–Pekar* equation (1.3) sharing the symmetry properties of V, we have

$$\ker \mathfrak{L}_\psi = \operatorname{span}\{\partial_x\psi, \partial_y\psi, \partial_z\psi\} \bigoplus \ker(\mathfrak{L}_\psi)_{|L^2_{\rm sym}(\mathbb{R}^3)}\,. \tag{1.8}$$

Where $L^2_{\rm sym}(\mathbb{R}^3)$ is the subspace of function in $L^2(\mathbb{R}^3)$ sharing the symmetry properties of V. For instance, in the general case where the three eigenvalues of M (or S) are distinct from each other and V is decreasing in the corresponding directions, $L^2_{\rm sym}(\mathbb{R}^3)$ is the subspace of functions that are even in these directions. On the other hand, if exactly two eigenvalues are equal, it is the subspace of cylindrical functions that are also even in the directions of the principal axis.

The main difficulty in proving (1.8) is that the operator $\mathfrak{L}_\psi$ is non-local and therefore the ordering of its eigenvalues is not obvious. The next step would be to prove that $\ker \mathfrak{L}_{\psi|L^2_{\rm sym}(\mathbb{R}^3)} = \{0\}$ which we only know for now in the weakly anisotropic regime (Theorem 1.7 below) and in the radial case (see [**Len09**]). We hope to come back to this problem in the future.

Acknowledgments
The author is grateful to M. Lewin for helpful discussions and advices. The author acknowledges financial support from the European Research Council under the European Community's Seventh Framework Program (FP7/2007-2013 Grant Agreement MNIQS 258023), and from the French ministry of research (ANR-10-BLAN-0101).

2. Elementary properties

We define the energy $\mathscr{E}^V$ as in (1.1) and consider, for all $\lambda > 0$, the minimization problem

$$I^V(\lambda) := \min_{\substack{\psi\in H^1(\mathbb{R}^3)\\ \|\psi\|_2^2=\lambda}} \mathscr{E}^V(\psi). \tag{1.9}$$

Let (e_1, e_2, e_3) be the principal axis of the medium, that is, such that each $e_i \in \mathbb{R}^3$ is a normalized eigenvector associated with the eigenvalue m_i of the real symmetric matrix M, where $0 < m_1 \leqslant m_2 \leqslant m_3 \leqslant 1$ with $m_1 < 1$ (otherwise the medium would be the vacuum), or associated with the eigenvalue s_i of the real symmetric matrix S where $0 \leqslant s_3 \leqslant s_2 \leqslant s_1 < 1$ in the simplified model.

We define the map $M \mapsto V$ as

$$\begin{aligned}\{0 < M \leqslant 1 \mid M \text{ symmetric real}\} &\to L^2(\mathbb{R}^3) + L^4(\mathbb{R}^3)\\ M &\mapsto V(x) = \frac{1}{|x|} - \frac{1}{\sqrt{\det(M^{-1})}|M^{1/2}x|}\end{aligned} \tag{1.10}$$

with, in particular, $M \equiv \mathrm{Id} \mapsto V \equiv \bar{0}$ which corresponds to the vacuum. And, in the simplified model, $S \mapsto V$ is defined as

$$\begin{aligned} \{0 \leqslant S < 1 \mid S \text{ symmetric real}\} &\to L^2(\mathbb{R}^3) + L^4(\mathbb{R}^3) \\ S &\mapsto V(x) = |(1-S)^{-1}x|^{-1} \end{aligned} \tag{1.11}$$

with, in particular, $S \equiv 0 \mapsto V \equiv V_0$. We denote the isotropic potentials by $V_c(x) = (1-c)|x|^{-1}$, for $0 \leqslant c \leqslant 1$, and I_c^V the associated minimization problem.

Both maps are well-defined. Indeed, let V be as in (1.10) or (1.11) then one can easily show that there exist $a > b \geqslant 0$ such that

$$\forall x \in \mathbb{R}^3 \backslash \{0\}, \quad 0 \leqslant b|x|^{-1} \leqslant V(x) \leqslant a|x|^{-1} \leqslant |x|^{-1}. \tag{1.12}$$

Consequently, $V \in L^2(\mathbb{R}^3) + L^4(\mathbb{R}^3)$. Moreover, if we restrict ourselves to $0 < M < 1$ then there exist $a > b > 0$ such that

$$\forall x \in \mathbb{R}^3 \backslash \{0\}, \quad 0 < b|x|^{-1} \leqslant V(x) \leqslant a|x|^{-1} \leqslant |x|^{-1}. \tag{1.13}$$

Lemma 1.1. *Let $M \mapsto V$ be defined as in* (1.10)*, $S \mapsto V$ as in* (1.11) *and let f, g be two functions in $H^1(\mathbb{R}^3)$. Then $V \star (fg) \in W^{1,\infty}$ and, for any $0 < \alpha < 1$, we have*

(1) local Lipschitzity of

$$\begin{aligned} \{\alpha < M \leqslant 1 \mid M \textit{ symmetric real}\} \times H^1 \times H^1 &\to W^{1,\infty} \\ (M, f, g) &\mapsto V \star (fg), \end{aligned}$$

(2) uniform Lipschitzity of

$$\begin{aligned} \{0 \leqslant S < \alpha \mid S \textit{ symmetric real}\} \times H^1 \times H^1 &\to W^{1,\infty} \\ (S, f, g) &\mapsto V \star (fg). \end{aligned}$$

Proof of Lemma 1.1. First, for any $f \in L^2(\mathbb{R}^3)$ and $g \in H^1(\mathbb{R}^3)$, by (1.12) together with Hardy's inequality, $|V \star (fg)(x)| \leqslant (|\cdot|^{-1} \star |fg|)(x) \leqslant 2\|f\|_2 \|\nabla g\|_2$ holds. Consequently, for any $f, g \in H^1(\mathbb{R}^3)$, we have

$$\begin{aligned} \|V \star (fg)\|_{W^{1,\infty}} &\leqslant \|V \star (fg)\|_\infty + \|V \star (g\nabla f)\|_\infty + \|V \star (f\nabla g)\|_\infty \\ &\leqslant 2\|f\|_2 \|\nabla g\|_2 + 4\|\nabla f\|_2 \|\nabla g\|_2 \leqslant 6\|f\|_{H^1} \|g\|_{H^1}. \end{aligned}$$

Thus $V \star (fg)$ is in $W^{1,\infty}$. For the rest of the proof, we denote by $\|M\|$ the spectral norm of M and fix an α such that $0 < \alpha < 1$.

For $(S,T) \in \{0 \leqslant M < \alpha \mid M \text{ symmetric real}\}^2$, $f \in L^2(\mathbb{R}^3)$, $g \in H^1(\mathbb{R}^3)$ and $x \in \mathbb{R}^3$, we have

$$\begin{aligned}
|(V_S - V_T) \star (fg)(x)| &\leqslant \left| \frac{|(1-T)^{-1}\cdot| - |(1-S)^{-1}\cdot|}{|(1-S)^{-1}\cdot||(1-T)^{-1}\cdot|} \right| \star |fg|(x) \\
&\leqslant \frac{|[(1-T)^{-1} - (1-S)^{-1}]\cdot|}{|\cdot|^2} \star |fg|(x) \\
&\leqslant \frac{|(1-S)^{-1}(T-S)(1-T)^{-1}\cdot|}{|\cdot|^2} \star |fg|(x) \\
&\leqslant \left\|(1-S)^{-1}\right\| \|T-S\| \left\|(1-T)^{-1}\right\| \frac{1}{|\cdot|} \star |fg|(x) \\
&\leqslant 2(1-\alpha)^{-2} \|f\|_2 \|\nabla g\|_2 \|S-T\|.
\end{aligned}$$

Thus, for any $f, g \in H^1(\mathbb{R}^3)$, we have

$$\|(V_S - V_T) \star (fg)\|_{W^{1,\infty}} \leqslant 6(1-\alpha)^{-2} \|f\|_{H^1} \|g\|_{H^1} \|S-T\|,$$

which concludes the proof of *(2)*.

For $(M,N) \in \{\alpha < M \leqslant 1 \mid M \text{ symmetric real}\}^2$, we have

$$\begin{aligned}
M^{1/2} - N^{1/2} &= \pi^{-1} \int_0^\infty \left(\frac{M}{s+M} - \frac{N}{s+N} \right) \frac{\mathrm{d}s}{\sqrt{s}} \\
&= \pi^{-1} \int_0^\infty \frac{1}{s+M} (M-N) \frac{1}{s+N} \sqrt{s}\, \mathrm{d}s,
\end{aligned}$$

which leads to

$$\begin{aligned}
\left\| M^{\frac{1}{2}} - N^{\frac{1}{2}} \right\| \leqslant \frac{\|M-N\|}{\pi} \int_0^\infty \frac{\sqrt{s}}{(s+\alpha)^2}\, \mathrm{d}s &= \frac{\|M-N\|}{\pi\sqrt{\alpha}} \int_0^\infty \frac{\sqrt{s}}{(s+1)^2}\, \mathrm{d}s \\
&= \frac{\|M-N\|}{2\sqrt{\alpha}}.
\end{aligned}$$

Moreover, with a similar computation and since $\det M, \det N > \alpha^3$, we obtain

$$\left| \sqrt{\det M} - \sqrt{\det N} \right| \leqslant \frac{|\det M - \det N|}{2\alpha^{3/2}}.$$

Thus, for $f \in L^2(\mathbb{R}^3)$, $g \in H^1(\mathbb{R}^3)$ and $x \in \mathbb{R}^3$, we have

$$\begin{aligned}
|(V_M - V_N) \star (fg)(x)| &\leqslant \frac{1}{\sqrt{\det N^{-1}}} |fg| \star \frac{\left||M^{1/2}\cdot| - |N^{1/2}\cdot|\right|}{|M^{1/2}\cdot|\,|N^{1/2}\cdot|}(x) \\
&\quad + \left| \frac{1}{\sqrt{\det N^{-1}}} - \frac{1}{\sqrt{\det M^{-1}}} \right| |fg| \star \left|M^{1/2}\cdot\right|^{-1}(x) \\
&\leqslant 2\sqrt{\det N} \left\|M^{-1}\right\|^{1/2} \left\|N^{-1}\right\|^{1/2} \|f\|_2 \|\nabla g\|_2 \left\|M^{1/2} - N^{1/2}\right\| \\
&\quad + 2\left\|M^{-1}\right\|^{1/2} \|f\|_2 \|\nabla g\|_2 \left|\sqrt{\det N} - \sqrt{\det M}\right| \\
&\leqslant \left(\|M - N\| + \alpha^{-1/2} |\det N - \det M|\right) \alpha^{-3/2} \|f\|_2 \|\nabla g\|_2 .
\end{aligned}$$

Finally, the determinant being locally Lipschitz, we obtain that $M \mapsto V \star (fg)$ is locally Lipschitz. $\square$

Since M^{-1} is real and symmetric, there exists $R \in O(3)$ such that

$$R^T M R = \operatorname{diag}(m_3, m_2, m_1)$$

and so, for any $x \in \mathbb{R}^3$, after a simple computation, we have

$$V(Rx) = |x|^{-1} - \left|\operatorname{diag}\left((m_1 m_2)^{-1/2}, (m_1 m_3)^{-1/2}, (m_2 m_3)^{-1/2}\right) x\right|^{-1},$$

where $0 < \sqrt{m_1 m_2} \leqslant \sqrt{m_1 m_3} \leqslant \sqrt{m_2 m_3} \leqslant 1$ and $\sqrt{m_1 m_3} < 1$ since $m_1 < 1$. Thus, we can consider, without any loss of generality, that

$$\begin{cases} M = \operatorname{diag}(m_1, m_2, m_3),\ 0 < m_3 \leqslant m_2 \leqslant m_1 \leqslant 1 \text{ and } m_2 < 1, \\ M \mapsto V(x) = \dfrac{1}{|x|} - \dfrac{1}{|M^{-1}x|} \end{cases} \tag{1.14}$$

Similarly, for the simplified model, we can also assume that

$$V(x) = |\operatorname{diag}(1 - s_1, 1 - s_2, 1 - s_3)^{-1} x|^{-1}, \qquad 0 \leqslant s_3 \leqslant s_2 \leqslant s_1 < 1. \tag{1.15}$$

For clarity, from now on we denote by $\mathscr{E}_M$ (resp. $\mathscr{E}_S$) the energy and by $I_M(\lambda)$ (resp. $I_S(\lambda)$) the minimization problem since V depends only on the matrix M (resp. on the matrix S). However, for shortness, we will omit the subscripts when no confusion is possible.

LEMMA 1.2. *Let $\psi \in H^1(\mathbb{R}^3)$ be a solution of the equation* (1.3)*, for V defined as in* (1.14) *or in* (1.15)*, then $(x, y, z) \mapsto \psi(\pm x, \pm y, \pm z)$ are $H^1(\mathbb{R}^3)$-solutions to* (1.3).

PROOF OF LEMMA 1.2. This follows from the symmetry properties of V. $\square$

3. Existence of minimizers

We prove in this section the existence of minimizers for the minimization problems. As preparation, we first give some properties of these variational problems.

LEMMA 1.3. *Let V be defined as in* (1.14) *or* (1.15) *and I be defined as in* (1.9). *Then*

$$I(\lambda) = \lambda^3 I(1) < 0, \text{ if } \lambda > 0. \tag{1.16}$$

Consequently,

(1) $\lambda \mapsto I(\lambda)$ is C^∞ on $\mathbb{R}^+$,

(2) $I(\lambda) < I(\lambda - \lambda') + I(\lambda')$, for any λ et λ' such that $0 < \lambda' < \lambda$,

and, in particular,

(3) $I(\lambda) < I(\lambda')$, for any $0 \leqslant \lambda' < \lambda$.

PROOF OF LEMMA 1.3. Let $\psi \in H^1(\mathbb{R}^3)$ with $\|\psi\|^2_{L^2(\mathbb{R}^3)} = 1$, then we have $\psi_\lambda := \lambda^2 \psi(\lambda \cdot) \in H^1(\mathbb{R}^3)$ and $\|\psi_\lambda\|^2_{L^2(\mathbb{R}^3)} = \lambda$ and, by a direct computation, $\mathscr{E}(\psi_\lambda) = \lambda^3 \mathscr{E}(\psi)$ which leads to $I(\lambda) = \lambda^3 I(1)$. If we now define $\psi_t = t^{3/2}\psi(t\cdot)$ and use (1.13), we find that

$$\begin{aligned}
\mathscr{E}(\psi_t) &\leqslant \frac{1}{2}\|\nabla \psi_t\|^2_{L^2} - \frac{b}{2}\left\||\psi_t|^2\left(|\psi_t|^2 \star |\cdot|^{-1}\right)\right\|^2_{L^2} \\
&\leqslant \frac{t^2}{2}\|\nabla \psi\|^2_{L^2} - \frac{bt}{2}\left\||\psi|^2\left(|\psi|^2 \star |\cdot|^{-1}\right)\right\|^2_{L^2},
\end{aligned}$$

and taking t small enough leads to the claimed strict negativity. The rest follows immediately. □

LEMMA 1.4. *Let V be defined as in* (1.14) *or* (1.15). *Let I be as in* (1.9) *and let $\lambda > 0$. Then $I(t\lambda) > tI(\lambda)$, for all $t \in (0,1)$.*

PROOF OF LEMMA 1.4. Let $t \in (0,1)$. By Lemma 1.3, $0 > I(t\lambda) = t^3 I(\lambda) > tI(\lambda)$. □

These two lemmas imply the existence of minimizers and the compactness of minimizing sequences, as stated in the following theorem which gives also some properties of these minimizers.

THEOREM 1.5 (Existence of a minimizer). *Let V be as in* (1.14) *or* (1.15) *and $\lambda > 0$. Then $I(\lambda)$ has a minimizer and any minimizing sequence strongly converges in $H^1(\mathbb{R}^3)$ to a minimizer, up to extraction of a subsequence and after an appropriate space translation.*

Moreover for any minimizer ψ, we have

(1) ψ *is a* $H^2(\mathbb{R}^3)$*-solution of the Choquard–Pekar equation* (1.3) *with* $-\mu = \frac{d}{d\lambda}I(\lambda) < 0$ *being the smallest eigenvalue of the self-adjoint operator* $H_\psi := -\Delta/2 - |\psi|^2 \star V$*, which is simple;*

(2) $$\mu\lambda = -\lambda\frac{d}{d\lambda}I(\lambda) = -3\lambda^3 I(1) = \frac{3}{2}\|\nabla\psi\|_2^2 = \frac{3}{4}\left\langle V \star |\psi|^2, |\psi|^2\right\rangle; \qquad (1.17)$$

(3) $|\psi|$ *is a minimizer and* $|\psi| > 0$*;*

(4) $\psi = z|\psi|$ *for a given* $|z| = 1$*.*

For the isotropic potentials V_c, Lieb proved several of these statements in [**Lie77**] using only the fact that $|x|^{-1}$ is radially decreasing. In the general case, the proof is now standard and follows from Lions' concentration-compactness method [**Lio84a, Lio84b**]. A sketch is given in Section 7.1 of the Appendix. For a related result dealing with the case where $|\psi|^2$ is replaced by $|\psi|^p$ in the energy (1.1) see [**MS13**].

4. Uniqueness in a weakly anisotropic material

We recall that the uniqueness of the minimizer, up to phases and space translations, in the isotropic case, was proven by Lieb in [**Lie77**]. In this section, we extend this result to the case of *weakly anisotropic materials*, meaning that we consider static dielectric matrices close to an homothecy.

We first prove the continuity of $I_M(\lambda)$, with respect to (M, λ), which we will need in the proof of uniqueness.

Lemma 1.6 (Minimums' convergence). *Let* V *be defined as in* (1.14) *or* (1.15), I *be defined as in* (1.9) *and* $(\lambda, \lambda') \in \left(\mathbb{R}_+^*\right)^2$*. Then*

$$I_{M'}(\lambda') \xrightarrow[\substack{\|M'-M\|\to 0 \\ |\lambda'-\lambda|\to 0}]{} I_M(\lambda).$$

Thus, the continuity of the corresponding Euler-Lagrange multiplier, $-\mu_{M',\lambda'}$*, holds as well:*

$$\mu_{M',\lambda'} \xrightarrow[\substack{\|M'-M\|\to 0 \\ |\lambda'-\lambda|\to 0}]{} \mu_{M,\lambda}.$$

Proof of Lemma 1.6. Let ψ (resp. ψ') be a minimizer of $I_M(\lambda)$ (resp. $I_{M'}(\lambda)$) for a given $\lambda > 0$.

First, for any $\varphi \in H^1(\mathbb{R}^3)$, we have

$$|\mathcal{E}_M(\varphi) - \mathcal{E}_{M'}(\varphi)| = \frac{1}{2}\left|\left\langle|\varphi|^2, |\varphi|^2 \star (V - V')\right\rangle\right| \leqslant \frac{1}{2}\left\||\varphi|^2 \star (V - V')\right\|_\infty \|\varphi\|_2^2 .$$

Thus, by Lemma 1.1, $M \mapsto \mathcal{E}_M(\varphi)$ is Lipschitz for any $\varphi \in H^1(\mathbb{R}^3)$. Moreover

$$\mathcal{E}_M(\psi) - \mathcal{E}_{M'}(\psi) \leqslant I_M(\lambda) - I_{M'}(\lambda) \leqslant \mathcal{E}_M(\psi') - \mathcal{E}_{M'}(\psi'),$$

which implies that $M \mapsto I_M(\lambda)$ is Lipschitz for any $\lambda > 0$.

Thanks to Lemma 1.3, we conclude the proof of the convergence of I since

$$|I_M(\lambda) - I_{M'}(\lambda')| \lesssim |I_M(1)| \left|\lambda^3 - (\lambda')^3\right| + \|M - M'\|.$$

Then, the equality $-\mu_{M,\lambda} = 3\lambda^2 I_M(1)$ gives the convergence of the $\mu_{M',\lambda'}$'s. □

We now give our theorem of uniqueness in the weakly anisotropic case.

Theorem 1.7 (Uniqueness and non-degeneracy in the weakly anisotropic case).
Let $\lambda > 0$.

i. Let $0 < s < 1$. There exists $\varepsilon > 0$ such that, for every real symmetric 3×3 matrix $0 < M < 1$ with $\|M - s \cdot \mathrm{Id}\| < \varepsilon$, the minimizer ψ of the minimization problem $I_M(\lambda)$, for $V(x) = |x|^{-1} - |M^{-1}x|^{-1}$ as in (1.14), is unique up to phase and space translations.

ii. Let $0 \leqslant s < 1$. There exists $\varepsilon > 0$ such that, for every real symmetric 3×3 matrix $0 \leqslant S < 1$ with $\|S - s \cdot \mathrm{Id}\| < \varepsilon$, the minimizer ψ of the minimization problem $I_S(\lambda)$, for $V(x) = |(1 - S)^{-1}x|^{-1}$ as in (1.15), is unique up to phase and space translations.

Moreover, in both cases, the minimizer is even along each eigenvectors of M and $\ker \mathfrak{L}_\psi = \operatorname{span}\{\partial_x\psi, \partial_y\psi, \partial_z\psi\}$, where $\mathfrak{L}_\psi$ is the linearized operator defined in (1.4).

The proof of this theorem is based on a perturbative argument around the isotropic case, using the implicit functions theorem. The fundamental nondegeneracy result in the isotropic case, proved by Lenzmann in [**Len09**], is a key ingredient of our proof.

Proof of Theorem 1.7. The proof of ii being similar to the one of i, we will only give the latter. Let us fix $0 < s < 1$, define

$$\mathscr{D} := \{0 < M < 1 \mid M \text{ symmetric real}\}$$

and denote by Q the unique positive minimizer of the isotropic minimization problem $I(\lambda) := I_{s\cdot\mathrm{Id}}(\lambda)$ for $V(x) = V_{s\cdot\mathrm{Id}}(x) = (1-s)|x|^{-1}$, which is radial and solves (1.3):

$$-\frac{1}{2}\Delta Q + \mu Q - (|Q|^2 \star V)Q = 0,$$

with $\|Q\|_2^2 = \lambda$. There λ is fixed hence is $\mu := \mu_{s\cdot\mathrm{Id},\lambda} > 0$ by Lemma 1.3.

Step 1: Implicit function theorem and local uniqueness. By Proposition 5 in [**Len09**], we know that the linearized operator $\mathfrak{L}_Q$ given by

$$\mathfrak{L}_Q\xi = -\frac{1}{2}\Delta\xi + \mu\xi - \left(V \star |Q|^2\right)\xi - 2Q\left(V \star (Q\xi)\right), \tag{1.18}$$

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

$$\ker \mathfrak{L}_Q = \operatorname{span}\left\{\partial_{x_1}Q, \partial_{x_2}Q, \partial_{x_3}Q\right\}. \tag{1.19}$$

Let us define u as

$$\begin{aligned} H^1(\mathbb{R}^3,\mathbb{R}) \times \mathscr{D} &\xrightarrow{u} L^2(\mathbb{R}^3,\mathbb{R}) \\ (\psi, M) &\mapsto -\left(|\psi|^2 \star V\right)\psi \end{aligned}$$

and G as

$$\begin{aligned} (\ker \mathfrak{L}_Q)^\perp \times \mathscr{D} &\xrightarrow{G} H^1(\mathbb{R}^3,\mathbb{R}) \\ (\psi, M) &\mapsto \psi + (-\Delta/2 + \mu_M)^{-1}\, u(\psi, M), \end{aligned}$$

where $(\ker \mathfrak{L}_Q)^\perp$ is the orthogonal of $\ker \mathfrak{L}_Q$ for the scalar product of $L^2(\mathbb{R}^3)$, which we endow with the norm of $H^1(\mathbb{R}^3)$, and $\mu_M := \mu_{M,\lambda} = 3\lambda^2 I_M(1)$. We emphasize here that we consider real valued functions, meaning that we are constructing a branch of real valued solutions. Moreover, $G(\psi, M) = 0$ is equivalent to $-\frac{1}{2}\Delta\psi + \mu\psi - (|\psi|^2 \star V)\psi = 0$. Differentiating with respect to x_i, for $i = 1, 2, 3$, we get $\mathfrak{L}_\psi \partial_{x_i}\psi = 0$, for $i = 1, 2, 3$, and thus $\operatorname{span}\{\partial_x\psi, \partial_y\psi, \partial_z\psi\} \subset \ker \mathfrak{L}_\psi$.

By the Hardy-Littlewood-Sobolev and Sobolev inequalities, u is well defined. Moreover, splitting $u(\psi, M) - u(\psi', M')$ into three pieces and using (1.13) together with the Hardy inequality, one obtains

$$\begin{aligned} \|u(\psi, M) - u(\psi', M')\|_{L^2} &\leqslant \left\|V \star |\psi|^2\right\|_{L^\infty} \|\psi - \psi'\|_{L^2} + \left\|(V - V') \star |\psi|^2\right\|_{L^\infty} \|\psi'\|_{L^2} \\ &\quad + \left\|V' \star \left((|\psi| - |\psi'|)(|\psi| + |\psi'|)\right)\right\|_{L^\infty} \|\psi'\|_{L^2}. \end{aligned}$$

Therefore, using Lemma 1.1, u is locally Lipschitz on $H^1(\mathbb{R}^3,\mathbb{R}) \times \mathscr{D}$. Then, since $(-\Delta/2 + \mu_M)^{-1}$ maps $L^2(\mathbb{R}^3)$ onto $H^2(\mathbb{R}^3) \subset H^1(\mathbb{R}^3)$, G is also well defined. Moreover, since $|||(-\Delta + \nu)^{-1}|||_{L^2 \to H^2} \leqslant \max\{1, \nu^{-1}\}$ (for $\nu > 0$) and

$$(-\Delta/2 + a)^{-1} - (-\Delta/2 + b)^{-1} = (b - a)\,(-\Delta/2 + a)^{-1}\,(-\Delta/2 + b)^{-1},$$

for all $a, b > 0$, we have

$$\begin{aligned} &\|G(\psi, M) - G(\psi', M')\|_{H^1} \\ &\qquad \leqslant \|\psi - \psi'\|_{H^1} + \left\|(-\Delta/2 + \mu_M)^{-1}\left(u(\psi, M) - u(\psi', M')\right)\right\|_{H^1} \\ &\qquad\quad + |\mu_{M'} - \mu_M| \left\|(-\Delta/2 + \mu_M)^{-1}\left(-\Delta/2 + \mu_{M'}\right)^{-1} u(\psi', M')\right\|_{H^1} \\ &\qquad \lesssim \|\psi - \psi'\|_{H^1} + \max\{2, (\mu_M)^{-1}\}\, \|u(\psi, M) - u(\psi', M')\|_{L^2} \\ &\qquad\quad + \max\{2, (\mu_M)^{-1}\} \max\{2, (\mu_{M'})^{-1}\}\, \|u(\psi', M')\|_{L^2}\, \|M' - M\|, \end{aligned}$$

which proves that G is also locally Lipschitz.

A simple computation shows that

$$\partial_\psi u(\psi, M)\xi = -\left(|\psi|^2 \star V\right)\xi - 2\psi\left((\psi\xi) \star V\right), \tag{1.20}$$

acting on $\xi \in (\ker \mathfrak{L}_Q)^\perp$, and that

$$\partial_\psi G(\psi, M) = 1 + (-\Delta/2 + \mu_M)^{-1}\,\partial_\psi u(\psi, M). \tag{1.21}$$

We claim $\partial_\psi G(\varphi, M)$, defined from $(\ker \mathfrak{L}_Q)^\perp \times \mathscr{D}$ into $\mathcal{L}\left((\ker \mathfrak{L}_Q)^\perp, L^2(\mathbb{R}^3, \mathbb{R})\right)$, to be continuous. Indeed,

$$\begin{aligned}\|\partial_\psi u(\psi, M)\xi\|_{L^2} &\leqslant \|\xi\|_{L^2}\left\|V \star |\psi|^2\right\|_{L_\infty} + 2\|\psi\|_{L^2}\|(\psi\xi) \star V\|_{L^\infty}\\ &\leqslant 3\|\psi\|_{H^1}\|\psi\|_{L^2}\|\xi\|_{L^2},\end{aligned}$$

thus $\partial_\psi u(\psi, M)\xi \in L^2(\mathbb{R}^3, \mathbb{R})$ for any $(\psi, M, \xi) \in (\ker \mathfrak{L}_Q)^\perp \times \mathscr{D} \times (\ker \mathfrak{L}_Q)^\perp$.

Splitting again the term into pieces and using (1.13), for $\xi \in L^2(\mathbb{R}^3, \mathbb{R})$, one obtains

$$\begin{aligned}&\|\partial_\psi u(\psi, M)\xi - \partial_1 u(\psi', M')\xi\|_{L^2}\\ &\qquad\leqslant \left\|V \star \left(|\psi|^2 - |\psi'|^2\right)\right\|_{L^\infty}\|\xi\|_{L^2} + \left\|(V - V') \star |\psi'|^2\right\|_{L^\infty}\|\xi\|_{L^2}\\ &\qquad\quad + 2\|V \star (\psi\xi)\|_{L^\infty}\|\psi - \psi'\|_{L^2} + 2\|V \star ((\psi - \psi')\xi)\|_{L^\infty}\|\psi'\|_{L^2}\\ &\qquad\quad + 2\|(V - V') \star (\psi'\xi)\|_{L^\infty}\|\psi'\|_{L^2}\\ &\qquad = O\left(\|(\psi, M) - (\psi', M')\|_{H^1 \times \mathscr{D}}\right)\|\xi\|_{L^2}.\end{aligned}$$

Then, since

$$\begin{aligned}&\|\partial_\psi G(\psi, M)\xi - \partial_\psi G(\psi', M')\xi\|_{H^1}\\ &\qquad\lesssim \max\{2, (\mu_M)^{-1}\}\|\partial_\psi u(\psi, M) - \partial_\psi u(\psi', M')\|_{L^2}\\ &\qquad\quad + \max\{2, (\mu_M)^{-1}\}\max\{2, (\mu_{M'})^{-1}\}\|\partial_\psi u(\psi', M')\|_{L^2}\|M' - M\|,\end{aligned}$$

we have

$$|\!|\!|\partial_\psi G(\psi, M) - \partial_\psi G(\psi', M')|\!|\!| \to 0, \text{ if } \|(\psi, M) - (\psi', M')\|_{H^1 \times \mathscr{D}} \to 0.$$

This concludes the proof of the continuity of $\partial_\psi G(\varphi, M)$ from $(\ker \mathfrak{L}_Q)^\perp \times \mathscr{D}$ into $\mathcal{L}\left((\ker \mathfrak{L}_Q)^\perp, H^1(\mathbb{R}^3, \mathbb{R})\right)$.

We now apply the implicit function theorem to G. Indeed, by the definition of $(\ker \mathfrak{L}_Q)^\perp$, the restriction of $\mathfrak{L}_Q$ to $(\ker \mathfrak{L}_Q)^\perp$ has a trivial kernel. On the other hand, the operator $(-\Delta/2 + \mu_M)^{-1}\,\partial_\psi u(Q, s \cdot \mathrm{Id})$ is compact on $L^2(\mathbb{R}^3)$ (see section 7.2 in Appendix), therefore -1 does not belong to its spectrum. We deduce from this the existence of the inverse operator

$$\left(\partial_\psi G(Q, s \cdot \mathrm{Id})\right)^{-1} : \mathrm{Ran}(G) \subset H^1(\mathbb{R}^3, \mathbb{R}) \to (\ker \mathfrak{L}_Q)^\perp. \tag{1.22}$$

Then, by the continuity of G and $\partial_\psi G$, the existence of $(\partial_\psi G(Q_s, s\cdot \mathrm{Id}))^{-1}$ and since $G(Q, s\cdot\mathrm{Id}) = 0$, the inverse function theorem 1.2.1 of **[Cha05]** implies that there exist $\delta, \varepsilon > 0$ such that there exists a unique $\psi(M) \in (\ker \mathfrak{L}_Q)^\perp$ satisfying:

$$G(\psi(M), M) = 0 \quad \text{for } \|M - s\cdot\mathrm{Id}\| \leqslant \varepsilon \text{ and } \|\psi(M) - Q\|_{H^1} \leqslant \delta. \tag{1.23}$$

Moreover, the map $M \mapsto \psi(M)$ is continuous.

Additionally, $\ker \partial_\psi G(\psi(M), M) = \{0\}$, i.e. $\ker_{|(\ker \mathfrak{L}_Q)^\perp} \mathfrak{L}_\psi = \{0\}$ which leads to $\dim\ker(\mathfrak{L}_\psi) \leqslant 3$ since $\dim\ker(\mathfrak{L}_Q) = 3$ by (1.19).

We now claim that $\psi(M)$ is symmetric with respect to the three eigenvectors of M, $\{e_i\}_{i=1,2,3}$, and consequently that, for $i = 1, 2, 3$, $\partial_{x_i}\psi(M)$ is odd along e_i and even along e_j for $j \neq i$. Indeed V being symmetric, the eight functions $(x, y, z) \mapsto \psi(M)(\pm x, \pm y, \pm z)$, which are in $(\ker \mathfrak{L}_Q)^\perp$, are zeros of $G(\cdot, M)$. If $\psi(M)$ were not symmetric with respect to each e_i, then at least two of the functions $(x, y, z) \mapsto \psi(M)(\pm x, \pm y, \pm z)$ would be distinct functions but both verifying (1.23), since Q is symmetric with respect to each e_i, which is impossible by local uniqueness.

Thus the $\partial_{x_i}\psi(M)$'s are orthogonal and we have $\dim \mathrm{span}\{\partial_x\psi, \partial_y\psi, \partial_z\psi\} = 3$. Since $\mathrm{span}\{\partial_x\psi, \partial_y\psi, \partial_z\psi\} \subset \ker\mathfrak{L}_\psi$, this leads to $\dim\ker(\mathfrak{L}_\psi) \geqslant 3$. Which proves that $\ker \mathfrak{L}_\psi = \mathrm{span}\{\partial_x\psi, \partial_y\psi, \partial_z\psi\}$.

Let us emphasize that, at this point, we do not know the masses $\|\psi(M)\|_2^2$ of those $\psi(M)$. Note also that we could prove here that $|\psi| > 0$, since $-\mu_M$ stays the first eigenvalue by continuity and with a Perron–Frobenius type argument, but we do not give the details here since this fact will be a consequence of Step 2.

Step 2: Global uniqueness. Let $(M_n)_n$ be a sequence of matrices in $\mathscr{D}$ such that $M_n \underset{n\to\infty}{\longrightarrow} s\cdot\mathrm{Id}$ and let $(\psi_{M_n})_n$ be a sequence of minimizers of $(I_{M_n}(\lambda))_n$ which we can suppose, up to phase, strictly positive by Theorem 1.5 and, up to a space translation (for each M_n), in $(\ker\mathfrak{L}_Q)^\perp$. Indeed, for any $\psi \in H^1(\mathbb{R}^3)$, let us define the continuous function

$$f(\tau) := \int \nabla Q(\cdot)\psi(\cdot - \tau)$$

which is bounded, by the Cauchy-Schwarz inequality. Then

$$\int f(\tau)\,\mathrm{d}\tau = \int \psi(x) \int \nabla Q(x - \tau)\,\mathrm{d}\tau\,\mathrm{d}x = 0$$

since $\int \nabla Q = 0$. Thus, f being continuous, there exists τ such that

$$f(\tau) = \int \psi(x - \tau)\nabla Q(x)\,\mathrm{d}x = 0,$$

i.e. $\psi(\cdot - \tau) \in (\ker\mathfrak{L}_Q)^\perp$ since $\ker\mathfrak{L}_Q = \mathrm{span}\{\partial_{x_1}Q, \partial_{x_2}Q, \partial_{x_3}Q\}$.

By continuity of $(I_{M_n}(\lambda))_n$, given by Lemma 1.6, $(\psi_{M_n})_n$ is a minimizing sequence of $I_{s\cdot\mathrm{Id}}(\lambda)$. So, by Theorem 1.5, $(\psi_{M_n})_n$ strongly converges in $H^1(\mathbb{R}^3)$ to a minimizer of $I_{s\cdot\mathrm{Id}}(\lambda)$, up to extraction of a subsequence. But, since the ψ_{M_n} are positive and in $(\ker \mathfrak{L}_Q)^\perp$, they converge to a positive minimizer of $I_{s\cdot\mathrm{Id}}(\lambda)$ in $(\ker \mathfrak{L}_Q)^\perp$ which is Q.

So, there exists $\varepsilon' \leqslant \varepsilon$ such that if $\|M - s\cdot\mathrm{Id}\|_\infty \leqslant \varepsilon'$, then each ψ_{M_n} verifies $G(\psi_{M_n}, M_n) = 0$, by definition of $(\psi_{M_n})_n$, and $\|\psi_{M_n} - Q\|_{H^1} \leqslant \delta$ i.e. verifies (1.23). So the ψ_{M_n} are unique (up to phases and spaces translation). Which concludes the proof of Theorem 1.7.

Moreover, we now know that, in fact, the masses $\|\psi(M_n)\|_2^2$ of the unique $\psi(M_n)$ found in the local result were in fact all equal to λ. We also proved incidentally that our choice of translation to obtain $(\psi_{M_n})_n \subset (\ker \mathfrak{L}_Q)^\perp$ was, in fact, unique. □

5. Rearrangements and symmetries

The goal of this section is to prove that minimizers are symmetric and strictly decreasing in the directions along which V is decreasing, without assuming that V is close to the isotropic case as we did in the previous section. More precisely, we will consider here the general anisotropic case $m_3 \leqslant m_2 \leqslant m_1$ (resp. $s_3 \leqslant s_2 \leqslant s_1$) and, in particular, the two cylindrical cases $m_3 = m_2 < m_1$ (resp. $s_3 = s_2 < s_1$) and $m_3 < m_2 = m_1$ (resp. $s_3 < s_2 = s_1$). Our main result in this section is Theorem 1.9 below. As a preparation, we first give conditions for V to be its own Steiner symmetrization.

As in [**Cap14**], for f defined on $\mathbb{R}^n = \mathrm{span}\{e_1, \dots, e_n\}$, we denote:

— by f^* its *Schwarz symmetrization*, for $n \geqslant 1$;

— by $\mathrm{St}_{i_1,\dots,i_k}(f)$ its *Steiner symmetrization (in codimension k) with respect to the subspace spanned by* $e_{i_1}, \dots, e_{i_k}$, for $n \geqslant 2$ and $1 \leqslant k < n$.

Let us remark that the Steiner symmetrization $\mathrm{St}_{i_1,\dots,i_k}(f)$ of f is the Schwarz symmetrization of the function $(x_{i_1}, \cdots, x_{i_k}) \mapsto f(x_1, \cdots, x_n)$.

Proposition 1.8 (Criterion for V to be its own Steiner symmetrization).

(1) Let V be given by (1.14)*, with* $0 < m_3 \leqslant m_2 \leqslant m_1 < 1$*. Then* $V = \mathrm{St}_1(V)$ *(thus V is e_1-symmetric strictly decreasing). Moreover, for $k \in \{2,3\}$, $V = \mathrm{St}_k(V)$ (thus V is e_k-symmetric strictly decreasing) if and only if*

$$m_1^3 \leqslant m_k^2. \tag{1.24$_k$}$$

Moreover,

i. *if* $m_3 < m_2 = m_1$*, then* $V = \mathrm{St}_{1,2}(V)$*. Thus* V *is* (e_1, e_2)*-radial strictly decreasing.*

ii. *if* $m_3 = m_2 < m_1$*, then* $V = \mathrm{St}_{2,3}(V)$ *— thus* V *is* (e_2, e_3)*-radial strictly decreasing — if and only if*

$$m_1^3 \leqslant m_2^2 = m_3^2; \tag{1.25}$$

(2) Let V *be given by* (1.15)*, with* $0 \leqslant s_3 \leqslant s_2 \leqslant s_1 < 1$*. Then* $V = \mathrm{St}_k(V)$ *(thus* V *is* e_k*-symmetric strictly decreasing) for* $k = 1, 2, 3$*. Moreover,*

i. *if* $s_3 < s_2 = s_1$*, then* $V = \mathrm{St}_{1,2}(V)$*. Thus* V *is* (e_1, e_2)*-radial strictly decreasing;*

ii. *if* $s_3 = s_2 < s_1$*, then* $V = \mathrm{St}_{2,3}(V)$*. Thus* V *is* (e_2, e_3)*-radial strictly decreasing.*

Proof of Proposition 1.8. Suppose V is given by (1.14), then it obviously has the claimed properties of symmetry and, moreover, the cylindrical ones in cases *i.* and *ii.*. So the proof that V is equal to its symmetrization is reduced to the proof of decreasing properties.

For any $x \neq 0$ and $k = 1, 2, 3$, we have

$$\partial_{|x_k|} V(x_1, x_2, x_3) = \frac{m_k^{-2}|x_k|}{(m_1^{-2}x_1^2 + m_2^{-2}x_2^2 + m_3^{-2}x_3^2)^{3/2}} - \frac{|x_k|}{(x_1^2 + x_2^2 + x_3^2)^{3/2}}. \tag{1.26}$$

Thus, $V = \mathrm{St}_k(V)$ and V is radially decreasing with respect to x_k if and only if

$$0 \leqslant (m_1^{-2} - m_k^{-4/3})x_1^2 + (m_2^{-2} - m_k^{-4/3})x_2^2 + (m_3^{-2} - m_k^{-4/3})x_3^2 \quad \text{a.e. on } \mathbb{R}^3$$

which is equivalent to $m_1 \leqslant m_k^{2/3}$. Consequently, $V = \mathrm{St}_1(V)$ always holds.

If $m_3 = m_2 < m_1$, denoting $u = |(x_2, x_3)|$, and computing $\partial_u V$, we obtain that $V = \mathrm{St}_{2,3}(V)$ if and only if $m_1 \leqslant m_2^{2/3} = m_3^{2/3}$, in which case V is (e_2, e_3)-radial decreasing.

If $m_3 < m_2 = m_1$, denoting $u = |(x_1, x_2)|$, and computing $\partial_u V$, we obtain that $V = \mathrm{St}_{1,2}(V)$ if and only if $m_3 \leqslant m_2^{2/3} = m_1^{2/3}$, which always holds thus V is (e_1, e_2)-radial decreasing.

We now need to prove the strict monotonicity. Thanks to (1.26), $\nabla V = 0$ holds only on measure-zero sets (note that we use the computation but do not use any condition on m_1, m_2 and m_3 except that they are strictly less than 1). Thus $|\{V = t\}| = 0$ for any $t \in \mathbb{R}_+$ and then $|\{V^* = t\}| = 0$ for any $t \in \mathbb{R}_+$. Hence V^* is radially strictly decreasing. Same results of strict decreasing hold for Steiner symmetrizations since, as noted before, a Steiner symmetrization is a Schwarz symmetrization on a subspace.

The proof for V given by (1.15) is very similar and easier. □

We now state our main result about the symmetries of minimizers.

THEOREM 1.9 (Symmetries of minimizers). *Let $\lambda > 0$.*

(1) Let V be given by (1.14) and $\psi_M \geqslant 0$ be a minimizer of $I_M(\lambda)$. Then, up to a space translation, ψ_M is e_1-symmetric strictly decreasing. If $m_1^3 \leqslant m_2^2$ as in (1.24_2), then ψ_M is also e_2-symmetric strictly decreasing. Finally, if $m_1^3 \leqslant m_3^2$ as in (1.24_3), then ψ_M is additionally e_3-symmetric strictly decreasing. Moreover,

i. if $m_3 < m_2 = m_1$, then ψ_M is cylindrical strictly decreasing *with axis e_3. Meaning that ψ_M is (e_1, e_2)-radial strictly decreasing. If additionally (1.24_3) holds, then ψ_M is* cylindrical-even strictly decreasing *with axis e_3. This means that ψ_M is* cylindrical strictly decreasing *with axis e_3 and e_3-symmetric strictly decreasing;*

ii. if $m_3 = m_2 < m_1$ and $m_1^3 \leqslant m_2^2 = m_3^2$ as in (1.25), then ψ_M is cylindrical-even strictly decreasing *with axis e_1.*

(2) Let V be given by (1.15) and $\psi_S \geqslant 0$ be a minimizer of $I_S(\lambda)$. Then, up to a space translation, ψ_S is e_k-symmetric strictly decreasing for $k = 1, 2, 3$. Moreover,

i. if $s_3 < s_2 = s_1$, then ψ_S is cylindrical-even strictly decreasing *with axis e_3;*

ii. If $s_3 = s_2 < s_1$, then ψ_S is cylindrical-even strictly decreasing *with axis e_1.*

To prove the symmetry properties of the minimizers, we need symmetrizations of a minimizer to be minimizers, which is proved in the following lemma.

LEMMA 1.10. *Suppose that V, given by (1.14) or by (1.15), verifies one of the* symmetric strictly decreasing *property (resp.* radial strictly decreasing *property) described in Proposition 1.8, and define ψ^{St} the symmetrization of ψ corresponding to this symmetric strictly decreasing property of V.*

If ψ is a minimizer then ψ^{St} too. Moreover the following equalities hold

i. $\|\nabla\psi\|_2^2 = \left\|\nabla\psi^{\mathrm{St}}\right\|_2^2$,

ii. $\left\langle|\psi|^2, |\psi|^2 \star V\right\rangle_2 = \left\langle|\psi^{\mathrm{St}}|^2, |\psi^{\mathrm{St}}|^2 \star V\right\rangle_2$.

PROOF OF LEMMA 1.10. On one hand, since the symmetrization conserves the L^2 norm and ψ is a minimizer, we have $\mathscr{E}(\psi) \leqslant \mathscr{E}(\psi^{\mathrm{St}})$. On the other hand, given the Riesz inequality (see [**Bur96**]), the fact that the kinetic energy is decreasing under symmetrizations (see Theorem 2.1 in [**Cap14**]) and since $V = V^{\mathrm{St}}$ by Proposition 1.8, we have $\mathscr{E}(\psi) \geqslant \mathscr{E}(\psi^{\mathrm{St}})$. So finally $I(\lambda) = \mathscr{E}(\psi) =$

$\mathscr{E}(\psi^{\mathrm{St}})$. Consequently, given (1.17) in Theorem 1.5 and that minimizers ψ and ψ^{St} have the same Lagrange multiplier $\mu = -3\lambda^2 I(1)$, we immediately obtain both equalities. □

Using the analycity of minimizers (Lemma 1.12) we can now prove the strict monotonicity of Steiner symmetrizations of minimizers.

LEMMA 1.11. *Let $\lambda > 0$ and ψ be a real minimizer of $I(\lambda)$ for V given by* (1.14) *or by* (1.15)*, then ψ^* is radially strictly decreasing. Moreover, for any permutation $\{i, j, k\}$ of $\{1, 2, 3\}$, we have*

i. for any $x \in \operatorname{span}\{e_j, e_k\}$, $\mathrm{St}_i(\psi)(x, \cdot)$ is radially strictly decreasing,

ii. for any $x \in \operatorname{span}\{e_i\}$, $\mathrm{St}_{j,k}(\psi)(x, \cdot)$ is radially strictly decreasing.

PROOF OF LEMMA 1.11. By Theorem 1.5, ψ is in $H^2(\mathbb{R}^3, \mathbb{R})$ and a solution of (1.3) with a real Lagrange multiplier μ. Then, by the following lemma (proved in the Section 7.3 of the Appendix), ψ is real analytic.

LEMMA 1.12. *Any $\psi \in H^2(\mathbb{R}^3, \mathbb{R})$ solution of* (1.3) *for $\mu \in \mathbb{R}$ is analytic.*

Thus $|\{\psi = t\}| = 0$ for any $t \in \mathbb{R}_+$ and this is equivalent to $|\{\psi^* = t\}| = 0$ for any $t \in \mathbb{R}_+$. Hence ψ^* is radially strictly decreasing.

Given that for any $1 \leqslant k < 3$ and any $x \in \mathbb{R}^{3-k}$, $\psi(x, \cdot)$ is analytic and since a Steiner symmetrization is a Schwarz symmetrization, we obtain *ii.* and *iii.* by the same reasoning to $\psi(x, \cdot)$. □

Finally, to prove our Theorem 1.9 on the symmetries of minimizers, we need a result on the case of equality in Riesz' inequality for Steiner's symmetrizations. We emphasize that different Steiner symmetrizations do not commute in general. However, if the Steiner symmetrizations are made with respect to the vectors of an orthogonal basis then the radial strictly decreasing properties are preserved.

For shortness, we write $u^{\mathrm{St}_k} := \mathrm{St}_k(u)$ and, in cylindrical cases, $u^{\mathrm{St}_{1,2}} := \mathrm{St}_{1,2}(u)$ and $u^{\mathrm{St}_{2,3}} := \mathrm{St}_{2,3}(u)$.

PROPOSITION 1.13 (Steiner symmetrization: case of equality for g strictly decreasing). *Let f, g, h be three measurable functions on $\mathbb{R}^3$ such that $g > 0$ and $f, h \geqslant 0$ where $0 \neq f \in L^p(\mathbb{R}^3)$, with $1 \leqslant p \leqslant +\infty$, and $0 \neq h \in L^q(\mathbb{R}^3)$, with $1 \leqslant q \leqslant +\infty$. Define*

$$J(f, g, h) = \frac{1}{2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} f(x) g(x-y) h(y)\, dx\, dy \leqslant \infty.$$

(1) Let (i, j, k) be a permutation of $(1, 2, 3)$ and $J\left(f^{\mathrm{St}_i}, g, h^{\mathrm{St}_i}\right) < \infty$. If for any $(x_j, x_k) \in \mathbb{R}^2$ the functions g, f^{St_i} and h^{St_i} are all strictly decreasing with

respect to $|x_i|$, then

$$J(f,g,h) = J\left(f^{\mathrm{St}_i}, g, h^{\mathrm{St}_i}\right) \Leftrightarrow \exists\, a \in \mathbb{R}^3, \begin{cases} f = f^{\mathrm{St}_i}(\cdot - a), \\ h = h^{\mathrm{St}_i}(\cdot - a), \end{cases} \quad \text{a.e. on } \mathbb{R}^3.$$

(2) *Let (i,j,k) be a permutation of $(1,2,3)$ and $J\left(f^{\mathrm{St}_{j,k}}, g, h^{\mathrm{St}_{j,k}}\right) < \infty$. If for any $x_i \in \mathbb{R}$ the functions g, $f^{\mathrm{St}_{j,k}}$ and $h^{\mathrm{St}_{j,k}}$ are all radially strictly decreasing with respect to (x_j, x_k), then*

$$J(f,g,h) = J\left(f^{\mathrm{St}_{j,k}}, g, h^{\mathrm{St}_{j,k}}\right) \Leftrightarrow \exists\, a \in \mathbb{R}^3, \begin{cases} f = f^{\mathrm{St}_{j,k}}(\cdot - a), \\ h = h^{\mathrm{St}_{j,k}}(\cdot - a), \end{cases} \text{a.e. on } \mathbb{R}^3.$$

(3) *Let* St *and* St′ *be two Steiner symmetrizations, acting on two orthogonal directions, $T = \mathrm{St}' \circ \mathrm{St}$ and $J\left(f^T, g, h^T\right) < \infty$. If the functions g, f^{St}, h^{St} are all radially strictly decreasing in the direction (or the plane) of* St*, and g, $f^{\mathrm{St}'}$ and $h^{\mathrm{St}'}$ are all radially strictly decreasing in the direction (or the plane) of* St′*, then*

$$J(f,g,h) = J\left(f^T, g, h^T\right) \Leftrightarrow \exists\, a \in \mathbb{R}^3, \begin{cases} f = f^T(\cdot - a), \\ h = h^T(\cdot - a). \end{cases} \quad \text{a.e. on } \mathbb{R}^3.$$

PROOF OF PROPOSITION 1.13. The implications $\Leftarrow$ all follow from a simple changes of variable. We show the implications $\Rightarrow$ and start with *(1)*. Define, for any permutation (i,j,k) of $(1,2,3)$ and any $(x_j, x_j', x_k, x_k') \in \mathbb{R}^4$, the functions

$$J_i(f,g,h)(x_j, x_j', x_k, x_k') = \frac{1}{2}\int_{\mathbb{R}}\int_{\mathbb{R}} f(X) g(X - X') h(X')\, \mathrm{d}x_i\, \mathrm{d}x_i',$$

where $X = (x_1, x_2, x_3)$ and $X' = (x_1', x_2', x_3')$. We claim that for almost all $(x_j, x_j', x_k, x_k') \in \mathbb{R}^4$, we have

$$J_i(f,g,h)(x_j, x_j', x_k, x_k') = J_i(f^{\mathrm{St}_i}, g, h^{\mathrm{St}_i})(x_j, x_j', x_k, x_k').$$

Indeed, assume that there exists a non-zero measure set $E \subset \mathbb{R}^2 \times \mathbb{R}^2$ such that $J_i(f,g,h)(y,y') \neq J_i(f^{\mathrm{St}_i}, g, h^{\mathrm{St}_i})(y,y')$ for any $(y,y') \in E$. Thus, by Riesz inequality on $\mathbb{R}$, $J_i(f,g,h) < J_i(f^{\mathrm{St}_i}, g, h^{\mathrm{St}_i})$ necessarily holds on E, since $g = g^{\mathrm{St}_i}$, and consequently $J(f,g,h) < J(f^{\mathrm{St}_i}, g, h^{\mathrm{St}_i})$, reaching a contradiction.

We now use the following result of Lieb [**Lie77**]:

LEMMA 1.14 ([**Lie77**, Lemma 3]: Case of equality in Riesz' inequality for g strictly decreasing). *Suppose g is a positive spherically symmetric strictly decreasing function on $\mathbb{R}^n$, $f \in L^p(\mathbb{R}^n)$ and $h \in L^q(\mathbb{R}^n)$ are two nonnegative functions, with $p, q \in [1; +\infty]$, such that $J(f^*, g, h^*) < \infty$. Then*

$$J(f,g,h) = J(f^*, g, h^*) \Rightarrow \exists\, a \in \mathbb{R}^n, f = f^*(\cdot - a) \text{ and } h = h^*(\cdot - a) \text{ a.e.}$$

Thus, for almost all $(y,y')\in\mathbb{R}^2\times\mathbb{R}^2$, there exists $a_i(y,y')\in\mathbb{R}$ such that

$$f(y,x_i)=f^{\mathrm{St}_i}\left(y,x_i-a_i(y,y')\right)$$

and $h(y',x_i)=h^{\mathrm{St}_i}\left(y',x_i-a_i(y,y')\right)$, for almost all $x_i\in\mathbb{R}$. Using now the assumed strict monotonicity of $f^{\mathrm{St}_i}(y,\cdot)$ and $h^{\mathrm{St}_i}(y',\cdot)$, it follows that a_i does not depend on (y,y'), and *(1)* is proved.

The case *(2)* is very similar, defining this time

$$J_{j,k}(f,g,h)(x_i,x_i')=\frac{1}{2}\left\langle f(\cdot,x_i),g(\cdot,x_i-x_i')\star h(\cdot,x_i')\right\rangle_{L^2(\mathbb{R}^2)},$$

for all $(x_i,x_i')\in\mathbb{R}^2$.

We now prove *(3)*. Let St be one of the Steiner's symmetrization described *(1)* and *(2)* and the same for St$'$. We claim that

$$J_{\mathrm{St}}(f,g,h)=J_{\mathrm{St}}(f^{\mathrm{St}},g,h^{\mathrm{St}})\text{ and }J_{\mathrm{St}'}(f,g,h)=J_{\mathrm{St}'}(f^{\mathrm{St}'},g,h^{\mathrm{St}'}),\ a.e..$$

Indeed, Riesz inequality gives $J(f,g,h)\leqslant J(f^{\mathrm{St}},g,h^{\mathrm{St}})\leqslant J(f^T,g,h^T)$. Since first and third terms are equal, the three of them are. From the first equality, there exists $a\in\mathbb{R}^\ell$ $(\ell=1,2)$ such that $f=f^{\mathrm{St}}(\cdot-a,\cdot)$ and $h=h^{\mathrm{St}}(\cdot-a,\cdot)$. Then, since St and St$'$ act on orthogonal directions, we have

$$J(f^T,g,h^T)=J\left(f^{\mathrm{St}'}(\cdot+a,\cdot),g,h^{\mathrm{St}'}(\cdot+a,\cdot)\right)=J(f^{\mathrm{St}'},g,h^{\mathrm{St}'})$$

and so the second claim holds true too. Then we have

$$\begin{cases} f^T\left(y-(a',a)\right)=\left(f^{\mathrm{St}}(x-a,\cdot)\right)^{\mathrm{St}'}(z-a')=f^{\mathrm{St}'}(x,z-a') \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad =f(x,z)=f(y), \\ h^T\left(y-(a',a)\right)=\left(h^{\mathrm{St}}(x-a,\cdot)\right)^{\mathrm{St}'}(z-a')=h^{\mathrm{St}'}(x,z-a') \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad =h(x,z)=h(y), \end{cases}$$

for almost every $y:=(x,z)\in\mathbb{R}^3$ □

We now have all the ingredients to prove Theorem 1.9.

Proof of Theorem 1.9. Let ψ be a minimizer and ψ^{St} one (or a composition) of its Steiner symmetrizations with a direction (or a plane) for which $V=V^{\mathrm{St}}$.

We take $f=h=|\psi|^2\in$ and $g=V$. So we have $f=h>0$ (thanks to Theorem 1.5), $g>0$ (thanks to (1.13)) and $J(f^{\mathrm{St}},V,f^{\mathrm{St}})$ finite. Indeed by the Hardy-Littlewood-Sobolev inequality and (1.13), $J(f^{\mathrm{St}},V,f^{\mathrm{St}})\lesssim\left\|f^{\mathrm{St}}\right\|_{6/5}^2=\|f\|_{6/5}^2<+\infty$ since $f\in H^1(\mathbb{R}^3)$. Moreover, the assumption on the m_k's gives that $g=g^{\mathrm{St}}$ is radially strictly decreasing by Proposition 1.8, and the strict monotonicity of $f^{\mathrm{St}}=h^{\mathrm{St}}$ is obtained by Lemma 1.11.

Finally, by Lemma 1.10, ψ^{St} is a minimizer and

$$J(|\psi|^2, V, |\psi|^2) = J\left((|\psi|^2)^{\mathrm{St}}, (V)^{\mathrm{St}}, (|\psi|^2)^{\mathrm{St}}\right) = J\left((|\psi|^2)^{\mathrm{St}}, V, (|\psi|^2)^{\mathrm{St}}\right).$$

By Proposition 1.13, there exists a such that $|\psi|^2 = (|\psi|^2)^{\mathrm{St}}(\cdot - a) = (|\psi|^{\mathrm{St}})^2(\cdot - a)$ holds a.e. thus $\psi = \psi^{\mathrm{St}}(\cdot - a)$ since $\psi \geqslant 0$. This concludes the proof of Theorem 1.9. □

6. Study of the linearized operator

In this section we study the linearized operator $\mathfrak{L}_Q$, on $L^2(\mathbb{R}^3)$ with domain $H^2(\mathbb{R}^3)$, associated with the Euler-Lagrange equation $-\Delta Q + Q - (|Q|^2 \star V)Q = 0$ (1.3), which is given by

$$\boxed{\mathfrak{L}_Q \xi = -\Delta\xi + \xi - \left(V \star |Q|^2\right)\xi - 2Q\left(V \star (Q\xi)\right),} \tag{1.27}$$

and we give partial characterization of its kernel. We first consider the true model (1.14) for which, following the scheme in **[Len09]**, we will use a Perron–Frobenius argument on subspaces adapted to the symmetries of the problem. The main difficulty will stand in dealing with the non-local operator $Q\left(V \star (Q\xi)\right)$ and, in particular, with proving that this operator is positivity improving. The fundamental use of Newton's theorem in the proof of this property in the isotropic case does not work here, therefore we need a new argument. Our proof will rely on the conditions (1.24_k)'s for which V is e_k-symmetric strictly decreasing for each k (see Proposition 1.8). Then we discuss in a similar way the cylindrical case for the simplified model (1.15), which will need another argument.

6.1. The linearized operator in the symmetric decreasing case. We consider the general case for V, given by (1.14), verifying the three conditions (1.24_k), for $k = 1, 2, 3$, and define the subspaces of $L^2(\mathbb{R}^3)$

$$L^2_{\tau_x,\tau_y,\tau_z} := \left\{ f \in L^2(\mathbb{R}^3) \;\middle|\; \begin{aligned} f(-x,y,z) &= \tau_x f(x,y,z), \\ f(x,-y,z) &= \tau_y f(x,y,z), \\ f(x,y,-z) &= \tau_z f(x,y,z) \end{aligned} \right\}, \tag{1.28}$$

obtained by choosing $\tau_x, \tau_y, \tau_z \in \{\pm 1\}$. We prove the following theorem which is basically saying that the kernel of the linearized operator around solutions is reduced to the kernel on functions that are even in all three directions.

THEOREM 1.15. *Let V, be given by* (1.14)*, verifying* (1.24_k)*, for all k, and let Q be a positive and symmetric strictly decreasing (with respect to each e_k separately) solution of* (1.3)*. Then*

$$\ker \mathfrak{L}_Q = \operatorname{span}\{\partial_x Q, \partial_y Q, \partial_z Q\} \bigoplus \ker\left(\mathfrak{L}_Q\right)_{|L^2_{+,+,+}}. \tag{1.29}$$

For instance, Q could be a minimizer for $I_M(\lambda)$.

The proof of this result is inspired by Lenzmann's proof in [**Len09**] of the fundamental similar result for the linearized operator in the radial case which corresponds to $m_1 = m_2 = m_3$. In that case, Lenzmann proved that

$$\ker\left(\mathfrak{L}_Q\right)_{|L^2_{+,+,+}} = \{0\}.$$

Note that by the result of Section 4, we know that this is still true in the weakly anisotropic case. Moreover, a theorem similar to Theorem 1.15 holds true for the simplified model (1.15) (with no conditions on the matrix S) but we do not state it here for shortness.

The rest of this Section 6.1 being dedicated to the proof of the theorem, let V and Q verify the assumptions of Theorem 1.15 for the entire Section 6.1.

6.1.1. *Direct sum decomposition.* First, one can easily verify that $\mathfrak{L}_Q$ stabilizes the spaces $L^2_{\tau_x,\tau_y,\tau_z}$. Let us then introduce the direct sum decomposition

$$L^2(\mathbb{R}^3) = L^2_{x-} \oplus L^2_{x+} = L^2_{y-} \oplus L^2_{y+} = L^2_{z-} \oplus L^2_{z+}$$

where

$$\begin{cases} L^2_{x-} := \bigoplus\limits_{\tau_y,\tau_z=\pm} L^2_{-,\tau_y,\tau_z}, & L^2_{x+} := \bigoplus\limits_{\tau_y,\tau_z=\pm} L^2_{+,\tau_y,\tau_z} \\ L^2_{y-} := \bigoplus\limits_{\tau_x,\tau_z=\pm} L^2_{\tau_x,-,\tau_z}, & L^2_{y+} := \bigoplus\limits_{\tau_x,\tau_z=\pm} L^2_{\tau_x,+,\tau_z} \\ L^2_{z-} := \bigoplus\limits_{\tau_x,\tau_y=\pm} L^2_{\tau_x,\tau_y,-}, & L^2_{z+} := \bigoplus\limits_{\tau_x,\tau_y=\pm} L^2_{\tau_x,\tau_y,+}. \end{cases}$$

We claim that those spaces — with corresponding projectors P^{x-}, P^{x+}, P^{y-}, P^{y+}, P^{z-} and P^{z+} — reduce the linearized operator $\mathfrak{L}_Q$ (see [**Tes09**] for a definition of reduction), where

$$P^{x\pm}\psi(x,y,z) = \frac{\psi(x,y,z) \pm \psi(-x,y,z)}{2}$$

and similarly for the other projections. The reduction property is straightforward for $-\Delta + 1 - (V \star |Q|^2)$. Moreover, since Q is even in x, we have

$$\begin{aligned} V \star (QP^{x\pm}\psi) &= \frac{V \star (Q\psi) \pm V \star (Q\psi(-\cdot,\cdot,\cdot))}{2} \\ &= \frac{V \star (Q\psi) \pm [V \star (Q\psi)](-\cdot,\cdot,\cdot)}{2} = P^{x\pm}[V \star (Q\psi)] \end{aligned}$$

and, Q being also even in y and in z, we obtain the result for the other projections. Thus we can apply [**Tes09**, Lemma 2.24] which gives us that

$$\mathfrak{L}_Q = \mathfrak{L}_Q^{x-} \oplus \mathfrak{L}_Q^{x+} = \mathfrak{L}_Q^{y-} \oplus \mathfrak{L}_Q^{y+} = \mathfrak{L}_Q^{z-} \oplus \mathfrak{L}_Q^{z+},$$

with the six operators $\mathfrak{L}_Q^w$, for $w \in \{x-, x+, y-, y+, z-, z+\}$, being self-adjoint operators on the corresponding $L^2(\mathbb{R}^3)$ spaces with domains $P^w H^2(\mathbb{R}^3)$. Note that $P^{x-}H^2(\mathbb{R}^3) = H^2_{x-}(\mathbb{R}^3) := H^2(\mathbb{R}^3) \cap L^2_{x-}(\mathbb{R}^3)$ and similarly for P^{y-} and P^{z-}.

Let us then redefine from now on the operator $\mathfrak{L}_Q^{x-}$ (resp. $\mathfrak{L}_Q^{y-}$ and $\mathfrak{L}_Q^{z-}$) by restricting it to x-odd (resp. y-odd and z-odd) functions through the isomorphic identifications $L^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2) \approx L^2_{x-}(\mathbb{R}^3)$ and $H^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2) \approx H^2_{x-}(\mathbb{R}^3)$. Thus, $\mathfrak{L}_Q^{x-}$, as an operator on $L^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2)$ with domain $H^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2)$, can be written

$$\mathfrak{L}_Q^{x-} = -\Delta + 1 + \Phi_{(x-)} + W_{(x-)}$$

where the strictly negative multiplication local operator, on $\mathbb{R}_+ \times \mathbb{R}^2$, is

$$\begin{aligned}\Phi_{(x-)}(x, Y) &= -\left(V \star |Q|^2\right)(x, Y) \\ &= -\int_{\mathbb{R}_+ \times \mathbb{R}^2} [V(x - x', Y - Y') + V(x + x', Y - Y')] \times \\ &\qquad\qquad \times Q^2(x', Y') \,\mathrm{d}Y' \,\mathrm{d}x'\end{aligned}$$

and the non-local term $W_{(x-)}$, on $\mathbb{R}_+ \times \mathbb{R}^2$, is

$$\begin{aligned}&(W_{(x-)} f)(x, Y) \\ &\quad = -2Q(x, Y) \int_{\mathbb{R}_+ \times \mathbb{R}^2} [V(x - x', Y - Y') - V(x + x', Y - Y')] \times \\ &\qquad\qquad \times Q(x', Y') f(x', Y') \,\mathrm{d}Y' \,\mathrm{d}x'.\end{aligned}$$

The same properties hold for $\mathfrak{L}_Q^{y-}$ and $\mathfrak{L}_Q^{z-}$ with corresponding $\Phi_{(y-)}$, $W_{(y-)}$, $\Phi_{(z-)}$ and $W_{(z-)}$.

The key fact to deal with the non-local operator, in order to adapt Lenzmann's proof to anisotropic case, is the positivity improving property of the $-W_{(-)}$'s.

Lemma 1.16. *The operator $-W_{(x-)}$ is positivity improving on $L^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2)$. The same holds true for $-W_{(y-)}$ and $-W_{(z-)}$ on corresponding spaces.*

Proof of Lemma 1.16. Since $X \mapsto V(X, Y)$ is $|X|$-strictly decreasing, due to conditions (1.24_k), and $x + x' > |x - x'|$ on $(\mathbb{R}_+)^2$, we obtain, for $x, x' > 0$ and $(Y, Y') \in \left(\mathbb{R}^2\right)^2$, that $V(x - x', Y - Y') - V(x + x', Y - Y') > 0$. Moreover $Q > 0$. Thus, $-W_{(-)}$ is positivity improving on $L^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2)$. □

6.1.2. *Perron–Frobenius property.* We can now prove that the three operators $\mathfrak{L}_Q^{x-}$, $\mathfrak{L}_Q^{y-}$ and $\mathfrak{L}_Q^{z-}$ verify a Perron–Frobenius property.

Proposition 1.17 (Perron–Frobenius properties). *The operator $\mathfrak{L}_Q^{x-}$ is self-adjoint on $L^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2)$ with domain $H^2_{x-}(\mathbb{R}_+ \times \mathbb{R}^2)$, is bounded below and has* *the Perron–Frobenius property: if* λ_0^{x-} *denotes the lowest eigenvalue of* $\mathfrak{L}_Q^{x-}$*, then* λ_0^{x-} *is simple and the corresponding eigenfunction* ψ_0^{x-} *is strictly positive.*

The same holds true for $\mathfrak{L}_Q^{y-}$ *and* $\mathfrak{L}_Q^{z-}$ *with the corresponding domains, lowest eigenvalues and eigenfunctions.*

Proof of Proposition 1.17. We follow the proof's structure of [**Len09**, Lemma 8]. Moreover, we only write the proof for $\mathfrak{L}_Q^{x-}$ thus the superscripts and subscripts "$x-$" will everywhere in this proof be replaced by "$-$" for simplicity. The argument is the same for the other directions.

Self-adjointness. We have $Q \in H^2(\mathbb{R}^3) \subset C^0(\mathbb{R}^3) \cap L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ and, by (1.13), $V \star |Q|^2$ is in $L^4(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ since $V = V_2 + V_4 \in L^2(\mathbb{R}^3) + L^4(\mathbb{R}^3)$. Defining, for any $f \in L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$, $\tilde{f} \in L^2_-(\mathbb{R}^3)$ by $f(x,\cdot) = \tilde{f}(x,\cdot)$ for $x \geqslant 0$, we have $2\langle f, g\rangle_{L^2_-(\mathbb{R}_+\times\mathbb{R}^2)} = \langle \tilde{f}, \tilde{g}\rangle_{L^2_-(\mathbb{R}^3)}$ and so $\Phi_{(-)} + 1$ is bounded on $L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$. Moreover, by Young inequalities, for any $\xi \in L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$,

$$\|V \star (Q\tilde{\xi})\|_{L^\infty} \leqslant (\|V_4\|_{L^4} \|Q\|_{L^4} + \|V_2\|_{L^2} \|Q\|_{L^\infty}) \|\tilde{\xi}\|_{L^2}$$

holds. Thus, for $p \in [2, \infty]$, we have

$$\begin{aligned}\left\|W_{(-)}\xi\right\|_{L^p(\mathbb{R}_+\times\mathbb{R}^2)} &\leqslant 2\|Q\|_{L^p(\mathbb{R}_+\times\mathbb{R}^2)} \|V \star (Q\tilde{\xi})\|_{L^\infty(\mathbb{R}_+\times\mathbb{R}^2)}\\ &\leqslant \|Q\|_{L^p} \|V \star (Q\tilde{\xi})\|_{L^\infty}\end{aligned}$$

and $W_{(-)}\xi \in L^2_-(\mathbb{R}_+ \times \mathbb{R}^2) \cap L^\infty(\mathbb{R}_+ \times \mathbb{R}^2)$. Consequently, $1 + \Phi_{(-)} + W_{(-)}$ and, thus, $\mathfrak{L}_Q^-$ is bounded below on $L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$.

Finally, we deduce the self-adjointness of the operator $\mathfrak{L}_Q^-$ on $L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$ with domain $H^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$ from the self-adjointness of the operator $\mathfrak{L}_Q^-$ on $L^2_-(\mathbb{R}^3)$ with domain $H^2_-(\mathbb{R}^3)$.

Positivity improving. We know (see the proof of Lemma 1.30 in the Appendix) that

$$(-\Delta + \mu)^{-1}\xi(X) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{e^{-\sqrt{\mu}|X-Y|}}{|X-Y|}\xi(Y)\,\mathrm{d}Y,$$

for all $\mu > 0$ and all $\xi \in L^2(\mathbb{R}^3)$. Consequently, for $\xi \in L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$ and $(x, \tilde{x}) \in \mathbb{R}_+ \times \mathbb{R}^2$, we have

$$\begin{aligned}&(-\Delta + \mu)^{-1}\xi(x, \tilde{x})\\ &\qquad = \frac{1}{4\pi}\int_{\mathbb{R}_+\times\mathbb{R}^2} \left[\frac{e^{-\sqrt{\mu}|(x-y,\tilde{x}-\tilde{y})|}}{|(x-y,\tilde{x}-\tilde{y})|} - \frac{e^{-\sqrt{\mu}|(x+y,\tilde{x}-\tilde{y})|}}{|(x+y,\tilde{x}-\tilde{y})|}\right]\xi(y,\tilde{y})\,\mathrm{d}y\,\mathrm{d}\tilde{y}.\end{aligned}$$

Thus, with the same arguments as in the proof of Lemma 1.16, $(-\Delta + \mu)^{-1}$ is positivity improving on $L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$ for all $\mu > 0$. Moreover, $-(\Phi_{(-)} + W_{(-)})$ is positivity improving on $L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$ since $-\Phi_{(-)}$ is a positive multiplication operator and $-W_{(-)}$ is positivity improving by Lemma 1.16. Then similarly to the proof of [**Len09**, Lemma 8], for $\mu \gg 1$,we have

$$\left(\mathfrak{L}_Q^- + \mu\right)^{-1} = (-\Delta + \mu + 1)^{-1} \cdot \left(1 + (\Phi_{(-)} + W_{(-)})(-\Delta + \mu + 1)^{-1}\right)^{-1}.$$

Since $(\Phi_{(-)} + W_{(-)})$ is bounded, we have

$$\left\|(\Phi_{(-)} + W_{(-)})(-\Delta + \mu)^{-1}\right\|_{L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)} < 1,$$

for μ large enough. This implies, for $\mu \gg 1$, by Neumann's expansion that

$$\left(\mathfrak{L}_Q^- + \mu\right)^{-1} = (-\Delta + \mu + 1)^{-1} \sum_{p=0}^{\infty} \left[-(\Phi_{(-)} + W_{(-)})(-\Delta + \mu + 1)^{-1}\right]^p,$$

which is consequently positivity improving on $L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$ for $\mu \gg 1$.

Conclusion. We choose $\mu \gg 1$ such that $(\mathfrak{L}_Q^- + \mu)^{-1}$ is positivity improving and bounded. Then, by [**RS78**, Thm XIII.43], the largest eigenvalue $\sup \sigma((\mathfrak{L}_Q^- + \mu)^{-1})$ is simple and the associated eigenfunction $\psi_0^- \in L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$ is strictly positive. Since, for any $\psi \in L^2_-(\mathbb{R}_+ \times \mathbb{R}^2)$, having ψ being an eigenfunction of $\mathfrak{L}_Q^-$ for the eigenvalue λ is equivalent to having ψ being an eigenfunction of $(\mathfrak{L}_Q^- + \mu)^{-1}$ for the eigenvalue $(\lambda + \mu)^{-1}$, we have proved Proposition 1.17. □

6.1.3. *Proof of Theorem 1.15.* Differentiating, with respect to x the Euler-Lagrange equation $-\Delta Q + Q - (|Q|^2 \star V)Q = 0$ (1.3), we obtain $\mathfrak{L}_Q \partial_x Q \equiv 0$. Moreover, Q is positive *symmetric strictly decreasing*, thus $\partial_x Q \in L^2_{x-}(\mathbb{R}^3)$, and this shows that $\mathfrak{L}_Q^{x-} \partial_x Q \equiv 0$. Then, $Q > 0$ being *symmetric strictly decreasing*, $\partial_x Q < 0$ on $\mathbb{R}_+ \times \mathbb{R}^2$ and, by the Perron–Frobenius property, it is (up to sign) the unique eigenvector associated with the lowest eigenvalue of $\mathfrak{L}_Q^{x-}$, namely $\lambda_0^{x-} = 0$. Since $\mathfrak{L}_Q^{x-}$ acts on $L^2_{x-} := \bigoplus_{\tau_y, \tau_z = \pm} L^2_{-,\tau_y,\tau_z}$, we obtain

$$\begin{cases} \ker\left(\mathfrak{L}_Q\right)_{|L^2_{-,+,+}(\mathbb{R}^3)} = \operatorname{span}\{\partial_x Q\}; \\ \ker\left(\mathfrak{L}_Q\right)_{|L^2_{-,-,+}(\mathbb{R}^3)} = \ker\left(\mathfrak{L}_Q\right)_{|L^2_{-,+,-}(\mathbb{R}^3)} = \ker\left(\mathfrak{L}_Q\right)_{|L^2_{-,-,-}(\mathbb{R}^3)} = \{0\}. \end{cases}$$

This the exact same arguments for the two other directions we finally obtain that

$$\ker \mathfrak{L}_Q = \operatorname{span}\{\partial_x Q, \partial_y Q, \partial_z Q\} \bigoplus \ker\left(\mathfrak{L}_Q\right)_{|L^2_{+,+,+}(\mathbb{R}^3)}.$$

Which concludes the proof of Theorem 1.15. □

6.2. The linearized operator in the cylindrical case for the simplified model. We now consider the case where the static dielectric matrix has exactly two identical eigenvalues. Obviously, Theorem 1.15 holds and it tells us that the kernel is reduced to the kernel on functions that are even in the z-direction and even in any direction of the plane orthogonal to z. However, this does not tell us that it is reduced to the kernel on cylindrical functions, which is what we are interested in. Indeed, instead of the kernel of $\mathfrak{L}_Q$ on $L^2_{+,+,+}(\mathbb{R}^3)$, we want the remaining term in the direct sum to be the kernel on $L^2_{\mathrm{rad},+}(\mathbb{R}^3)$, namely the subset of cylindrical functions that are also even in the direction of their principal axis.

Unfortunately, our method fails to prove it for V given by (1.14) since we are not able to prove a positivity improving property for the non local operator. Therefore, in this section, we will only consider the simplified model where V is given by (1.15).

We use the cylindrical coordinates (r, θ, z) where e_z is the vector orthogonal to the plane of symmetry. Namely, $e_z = e_3$ if $s_3 < s_2 = s_1$ and $e_z = e_1$ if $s_3 = s_2 < s_1$. We then define the following subspaces

$$
\begin{aligned}
L^2_\tau(\mathbb{R}^3) &:= \left\{ f \in L^2(\mathbb{R}^3) \,|\, f(x,y,-z) = \tau f(x,y,z) \right\}, \qquad \text{for } \tau = \pm; \\
L^2_+(\mathbb{R}_+ \times \mathbb{R}) &:= \left\{ f \in L^2(\mathbb{R}_+ \times \mathbb{R}, r\,\mathrm{d}r\,\mathrm{d}z) \,|\, f(r,-z) = f(r,z) \right\}; \\
L^2_{\mathrm{rad},+}(\mathbb{R}^3) &:= L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \left\{ Y_0^+ \right\}.
\end{aligned} \tag{1.30}
$$

Thus $L^2_{\mathrm{rad},+}(\mathbb{R}^3)$ is the space of square-integrable functions which are even in z and radial in the (x, y) plane.

Theorem 1.18. *Let V be given by* (1.15) *with S having one eigenvalue of multiplicity* 2 *and let Q be a* cylindrical-even decreasing *and positive solution of* (1.3). *Then*

$$
\ker \mathfrak{L}_Q = \operatorname{span}\{\partial_x Q, \partial_y Q, \partial_z Q\} \oplus \ker (\mathfrak{L}_Q)_{|L^2_{\mathrm{rad},+}(\mathbb{R}^3)}. \tag{1.31}
$$

For instance, Q could be a minimizer for $I_S(\lambda)$.

Several parts of the proof of this theorem being identical to the ones in the proof of Theorem 1.15, we will only give the details for the parts that differ.

6.2.1. *Cylindrical decomposition.* Since V is *cylindrical-even strictly decreasing* by Proposition 1.8 and since minimizers are *cylindrical-even strictly decreasing* by Proposition 1.9, $\mathfrak{L}_Q$ commutes with rotation in the plane of symmetry. Let us then introduce the direct sum decomposition

$$
L^2(\mathbb{R}^3) = L^2_-(\mathbb{R}^3) \oplus \bigoplus_{n \geqslant 0, \sigma = \pm} L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \{Y_n^\sigma\}, \tag{1.32}
$$

with

$$
\begin{cases}
Y_0^+ \equiv (2\pi)^{-\frac{1}{2}};\ Y_0^- \equiv 0; \\
Y_n^+ \equiv \pi^{-\frac{1}{2}} \cos(n\cdot);\ Y_n^- \equiv \pi^{-\frac{1}{2}} \sin(n\cdot), \quad \text{for } n \geqslant 1.
\end{cases} \tag{1.33}
$$

The operator $\mathfrak{L}_Q$ stabilizes $L^2_-(\mathbb{R}^3)$ and the spaces $L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \{Y_n^\sigma\}$.

Let us immediately decompose the potential V in order to give the fundamental property in the cylindrical case (Proposition 1.19 below), which is what allows us to adapt the original work of Lenzmann, namely the strict positivity of each z-odd terms of the cylindrical decomposition of V. For any $\mathbf{r} = (r, \varphi, z) \in \mathbb{R}^3$ and $\mathbf{r}' = (r', \varphi', z') \in \mathbb{R}^3$, defining $\rho := (r - r', 0, z - z')$ and $\theta := \varphi - \varphi'$, we have, as soon as $(r', z') \neq (r, z)$:

$$\theta \mapsto V(\mathbf{r} - \mathbf{r}') = \frac{1}{\sqrt{\left|(1-S)^{-1}\rho\right|^2 + 2(1-s_2)^{-2} r r'(1-\cos\theta)}} > 0, \tag{1.34}$$

which is in $C^\infty(\mathbb{R})$, 2π-periodic and even. Thus, for any $\mathbf{r} \neq \mathbf{r}'$,

$$V(\mathbf{r} - \mathbf{r}') = \sum_{n=0}^{\infty} v_n(r, r', z - z') Y_n^+(\varphi - \varphi'),$$

with

$$v_n(r, r', z - z') = \int_{-\pi}^{\pi} V(\mathbf{r} - \mathbf{r}') Y_n^+(\theta)\,\mathrm{d}\theta = 2\int_0^{\pi} V(\mathbf{r} - \mathbf{r}') Y_n^+(\theta)\,\mathrm{d}\theta. \tag{1.35}$$

PROPOSITION 1.19. *Let V be given by* (1.15)*, the Y_n^+'s by* (1.33) *and the v_n's by* (1.35) *for any $(n, r, r', z, z') \in \mathbb{N} \times \mathbb{R}_+^* \times \mathbb{R}_+^* \times \mathbb{R} \times \mathbb{R}$. Then*

$$v_n(r, r', z - z') > 0, \qquad \forall (n, r, r', z, z') \in \mathbb{N} \times \mathbb{R}_+^* \times \mathbb{R}_+^* \times \mathbb{R} \times \mathbb{R}.$$

PROOF OF PROPOSITION 1.19. Defining for $r, r' > 0$,

$$\begin{aligned} m^\pm &:= \sqrt{\left(\frac{r + r'}{1 - s_2}\right)^2 + \left(\frac{z - z'}{1 - s_z}\right)^2} \pm \sqrt{\left(\frac{r - r'}{1 - s_2}\right)^2 + \left(\frac{z - z'}{1 - s_z}\right)^2} \\ &= \max_{\varphi - \varphi'} \left|(1-S)^{-1}(\mathbf{r} - \mathbf{r}')\right| \pm \min_{\varphi - \varphi'} \left|(1-S)^{-1}(\mathbf{r} - \mathbf{r}')\right| > 0, \end{aligned}$$

we note that $m^+ > m^-$ and obtain

$$V(\mathbf{r} - \mathbf{r}') = \frac{2}{m^+} \frac{1}{\sqrt{1 - 2\frac{m^-}{m^+}\cos\theta + \left(\frac{m^-}{m^+}\right)^2}}.$$

We now give the explicit expansion of $(1 - 2t\cos\theta + t^2)^{-1/2}$ in the following lemma.

LEMMA 1.20. *For $(0, 1) \neq (\theta, t) \in \mathbb{R} \times [0, 1]$, we have*

$$\begin{aligned} \frac{1}{\sqrt{1 - 2t\cos\theta + t^2}} &= \sum_{k=0}^{\infty} \beta_{0,2k} t^{2k} Y_0^+(\theta) + \sum_{n=1}^{\infty} \sum_{k=n}^{\infty} \beta_{2n,2k} t^{2k} Y_{2n}^+(\theta) \\ &\quad + \sum_{n=0}^{\infty} \sum_{k=n}^{\infty} \beta_{2n+1,2k+1} t^{2k+1} Y_{2n+1}^+(\theta). \end{aligned} \tag{1.36}$$

with

$$\begin{cases} \beta_{0,2k} = \sqrt{2\pi}\dfrac{\binom{2k}{k}^2}{2^{4k}} > 0, & 0 \leqslant k; \\ \beta_{2n,2k} = 2\sqrt{\pi}\dfrac{\binom{2(k+n)}{k+n}\binom{2(k-n)}{k-n}}{2^{4k}} > 0, & 0 < n \leqslant k; \\ \beta_{2n+1,2k+1} = 2\sqrt{\pi}\dfrac{\binom{2(k+n+1)}{k+n+1}\binom{2(k-n)}{k-n}}{2^{4k+2}} > 0, & 0 \leqslant n \leqslant k. \end{cases}$$

PROOF OF LEMMA 1.20. The proof of this lemma is entirely inspired by the original computation of Legendre[1] in his famous *mémoire* [**Le 84**] where he introduced the polynomials that are nowadays called after him. Let us first rewrite the fraction, for $(0,1) \neq (\theta, t) \in \mathbb{R} \times [0,1]$:

$$\frac{1}{\sqrt{1-2t\cos\theta+t^2}} = (1-e^{\mathrm{i}\theta}t)^{-1/2}(1-e^{-\mathrm{i}\theta}t)^{-1/2}.$$

Then, since $\Gamma(1/2-p) = \frac{(-4)^p p!}{(2p)!}\Gamma(1/2)$ and using the following expansion

$$(1-x)^{-1/2} = \sum_{p=0}^{\infty} \frac{\Gamma(1/2)}{\Gamma(1/2-p)\Gamma(p+1)}(-x)^p = \sum_{p=0}^{\infty} \frac{\binom{2p}{p}}{2^{2p}}x^p,$$

we obtain:

$$\begin{aligned} \frac{1}{\sqrt{1-2t\cos\theta+t^2}} &= \sum_{(p,q)\in\mathbb{N}^2} \frac{\binom{2p}{p}\binom{2q}{q}}{2^{2(p+q)}} e^{\mathrm{i}(p-q)\theta}t^{p+q} \\ &= \sum_{\substack{k=0 \\ k \text{ even}}}^{\infty} \sum_{\substack{n=-k \\ n \text{ even}}}^{k} \frac{\binom{k+n}{(k+n)/2}\binom{k-n}{(k-n)/2}}{2^{2k}} e^{\mathrm{i}n\theta}t^k \\ &\quad + \sum_{\substack{k=1 \\ k \text{ odd}}}^{\infty} \sum_{\substack{n=-k \\ n \text{ odd}}}^{k} \frac{\binom{k+n}{(k+n)/2}\binom{k-n}{(k-n)/2}}{2^{2k}} e^{\mathrm{i}n\theta}t^k \\ &= \sum_{k=0}^{\infty} \frac{\binom{2k}{k}^2}{2^{4k}} t^{2k} + \sum_{k=0}^{\infty}\sum_{n=1}^{k} \frac{\binom{2(k+n)}{k+n}\binom{2(k-n)}{k-n}}{2^{4k}} 2\cos(2n\theta)t^{2k} \\ &\quad + \sum_{k=0}^{\infty}\sum_{n=0}^{k} \frac{\binom{2(k+n+1)}{k+n+1}\binom{2(k-n)}{k-n}}{2^{4k+2}} 2\cos((2n+1)\theta)t^{2k+1} \\ &= \sum_{k=0}^{\infty} \frac{\binom{2k}{k}^2}{2^{4k}} t^{2k} + \sum_{n=1}^{\infty}\sum_{k=n}^{\infty} \frac{\binom{2(k+n)}{k+n}\binom{2(k-n)}{k-n}}{2^{4k}} 2\cos(2n\theta)t^{2k} \end{aligned}$$

1. or Legendre and Laplace, according to a famous paternity controversy.

$$+\sum_{n=0}^{\infty}\sum_{k=n}^{\infty}\frac{\binom{2(k+n+1)}{k+n+1}\binom{2(k-n)}{k-n}}{2^{4k+2}}2\cos((2n+1)\theta)t^{2k+1}.$$

With the definition of the Y_n^+'s, this concludes the proof of Lemma 1.20. □

Defining all the others $\beta_{p,q}$'s to be zero, this proves Proposition 1.19:

$$v_n(r,r',z-z') = \frac{2}{m^+}\sum_{k=n}^{\infty}\beta_{n,k}\left(\frac{m^-}{m^+}\right)^k > 0,$$

for $n \geqslant 0$, $r, r' > 0$ and $z, z' \in \mathbb{R}$. Moreover, for $\mathbf{r} \neq \mathbf{r}'$, we have

$$V(\mathbf{r}-\mathbf{r}') = \sum_{n=0}^{\infty}\frac{2}{m^+}\left(\sum_{k=n}^{\infty}\beta_{n,k}\left(\frac{m^-}{m^+}\right)^k\right)Y_n^+(\theta).$$

□

Remark 1.21. (The anisotropic potential (1.14)) If we define v_n in a similar fashion for the true model based on (1.14), even with the conditions (1.24$_k$) and (1.25), the v_n's have no sign for $n \geqslant 2$, since we have

$$v_n(r,r',z-z') = \sum_{k=n}^{\infty}2\beta_{n,k}\left(\frac{1}{m_{Id}^+}\left(\frac{m_{Id}^-}{m_{Id}^+}\right)^k - \frac{1}{m_M^+}\left(\frac{m_M^-}{m_M^+}\right)^k\right)$$

which changes sign for $n \geqslant 2$. This is why our method fails if V is given by (1.14). Note that the strict positivity however holds true for v_0 and for v_1 if $r, r' > 0$, which is straightforward using (1.35).

As proved in the last Section, $L^2_-(\mathbb{R}^3)$, with corresponding projectors P^-, reduces $\mathfrak{L}_Q$. We claim that the spaces $L^2_+(\mathbb{R}_+\times\mathbb{R})\otimes\{Y_n^\sigma\}$, with corresponding projectors

$$P^+_{n,\sigma}\psi(r,\varphi,z) = \left(\int_0^{2\pi}\frac{\psi(r,\varphi',z)+\psi(r,\varphi',-z)}{2}Y_n^\sigma(\varphi')\,\mathrm{d}\varphi'\right)Y_n^\sigma(\varphi),$$

also reduce $\mathfrak{L}_Q$. Given that $(V\star|Q|^2)$ is radial and z-odd, that $\frac{\mathrm{d}^2}{\mathrm{d}\varphi^2}Y_n^\sigma = -n^2Y_n^\sigma$ and that

$$\Delta = \frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{\partial^2}{\partial z^2}+\frac{1}{r^2}\frac{\partial^2}{\partial\varphi^2}, \tag{1.37}$$

we have

$$\left[-\Delta+1-\left(V\star|Q|^2\right)\right](fY_n^\sigma) = \left[-\Delta_{(n)}+1-\left(V\star|Q|^2\right)\right](f)Y_n^\sigma, \tag{1.38}$$

for any $f \in L^2_+(\mathbb{R}_+\times\mathbb{R})$, and so belonging to $L^2_+(\mathbb{R}_+\times\mathbb{R})\otimes\{Y_n^\sigma\}$, and where

$$-\Delta_{(n)} := -\frac{\partial^2}{\partial r^2}-\frac{1}{r}\frac{\partial}{\partial r}-\frac{\partial^2}{\partial z^2}+\frac{n^2}{r^2}.$$

Thus the reduction property follows for $-\Delta + 1 - (V \star |Q|^2)$. Moreover, since $V \star (Q\cdot)$ and $P^+_{n,\sigma}$ are linear and using the decomposition

$$\psi(r,\varphi,z) = c^-(r,\varphi,z) + \sum_{n\geqslant 0,\sigma=\pm} c^+_{n,\sigma}(r,z) Y^\sigma_n(\varphi),$$

we have to prove that

$$V \star (Q P^+_{n',\sigma'} c^+_{n,\sigma} Y^\sigma_n) = P^+_{n',\sigma'}\left(V \star (Q c^+_{n,\sigma} Y^\sigma_n)\right),$$

for any $n, n' \geqslant 0$ and $\sigma, \sigma' = \pm$, in order to conclude. We have

$$\begin{aligned}
&\left[V \star (Q c^+_{n,\sigma} Y^\sigma_n)\right](r,\varphi,z) \\
&\quad = \int_{\mathbb{R}_+}\int_{-\pi}^{\pi}\int_{\mathbb{R}} Q(r',z') c^+_{n,\sigma}(r',z') Y^\sigma_n(\varphi') V(\mathbf{r}-\mathbf{r}') r' \,\mathrm{d}z' \,\mathrm{d}\varphi' \,\mathrm{d}r' \\
&\quad = \sqrt{\gamma_n \pi}\left(\int_{\mathbb{R}_+}\int_{\mathbb{R}} Q(r',z') c^+_{n,\sigma}(r',z') v_n(r,r',z-z') r' \,\mathrm{d}z' \,\mathrm{d}r'\right) Y^\sigma_n(\varphi),
\end{aligned} \tag{1.39}$$

with $\gamma_n = 2^{\mathbb{1}_{\{n=0\}}}$. Then using the parity of v_n with respect to its third variable (which is straightforward with (1.35)), we obtain $V \star (Q c^+_{n,\sigma} Y^\sigma_n) \in L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \{Y^\sigma_n\}$ and the reduction property follows. Thus we can apply [**Tes09**, Lemma 2.24] which gives us that

$$\mathfrak{L}_Q = \mathfrak{L}^- \oplus \bigoplus_{n\geqslant 0,\sigma=\pm} \mathfrak{L}^+_{n,\sigma},$$

with $\mathfrak{L}^- = \mathfrak{L}^{z-}_Q$ being the same operator as before and each $\mathfrak{L}^+_{n,\sigma}$ a self-adjoint operator on $L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \{Y^\sigma_n\}$ with domain $P^+_{n,\sigma} H^2(\mathbb{R}^3)$. For shortness, we now omit the Q subscript in the decomposition $\mathfrak{L}_Q$.

Given (1.38) and (1.39), for any $n \geqslant 0$ we note $\mathfrak{L}^+_n$ the operator on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$ such that $\mathfrak{L}^+_{n,+}(f Y^+_n) = \mathfrak{L}^+_n(f) Y^+_n$ and $\mathfrak{L}^+_{n,-}(f Y^-_n) = \mathfrak{L}^+_n(f) Y^-_n$. This operator is

$$\mathfrak{L}^+_n = -\Delta_{(n)} + 1 + \Phi + W_{(n)}$$

where Φ is the strictly negative multiplication local potential, on $\mathbb{R}_+ \times \mathbb{R}$,

$$\begin{aligned}
\Phi(r,z) &= -\left(V \star |Q|^2\right)(r,z) \\
&= -\sqrt{2\pi}\int_{\mathbb{R}_+\times\mathbb{R}} |Q(r',z')|^2 v_0(r,r',z-z') r' \,\mathrm{d}z' \,\mathrm{d}r' < 0
\end{aligned}$$

and $W_{(n)}$ is the non-local operator, on $\mathbb{R}_+ \times \mathbb{R}$,

$$(W_{(n)} f)(r,z) = -2Q(r,z)\int_{\mathbb{R}_+\times\mathbb{R}} Q(r',z') f(r',z') v_n(r,r',z-z') r' \,\mathrm{d}z' \,\mathrm{d}r'. \tag{1.40}$$

Similarly to the non-cylindrical case, we need to prove that $-W_{(n)}$ is positivity improving on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$ and this is where the result of Proposition 1.19 is needed.

LEMMA 1.22. *For $n \geqslant 0$, the operator $-W_{(n)}$ is positivity improving on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$.*

PROOF OF LEMMA 1.22. Given the definition (1.40) of $-W_{(n)}$, the fact that the v_n's are strictly positive as soon as $r, r' > 0$ (by Proposition 1.19) and that $Q > 0$, it follows that $-W_{(n)}$ is positivity improving on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$ for any $n \geqslant 0$. □

6.2.2. *Perron–Frobenius property.* We now prove that the $\mathfrak{L}_n^+$'s verify the Perron–Frobenius property.

PROPOSITION 1.23 (Perron–Frobenius properties). *For $n > 0$, the $\mathfrak{L}_n^+$'s are essentially self-adjointness on $C_0^\infty(\mathbb{R}_+ \times \mathbb{R})$ and bounded below.*

Moreover they have the Perron–Frobenius property: if λ_0^n denotes the lowest eigenvalue of $\mathfrak{L}_n^+$, then λ_0^n is simple and the corresponding eigenfunction ψ_0^n is strictly positive.

PROOF OF PROPOSITION 1.23. We follow the proof's structure of [**Len09**, Lemma 8].

Self-adjointness. We still have $V \star |Q|^2 \in L^4(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$. Moreover, defining $\mathring{f}(r, \cdot, z) = f(r, z) Y_n^+ \in L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \{Y_n^+\} \subset L^2(\mathbb{R}^3)$, for any $f \in L^2_+(\mathbb{R}_+ \times \mathbb{R})$, we have $\langle f, g \rangle_{L^2_+(\mathbb{R}_+ \times \mathbb{R})} = \langle \mathring{f}, \mathring{g} \rangle_{L^2(\mathbb{R}^3)}$ and, consequently, that $\Phi + 1$ is a bounded operator on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$. Then, for any $\xi \in L^2_+(\mathbb{R}_+ \times \mathbb{R})$ and $p \in [2, \infty]$, we have

$$\left\| W_{(n)} \xi \right\|_{L^p(\mathbb{R}_+ \times \mathbb{R})} \leqslant \|Q\|_{L^p} \, \|V \star (Q \mathring{\xi})\|_{L^\infty}.$$

Thus $W_{(n)} \xi \in L^2_+(\mathbb{R}_+ \times \mathbb{R}) \cap L^\infty(\mathbb{R}_+ \times \mathbb{R})$ and, finally, $1 + \Phi + W_{(n)}$ and, thus, $\mathfrak{L}_n^+$ are bounded below on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$. Furthermore, it is known that $-\Delta_{(n)}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}_+ \times \mathbb{R})$ provided that $n > 0$. Thus, given that $1 + \Phi + W_{(n)}$ is bounded (so $-\Delta_{(n)}$-bounded of relative bound zero), symmetric (moreover self-ajoint) and that its domain contains the domain of $-\Delta_{(n)}$, we obtain by the Rellich-Kato theorem the essentially self-adjointness of $\mathfrak{L}_n^+$ on $C_0^\infty(\mathbb{R}_+ \times \mathbb{R})$.

Positivity improving. We claim that $e^{t\Delta_{(n)}}$ is positivity improving for all $t > 0$ on $L^2(\mathbb{R}_+ \times \mathbb{R})$. Indeed we have the explicit formula for the integral kernel $e^{t\Delta}$ on $\mathbb{R}^3$, namely,

$$e^{t\Delta}(x, y) = (4\pi t)^{-3/2} e^{-\frac{|x-y|^2}{4t}} = (4\pi t)^{-3/2} e^{-\frac{r^2 + r'^2 + (z-z')^2}{4t}} e^{\frac{rr'}{2t} \cos(\varphi - \varphi')}, \tag{1.41}$$

for all $x := (r, \varphi, z)$ and $y := (r', \varphi', z')$. On the other hand we have

$$e^{x\cos\theta} = \sqrt{2\pi} \sum_{m=0}^{\infty} \sqrt{2}^{\delta_{\{m\geqslant 1\}}} I_m(x) Y_m^+(\theta), \quad \forall x \in \mathbb{R}, \tag{1.42}$$

where $I_n(x) = \pi^{-1} \int_0^\pi \exp(x\cos\theta)\cos(n\theta)\,\mathrm{d}\theta$ are the modified Bessel functions of the first kind, that are strictly positive for $n \geqslant 0$ and $x > 0$. From these two relations, we deduce the integral kernel $e^{t\Delta_{(n)}}$ acting on $L^2(\mathbb{R}_+ \times \mathbb{R})$ and that it is positive, which are the two points of the following lemma.

Lemma 1.24. *Let $f \in L^2(\mathbb{R}_+ \times \mathbb{R})$, $r, r' > 0$ and $n \geqslant 0$. Then the integral kernel $e^{t\Delta_{(n)}}$ acting on $L^2(\mathbb{R}_+ \times \mathbb{R})$ verifies*

$$e^{t\Delta_{(n)}}((r,z),(r',z')) = \frac{\sqrt{2}^{-\delta_n^0}}{4\pi t^{3/2}} e^{-\frac{r^2+r'^2+z^2+z'^2}{4t}} I_n\left(\frac{rr'}{2t}\right) \exp\left(\frac{zz'}{2t}\right) > 0. \tag{1.43}$$

Proof of Lemma 1.24. Let $f \in L^2(\mathbb{R}_+ \times \mathbb{R})$. Using (1.41), for $n \geqslant 0$, we have

$$\begin{aligned}
&\left(e^{t\Delta}(fY_n^\sigma)\right)(r,\varphi,z) \\
&= (4\pi t)^{-3/2} \int_{\mathbb{R}_+\times\mathbb{R}} e^{-\frac{r^2+r'^2+(z-z')^2}{4t}} f(r',z') \left(\int_{-\pi}^{\pi} e^{\frac{rr'}{2t}\cos(\varphi-\varphi')} Y_n^\sigma(\varphi')\,\mathrm{d}\varphi'\right) r'\,\mathrm{d}r'\,\mathrm{d}z' \\
&= \frac{\sqrt{2}^{-\delta_n^0}}{4\pi t^{3/2}} \int_{\mathbb{R}_+\times\mathbb{R}} e^{-\frac{r^2+r'^2+z^2+z'^2}{4t}} f(r',z') I_n\left(\frac{rr'}{2t}\right) \exp\left(\frac{zz'}{2t}\right) r'\,\mathrm{d}r'\,\mathrm{d}z' Y_n^\sigma(\varphi).
\end{aligned}$$

Which allows to conclude the proof of Lemma 1.24. □

So, for all $n \geqslant 0$, $e^{t\Delta_{(n)}}$ is positivity improving on $L^2(\mathbb{R}_+ \times \mathbb{R})$ for all $t > 0$ and consequently on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$. Then, by functional calculus, we have

$$\left(-\Delta_{(n)} + \mu\right)^{-1} = \int_0^\infty e^{-t\mu} e^{t\Delta_{(n)}}\,\mathrm{d}t, \quad \forall\, \mu > 0,$$

thus $(-\Delta_{(n)} + \mu)^{-1}$ is positivity improving on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$ for all $\mu > 0$.

Moreover we claim that $-(\Phi + W_{(n)})$ is positivity improving on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$ since $-\Phi$ is a positive multiplication operator and $-W_{(n)}$ is positivity improving on $L^2_+(\mathbb{R}_+ \times \mathbb{R})$.

The end of the proof uses the exact same arguments as in the proof of the Perron–Frobenius property in the non-cylindrical case (Proposition 1.17) and, consequently, this ends the proof of Proposition 1.23. □

6.2.3. *Proof of Theorem 1.18.* First, using the results of the previous Section, we have

$$\ker(\mathfrak{L}_Q)_{|L^2_-(\mathbb{R}^3)} = \ker(\mathfrak{L}_Q)_{|L^2_{+,+,-}(\mathbb{R}^3)} = \operatorname{span}\{\partial_z Q\}$$

and $\mathfrak{L}_Q \partial_x Q \equiv \mathfrak{L}_Q \partial_y Q \equiv 0$. But now Q is furthermore *cylindrical-even*, thus $\partial_x Q = \frac{x}{r}\partial_r Q \in L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \left\{Y_1^+\right\}$ and $\partial_y Q = \frac{y}{r}\partial_r Q \in L^2_+(\mathbb{R}_+ \times \mathbb{R}) \otimes \left\{Y_1^-\right\}$, which implies that $\mathfrak{L}_1^+ \partial_r Q \equiv 0$. Then, $Q > 0$ being *cylindrical-even strictly decreasing*, $\partial_r Q < 0$ on $\mathbb{R}_+ \times \mathbb{R}$ and, by the Perron–Frobenius property (Proposition 1.23), it is (up to sign) the unique eigenvector associated with the lowest eigenvalue of $\mathfrak{L}_1^+$, namely $\lambda_0^1 = 0$. Consequently, $\partial_x Q$ (resp. $\partial_y Q$) is the unique eigenvector — up, in addition, to rotations in the cylindrical plane — associated with the lowest eigenvalue $\lambda_0^{1,+} = 0$ (resp. $\lambda_0^{1,-} = 0$) of $\mathfrak{L}_{1,+}^+$ (resp. $\mathfrak{L}_{1,-}^+$). To summarize, we know at this point that

$$\ker \mathfrak{L}_Q = \operatorname{span}\left\{\partial_x Q, \partial_y Q, \partial_z Q\right\} \oplus \ker(\mathfrak{L}_Q)_{|L^2_{\mathrm{rad},+}(\mathbb{R}^3)} \oplus \bigoplus_{\substack{n\geqslant 2\\ \sigma=\pm}} \ker(\mathfrak{L}_Q)_{|L^2_+(\mathbb{R}_+\times\mathbb{R})\otimes\{Y_n^\sigma\}},$$

and we have to deal with the higher orders. The end of the paper is devoted to the proof that

$$\ker \mathfrak{L}_{n,\sigma}^+ = \{0\}, \quad \forall n \geqslant 2, \sigma = \pm. \tag{1.44}$$

For $n \geqslant 2$, let $0 < \varphi^n \in L^2_+(\mathbb{R}_+ \times \mathbb{R})$ be an eigenvector of $\mathfrak{L}_n^+$ associated with λ_0^n. Then $\varphi^n Y_n^+$ (resp. $\varphi^n Y_n^-$) is an eigenvector of $\mathfrak{L}_{n,+}^+$ (resp. $\mathfrak{L}_{n,-}^+$) associated to the eigenvalue $\lambda_0^{n,+} = \lambda_0^n$ (resp. $\lambda_0^{n,-} = \lambda_0^n$). Thus, for $n \geqslant 2$ and $\sigma = \pm$, we have

$$\begin{aligned}
&\lambda_0^{1,\sigma} - \lambda_0^{n,\sigma} \\
&\quad \leqslant \left\langle \varphi^n, \mathfrak{L}_1^+ \varphi^n \right\rangle_{L^2(\mathbb{R}_+\times\mathbb{R})} - \left\langle \varphi^n, \mathfrak{L}_n^+ \varphi^n \right\rangle_{L^2(\mathbb{R}_+\times\mathbb{R})} \\
&\quad \leqslant -\int_{\mathbb{R}_+\times\mathbb{R}} \frac{n^2-1}{r^2} \left(\varphi^n(r,z)\right)^2 r \,\mathrm{d}r\,\mathrm{d}z \\
&\qquad + 2 \iint_{(\mathbb{R}_+\times\mathbb{R})^2} [Q\varphi^n](r,z)[Q\varphi^n](r',z')\left[v_n - v_1\right](r,r',z-z') r r' \,\mathrm{d}z\,\mathrm{d}z'\,\mathrm{d}r\,\mathrm{d}r'.
\end{aligned}$$

Since $Q > 0$ and $\varphi^n > 0$ (by the Perron–Frobenius property in Proposition 1.23), in order to prove that $\lambda_0^{n,\sigma} > \lambda_0^{1,\sigma}$, it is sufficient to prove that $v_n < v_1$ almost everywhere on $(\mathbb{R}_+ \times \mathbb{R})^2$. Using the explicit formula (1.34) for V, this is equivalent to prove that

$$T_n := \int_0^\pi \frac{\cos(n\theta) - \cos\theta}{\sqrt{K + 2a_2^2 r r'(1-\cos\theta)}} \,\mathrm{d}\theta < 0,$$

for a.e. $(r,z), (r',z') \in (\mathbb{R}_+ \times \mathbb{R})^2$, where $K = |(1-S)^{-1}(r-r',0,z-z')|^2$ and $a_2 = 1 - s_2$ (where we recall that s_2 is the second largest eigenvalue of S).

First, let us remark that the points $\left\{2\frac{k}{n-1}\pi\right\}_{k\in\mathbb{Z}}$ and $\left\{2\frac{k}{n+1}\pi\right\}_{k\in\mathbb{Z}}$ are the zeros of $\cos(n\cdot)-\cos(\cdot)$ and that the function

$$g=\left[K+2(1-s_2)^{-2}rr'(1-\cos(\cdot))\right]^{-1/2}$$

is strictly decreasing on $]0,\pi[$. Let us define, $\theta_{2\lfloor n/2\rfloor}:=\pi$ and, for k an integer in $[0,\lfloor n/2\rfloor-1]$, $\theta_{2k}:=2\frac{k}{n-1}\pi$ and $\theta_{2k+1}:=2\frac{k+1}{n+1}\pi$ which are all the zeros of $\cos(n\cdot)-\cos(\cdot)$ in $[0,\pi]$, except $\theta_{2\lfloor n/2\rfloor}$ if n is even. Then, noticing that $\cos(n\cdot)-\cos(\cdot)$ is strictly negative on intervals $]\theta_{2k},\theta_{2k+1}[$, strictly positive on intervals $]\theta_{2k+1},\theta_{2k+2}[$ and that $n\theta_{2k}=2k\pi+\theta_{2k}$, we have

$$\begin{aligned}T_n&=\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor-1}\int_{\theta_{2k}}^{\theta_{2k+1}}\underbrace{g(\theta)}_{>g(\theta_{2k+1})>0}\underbrace{(\cos(n\theta)-\cos\theta)}_{<0}\,\mathrm{d}\theta+\int_{\theta_{2k+1}}^{\theta_{2k+2}}\underbrace{g(\theta)}_{0<\cdot<g(\theta_{2k+1})}\underbrace{(\cos(n\theta)-\cos\theta)}_{>0}\,\mathrm{d}\theta\\&<\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor-1}g(\theta_{2k+1})\int_{\theta_{2k}}^{\theta_{2k+2}}(\cos(n\theta)-\cos\theta)\ \mathrm{d}\theta.\end{aligned}$$

If $n=2$ or $n=3$, this immediately leads to $T_n<0$. Otherwise, if $n\geqslant 4$, we have

$$\begin{aligned}T_n&<\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor-1}g(\theta_{2k+1})\int_{\theta_{2k}}^{\theta_{2k+2}}(\cos(n\theta)-\cos\theta)\ \mathrm{d}\theta\\&<-\frac{n-1}{n}\left(\sum_{k=0}^{\lfloor\frac{n}{2}\rfloor-2}g(\theta_{2k+1})\sin\theta_{2k+2}-\sum_{k=1}^{\lfloor\frac{n}{2}\rfloor-1}g(\theta_{2k+1})\sin\theta_{2k}\right)\\&<-\frac{n-1}{n}\sum_{k=1}^{\lfloor\frac{n}{2}\rfloor-1}\underbrace{\left[g(\theta_{2k-1})-g(\theta_{2k+1})\right]}_{>0}\underbrace{\sin\theta_{2k}}_{>0}<0.\end{aligned}$$

Thus we have just proved, for $n\geqslant 2$ and $\sigma=\pm$, that $\lambda_0^{n,\sigma}>\lambda_0^{1,\sigma}=0$, consequently $\ker\mathfrak{L}^+_{n,\sigma}=\{0\}$.

This concludes the proof of Theorem 1.18. $\square$

7. Appendix

This appendix is devoted to the proof of the existence of minimizers and of two technical results used in the core of the paper.

7.1. Proof of Theorem 1.5. This follows from Lions' concentration-compactness method [**Lio84a, Lio84b**] that we will present in another way, following [**Lew10**].

Preliminary results. To overcome the lack of radially decreasing properties, we need to introduce the largest possible mass of weak limits of any sequence $\{\psi_n\}$ bounded in $L^2(\mathbb{R}^3)$, up to subsequences and space translations. Let $\boldsymbol{\psi} = \{\psi_n\}$ be a bounded sequence in $L^2(\mathbb{R}^d)$, we define the following number

$$\mathbf{m}(\boldsymbol{\psi}) = \sup_{\psi} \int_{\mathbb{R}^d} |\psi|^2 \ , \tag{1.45}$$

where the sup is taken over the functions ψ for which there exist a sequence $\{x_k\} \subset \mathbb{R}^d$ and a subsequence ψ_{n_k} of ψ_n such that $\psi_{n_k}(\cdot + x_k) \rightharpoonup \psi$ weakly in $L^2(\mathbb{R}^d)$.

We first give an estimate that we will need later and a characterization of being of null highest local mass.

Lemma 1.25 (A subcritical estimate). *Let $\boldsymbol{\psi} = \{\psi_n\}$ be a bounded sequence in $H^1(\mathbb{R}^d)$, with $d \geqslant 3$. Then there exists a constant C_d, independent of $\boldsymbol{\psi}$, such that*

$$\limsup_{n\to\infty} \int_{\mathbb{R}^d} |\psi_n|^{2+\frac{4}{d}} \leqslant C_d \mathbf{m}(\boldsymbol{\psi})^{\frac{2}{d}} \limsup_{n\to\infty} \|\psi_n\|^2_{H^1(\mathbb{R}^d)}.$$

Proof of Lemma 1.25. The proof is essentially due to Lions (see [**Lio84b**]). Let us consider the tiling $C_z = \prod_{j=1}^{d} [z_j, z_j + 1)$ of the whole space $\mathbb{R}^d = \bigcup_{z\in\mathbb{Z}^d} C_z$. By Hölder's inequality on each C_z, we obtain that

$$\int_{\mathbb{R}^d} |\psi_n|^q = \sum_{z\in\mathbb{Z}^d} \int_{C_z} |\psi_n|^q \leqslant \sum_{z\in\mathbb{Z}^d} \|\psi_n\|^{q\theta}_{L^2(C_z)} \|\psi_n\|^{q(1-\theta)}_{L^{p^\star}(C_z)} ,$$

where $p^\star = 2 + 4/(d-2)$ and $1/q = \theta/2 + (1-\theta)/p^\star$. We now choose $q(1-\theta) = 2$, for which $q = 2 + 4/d$. Then, by the Sobolev embeddings, in each C_z, one gets

$$\|\psi_n\|^2_{L^{p^\star}(C_z)} \leqslant C_d \left(\|\psi_n\|^2_{L^2(C_z)} + \|\nabla\psi_n\|^2_{L^2(C_z)} \right) ,$$

with C_d being independent of z. This finally leads to

$$\int_{\mathbb{R}^d} |\psi_n|^{2+\frac{4}{d}} \leqslant C_d \left(\sup_{z\in\mathbb{Z}^d} \|\psi_n\|^2_{L^2(C_z)} \right)^{\frac{2}{d}} \|\psi_n\|^2_{H^1(\mathbb{R}^d)} .$$

Passing now to the limit, we obtain

$$\limsup_{n\to\infty}\int_{\mathbb{R}^d}|\psi_n|^{2+\frac{4}{d}} \leqslant C_d\left(\limsup_{n\to\infty}\sup_{z\in\mathbb{Z}^d}\|\psi_n\|^2_{L^2(C_z)}\right)^{\frac{2}{d}}\limsup_{n\to\infty}\|\psi_n\|^2_{H^1(\mathbb{R}^d)}. \quad (1.46)$$

Let $\{z_n\}\subset\mathbb{R}^d$ be such that

$$\lim_{n\to\infty}\int_{C_{z_n}}|\psi_n|^2 = \limsup_{n\to\infty}\sup_{z\in\mathbb{Z}^d}\int_{C_z}|\psi_n|^2.$$

Then, $\{\psi_n\}$ being bounded in $H^1(\mathbb{R}^d)$, $\{\psi_n(\cdot+z_n)\}$ is bounded too and there exists a subsequence such that $\psi_{n_k}(\cdot+\ z_{n_k})\rightharpoonup\psi$ weakly in $H^1(\mathbb{R}^d)$. But, by the Rellich-Kondrachov Theorem [**LL01**, Section 8.9], this convergence is strong in $L^2(C_0)$ and finally

$$\begin{aligned}\limsup_{n\to\infty}\sup_{z\in\mathbb{Z}^d}\int_{C_z}|\psi_n|^2 = \lim_{n\to\infty}\int_{C_{z_n}}|\psi_n|^2 &= \lim_{n_k\to\infty}\int_{C_0}|\psi_{n_k}(\cdot+z_{n_k})|^2 \\ &= \int_{C_0}|\psi|^2 \leqslant \int_{\mathbb{R}^d}|\psi|^2 \leqslant \mathbf{m}(\boldsymbol{\psi}).\end{aligned} \quad (1.47)$$

This concludes the proof of Lemma 1.25. □

LEMMA 1.26 (Characterization of null mass). *Let $\boldsymbol{\psi}=\{\psi_n\}$ be a bounded sequence in $H^1(\mathbb{R}^d)$, with $d\geqslant 3$. The following assertions are equivalent:*

i. $\mathbf{m}(\boldsymbol{\psi})=0$*;*

ii. $\lim_{n\to\infty}\sup_{z\in\mathbb{Z}^d}\int_{C_z}|\psi_n|^2=0$*;*

iii. $\forall\, R>0,\ \lim_{n\to\infty}\sup_{x\in\mathbb{R}^d}\int_{B(x,R)}|\psi_n|^2=0$*;*

iv. $\psi_n\to 0$ *strongly in* $L^p(\mathbb{R}^d)$ *for all* $p\in]2,p^\star[$*, with* $p^\star=2d/(d-2)$ *.*

PROOF OF LEMMA 1.26. We will follow the proof in [**Lew10**]. First, if $\mathbf{m}(\boldsymbol{\psi})=0$, then the estimate (1.47) leads to

$$\limsup_{n\to\infty}\sup_{z\in\mathbb{Z}^d}\int_{C_z}|\psi_n|^2=0,$$

hence *ii.* and *i.*⇒*ii.* is proved.

Second, if *ii.* holds true, then the estimate (1.46) gives

$$\|\psi_n\|_{L^{2+\frac{4}{d}}(\mathbb{R}^d)}\underset{n\to\infty}{\longrightarrow}0.$$

Since, by the Sobolev embedding, $\{\psi_n\}$ is bounded in $L^p(\mathbb{R}^d)$ for any $p\in[2,p^\star]$, we conclude that *ii.*⇒*iv.* by Hölder's inequality.

Suppose now that *iv.* holds true. Let $\{x_{n_k}\} \subset \mathbb{R}^d$ and ψ be such that $\psi_{n_k}(\cdot + x_{n_k}) \rightharpoonup \psi$ weakly in $H^1(\mathbb{R}^d)$. Since for any $2 < p < p^\star$, we have

$$\|\psi_{n_k}(\cdot + x_{n_k})\|_{L^p(\mathbb{R}^d)} = \|\psi_{n_k}\|_{L^p(\mathbb{R}^d)} \to 0,$$

then $\psi_{n_k}(\cdot + x_{n_k}) \to 0$ strongly in $L^p(\mathbb{R}^d)$. Then, by uniqueness of the weak-limit, we obtain $\psi = 0$ hence $\mathbf{m}(\boldsymbol{\psi}) = 0$ and *iv.*$\Rightarrow$*i.* is proved.

Since any ball of fixed radius R can be covered by a finite union of C_z's, the implication *ii.*$\Rightarrow$*iii.* holds true.

Finally, since the size of the C_z's is fixed, we obtain *iii.*$\Rightarrow$*ii.* by choosing a R large enough. This concludes the proof of Lemma 1.26. $\square$

We now give a lemma which is going to be useful in the proof of the existence of minimizers.

LEMMA 1.27. *Let $p \geqslant 1$. If $f_n \to f$ strongly in $L^p(K)$ for any compact $K \subset \mathbb{R}^3$ and there exists $C > 0$ such that $\|f_n\|_{L^p} \leqslant C$ for all n, then $f_n \rightharpoonup f$ weakly in $L^p(\mathbb{R}^3)$.*

PROOF OF LEMMA 1.27. Let $g \in L^q(\mathbb{R}^3)$ with $1/p + 1/q = 1$. For a given ε, let $R > 0$ be such that $(C + \|f\|_{L^p}) \|g\|_{L^q({}^c B_R)} \leqslant \varepsilon$ and then n be such that $\|f_n - f\|_{L^p(B_R)} \|g\|_{L^q} \leqslant \varepsilon$, by strong convergence. Then

$$\langle f_n - f, g\rangle_{L^p,L^q} \leqslant \|f_n - f\|_{L^p(B_R)} \|g\|_{L^q} + (C + \|f\|_{L^p}) \|g\|_{L^q({}^c B_R)} \leqslant 2\varepsilon.$$

Therefore we have proved the lemma. $\square$

Existence of minimizers. Our strategy to prove the existence of minimizers will be to first prove that

$$\mathscr{E}(\psi_n) - \mathscr{E}(\psi_n - \psi) \underset{n\to\infty}{\longrightarrow} \mathscr{E}(\psi)$$

where ψ is the weak limit in $H^1(\mathbb{R}^3)$ of a minimizing sequence $(\psi_n)_n$. Denoting $\lambda' := \|\psi\|_2^2$, we also know that $\lambda' \leqslant \lambda$ by weak convergence. We will then prove that ψ is a minimizer of $I(\lambda')$ and that $I(\lambda - \lambda') + I(\lambda') = I(\lambda)$, which finally leads to $\lambda' = \lambda$.

We first claim that $\mathbf{m}(\boldsymbol{\psi}) > 0$. Indeed, suppose $\mathbf{m}(\boldsymbol{\psi}) = 0$, then $\psi_n \to 0$ strongly in L^p for any $p \in]2, 6[$ by Lemma 1.26 and in particular in $L^{12/5}$. Consequently, by the Hardy-Littlewood-Sobolev inequality and (1.13), the Coulomb term of $\mathscr{E}$ converges to 0, which leads to $2\mathscr{E}(\psi_n) = \|\nabla\psi_n\|_2^2 + o(1)$. So $I(\lambda) \geqslant 0$, which contradicts Lemma 1.3.

Since $\mathbf{m}(\{\psi_n\}) > 0$, there exist a function $\psi \neq 0$, a sequence $(y_k)_k \subset \mathbb{R}^3$ and a subsequence n_k such that $\psi_{n_k}(\cdot + y_k) \rightharpoonup \psi$ in L^2. The sequence $(\psi_{n_k}(\cdot + y_k))_k$

being also a minimizing sequence, we assume in the following for simplicity of notation that $\psi_n \rightharpoonup \psi \neq 0$ with $\|\psi\|_2^2 = \lambda'$.

We can now prove the following equality:

Lemma 1.28.

$$\mathscr{E}(\psi_n) = \mathscr{E}(\psi) + \mathscr{E}(\psi_n - \psi) + o(1) \tag{1.48}$$

Proof of Lemma 1.28. By weak convergence of $\nabla\psi_n$,

$$\begin{aligned}\|\nabla\psi_n - \nabla\psi\|_2^2 &= \|\nabla\psi_n\|_2^2 + \|\nabla\psi\|_2^2 - 2\Re\langle\nabla\psi_n, \nabla\psi\rangle \\ &= \|\nabla\psi_n\|_2^2 - \|\nabla\psi\|_2^2 + o(1).\end{aligned}$$

We now deal with the coulomb term. We introduce the bilinear form

$$D(f,g) := \frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f(x)g(y)V(x-y)\,\mathrm{d}y\,\mathrm{d}x,$$

and we show that

$$D(|\psi_n|^2, |\psi_n|^2) = D(|\psi|^2, |\psi|^2) + D(|\psi_n - \psi|^2, |\psi_n - \psi|^2) + o(1). \tag{1.49}$$

To do so we give two results of convergence.

Since $\psi_n \rightharpoonup \psi$ weakly in $H^1(\mathbb{R}^3)$, by the Rellich-Kondrachov Theorem [**LL01**, Section 8.9], $|\psi_n|^2 \to |\psi|^2$ strongly in $L^p(K)$ for $1 \leqslant p < 3$ and any compact K. On the other hand, by the Sobolev embeddings, $\||\psi_n|^2\|_{L^p}$ is uniformly bounded for $p \in [1,3]$. With these two properties, by Lemma 1.27, $|\psi_n|^2 \rightharpoonup |\psi|^2$ weakly in $L^p(\mathbb{R}^3)$ for any $1 \leqslant p < 3$.

With the same kind of arguments as in Lemma 1.27, we obtain that $\psi_n\overline{\psi} \to |\psi|^2$ strongly in $L^1(\mathbb{R}^3)$. On the other hand $\left\|\psi_n\overline{\psi} - |\psi|^2\right\|_{L^q} \leqslant \|\psi_n\|_{L^{2q}}\|\psi\|_{L^{2q}} + \|\psi^2\|_{L^q}$, for any $q \in [1,3[$, which is uniformly bounded. Finally, by interpolation, for any $1 \leqslant r \leqslant q < 3$ and $\theta + (1-\theta)/q = 1/r$, we have

$$\left\|\psi_n\overline{\psi} - \psi^2\right\|_{L^r(\mathbb{R}^3)} \leqslant \left\|\psi_n\overline{\psi} - \psi^2\right\|_{L^1(\mathbb{R}^3)}^{\theta}\left\|\psi_n\overline{\psi} - \psi^2\right\|_{L^q(\mathbb{R}^3)}^{1-\theta} \xrightarrow[n\to\infty]{} 0,$$

which means that $\psi_n\overline{\psi} \to |\psi|^2$ strongly in L^p for any $1 \leqslant p < 3$.

We also recall that $|\psi|^2 \star V \in L^4(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ (see (1.13)) and now prove (1.49). First, since $|\psi_n|^2 \rightharpoonup |\psi|^2$ weakly in $L^{4/3}$ and $|\psi|^2 \star V$ is in L^4, one has

$$\int_{\mathbb{R}^3} |\psi_n|^2(|\psi|^2 \star V) \to \int_{\mathbb{R}^3} |\psi|^2(|\psi|^2 \star V).$$

This leads to

$$D(|\psi_n|^2 - |\psi|^2, |\psi_n|^2 - |\psi|^2) - D(|\psi_n|^2, |\psi_n|^2) = D(|\psi|^2, |\psi|^2) - 2D(|\psi_n|^2, |\psi|^2),$$

and consequently to

$$D(|\psi_n|^2 - |\psi|^2, |\psi_n|^2 - |\psi|^2) + D(|\psi|^2, |\psi|^2) - D(|\psi_n|^2, |\psi_n|^2) \xrightarrow[n\to\infty]{} 0.$$

Second, a simple computation gives

$$\frac{1}{4}\left[D(|\psi_n|^2-|\psi|^2,|\psi_n|^2-|\psi|^2)-D(|\psi_n-\psi|^2,|\psi_n-\psi|^2)\right]$$
$$=D(\psi_n\psi-|\psi|^2,\psi_n\psi-|\psi|^2)+D(|\psi|^2-|\psi_n|^2,\psi_n\psi-|\psi|^2).$$

But since $\|\psi_n\psi-|\psi|^2\|_{L^{4/3}}\to 0$ and

$$\left\|(\psi_n\psi-|\psi|^2)\star V\right\|_{L^4}\leqslant\left\|\psi_n\psi-|\psi|^2\right\|_{L^{4/3}}\|V_2\|_{L^2}+\left\|\psi_n\psi-|\psi|^2\right\|_{L^1}\|V_4\|_{L^4}\to 0,$$

where $V=V_2+V_4\in L^2(\mathbb{R}^3)+L^4(\mathbb{R}^3)$, we have

$$D(\psi_n\psi-|\psi|^2,\psi_n\psi-|\psi|^2)\leqslant\left\|\psi_n\psi-|\psi|^2\right\|_{L^{4/3}(\mathbb{R}^3)}\left\|(\psi_n\psi-|\psi|^2)\star V\right\|_{L^4(\mathbb{R}^3)}\to 0$$

and

$$D(|\psi|^2-|\psi_n|^2,\psi_n\psi-|\psi|^2)\leqslant\left(\left\||\psi_n|^2\right\|_{L^{4/3}}+\left\||\psi|^2\right\|_{L^{4/3}}\right)\left\|(\psi_n\psi-|\psi|^2)\star V\right\|_{L^4}\to 0.$$

We have finally proved (1.49) which concludes the proof of Lemma 1.28. □

We now prove that ψ is a minimizer of $I(\lambda')$ and that $I(\lambda-\lambda')+I(\lambda')=I(\lambda)$. First, Lemma 1.28 gives, for any n, that

$$\mathscr{E}(\psi_n)\geqslant\mathscr{E}(\psi)+I\left(\|\psi_n-\psi\|_2^2\right)+o(1).$$

Since $\|\psi_n-\psi\|_2^2=\lambda+\lambda'-2\Re\langle\psi_n,\psi\rangle\to\lambda-\lambda'$ and $\lambda\mapsto I(\lambda)$ is continuous, we conclude that

$$I(\lambda-\lambda')+I(\lambda')\leqslant I(\lambda-\lambda')+\mathscr{E}(\psi)\leqslant I(\lambda).$$

On the other hand, by Lemma 1.3, we have the inequality

$$I(\lambda)\leqslant I(\lambda-\lambda')+I(\lambda').$$

This immediately gives

$$I(\lambda-\lambda')+I(\lambda')=I(\lambda) \tag{1.50}$$

and $\mathscr{E}(\psi)=I(\lambda')$, that is, ψ is a minimizer of $I(\lambda')=I\left(\|\psi\|_2^2\right)$.

We now conclude the proof of the existence of minimizers by proving that $\lambda'=\lambda$. By Lemma 1.3 we then have $(\lambda-\lambda')^3+(\lambda')^3=\lambda^3$ which is only possible if $\lambda'=0$ or $\lambda'=\lambda$. Since $\lambda'\neq 0$, we have just proved the existence of minimizers.

Convergence of all the minimizing sequences. The fact that any minimizing sequence strongly converges in $H^1(\mathbb{R}^3)$ to a minimizer follows directly from the following compactness criterion.

LEMMA 1.29 (Compactness criterion). *Let $\{\psi_n\}$ be a minimizing sequence for $I(\lambda)$ such that $\psi_n \rightharpoonup \psi$ weakly in $H^1(\mathbb{R}^3)$. Then*

$$\psi_n \to \psi \text{ strongly in } H^1(\mathbb{R}^3) \Leftrightarrow \int_{\mathbb{R}^3} |\psi|^2 = \lambda.$$

Moreover, if this criterion is verified then ψ is a minimizer of $I(\lambda)$.

PROOF OF LEMMA 1.29. By assumption, for any n, we have $\|\psi_n\|_{L^2}^2 = \lambda$. So if we suppose the strong convergence in $H^1(\mathbb{R}^3)$ of $(\psi_n)_n$, we have $\lambda = \|\psi_n\|_{L^2}^2 \to \|\psi\|_{L^2}^2$.

We now prove the converse implication. For that we will prove that $\mathscr{E}(\psi_n)$ (resp. that the Coulomb term of $\mathscr{E}(\psi_n)$) converges in $L^2(\mathbb{R}^3)$ to $\mathscr{E}(\psi)$ (resp. to the Coulomb term of $\mathscr{E}(\psi_n)$), which implies the same convergence for the kinetic term of $\mathscr{E}(\psi_n)$. Suppose that $\|\psi\|_{L^2}^2 = \lambda$. By the weak convergence $\psi_n \rightharpoonup \psi$ in $L^2(\mathbb{R}^3)$, we have

$$\|\psi_n - \psi\|_{L^2}^2 = \|\psi_n\|_{L^2}^2 + \|\psi\|_{L^2}^2 - 2\Re\langle\psi_n, \psi\rangle = 2\lambda - 2\Re\langle\psi_n, \psi\rangle \to 0.$$

On another hand, by the Sobolev embedding, $\psi_n - \psi$ is bounded in $L^6(\mathbb{R}^3)$, wich leads by interpolation to the strong convergence $\psi_n \to \psi$ in $L^p(\mathbb{R}^3)$ for any $p \in [2, 6[$ and in particular in $L^{12/5}(\mathbb{R}^3)$. Since $|\int_{\mathbb{R}^3} f\,(g \star V)| \leqslant C\,\|f\|_{L^{6/5}}\,\|g\|_{L^{6/5}}$ for any $f, g \in L^{6/5}(\mathbb{R}^3)$ (by the Hardy-Littlewood-Sobolev inequality and (1.13)), the Coulomb term of $\mathscr{E}$ is then continuous for the strong topology of $L^{12/5}(\mathbb{R}^3)$ and

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} |\psi_n(x)|^2 \left(|\psi_n|^2 \star V\right)(x)\,\mathrm{d}x = \int_{\mathbb{R}^3} |\psi(x)|^2 \left(|\psi|^2 \star V\right)(x)\,\mathrm{d}x. \tag{1.51}$$

Secondly, we have $\lim_{n\to\infty} \|\nabla\psi_n\|_{L^2}^2 \geqslant \|\nabla\psi\|_{L^2}^2$ by the weak convergence $\nabla\psi_n \rightharpoonup \nabla\psi$ in $L^2(\mathbb{R}^3)$. This, combined with (1.51) and recalling that $\{\psi_n\}$ is a minimizing sequence of $I(\lambda)$, leads to

$$I(\lambda) \geqslant \lim_{n\to\infty} \mathscr{E}(\psi_n) \geqslant \mathscr{E}(\psi) \geqslant I(\lambda).$$

So we have in fact an equality between the three terms and, combining this again with (1.51), leads to $\|\nabla\psi_n\|_{L^2} \to \|\nabla\psi\|_{L^2}$. We finally obtain the strong convergence $\nabla\psi_n \to \nabla\psi$ in $L^2(\mathbb{R}^3)$ recalling that we had the weak convergence already. $\square$

We now prove the remaining properties. Let ψ be a minimizer of $I(\lambda)$.

Proof that ψ is an $H^2(\mathbb{R}^3)$-solution of (1.3). We first show that it is a solution in $H^{-1}(\mathbb{R}^3)$. Let $\chi \in H^1(\mathbb{R}^3)$. For $\varepsilon \in \mathbb{R}$ small enough such that $\|\psi + \varepsilon\chi\|_{L^2(\mathbb{R}^3)} > 0$, we define $\psi_\varepsilon \in H^1(\mathbb{R}^3)$ as

$$\psi_\varepsilon := \sqrt{\lambda}\frac{\psi + \varepsilon\chi}{\|\psi + \varepsilon\chi\|_{L^2(\mathbb{R}^3)}}.$$

Thus $\|\psi_\varepsilon\|_2^2 = \lambda$ and a straightforward computation gives

$$\mathscr{E}(\psi_\varepsilon) = \mathscr{E}(\psi) + \varepsilon\Re\left[\int_{\mathbb{R}^3}\left(-\Delta\overline{\psi} - 2(|\psi|^2 \star V)\overline{\psi} + 2\mu\overline{\psi}\right)\chi\right] + O(\varepsilon^2),$$

with

$$-2\mu := \frac{1}{\lambda}\left(\|\nabla\psi\|_{L^2(\mathbb{R}^3)}^2 - 2\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}|\psi(x)|^2|\psi(y)|^2V(x-y)\,\mathrm{d}y\,\mathrm{d}x\right).$$

Replacing χ by $\mathrm{i}\chi$, we get the same result except for having the imaginary part instead of the real part. Since ψ is a minimizer, we conclude that ψ is a solution of (1.3) in $H^{-1}(\mathbb{R}^3)$.

Since $|\psi|^2 \star V \in L^4(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, the Rellich-Kato Theorem [**RS75**, Section X.12] implies that H_ψ is self-adjoint with domain $H^2(\mathbb{R}^3)$. Moreover,

$$|\langle\psi, H_\psi\varphi\rangle| = |\langle\mu\psi, \varphi\rangle| \leqslant |\mu|\,\|\varphi\|_{L^2}\,\|\psi\|_{L^2}$$

for any $\varphi \in H^2(\mathbb{R}^3)$. Thus $\psi \in D(H_\psi^\star) = D(H_\psi) = H^2(\mathbb{R}^3)$ and we conclude that $\psi \in H^2(\mathbb{R}^3)$.

Proof that $\boldsymbol{\mu = -\frac{d}{d\lambda}I(\lambda) > 0}$ and norms equalities. Let ψ be a minimizer of $I(\lambda)$, then for any $\varepsilon \in (-1,1)$,

$$\mathscr{E}(\sqrt{1+\varepsilon}\psi) = \mathscr{E}(\psi) - \varepsilon\mu\lambda + O(\varepsilon^2).$$

Moreover, by Lemma 1.3, one has $I((1+\varepsilon)\lambda) = I(\lambda)(1+3\varepsilon) + O(\varepsilon^2)$ thus

$$0 \leqslant \mathscr{E}(\sqrt{1+\varepsilon}\psi) - I((1+\varepsilon)\lambda) = -\varepsilon\left(\mu\lambda + 3I(\lambda)\right) + O(\varepsilon^2),\ \text{for any } \varepsilon \in (-1,1).$$

Then, sending ε to 0^+ and 0^-, we obtain $\mu\lambda = -3I(\lambda)$ and Lemma 1.3 leads to $\mu = -3\lambda^2 I(1) = -\frac{d}{d\lambda}I(\lambda) > 0$. Thus, ψ being a minimizer and a solution of (1.3), we have

$$\|\nabla\psi\|_2^2 - 2\left\langle V \star |\psi|^2, |\psi|^2\right\rangle = -2\mu\lambda = 6I(\lambda) = 3\|\nabla\psi\|_2^2 - 3\left\langle V \star |\psi|^2, |\psi|^2\right\rangle.$$

This gives (1.17).

Proof that $|\boldsymbol{\psi}|$ is a minimizer and $|\boldsymbol{\psi}| > \mathbf{0}$. Since

$$\|\nabla|\varphi|\|_{L^2(\mathbb{R}^3)} \leqslant \|\nabla\varphi\|_{L^2(\mathbb{R}^3)}\,,$$

for any $\varphi \in H^1(\mathbb{R}^3)$, and ψ being a minimizer, it is straightforward that $|\psi|$ is also a minimizer. Consequently $|\psi|$ is a $H^2(\mathbb{R}^3)$-solution of (1.3) with the same μ. Moreover, $0 \not\equiv |\psi| \in H^2(\mathbb{R}^3)$, since $0 \not\equiv \psi$, and $W := -2|\psi|^2 \star V + 2\mu \in L^\infty(\mathbb{R}^3)$. We then use the following lemma to conclude that $|\psi| > 0$.

LEMMA 1.30. *Let $W \in L^1_{loc}(\mathbb{R}^3)$ such that there exists $C \in \mathbb{R}$ such that $W \leqslant C$. If $0 \not\equiv \varphi \in H^2(\mathbb{R}^3)$ is such that $\varphi \geqslant 0$ and $(-\Delta + W)\varphi \geqslant 0$ then $\varphi > 0$.*

REMARK 1.31. This lemma is of course a special case of [**LL01**, Theorem 9.10] or of results in [**RS78**, Section XIII.12] but we give here a more adapted and easier version.

PROOF OF LEMMA 1.30. Let $\kappa^2 > \max(C, 0)$. We define $0 \leqslant (-\Delta + \kappa^2)\varphi := g \in L^2(\mathbb{R}^3)$ because $\varphi \in H^2(\mathbb{R}^3)$. But $g \geqslant (\kappa^2 - C)\varphi \not\equiv 0$ and so $g \not\equiv 0$. Since $\hat{\varphi} = (|k|^2 + \kappa^2)^{-1}\hat{g}$ and using Yukawa's formula giving the inverse Fourier transform of $k \mapsto (|k|^2 + \kappa^2)^{-1}$, one obtains $\varphi(x) = (4\pi)^{-1}\int_{\mathbb{R}^3} e^{-\kappa|x-y|}|x-y|^{-1}g(y)\,\mathrm{d}y$ and finally $\varphi > 0$. □

Proof that $-\boldsymbol{\mu}$ is the lowest eigenvalue, $\boldsymbol{\psi} = \boldsymbol{z}|\boldsymbol{\psi}|$ and $-\boldsymbol{\mu}$ is simple. Those results come from the following lemma.

LEMMA 1.32. *Let $H = -\Delta + W$ with $W \in L^\infty(\mathbb{R}^3)$ with a strictly negative lower eigenvalue ν. Then ν is simple and the associated eigenfunction φ_ν is strictly positive up to a phase vector.*

Moreover, for any $0 \not\equiv u \geqslant 0$ and λ such that $Hu = \lambda u$, then $\lambda = \nu$.

PROOF OF LEMMA 1.32. Given that $W \in L^\infty(\mathbb{R}^3)$, H is self-adjoint with domain $H^2(\mathbb{R}^3)$. Thus $0 \not\equiv \varphi_\nu \in H^2(\mathbb{R}^3)$ and $\langle H|\varphi_\nu|, |\varphi_\nu|\rangle \leqslant \langle H\varphi_\nu, \varphi_\nu\rangle$. Moreover, since

$$\nu = \inf_{\varphi\in D, \|\varphi\|=1} \langle H\varphi, \varphi\rangle,$$

$|\varphi_\nu|$ is also a ground state of H and Lemma 1.30 gives that $|\varphi_\nu| > 0$.

Let suppose there exist two strictly positive normalized distinct ground states ψ_A et ψ_B of H. Then $\psi_A - \psi_B$ is also a ground state of H and, as before, $|\psi_A - \psi_B|$ too thus $|\psi_A - \psi_B| > 0$ everywhere. So either $\psi_A > \psi_B$ everywhere or $\psi_A < \psi_B$ everywhere. But this contradicts the fact that they are both normalized. We conclude that $|\varphi_\nu| / \|\varphi_\nu\|_2$ is the unique normalized strictly positive ground state.

If φ_ν is real valued (resp. purely imaginary valued), since $|\varphi_\nu| > 0$ and φ_ν is continuous ($H^2(\mathbb{R}^3) \hookrightarrow C^0(\mathbb{R}^3)$), we have $\varphi_\nu = \pm|\varphi_\nu|$ (resp. $\varphi_\nu = \pm\mathrm{i}|\varphi_\nu|$).

Otherwise, let us define $\psi_r \not\equiv 0$ and $\psi_i \not\equiv 0$ real valued such that $\varphi_\nu = \psi_r + \mathrm{i}\psi_i$. The operator H being real, $H\psi_r = \nu\psi_r$ and $H\psi_i = \nu\psi_i$ hold. Thus, as for $|\varphi_\nu|$ just above, $|\psi_r| > 0$ and $|\psi_i| > 0$ are two strictly positive ground states and consequently $|\psi_r| \propto |\psi_i| > 0$, by uniqueness of normalized strictly positive ground states. Moreover, since ψ_r and ψ_i are continuous (by continuity of φ_ν), $\psi_r = \pm|\psi_r|$ and $\psi_i = \pm|\psi_i|$. This leads to $\varphi_\nu = z|\varphi_\nu|$ and to the fact that ν is simple.

Let $0 \not\equiv u \geqslant 0$ and λ such that $Hu = \lambda u$. Since $|\varphi_\nu| > 0$ and $u \geqslant 0$ are two eigenfunctions, they are eigenfunctions of the same eigenvalue otherwise they should be orthogonal. Thus $\lambda = \nu$ and so $u \propto |\varphi_\nu| > 0$. □

Applying the second part of this lemma to $-\mu$ and its eigenfunction $|\psi| > 0$, we obtain that $-\mu$ is the lowest eigenvalue of H_ψ and is simple. Then, the first part of the lemma gives $\psi = z|\psi|$.

This concludes the proof ot Theorem 1.5. □

7.2. Compactness of the operator $\partial_\psi G(Q, s\cdot\mathbf{Id}) - 1$. The following lemma states the compactness result asserted in the proof of Theorem 1.7.

LEMMA 1.33. *Let V be given by* (1.14) *or* (1.15)*, $\psi \in H^1(\mathbb{R}^3)$ and $\mu > 0$. Then $\xi \mapsto (-\Delta + \mu)^{-1}\left[-\left(|\psi|^2 \star V\right)\xi - 2\psi\left((\psi\xi) \star V\right)\right]$ is a compact operator on $L^2(\mathbb{R}^3)$.*

PROOF. Since $|\psi|^2 \star V \in L^4(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$ and $(\mu + |\cdot|^2)^{-1} \in L^{3/2+\varepsilon}(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, by [**RS79**, Theorem XI.20], the operator $(-\Delta + \mu)^{-1}|\psi|^2 \star V$ is compact on $L^2(\mathbb{R}^3)$. For the second term, we first prove the following lemma:

LEMMA 1.34. *Let $1 \leqslant p, q, r < \infty$ such that $1 + 1/r = 1/p + 1/q$. If $f_n \rightharpoonup 0$ weakly in $L^p(\mathbb{R}^3)$ and $g \in L^q(\mathbb{R}^3)$ then $f_n \star g \to 0$ in $L^r_{loc}(\mathbb{R}^3)$.*

PROOF OF LEMMA 1.34. Since f_n converges weakly in $L^p(\mathbb{R}^3)$, f_n is bounded in $L^p(\mathbb{R}^3)$. Let B_R be a fixed ball of $\mathbb{R}^3$, and let $\varepsilon > 0$. Let $g' \in C^\infty_c(\mathbb{R}^3)$ be such that $\|g - g'\|_{L^q} \leqslant \varepsilon$. Since $g' \in C^\infty_c(\mathbb{R}^3) \subset L^{p'}(\mathbb{R}^3)$, we have $\int g'(x) f_n(y-x)\,\mathrm{d}x \to 0$ a.e.. Applying the dominated convergence theorem to $(\mathbb{1}_{B_R}(f_n \star g'))^r$, we obtain that $f_n \star g' \to 0$ in $L^r_{loc}(\mathbb{R}^3)$. Thus, for n big enough

$$\|f_n \star g\|_{L^r_{loc}} \leqslant \|f_n \star g'\|_{L^r_{loc}} + \|f_n \star (g - g')\|_{L^r_{loc}} \leqslant \varepsilon + \|f_n\|_{L^p}\|g - g'\|_{L^q} \leqslant \varepsilon(1 + C).$$

□

Since

$$\left\|\left|(\mu - \Delta)^{-1}\right|\right\|_{L^2 \to L^2} \leqslant \max\{1, \mu^{-1}\},$$

it then suffices to prove that $\xi \to \psi(\psi\xi_n) \star V$ is a compact operator on $L^2(\mathbb{R}^3)$ in order to prove that $(\mu - \Delta)^{-1}\xi \to \psi(\psi\xi_n) \star V$ is also a compact operator on

$L^2(\mathbb{R}^3)$. Let $\xi_n \rightharpoonup 0$ weakly in $L^2(\mathbb{R}^3)$. Since $\psi \in L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$, we have $\psi\xi_n \rightharpoonup 0$ weakly in $L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$ and then, given that $V \in L^2(\mathbb{R}^3) + L^4(\mathbb{R}^3)$, we have $\|(\psi\xi_n) \star V\|_{L^4} \leqslant C$ for all n. Then, using Lemma 1.34, we have

$$\begin{aligned}\|\psi(\psi\xi_n) \star V\|_{L^2} &\leqslant \|\mathbb{1}_{B_R}\psi(\psi\xi_n) \star V\|_{L^2} + \left\|\mathbb{1}_{B_R^c}\psi(\psi\xi_n) \star V\right\|_{L^2} \\ &\leqslant \|\psi\|_{L^4} \|(\psi\xi_n) \star V\|_{L^4_{loc}} + C\left\|\mathbb{1}_{B_R^c}\psi\right\|_{L^4}.\end{aligned}$$

Consequently, for any given ε, choosing the radius R of the B_R and n both big enough, we have $\|\psi(\psi\xi_n) \star V\|_{L^2} \leqslant \varepsilon$, thus $\|\psi(\psi\xi_n) \star V\|_{L^2} \to 0$. This concludes the proof of the Lemma 1.33. □

7.3. Real analicity of minimizers. We prove here Lemma 1.12.

Proof of Lemma 1.12. The function ψ is continuous and bounded since it belongs to $H^2(\mathbb{R}^3)$. Then the equation (1.3) and elliptic regularity give $\psi \in C^\infty(\mathbb{R}^3)$.

We define $V_\psi^A = 1/|A\cdot| \star |\psi|^2$, for any $\psi \in H^2(\mathbb{R}^3)$ and $A = \mathrm{diag}(a_1, a_2, a_3) > 0$ and have $-4\pi|\psi|^2 = \Delta V_\psi^{Id}$ and $V_\psi^{Id}(A\cdot) = \det(A) V^A_{\psi\circ A}$, thus, with $B = A^{-1}$,

$$\begin{aligned}-4\pi|\psi|^2 = -4\pi|\psi \circ B|^2(A\cdot) &= \sum_{i=1}^3 \partial_i^2 \left(V^{Id}_{\psi\circ B}\right)(A\cdot) \\ &= \sum_{i=1}^3 a_i^{-2}\partial_i^2\left[V^{Id}_{\psi\circ B}(A\cdot)\right] = \det(A)\sum_{i=1}^3 a_i^{-2}\partial_i^2 V_\psi^A.\end{aligned}$$

Noticing that $V_M = V_\psi^{Id} - V_\psi^M$, this yields

$$\begin{pmatrix} -\Delta & 0 & 0 \\ 0 & -\Delta & 0 \\ 0 & 0 & -\sum\limits_{i=1}^3 \varepsilon_i^{-2}\partial_i^2 \end{pmatrix}\begin{pmatrix}\psi \\ V_\psi^{Id} \\ V_\psi^M\end{pmatrix} = \begin{pmatrix} -2\mu\psi + 2V_\psi^{Id}\psi - 2V_\psi^M\psi \\ 4\pi\psi^2 \\ 4\pi(\det M)^{-1}\psi^2\end{pmatrix}. \tag{1.52}$$

This also proves that V_ψ^{Id} and V_ψ^M are in $H^2(\mathbb{R}^3) \cap C^\infty(\mathbb{R}^3)$. And we now follow a method (and the notations) of K. Kato in **[Kat96]** to prove that ψ, V_ψ^{Id} and V_ψ^M are analytic.

Let B and B' be open balls such that $\overline{B} \subset B'$ and $\overline{B'} \subset \mathbb{R}^3$, and r a *cut-off* function: $r \in C_c^\infty(\mathbb{R}^3)$ such that $0 \leqslant r \leqslant 1$, $\mathrm{supp}(r) \subset B'$ and $r \equiv 1$ on $\overline{B}$. We show by induction on $|\alpha|$ that there exist $A, C > 0$ such that $(H_{|\alpha|})$ holds for any multi-index α, where

$$(H_{|\alpha|}) : \max\left\{\left\|r^{|\alpha|}\partial^\alpha\psi\right\|_{H^2(B')}, \left\|r^{|\alpha|}\partial^\alpha V_\psi^{Id}\right\|_{H^2(B')}, \left\|r^{|\alpha|}\partial^\alpha V_\psi^M\right\|_{H^2(B')}\right\} \leqslant CA^{|\alpha|}|\alpha|!$$

In addition to some results of **[Kat96]**, we will need the following generalization of Proposition 2.3 in Kato's paper.

Lemma 1.35. *Let Ω be a domain of $\mathbb{R}^3$ and $a_1 \geqslant a_2 \geqslant a_3 \geqslant 1$. Then*

$$\|\partial^\alpha v\|_{H^2(\Omega)} \leqslant a_1^2 \left\| \sum_{k=1}^{3} a_k^{-2} \partial_k^2 v \right\|_{H^2(\Omega)}$$

holds for any $v \in H_0^4(\Omega)$ and any multi-index α such that $|\alpha| = 2$.

Proof of Lemma 1.35. Adapting the proof in [**Kat96**], from Plancherel's theorem and for any $v \in C_0^\infty(\Omega)$ and $i, j \in \{1,2,3\}$, we have

$$\begin{aligned}\|\partial_{ij} v\|_{H^2(\Omega)} &= a_i a_j \left\| \left(1 + |\xi|^2\right) a_i^{-1} \xi_i a_j^{-1} \xi_j \hat{v}(\xi) \right\|_{L^2(\mathbb{R}^3)} \\ &\leqslant a_1^2 \left\| \left(1 + |\xi|^2\right) \hat{v}(\xi) \sum_{k=1}^{3} a_k^{-2} \xi_k^2 \right\|_{L^2(\mathbb{R}^3)} = a_1^2 \left\| \sum_{k=1}^{3} a_k^{-2} \partial_k^2 v \right\|_{H^2(\Omega)}.\end{aligned}$$

□

Let $A \geqslant 1$ be an arbitrary constant, there exists a constant C such that, for $|\alpha| \leqslant 1$, we have

$$\max\left\{ \left\| r^{|\alpha|} \partial^\alpha \psi \right\|_{H^2(B')}, \left\| r^{|\alpha|} \partial^\alpha V_\psi^{Id} \right\|_{H^2(B')}, \left\| r^{|\alpha|} \partial^\alpha V_\psi^{M} \right\|_{H^2(B')} \right\} \leqslant C \leqslant C A^{|\alpha|} |\alpha|!.$$

We now suppose that $(H_{|\gamma|})$ holds for any γ such that $|\gamma| \leqslant n$. For shortness we will denote in the following $\|\cdot\| := \|\cdot\|_{H^2(B')}$. Let $|\alpha| = n - 1$ and $|\beta| = 2$.

Let $u \in H^2(\mathbb{R}^3) \cap C^\infty(\mathbb{R}^3)$ such that $\left\| r^{|\gamma|} \partial^\gamma u \right\| \leqslant C A^{|\gamma|} |\gamma|!$ for any $|\gamma| \leqslant n$. Then, using Proposition 2.2 of [**Kat96**], one has

$$\begin{aligned}&\left\| r^{n+1} \partial^{\alpha+\beta} u \right\| \\ &\qquad \leqslant \left\| \partial^\beta \left(r^{n+1} \partial^\alpha u \right) \right\| + n(n+1) C_1 \|\partial_i r \partial_j r\| \left\| r^{n-1} \partial^\alpha u \right\| \\ &\qquad\quad + (n+1) C_1 \left[\left\| r \partial^\beta r \right\| \left\| r^{n-1} \partial^\alpha u \right\| + \|\partial_i r\| \|r^n \partial_j \partial^\alpha u\| + \|\partial_j r\| \|r^n \partial_i \partial^\alpha u\| \right] \\ &\qquad \leqslant \left\| \partial^\beta \left(r^{n+1} \partial^\alpha u \right) \right\| + C C_1 A^{n-1} (n+1)! \, \|\partial_i r \partial_j r\| \\ &\qquad\quad + C C_1 A^{n-1} (n-1)! (n+1) \left[\left\| r \partial^\beta r \right\| + A n \left(\|\partial_i r\| + \|\partial_j r\| \right) \right] \\ &\qquad \leqslant \left\| \partial^\beta \left(r^{n+1} \partial^\alpha u \right) \right\| + C C_2 A^n (n+1)!,\end{aligned}$$

where we have used that $A \geqslant 1$ and defined

$$C_2 := \max_{1 \leqslant i,j \leqslant 3} C_1 \left(\|\partial_i r \partial_j r\| + \left\| r \partial^\beta r \right\| + \|\partial_i r\| + \|\partial_j r\| + \left\| r^2 \right\| \right).$$

Then, by Lemma 1.35 and [**Kat96**, Proposition 2.2], we have

$$\begin{aligned}
\left\|\partial^\beta\left(r^{n+1}\partial^\alpha u\right)\right\| &\leqslant \varepsilon_3^2\left\|\sum_{k=1}^3\varepsilon_k^{-2}\partial_k^2\left(r^{n+1}\partial^\alpha u\right)\right\| \\
&\leqslant \varepsilon_3^2\left\|r^{n+1}\partial^\alpha\left(\sum_{k=1}^3\varepsilon_k^{-2}\partial_k^2 u\right)\right\| \\
&\quad + \varepsilon_3^2\sum_{k=1}^3\varepsilon_k^{-2}\big(CA^n(n+1)!C_1\left[\|\partial_k r\partial_k r\| + \left\|r\partial_k^2 r\right\| + 2\|\partial_k r\|\right]\big)
\end{aligned}$$

since

$$\partial_k^2\left(r^{n+1}\partial^\alpha u\right) = r^{n+1}\partial^\alpha\partial_k^2 u+(n+1)\left[nr^{n-1}(\partial_k r)^2\partial^\alpha u + r^n\left(\partial_k^2 r\partial^\alpha u + 2\partial_k r\partial_k\partial^\alpha u\right)\right].$$

Thus, since $\varepsilon_k^{-2}\leqslant\varepsilon_1^{-2}$ and $C_1\left(\|\partial_k r\partial_k r\| + \|r\partial_k^2 r\| + 2\|\partial_k r\|\right)\leqslant C_2$, this leads to

$$\left\|r^{n+1}\partial^{\alpha+\beta}u\right\| \leqslant \varepsilon_3^2\left\|r^{n+1}\partial^\alpha\left(\sum_{k=1}^3\varepsilon_k^{-2}\partial_k^2 u\right)\right\| + \left(1+3\varepsilon_3^2\varepsilon_1^{-2}\right)CC_2A^n(n+1)!$$

And when $\varepsilon_3=\varepsilon_2=\varepsilon_1=1$, we have

$$\left\|r^{n+1}\partial^{\alpha+\beta}u\right\| \leqslant \left\|r^{n+1}\partial^\alpha(\Delta u)\right\| + 4CC_2A^n(n+1)!$$

Thanks to (1.52), we will conclude, using the following lemma, by applying the above results to u being ψ, V_ψ^{Id} or V_ψ^M.

LEMMA 1.36. *For any multi-index α, we have $\sum_{\gamma\leqslant\alpha}\binom{\alpha}{\gamma}|\gamma|!|\alpha-\gamma|! = (|\alpha|+1)!$.*

PROOF OF LEMMA 1.36. Using [**Kat96**, Proposition 2.1] and $|\alpha-\gamma| = ||\alpha|-|\gamma||$, one has

$$\sum_{\gamma\leqslant\alpha}\binom{\alpha}{\gamma}|\gamma|!|\alpha-\gamma|! = \sum_{k=0}^{|\alpha|}\sum_{\gamma\leqslant\alpha,|\gamma|=k}\binom{\alpha}{\gamma}|\alpha|!\binom{|\alpha|}{|\gamma|}^{-1} = \sum_{k=0}^{|\alpha|}|\alpha|! = (|\alpha|+1)!.$$

□

We first treat V_ψ^M (and $V_\psi^{M=Id}$), using Proposition 2.2 of [**Kat96**]. We have

$$\begin{aligned}
\det M\left\|r^{n+1}\partial^\alpha\left(\sum_{k=1}^3\varepsilon_k^{-2}\partial_k^2 V_\psi^M\right)\right\| &= 4\pi\left\|r^{n+1}\partial^\alpha(|\psi|^2)\right\| \\
&= 4\pi\left\|r^2\sum_{\gamma\leqslant\alpha}\binom{\alpha}{\gamma}r^{|\gamma|}\partial^\gamma\psi r^{|\alpha-\gamma|}\partial^{\alpha-\gamma}\overline{\psi}\right\|,
\end{aligned}$$

hence

$$\begin{aligned}\det M \left\| r^{n+1}\partial^\alpha \left(\sum_{k=1}^{3} \varepsilon_k^{-2}\partial_k^2 V_\psi^M \right) \right\| &\leqslant 4\pi C^2 C_1^2 \left\| r^2 \right\| \sum_{\gamma\leqslant\alpha} \left(\binom{\alpha}{\gamma} A^{|\gamma|}|\gamma|! A^{|\alpha-\gamma|}|\alpha-\gamma|! \right) \\ &\leqslant 4\pi C^2 C_1^2 \left\| r^2 \right\| A^{n-1} n! \\ &\leqslant 4\pi C^2 C_1 C_2 A^n (n+1)!.\end{aligned}$$

Thus

$$\left\| r^{n+1}\partial^{\alpha+\beta} V_\psi^M \right\| \leqslant C \left[\left(1 + 3\frac{\varepsilon_3^2}{\varepsilon_1^2} + \frac{4\pi\varepsilon_3^2 C C_1}{\det M} \right) C_2 \right] A^n (n+1)!.$$

Finally, if $A \geqslant \max\left\{1, 4C_2(1+\pi C C_1), C_2\left(1 + 3\frac{\varepsilon_3^2}{\varepsilon_1^2} + \frac{4\pi\varepsilon_3^2 C C_1}{\det M}\right)\right\}$,

$$\left\| r^{|\gamma|}\partial^\gamma V_\psi^M \right\|_{H^2(B')} \leqslant C A^{|\gamma|}|\gamma|! \quad \text{and} \quad \left\| r^{|\gamma|}\partial^\gamma V_\psi^{Id} \right\|_{H^2(B')} \leqslant C A^{|\gamma|}|\gamma|!,$$

for any γ such that $|\gamma| = n+1$.

We now deal with ψ. Similar computations give

$$\begin{aligned}\frac{1}{2}\left\| r^{n+1}\partial^\alpha (\Delta\psi) \right\| &\leqslant |\mu| \left\| r^{n+1}\partial^\alpha\psi \right\| + \left\| r^{n+1}\partial^\alpha (V_\psi^{Id}\psi) \right\| + \left\| r^{n+1}\partial^\alpha (V_\psi^M\psi) \right\| \\ &\leqslant |\mu| C_1 \left\| r^2 \right\| C A^{|\alpha|}|\alpha|! + 2C^2C_1^2 \left\| r^2 \right\| A^{|\alpha|}|\alpha|! \\ &\leqslant (|\mu| + 2CC_1)\, C C_2 A^n (n+1)!,\end{aligned}$$

thus

$$\left\| r^{n+1}\partial^{\alpha+\beta}\psi \right\| \leqslant 2\,(2 + |\mu| + 2CC_1)\, C C_2 A^n (n+1)!.$$

Finally, $(H_{|\gamma|})$ holds for any γ such that $|\gamma| = n+1$, if

$$A \geqslant \max\left\{1, 4C_2(1+\pi CC_1), 2(2+|\mu|+2CC_1)C_2, C_2\left(1 + 3\frac{\varepsilon_3^2}{\varepsilon_1^2} + \frac{4\pi\varepsilon_3^2 CC_1}{\det M}\right)\right\}.$$

This concludes the induction and the proof of Lemma 1.12. $\square$

PARTIE 2

Symmetry breaking in the periodic TFDW model

Ce chapitre est une version plus détaillée d'un article soumis

Julien Ricaud, *Symmetry Breaking in the Periodic Thomas-Fermi-Dirac-Von Weizsäcker Model*, ArXiv:1703.07284 (2017).

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.

Contents

1. Introduction

Symmetry breaking is a fundamental question in Physics which is largely discussed in the literature. In this second part of the thesis, 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

$$\int_{\mathbb{K}} |\nabla\sqrt{\rho}|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{K}} \rho^{\frac{5}{3}} - \frac{3}{4}c\int_{\mathbb{K}} \rho^{\frac{4}{3}} + \frac{1}{2}\int_{\mathbb{K}} (G\star\rho)\rho - \int_{\mathbb{K}} G\rho, \tag{2.1}$$

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 [**GS94, Fri97, BM99, BGM03, Sei06**] 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 second part of the thesis, 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 [**Le 93**] in the whole space.

The main novelty of this part of the thesis, is the regime of large c. The $\rho^{\frac{4}{3}}$ term in (2.1) favours concentration and we will prove that the electronic density concentrates at some points in the unit cell $\mathbb{K}$ in the limit $c \to \infty$ (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:

$$J_{\mathbb{R}^3}(\lambda) = \inf_{\substack{v\in H^1(\mathbb{R}^3)\\ \|v\|^2_{L^2(\mathbb{R}^3)}=\lambda}} \left\{\int_{\mathbb{R}^3} |\nabla v|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{R}^3} |v|^{\frac{10}{3}} - \frac{3}{4}\int_{\mathbb{R}^3} |v|^{\frac{8}{3}}\right\}. \tag{2.2}$$

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 (2.2) 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 second part of the thesis 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 [**Dir30**] in 1930 using an infinite non-interacting Fermi gas leading to the value $c_D := \sqrt[3]{6q^{-1}\pi^{-1}}$, where q is the number of spin states. For the spinless model (i.e. $q = 1$) that we are studying, this gives $c_D \approx 1.24$, which corresponds to the constant 0.93 generally appearing in the literature, namely, $\frac{3}{4}c_D \approx 0.93$. It is natural to use a constant $c > c_D$ in order to account for correlation effects. On the other hand, the famous Lieb-Oxford inequality [**Lie79, LO80, KH99, LS10**] suggests to take $\frac{3}{4}c_D \leqslant 1.64$. It has been argued in [**Per91, PW92, LP93**] 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 [**PBE96**]. However, this has recently been questioned in [**LL15**] by Lewin and Lieb. In any case, all physically reasonable choices lead to c of the order of 1.

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

There exist various works on the TFDW model for N electrons on the whole space $\mathbb{R}^3$. For example, Le Bris proved in [**Le 93**] that there exists $\varepsilon > 0$ such that minimizers exist for $N < Z + \varepsilon$, improving the result for $N \leqslant Z$ by Lions [**Lio87**]. It is also proved in [**Le 93**] that minimizers are unique for c small enough if $N \leqslant Z$. Non existence if N is large enough and Z small enough has been proved by Nam and Van Den Bosch in [**NVDB17**].

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 [**Frö54, Pei55**] while [**KL86, Lie86, KL87, LN95b, LN95a, LN96, FL11, GAS12**] 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 [**PN01**] for a one dimensional gas on a circle of finite length and in [**Pro05**] on toruses and spheres in dimension $d \leqslant 3$. On the whole space $\mathbb{R}^3$, symmetry breaking is proved in [**BG16**], namely, the minimizers are not radial for N large enough.

This part of the thesis 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. The Appendix collects some detailed proofs and some technical results.

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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 $\mathscr{L}_{\mathbb{K}}$ our lattice which is based on the natural basis $(\boldsymbol{e_1}, \boldsymbol{e_2}, \boldsymbol{e_3})$ 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 in this second part of the thesis is then the functional energy

$$\mathscr{E}_{\mathbb{K},c}(w) = \int_{\mathbb{K}} |\nabla w|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{K}} |w|^{\frac{10}{3}} - \frac{3}{4}c\int_{\mathbb{K}} |w|^{\frac{8}{3}} + \frac{1}{2}D_{\mathbb{K}}(|w|^2, |w|^2) - \int_{\mathbb{K}} G_{\mathbb{K}}|w|^2, \tag{2.3}$$

on the unit cell $\mathbb{K}$. Here

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

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

$$-\Delta G_{\mathbb{K}} = 4\pi\left(\sum_{k\in\mathscr{L}_{\mathbb{K}}}\delta_k - 1\right) \tag{2.4}$$

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

$$E_{\mathbb{K},\lambda}(c) = \inf_{\substack{w\in H^1_{\mathrm{per}}(\mathbb{K})\\ \|w\|^2_{L^2(\mathbb{K})}=\lambda}} \mathscr{E}_{\mathbb{K},c}(w), \tag{2.5}$$

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 [**CLL98**]), we study it for any λ.

Finally, for any $N \in \mathbb{N}\backslash\{0\}$, 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

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

2.1. Symmetry breaking. The main results presented in this second part of the thesis are the two following theorems.

THEOREM 2.1 (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 $0 \leqslant c < \delta$, the following holds:*

i. The minimizer w_c of the periodic TFDW problem $E_{\mathbb{K},\lambda}(c)$ in (2.5) *is* unique, *up to a phase factor. It is non constant, positive, in $H^2_{per}(\mathbb{K})$ and the unique ground-state eigenfunction of the $\mathbb{K}$-periodic self-adjoint operator*

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

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

THEOREM 2.2 (Symmetry breaking for large c). *Let $\mathbb{K}$ be the unit cube, c_{TF}, λ be two positive constants, and $N \geqslant 2$ be an integer. For c large enough, symmetry breaking occurs:*

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

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

$$c_n{}^{-\frac{3}{2}} w_{c_n}\left(R + \frac{\cdot}{c_n}\right) \underset{n\to\infty}{\longrightarrow} Q, \tag{2.6}$$

strongly in $L^p_{loc}(\mathbb{R}^3)$ for $2 \leqslant p < +\infty$, 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

$$J_{\mathbb{R}^3}(N^3\lambda) = \inf_{\substack{u\in H^1(\mathbb{R}^3)\\ \|u\|^2_{L^2(\mathbb{R}^3)}=N^3\lambda}} \left\{\int_{\mathbb{R}^3} |\nabla u|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{R}^3} |u|^{\frac{10}{3}} - \frac{3}{4}\int_{\mathbb{R}^3} |u|^{\frac{8}{3}}\right\}, \tag{2.7}$$

which must additionally minimize

$$S(N^3\lambda) = \inf_v \left\{\frac{1}{2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{|v(x)|^2|v(y)|^2}{|x-y|}\, dy\, dx - \int_{\mathbb{R}^3} \frac{|v(x)|^2}{|x|}\, dx\right\}, \tag{2.8}$$

where the minimization is performed among all possible minimizers of (2.7)*. Finally, when $c \to \infty$, $E_{N\cdot\mathbb{K},N^3\lambda}(c)$ has the expansion*

$$E_{N\cdot\mathbb{K},N^3\lambda}(c) = c^2 J_{\mathbb{R}^3}(N^3\lambda) + cS(N^3\lambda) + o(c). \tag{2.9}$$

Theorem 2.1 will be proved in Section 4 while Section 5 will be dedicated to the proof of Theorem 2.2. A natural question that comes with Theorem 2.2 is to know if c needs to be really large for the symmetry breaking to happen. We present some numerical answers to this question later in Section 2.3. Notice that the inequality $E_{N\cdot\mathbb{K},N^3\lambda}(c) < N^3 E_{\mathbb{K},\lambda}(c)$ in Theorem 2.2 is an immediate consequence of the first order expansion in (2.9)

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

which is proved in Proposition 2.37, since one has $J_{\mathbb{R}^3}(N^3\lambda) < N^3 J_{\mathbb{R}^3}(\lambda)$ as it will be proved in Proposition 2.16 of Section 3.

REMARK (Generalizations). For simplicity we have chosen to deal with a cubic lattice with one nucleus of charge 1 per unit cell, but the exact same results hold in a more general situation. We can take a charge Z larger than 1, several charges (of different values) per unit cell and a more general lattice than $\mathbb{Z}^3$. More precisely, the $\mathbb{K}$-periodic Coulomb potential $G_{\mathbb{K}}$ appearing in (2.3), in both $D_{\mathbb{K}}$ and $\int G|w|^2$, should then verify

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

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 and the charges and locations of the N_q nuclei in the unit cell $\mathbb{K}$ which can defined by three linearly independent vectors $(\boldsymbol{e_1}, \boldsymbol{e_2}, \boldsymbol{e_3})$.

Finally, in Theorem 2.2, denoting by $z_+ := \max_{1\leqslant i\leqslant N_q}\{z_i\} > 0$ the largest charge inside $\mathbb{K}$ and by $N_+ \geqslant 1$ 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

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

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

The functional to be considered is

$$u \mapsto \mathscr{J}_{\mathbb{R}^3}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{3}{5} c_{TF} \int_{\mathbb{R}^3} |u|^{\frac{10}{3}} - \frac{3}{4}\int_{\mathbb{R}^3} |u|^{\frac{8}{3}} \tag{2.10}$$

and the minimization problem (2.7) is

$$J_{\mathbb{R}^3}(\lambda) = \inf_{\substack{u\in H^1(\mathbb{R}^3)\\ \|u\|^2_{L^2(\mathbb{R}^3)}=\lambda}} \mathscr{J}_{\mathbb{R}^3}(u). \tag{2.11}$$

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

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

$$-\Delta Q + c_{TF}|Q|^{\frac{4}{3}}Q - |Q|^{\frac{2}{3}}Q = -\mu Q. \tag{2.12}$$

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

$$\forall\, 0 < \lambda' < \lambda, \qquad J_{\mathbb{R}^3}(\lambda) < J_{\mathbb{R}^3}(\lambda') + J_{\mathbb{R}^3}(\lambda - \lambda'). \tag{2.13}$$

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 (2.12) for any admissible $\mu > 0$. The proof of this theorem is the subject of Section 3.2.

THEOREM 2.4 (Uniqueness and non-degeneracy of positive solutions). *Let $c_{TF} > 0$. If $\frac{64}{15}c_{TF}\mu \geqslant 1$, then the Euler–Lagrange equation (2.12) has no non-trivial solution in $H^1(\mathbb{R}^3)$. For $0 < \frac{64}{15}c_{TF}\mu < 1$, the Euler–Lagrange equation (2.12) has, up to translations, a unique nonnegative solution $Q_\mu \not\equiv 0$ in $H^1(\mathbb{R}^3)$. This solution is radial decreasing and non-degenerate: the linearized operator*

$$L_\mu^+ = -\Delta + \frac{7}{3}c_{TF}|Q_\mu|^{\frac{4}{3}} - \frac{5}{3}|Q_\mu|^{\frac{2}{3}} + \mu \tag{2.14}$$

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

$$\operatorname{Ker} L_\mu^+ = \operatorname{span}\{\partial_{x_1}Q_\mu, \partial_{x_2}Q_\mu, \partial_{x_3}Q_\mu\}. \tag{2.15}$$

Note that the condition $\frac{64}{15}c_{TF}\mu \geqslant 1$ comes directly from Pohozaev's identity, see, e.g., [**BL83**, p. 318].

REMARK. The linearized operator L_μ for the Euler–Lagrange equation (2.12) 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 (2.14) while L_μ^- is the operator

$$L_\mu^- = -\Delta + c_{TF}|Q_\mu|^{\frac{4}{3}} - |Q_\mu|^{\frac{2}{3}} + \mu = H_{Q_\mu} + \mu. \tag{2.16}$$

The result about the lowest eigenvalue of the operator H_Q in Theorem 2.3 exactly gives that $\operatorname{Ker} L_\mu^- = \operatorname{span}\{Q_\mu\}$. Hence, Theorem 2.4 implies that

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

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 [**Lie77, TM99, Len09, FL13, FLS16, Ric16**]. An argument of this type relies on the fact that $\mu \mapsto M(\mu) := \|Q_\mu\|^2_{L^2(\mathbb{R}^3)}$ is a bijection, which is an easy result for models with trivial scalings like the non-linear Schrödinger equation with only one power nonlineartity. However, for the effective problem of this section, we are unable to prove that this mapping is a bijection.

In [**KOPV17**], 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

$$\int_{\mathbb{R}^3} \frac{1}{2}|\nabla u|^2 + \frac{1}{6}|u|^6 - \frac{1}{4}|u|^4. \tag{2.17}$$

They discussed at length the question of uniqueness of minimizers and could also not solve it for their model. An important difference between (2.17) 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 [**KOPV17**, 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 $(0; \frac{15}{64 c_{TF}})$ 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 2.5. *Let $\lambda > 0$ and $c_{TF} > 0$. There exist finitely many μ's for which the mass $M(\mu)$ of Q_μ is equal to λ.*

Proof of Proposition 2.5. By Theorem 2.3, we know that for any mass constraint $\lambda \in (0, +\infty)$, there exist at least one minimizer to the corresponding $J_{\mathbb{R}^3}(\lambda)$ minimization problem. Therefore, for any $\lambda \in (0, +\infty)$, there exists at least one μ such that the unique positive solution Q_μ to the associated Euler–Lagrange equation is a minimizer of $J_{\mathbb{R}^3}(\lambda)$ and thus is of mass $M(\mu) = \lambda$. We therefore obtain that $\left(0; \frac{15}{64 c_{TF}}\right) \ni \mu \mapsto M(\mu) \in (0; +\infty)$ is onto. Moreover, this map is real-analytic since the non-degeneracy in Theorem 2.4 and the analytic implicit function theorem give that $\mu \mapsto Q_\mu$ is real analytic. The map M being onto and real-analytic, then for any $\lambda \in (0;+\infty)$ there exists a finite number of μ's, which are all in $\left(0; \frac{15}{64c_{TF}}\right)$, 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 4.

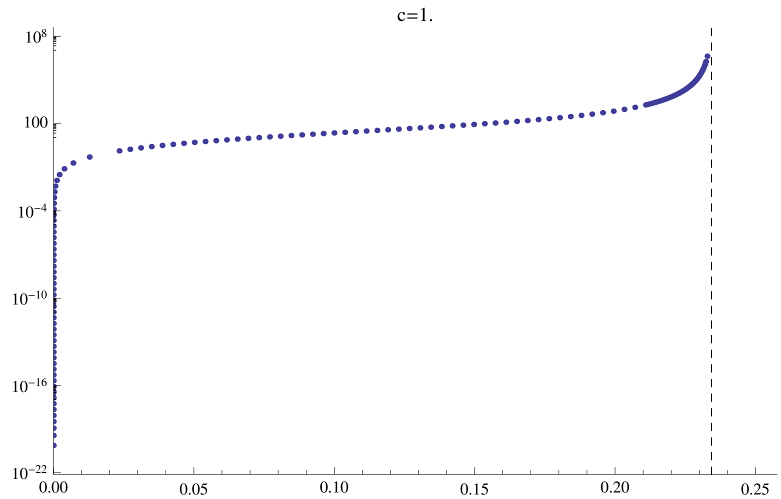


FIGURE 4. Plot of $\mu \mapsto \ln(M(\mu))$ on $\left(0; \frac{15}{64c_{TF}}\right)$.

CONJECTURE 2.6. The function

$$\begin{aligned} \left(0; \frac{15}{64c_{TF}}\right) &\to (0;+\infty) \\ \mu &\mapsto M(\mu) \end{aligned} \tag{2.18}$$

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

REMARK. Following the method of [**KOPV17**], one can prove there exist $C, C' > 0$ such that $M(\mu) = C\mu^{\frac{3}{2}} + o(\mu^{\frac{3}{2}})_{\mu\to 0^+}$ and $M(\mu) = C'(\mu-\mu_*)^{-3} + o\left((\mu-\mu_*)^{-3}\right)_{\mu\to\mu_*^-}$ where $\mu_* = \frac{15}{64c_{TF}}$.

REMARK 2.7. It should be possible to show that the energy $\mu \mapsto \mathscr{J}_{\mathbb{R}^3}(Q_\mu)$ 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 2.12) 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 lambda except at these finitely many points.

This conjecture on M is related to the stability condition on $(L_\mu^+)^{-1}$ that appears in works like [**Wei85, GSS87**]. Indeed, differentiating the Euler–Lagrange equation (2.12) with respect to μ, we obtain that $L_\mu^+(\frac{\mathrm{d}Q_\mu}{\mathrm{d}\mu}) = -Q_\mu$ which thus leads to

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

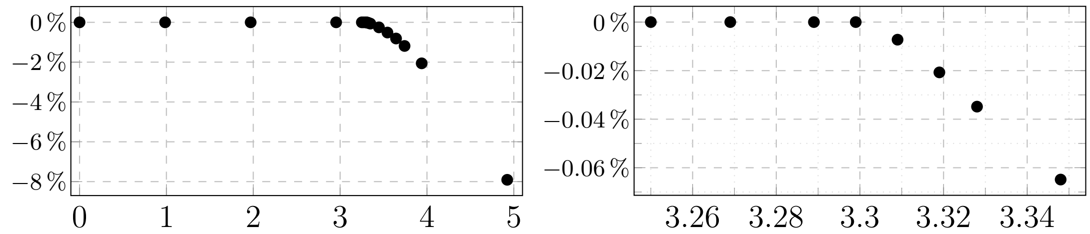
Thus our conjecture is that $\langle Q_\mu, \left(L_\mu^+\right)^{-1} Q_\mu\rangle < 0$ for all $0 < \mu < \frac{15}{64 c_{TF}}$ and this corresponds to the fact that all the solutions are local strict minimizers.

THEOREM 2.8. *If Conjecture 2.6 holds then, in the case of one charge per unit cell ($N_q = 1$) and 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 2.8 is the subject of Section 5.4.

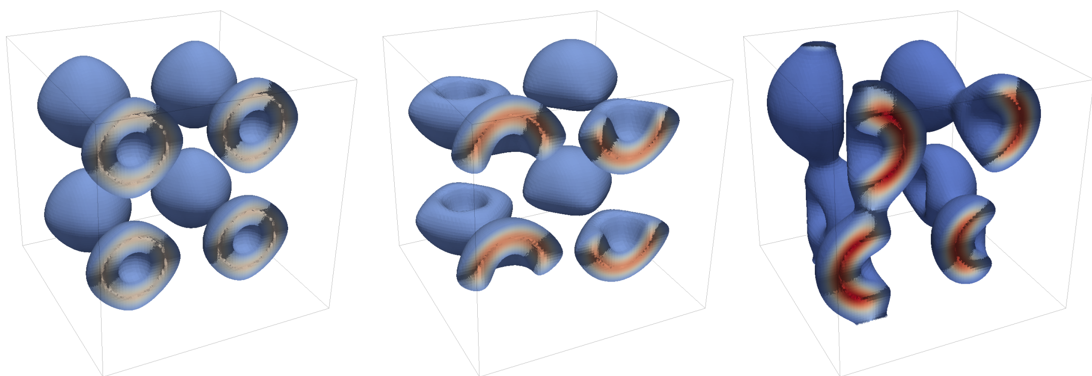
2.3. Numerical simulations. The occurrence of symmetry breaking is an important question in practical calculations. Concerning the general behavior of DFT on this matter, we refer to the discussion in [**SLHG99**] and the references therein.

Our numerical simulations have been run using the software *PROFESS v.3.0* [**CXH$^+$15**] which is based on pseudo-potentials (see Remark 2.9 below): we have used a (BCC) Lithium crystal of side-length 4Å (in order to be physically relevant as the two first alkali metals Lithium and Sodium organize themselves on BCC lattices with respective side length 3.51Å and 4.29Å) for which one electron is treated while the two others are included in the pseudo-potential, simulating therefore a lattice of pseudo-atoms with pseudo-charge $Z = \lambda = 1$. The relative gain of energy of 2-periodic minimizers compared to 1-periodic ones is plotted in Figure 5. Symmetry breaking occurs at about $c \approx 3.30$ which corresponds to $\frac{3}{4}c \approx 2.48$. More precisely, minimizing the $2\cdot\mathbb{K}$ problem and the $1\cdot\mathbb{K}$ problem result in the same minimum energy (up to a factor 8) if $c \lesssim 3.30$ while, for $c \gtrsim 3.31$, we have found (at least) one 2-periodic function for which the energy is lower than the minimal energy for the $1\cdot\mathbb{K}$ problem.



(a) $0 \leqslant c \leqslant 5$ (b) Zoom: $3.25 \leqslant c \leqslant 3.35$

FIGURE 5. Relative gain of energy $\frac{8E_{\mathbb{K},\lambda}(c)-E_{2\cdot\mathbb{K},8\lambda}(c)}{8E_{\mathbb{K},\lambda}(c)}$.



(a) $c = 3.35c_D \approx 3.30$ (b) $c = 3.36c_D \approx 3.31$ (c) $c = 3.50c_D \approx 3.45$

FIGURE 6. Electron density for $Z = 1$ and length side 4Å. Same "dark-blue to white to dark-red" density scale for (a), (b) and (c).
(a) The computed 2-periodic minimizer is still 1-periodic.
(b-c) The computed 2-periodic minimizer is not 1-periodic.

The plots of the computed minimizers presented in Figure 6 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 2.9 (Pseudo-potentials). The software *PROFESS v.3.0* that we used in our simulations is based on pseudo-potentials [**Joh73**]. 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 $-\int_{\mathbb{K}} G_{\rm ps}|w|^2$ where the $\mathbb{K}$-periodic function $G_{\rm ps}(x)$ behaves like $n/|x|$ when $|x| \to 0$. All our results apply to this case as well. More precisely, we only need that $G_{\rm ps}(x) - n/|x|$ 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 2.3 and Theorem 2.4. Since some steps of Theorem 2.3 (for example in the proof of Corollary 2.16) have to be proved for a slightly generalized model, we prove the whole theorem for such a generalized model. The generalization consists in the presence of the coefficient $c \geqslant 0$ in front of the non-convex term:

$$u \mapsto \mathscr{J}_{\mathbb{R}^3,c}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{R}^3} |u|^{\frac{10}{3}} - \frac{3}{4}c\int_{\mathbb{R}^3} |u|^{\frac{8}{3}} \tag{2.19}$$

and the minimization problem is then

$$J_{\mathbb{R}^3,c}(\lambda) = \inf_{\substack{u\in H^1(\mathbb{R}^3)\\ \|u\|^2_{L^2(\mathbb{R}^3)}=\lambda}} \mathscr{J}_{\mathbb{R}^3,c}(u). \tag{2.20}$$

The associated Euler–Lagrange equation in Theorem 2.3 obviously becomes

$$-\Delta Q + c_{TF}|Q|^{\frac{4}{3}}Q - c|Q|^{\frac{2}{3}}Q = -\mu Q, \quad \text{ in } H^{-1}(\mathbb{R}^3). \tag{2.21}$$

We first give a lemma on the functional $\mathscr{J}_{\mathbb{R}^3,c}$

LEMMA 2.10. *For $c \geqslant 0$, $c_{TF}, \lambda > 0$ and $u \in H^1(\mathbb{R}^3)$ such that $\|u\|_2^2 = \lambda$, we have*

$$\mathscr{J}_{\mathbb{R}^3,c}(u) \geqslant \|\nabla u\|^2_{L^2(\mathbb{R}^3)} - \frac{15}{64}\frac{\lambda}{c_{TF}}c^2. \tag{2.22}$$

REMARK 2.11. One can obtain a bound independent of c_{TF}: for any $a < 1$,

$$\mathscr{J}_{\mathbb{R}^3,c}(u) \geqslant a\,\|\nabla u\|^2_{L^2(\mathbb{R}^3)} - \frac{9\lambda^{\frac{5}{3}}{S_3}^2}{64(1-a)}c^2$$

where S_3 the Sobolev constant $\|u\|_{L^6(\mathbb{R}^3)} \leqslant S_3\,\|\nabla u\|_{L^2(\mathbb{R}^3)}$. See the proof in Section 6.3.

PROOF OF LEMMA 2.10. By Hölder's inequality

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

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

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

$\square$

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

Lemma 2.12 (A priori properties of $J_{\mathbb{R}^3,c}(\lambda)$). *Let $c_{TF}>0$, $c\geqslant 0$ and $\lambda>0$ be constants. We have*

$$-\frac{15}{64}\frac{\lambda}{c_{TF}}c^2 < J_{\mathbb{R}^3,c}(\lambda) = c^2 J_{\mathbb{R}^3,1}(\lambda) < 0. \tag{2.23}$$

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

Proof of Lemma 2.12. Let u be in the minimizing domain. Then, for any $\nu>0$, $\nu^{-\frac{3}{2}}u(\nu^{-1}\cdot)$ belongs to the minimizing domain too and

$$\mathscr{J}_{\mathbb{R}^3,c}(\nu^{-\frac{3}{2}}u(\nu^{-1}\cdot)) = \nu^{-2}\left(\int_{\mathbb{R}^3}|\nabla u|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{R}^3}|u|^{\frac{10}{3}} - \frac{3}{4}\nu c\int_{\mathbb{R}^3}|u|^{\frac{8}{3}}\right)$$

which is strictly negative for ν large enough since $c>0$, hence $J_{\mathbb{R}^3,c}(\lambda)<0$. Lemma 2.10 gives the lower bound in (2.23), which implies the continuity at $\lambda=0$. Moreover, after scaling, we have

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

where F is concave on $[0;+\infty)$, hence continuous on $(0;+\infty)$ on which it is also negative (because $J_{\mathbb{R}^3}$ is negative) and increasing. The continuity of F gives that $\lambda\mapsto J_{\mathbb{R}^3,c}(\lambda)$ is continuous as well. Moreover, if f is a concave non-decreasing negative function, we claim that $\lambda\mapsto\lambda f(\lambda^{2/3})$ is concave on $(0,\infty)$, which proves that our energy J is concave. To prove the claim we can regularize f by means of a convolution and then compute its second derivative, leading to

$$J'_{\mathbb{R}^3,c}(\lambda) = F(\lambda^{-2/3}) - \frac{2}{3}\lambda^{-2/3}F'(\lambda^{-2/3}) < 0, \qquad \forall\lambda>0,$$

and

$$J''_{\mathbb{R}^3,c}(\lambda) = -\frac{2}{9}\lambda^{-5/3}F'(\lambda^{-2/3}) + \frac{4}{9}\lambda^{-7/3}F''(\lambda^{-2/3}) \leqslant 0, \qquad \forall \lambda > 0.$$

$\square$

3.1. Proof of Theorem 2.3. We divide the proof into several steps for clarity.

Step 1: Large binding inequality.

LEMMA 2.13. *Let $c_{TF} \geqslant 0$ and $c > 0$ be constants. Then*

$$J_{\mathbb{R}^3,c}(\lambda) \leqslant J_{\mathbb{R}^3,c}(\lambda') + J_{\mathbb{R}^3,c}(\lambda - \lambda'), \qquad \forall\ 0 \leqslant \lambda' \leqslant \lambda. \tag{2.24}$$

PROOF OF LEMMA 2.13. To prove (2.24), let us fix $\varepsilon > 0$. By density of $C_c^\infty(\mathbb{R}^3)$ in $H^1(\mathbb{R}^3)$ and the continuity of $u \mapsto \mathscr{J}_{\mathbb{R}^3,c}(u)$ in $H^1(\mathbb{R}^3)$, let φ and χ be in $C_c^\infty(\mathbb{R}^3)$, respectively such that $\mathscr{J}_{\mathbb{R}^3,c}(\varphi) \leqslant J_{\mathbb{R}^3,c}(\lambda') + \varepsilon$, with $\|\varphi\|^2_{L^2(\mathbb{R}^3)} = \lambda'$, and $\mathscr{J}_{\mathbb{R}^3,c}(\chi) \leqslant J_{\mathbb{R}^3,c}(\lambda - \lambda') + \varepsilon$, with $\|\chi\|^2_{L^2(\mathbb{R}^3)} = \lambda - \lambda'$. Let $0 \neq v \in \mathbb{R}^3$ and define $u_R := \varphi + \chi(\cdot + Rv)$. Choose R large enough such that the supports of φ and $\chi(\cdot + Rv)$ are disjoints. Thus

$$\|u_R\|^2_{L^2(\mathbb{R}^3)} = \|\varphi + \chi(\cdot + Rv)\|^2_{L^2(\mathbb{R}^3)} = \|\varphi\|^2_{L^2(\mathbb{R}^3)} + \|\chi(\cdot + Rv)\|^2_{L^2(\mathbb{R}^3)} = \lambda.$$

So u_R belongs to the minimizing domain of $J_{\mathbb{R}^3,c}(\lambda)$. Moreover, since the supports are disjoint, we obtain that $\mathscr{J}_{\mathbb{R}^3,c}(u_R) = \mathscr{J}_{\mathbb{R}^3,c}(\varphi) + \mathscr{J}_{\mathbb{R}^3,c}(\chi)$. Thus

$$J_{\mathbb{R}^3,c}(\lambda) \leqslant \mathscr{J}_{\mathbb{R}^3,c}(u_R) = \mathscr{J}_{\mathbb{R}^3,c}(\varphi) + \mathscr{J}_{\mathbb{R}^3,c}(\chi) \leqslant J_{\mathbb{R}^3,c}(\lambda') + J_{\mathbb{R}^3,c}(\lambda - \lambda') + 2\varepsilon.$$

This concludes the proof of (2.24). $\square$

REMARK 2.14. The strict inequality in (2.24), which is important for applying Lions' concentration-compactness method, actually holds and is proved later in Proposition 2.16.

REMARK 2.15. The fact that $\lambda \mapsto J_{\mathbb{R}^3,c}(\lambda)$ is strictly decreasing on $[0; +\infty)$, proved in Lemma 2.12, also can be deduced directly (and only) from (2.24) and the strict negativity of $J_{\mathbb{R}^3,c}(\lambda)$.

Step 2: For any $\lambda, c > 0$, $J_{\mathbb{R}^3,c}(\lambda)$ has a minimizer. First, by rearrangement inequalities, we have $\mathscr{J}_{\mathbb{R}^3,c}(v) \geqslant \mathscr{J}_{\mathbb{R}^3,c}(v^*)$ for every $v \in H^1(\mathbb{R}^3)$, see [**LL01**, Theorem 7.8 & Lemma 7.17]. Therefore, one can restrict the minimization to nonnegative radial decreasing functions. Any minimizing sequence of nonnegative radial decreasing functions $(Q_n)_n$ is uniformly bounded in $H^1(\mathbb{R}^3)$ due to Lemma 2.10. Consequently, Q_n weakly converges in $H^1(\mathbb{R}^3)$, up to a subsequence, to a nonnegative radial decreasing function Q. Thus, by the compact embedding

$H^1_{rad}(\mathbb{R}^3) \hookrightarrow L^p(\mathbb{R}^3)$, for $2 < p < 6$, and since $\liminf \int_{\mathbb{R}^3} |\nabla Q_n|^2 \geqslant \int_{\mathbb{R}^3} |\nabla Q|^2$, we obtain

$$J_{\mathbb{R}^3,c}(\lambda') \leqslant \mathscr{J}_{\mathbb{R}^3,c}(Q) \leqslant \liminf \mathscr{J}_{\mathbb{R}^3,c}(Q_n) = J_{\mathbb{R}^3,c}(\lambda) \tag{2.25}$$

where $\lambda' := \|Q\|^2_{L^2(\mathbb{R}^3)} \leqslant \lambda$. Then, $\mathscr{J}_{\mathbb{R}^3,c}$ being strictly decreasing by Lemma 2.12, $\lambda' = \lambda$ and the limit is strong in $L^2(\mathbb{R}^3)$. This proves that the limit Q is a minimizer.

Moreover, the strong convergence holds in fact in $H^1(\mathbb{R}^3)$. Indeed, the strong convergence in $L^2(\mathbb{R}^3)$ — together with the Sobolev embeddings and the fact that Q_n is uniformly bounded in $H^1(\mathbb{R}^3)$ — implies the strong convergence in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$. Then, the fact that all terms in (2.25) are in fact equal gives the norm convergence $\|\nabla Q_n\|^2_{L^2(\mathbb{R}^3)} \to \|\nabla Q\|^2_{L^2(\mathbb{R}^3)}$. Together with the weak convergence of ∇Q_n in $L^2(\mathbb{R}^3)$, this leads to the strong convergence of ∇Q_n in $L^2(\mathbb{R}^3)$ and finally to the claimed strong convergence in $H^1(\mathbb{R}^3)$.

Step 3: Any minimizer is in $H^2(\mathbb{R}^3)$ and solves the E-L equation. Let Q be a minimizer. For any $f \in H^1(\mathbb{R}^3)$, we define

$$Q_\varepsilon = \frac{\sqrt{\lambda}}{\|Q + \varepsilon f\|_{L^2(\mathbb{R}^3)}}(Q + \varepsilon f).$$

We obviously have that $Q_\varepsilon \in H^1(\mathbb{R}^3)$ and $\|Q_\varepsilon\|^2_{L^2(\mathbb{R}^3)} = \lambda$. Moreover, Q being a minimizer of $J_{\mathbb{R}^3,c}(\lambda)$, we have $\frac{\mathrm{d}\mathscr{J}_{\mathbb{R}^3,c}}{\mathrm{d}\varepsilon}_{|Q} = 0$. Thus, computing $\mathscr{J}_{\mathbb{R}^3,c}(Q_\varepsilon)$ for f and $\mathrm{i}f$, we obtain that

$$\left\langle \left(-\Delta + c_{TF}|Q|^{4/3} - c|Q|^{2/3} + \mu\right) Q, f \right\rangle_{L^2(\mathbb{R}^3)} = 0,$$

with

$$\mu = -\frac{\|\nabla Q\|^2_{L^2(\mathbb{R}^3)} + c_{TF}\,\|Q\|^{10/3}_{L^{10/3}(\mathbb{R}^3)} - c\,\|Q\|^{8/3}_{L^{8/3}(\mathbb{R}^3)}}{\lambda}. \tag{2.26}$$

Finally, given that $u \in H^1(\mathbb{R}^3)$, equation (2.21) gives $u \in H^2(\mathbb{R}^3)$ by elliptic regularity.

Step 4: Strict binding inequality. As mentioned in Remark 2.14, we in fact have the following strict binding inequality.

PROPOSITION 2.16. *Let $c_{TF} > 0$, $\lambda > 0$ and $c > 0$.*

$$\forall\, 0 < \lambda' < \lambda,\ J_{\mathbb{R}^3,c}(\lambda) < J_{\mathbb{R}^3,c}(\lambda') + J_{\mathbb{R}^3,c}(\lambda - \lambda'). \tag{2.13}$$

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

$$J_{\mathbb{R}^3,c}(N^3\lambda) < N^3 J_{\mathbb{R}^3,c}(\lambda) < 0. \tag{2.27}$$

Proof of Proposition 2.16. By the same scaling as in Lemma 2.12, we have

$$J_{\mathbb{R}^3,c}(\lambda) = \lambda \inf_{\substack{u\in H^1(\mathbb{R}^3)\\ \|u\|^2_{L^2(\mathbb{R}^3)}=1}} \underbrace{\left\{\lambda^{-\frac{2}{3}} \|\nabla u\|^2_{L^2(\mathbb{R}^3)} + \frac{3}{5}c_{TF} \|u\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{R}^3)} - \frac{3}{4}c \|u\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)}\right\}}_{=:\mathscr{F}_\lambda(u)}. \tag{2.28}$$

Let $\lambda > \lambda' > 0$. The minimization problem

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

has by Step 2 — taking $\lambda = 1$ and making the replacements $\frac{3}{5}c_{TF} \leftrightarrow \frac{3}{5}c_{TF}\lambda'^{2/3} > 0$ and $\frac{3}{4} \leftrightarrow \frac{3}{4}\lambda'^{2/3} > 0$ under which the previous steps obviously hold — a minimizer $Q_{\lambda'} \not\equiv 0$ which, by Step 3, is in $H^2(\mathbb{R}^3)$ thus continuous and non constant. In particular, $\|\nabla Q_{\lambda'}\|_{L^2(\mathbb{R}^3)} > 0$ thus $\mathscr{F}_{\lambda'}(Q_{\lambda'}) > \mathscr{F}_\lambda(Q_{\lambda'})$, where $\mathscr{F}_\lambda$ is defined in (2.28). Therefore

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

and we finally obtain

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

as we wanted. □

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

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

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

$$J_{\mathbb{R}^3,c}(\lambda) \leqslant \mathscr{J}_{\mathbb{R}^3,c}\left(\sqrt{\lambda}{\alpha_0}^{3/2}v(\alpha_0\cdot)\right) = -\frac{9}{64}\lambda^{5/3}\frac{\left(c\|v\|^{8/3}_{8/3}\right)^2}{\|\nabla v\|^2_2 + \frac{3}{5}c_{TF}\|v\|^{10/3}_{10/3}\lambda^{2/3}}. \tag{2.29}$$

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

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

which leads, together with (2.24) and the fact that Q is a minimizer of $J_{\mathbb{R}^3,c}(\lambda)$, to

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

for any $\varepsilon \in (0;2)$. Using this last inequality together with the upper bound (2.29), we get for any $\varepsilon \in (0;1)$ that

$$\begin{aligned}
2\lambda\mu &\geqslant \frac{9}{64}\varepsilon^{2/3}(2-\varepsilon)^{5/3}\lambda^{5/3}\frac{\left(c\,\|v\|_{8/3}^{8/3}\right)^2}{\|\nabla v\|_2^2+\frac{3}{5}c_{TF}\,\|v\|_{10/3}^{10/3}\varepsilon^{2/3}(2-\varepsilon)^{2/3}\lambda^{2/3}}+O(\varepsilon)\\
&> \frac{9}{64}\varepsilon^{2/3}\lambda^{5/3}\frac{\left(c\,\|v\|_{8/3}^{8/3}\right)^2}{\|\nabla v\|_2^2+\frac{3}{5}2^{2/3}c_{TF}\,\|v\|_{10/3}^{10/3}\lambda^{2/3}}+O(\varepsilon).
\end{aligned}$$

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

Step 6: Positivity of nonnegative minimizers. Let $Q \geqslant 0$ be a minimizer. By Step 3, $0 \not\equiv Q \in H^2(\mathbb{R}^3) \subset C_0^0(\mathbb{R}^3)$ and $W := c_{TF}|Q|^{\frac{4}{3}} - c|Q|^{\frac{2}{3}} + \mu$ is in $L^\infty(\mathbb{R}^3)$. We can obtain that $Q > 0$ by [**LL01**, Theorem 9.10], by results in [**RS78**, Section XIII.12] or by Lemma 1.30

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

PROOF OF PROPOSITION 2.17. Let $0 \leqslant Q \in H^1(\mathbb{R}^3;\mathbb{R})$ be a minimizer of $J_{\mathbb{R}^3,c}(\lambda)$. We denote by Q^* its Schwarz rearrangement which is, as explained 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 (2.21). They are therefore real-analytic (see e.g. [**Mor58**]) 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 [**BZ88**, 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. ☐

Step 8: $-\mu$ is the lowest eigenvalue of H_Q, is simple, and $Q = z|Q|$. These are classical results, apply e.g. [**LL01**, Chapter 11] to $V_Q := c_{TF}|Q|^{\frac{4}{3}} - |Q|^{\frac{2}{3}}$ which is in $L^\infty(\mathbb{R}^3)$ by the previous steps.

More precisely, the function V_Q is in $L^\infty(\mathbb{R}^3)$ for any Q minimizer to $J_{\mathbb{R}^3}(\lambda)$ and, for such Q, $|Q|$ is also a minimizer. It also verifies, for a given $\mu > 0$, the Euler–Lagrange equation

$$H_Q|Q| = -\Delta|Q| + V_Q|Q| = -\mu|Q|.$$

We then have by [**LL01**, Corollary 11.9] that $|Q|$ is the unique minimizer (up to a constant phase) of

$$\inf_{\varphi}\left\{\int|\nabla\varphi(x)|^2+V_Q|\varphi(x)|^2\,\mathrm{d}x\,\middle|\int|\varphi|^2=\lambda\right\}$$

and $-\mu$ is equal to this infimum. This immediately gives that the lowest eigenvalue of H_Q is simple and is equal to $-\mu$.

Finally, Q verifying the Euler–Lagrange equation, it is an eigenfunction of H_Q with an associated eigenvalue given by (2.26)

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

But the lowest eigenvalue of H_Q being the Euler–Lagrange coefficient for $|Q|$, it verifies

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

Since $\|\nabla|Q|\|_{L^2(\mathbb{R}^3)}\leqslant\|\nabla Q\|_{L^2(\mathbb{R}^3)}$, by the convexity inequality for gradients (see Step 2), it implies that $\mu'\leqslant\mu$ which leads to $\mu'=\mu$ (because μ is the lowest eigenvalue of H_Q) and then it implies that there exists $z\in\mathbb{C}$ such that $Q=z|Q|$ because Q and $|Q|$ are eigenfunctions of H_Q associated with the same eigenvalue μ which is simple.

Step 9: Minimizing sequences are precompact up to a translations. Since the strict binding inequality (2.13) holds, this follows from a result of Lions in [**Lio84b**, Theorem I.2]. For completeness, we give a detailed proof of this known result in Section 6.1 of the Appendix.

This concludes the proof of Theorem 2.3.

□

This existence of minimizers gives us immediately the following continuity result.

COROLLARY 2.18. *On* $[0,+\infty)$, $c\mapsto J_{\mathbb{R}^3,\lambda}(c)$ *is continuous.*

PROOF OF COROLLARY 2.18. Let $0\leqslant c_1<c_2$ and, Q_1 and Q_2 be corresponding minimizers which exist by Theorem 2.3. By Lemma 2.10, $c_2\mapsto\|Q_2\|_{H^1(\mathbb{K})}$ is uniformly bounded on any bounded interval $[0;c_*]$, $c_*>0$, since

$$J_{\mathbb{R}^3,\lambda}(0)\geqslant J_{\mathbb{R}^3,\lambda}(c_2)=\mathscr{J}_{\mathbb{R}^3,c}(Q_2)\geqslant\|\nabla Q_2\|_{L^2(\mathbb{R}^3)}^2-\frac{15}{64}\frac{\lambda}{c_{TF}}{c_2}^2.$$

Therefore, by Lemma 2.13, we have for any $0 \leqslant c_1 < c_2 < c_* $ that

$$\begin{aligned} J_{\mathbb{R}^3,\lambda}(c_2) < J_{\mathbb{R}^3,\lambda}(c_1) \leqslant \mathscr{J}_{\mathbb{R}^3,c_1}(Q_2) &= J_{\mathbb{R}^3,\lambda}(c_2) + \frac{3}{4}(c_2 - c_1)\, \|Q_2\|_{L^{\frac{8}{3}}(\mathbb{K})}^{\frac{8}{3}} \\ &\leqslant J_{\mathbb{R}^3,\lambda}(c_2) + \frac{3}{4}(c_2 - c_1) C_1 \lambda^{5/6} \|Q_2\|_{H^1(\mathbb{K})} \\ &\leqslant J_{\mathbb{R}^3,\lambda}(c_2) + C_{c_*} \lambda^{5/6} \frac{3}{4}(c_2 - c_1) \end{aligned}$$

which gives the continuity and concludes the proof of Corollary 2.23. □

We now give the following decay result of positive continuous solutions (so, of solutions in $H^2(\mathbb{R}^3)$ for example) to the Euler–Lagrange equation. This result will be useful later.

Lemma 2.19 (Exponential decay of positive continuous solutions to the E–L equation (2.12)). *Let Q be a continuous positive solution to the Euler–Lagrange equation* (2.12)*, that vanishes as $|x|$ goes to infinity, with $-\mu < 0$ the associated Lagrange multiplier. Then for every $0 < \varepsilon < \mu$, there exists a constant C_ε such that*

$$0 < Q(x) \leqslant C_\varepsilon e^{-\sqrt{\mu - \varepsilon}|x|}. \tag{2.30}$$

Moreover, for any $p, q > 0$, there exist $C_{\varepsilon,p,q}, C_{\varepsilon,q}$ and $C'_{\varepsilon,q}$ such that

$$\int_{|x| \geqslant R} |Q(x)|^p \, dx \leqslant C_{\varepsilon,p,q} e^{-(p-q)\sqrt{\mu-\varepsilon}R}, \tag{2.31}$$

$$\int_{|x| \geqslant R} |\nabla Q(x)|^2 \, dx \leqslant C_{\varepsilon,q} e^{-(1-q)\sqrt{\mu-\varepsilon}R}, \tag{2.32}$$

$$\int_{|x| \geqslant R} |\Delta Q(x)|^2 \, dx \leqslant C'_{\varepsilon,q} e^{-(2-q)\sqrt{\mu-\varepsilon}R}. \tag{2.33}$$

Proof of Lemma 2.19. Let $0 < \varepsilon < \mu$. Then, by (2.12), we have

$$(-\Delta + (\mu - \varepsilon))Q = (-\varepsilon - c_{TF}|Q|^{\frac{4}{3}} + |Q|^{\frac{2}{3}})Q =: g$$

with $g(x) < 0$ for $|x| \geqslant R_\varepsilon$ for R_ε large enough. Indeed, $|Q|^{\frac{4}{3}}$ and $|Q|^{\frac{2}{3}}$ vanish as $|x|$ goes to infinity and $Q > 0$. Using the Yukawa potential, we obtain that

$$0 < Q(x) = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{e^{-\sqrt{\mu-\varepsilon}|x-y|}}{|x-y|} g(y) \, \mathrm{d}y \leqslant \frac{1}{4\pi} \int_{|y| \leqslant R_\varepsilon} \frac{e^{-\sqrt{\mu-\varepsilon}|x-y|}}{|x-y|} g(y) \, \mathrm{d}y.$$

Recalling that g is continuous, since Q is continuous, and that for any $|x| \geqslant 2R_\varepsilon$ and $|y| \leqslant R_\varepsilon$ we have $|x-y| \geqslant |x| - |y| \geqslant R_\varepsilon$, we have for $|x| \geqslant 2R_\varepsilon$ that

$$\begin{aligned} 0 < Q(x) &\leqslant \frac{1}{4\pi R_\varepsilon}\left(\sup_{B(0,R_\varepsilon)} g\right)\int_{|y|\leqslant R_\varepsilon} e^{-\sqrt{\mu-\varepsilon}|x-y|}\,\mathrm{d}y \\ &\leqslant \frac{1}{4\pi R_\varepsilon}\left(\sup_{B(0,R_\varepsilon)} g\right)\left(\int_{|y|\leqslant R_\varepsilon} e^{\sqrt{\mu-\varepsilon}|y|}\,\mathrm{d}y\right) e^{-\sqrt{\mu-\varepsilon}|x|}. \end{aligned}$$

The estimate $Q(x) \leqslant C_\varepsilon e^{-\sqrt{\mu-\varepsilon}|x|}$ on all $\mathbb{R}^3$ then follows from the fact that Q is bounded on $B(0, 2R_\varepsilon)$.

From (2.30) we obtain

$$\begin{aligned} \int_{|x|\geqslant R} |Q(x)|^p\,\mathrm{d}x \leqslant (C_\varepsilon)^p \int_{|x|\geqslant R} e^{-p\sqrt{\mu-\varepsilon}|x|}\,\mathrm{d}x &= 4\pi (C_\varepsilon)^p \int_R^\infty e^{-p\sqrt{\mu-\varepsilon}r} r^2\,\mathrm{d}r \\ &= P(R) e^{-p\sqrt{\mu-\varepsilon}R} \end{aligned}$$

where P is an order 2 polynomial with coefficients depending on ε and p. Thus, for any $q > 0$, $R \mapsto P(R)e^{-q\sqrt{\mu-\varepsilon}R}$ is bounded by a constant depending on ε, p and q. This leads to (2.31).

Multiplying (2.12) by χQ with $\chi \in C^\infty(\mathbb{R}^3)$, $0 \leqslant \chi \leqslant 1$, $\chi \equiv 1$ on $B(0,R)$, $\chi \equiv 0$ on $B(0, R-1)$ and $\|\nabla\chi\|_{L^\infty(\mathbb{R}^3)} \leqslant 2$ we obtain

$$\int_{\mathbb{R}^3} \chi|\nabla Q|^2 + \int_{\mathbb{R}^3} Q\nabla Q \cdot \nabla\chi = \int_{\mathbb{R}^3} \chi g Q - (\mu - \varepsilon)\int_{\mathbb{R}^3} \chi|\nabla Q|^2.$$

Since $\int_{\mathbb{R}^3} \chi g Q$ is non-positive for $R - 1 \geqslant R_\varepsilon$, it follows that

$$\begin{aligned} \int_{|x|\geqslant R} |\nabla Q(x)|^2\,\mathrm{d}x &\leqslant -\int_{|x|=R-1}^{|x|=R} \chi|\nabla Q(x)|^2\,\mathrm{d}x - \int_{|x|=R-1}^{|x|=R} Q(x)\nabla Q(x)\cdot\nabla\chi(x)\,\mathrm{d}x \\ &\leqslant \int_{|x|=R-1}^{|x|=R} |Q(x)||\nabla Q(x)||\nabla\chi(x)|\,\mathrm{d}x \\ &\leqslant 2\left(\int_{|x|=R-1}^{|x|=R} |Q(x)|^2\right)^{\frac12}\left(\int_{|x|=R-1}^{|x|=R} |\nabla Q(x)|^2\,\mathrm{d}x\right)^{\frac12} \\ &\leqslant 2\,\|\nabla Q\|_{L^2(\mathbb{R}^3)}\left(\int_{|x|\geqslant R-1} |Q(x)|^2\right)^{\frac12}. \end{aligned}$$

Thus, applying (2.31) for $p = 2$, we obtain (2.32).

By (2.12), we have

$$0 \leqslant \int_{|x|\geqslant R} |\Delta Q(x)|^2 \,\mathrm{d}x = \int_{|\cdot|\geqslant R} {c_{TF}}^2 |Q|^{\frac{14}{3}} + (1+2\mu c_{TF})|Q|^{\frac{10}{3}} + \mu^2|Q|^2$$
$$- 2\int_{|\cdot|\geqslant R} {c_{TF}}^2|Q|^4 - 2\mu|Q|^{\frac{8}{3}}.$$

Using (2.31), we see that largest term is due to $\mu^2|Q|^2$ and this leads to (2.33). □

3.2. Proof of Theorem 2.4. The uniqueness of radial solutions has been proved by Serrin and Tang in [**ST00**]. However, we need the non-degeneracy of the solution. Both uniqueness and non-degeneracy can be proved following line by line the method in [**LRN15**, Thm. 2] (the argument is detailed in Section 6.2 in the Appendix). One slight difference is the application of the moving plane method to prove that positive solutions are radial. Contrarily to [**LRN15**] we cannot use [**GNN81**, Thm. 2] because our function

$$F_\mu(y) = -c_{TF} y^{\frac{7}{3}} + y^{\frac{5}{3}} - \mu y \tag{2.34}$$

is not C^2. However, given that nonnegative solutions are positive, one can show that they are C^∞ and, therefore, we can apply [**Li91**, Thm. 1.1]. □

4. Regime of small c: uniqueness of the minimizer

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

Lemma 2.20 (The periodic Coulomb potential $G_{\mathbb{K}}$). *The function $G_{\mathbb{K}} - |\cdot|^{-1}$ is bounded on $\mathbb{K}$. Thus, there exits C such that for any $x \in \mathbb{K}\backslash\{0\}$, we have*

$$0 \leqslant G_{\mathbb{K}}(x) \leqslant \frac{C}{|x|}. \tag{2.35}$$

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

$$\widehat{G}_{\mathbb{K}}(\xi) = 4\pi \sum_{k\in\mathscr{L}_{\mathbb{K}}^*\backslash\{0\}} \frac{\delta_k(\xi)}{|k|^2} + \delta_0(\xi)\int_{\mathbb{K}} G_{\mathbb{K}}(x)\,dx \tag{2.36}$$

where $\mathscr{L}_{\mathbb{K}}^*$ is the reciprocal lattice of $\mathscr{L}_{\mathbb{K}}$. Hence, for any $f \not\equiv 0$ for which $D_{\mathbb{K}}(f,f)$ is defined, we have $D_{\mathbb{K}}(f,f) > 0$.

Proof of Lemma 2.20. The first part follows from the fact that

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

Indeed, $f(x) := \int_{\mathbb{K}} \frac{\mathrm{d}y}{|x-y|}$ is continuous — this can be seen from the fact that, for any $0 < |x - x_0| \leqslant \eta$, we have

$$\frac{|f(x) - f(x_0)|}{|x - x_0|} \leqslant \left\| |x - \cdot|^{-1} \right\|_{L^2(\mathbb{K})} \left\| |x_0 - \cdot|^{-1} \right\|_{L^2(\mathbb{K})} \leqslant 4\pi(|x_0| + \eta + R)$$

where R is such that $\mathbb{K} \subset B(0, R)$ — then the stated limit is obtained following the argument in [**LS77b**, VI.2]. It implies, together with the fact that both $G_{\mathbb{K}}$ and $|\cdot|^{-1}$ are bounded on the complementary in Q of any $B(0, R) \subset Q$ for $R > 0$, the bounds on $G_{\mathbb{K}}$. The positivity of $D_{\mathbb{K}}(f, f)$ comes directly from the expression of the Fourier transform since we choose $G_{\mathbb{K}}$ such that $\min\limits_{x \in \mathbb{K}} G_{\mathbb{K}}(x) = 0$ hence $\widehat{G}_{\mathbb{K}}(0) = \int_{\mathbb{K}} G_{\mathbb{K}} > 0$. We now prove the stated expression. For any $\xi \neq 0$, we have by (2.4) that

$$|\xi|^2 \widehat{G}_{\mathbb{K}}(\xi) = 4\pi \int_{\mathbb{R}^3} \sum_{k \in \mathscr{L}_{\mathbb{K}}^* \setminus \{0\}} e^{2\mathrm{i}\pi\langle k - \xi, x\rangle} \, \mathrm{d}x = 4\pi \sum_{k \in \mathscr{L}_{\mathbb{K}}^* \setminus \{0\}} \delta_k(\xi)$$

where we have used that

$$\sum_{\ell \in \mathscr{L}_{\mathbb{K}}} \delta_\ell = \frac{1}{|\mathbb{K}|} \sum_{k \in \mathscr{L}_{\mathbb{K}}^*} e^{2\mathrm{i}\pi\langle k, \cdot\rangle} \qquad \text{in } \mathscr{D}'(\mathbb{R}^3)$$

which we prove using the Fourier series of the Dirac comb $\sum\limits_{\ell \in \mathbb{Z}} \delta_\ell$, which is

$$\sum_{k \in \mathbb{Z}} e^{2\mathrm{i}\pi k x} = \sum_{\ell \in \mathbb{Z}} \delta_\ell(x) \qquad \text{in } \mathscr{D}'(\mathbb{R}).$$

Indeed, let denote A the application sending $\mathbb{Z}^3$ onto $\mathscr{L}_{\mathbb{K}}$ hence $|\mathbb{K}| = \det A$ and ${}^t A^{-1}$ sends $\mathbb{Z}^3$ onto $\mathscr{L}_{\mathbb{K}}^*$. For $\varphi \in C_c^\infty(\mathbb{R}^3)$, we have

$$\left\langle \sum_{k \in \mathscr{L}_{\mathbb{K}}^*} e^{2\mathrm{i}\pi\langle k, \cdot\rangle}, \varphi \right\rangle = \left\langle \sum_{k \in \mathbb{Z}^3} e^{2\mathrm{i}\pi\left\langle k, A^{-1}\cdot\right\rangle}, \varphi \right\rangle = |\mathbb{K}| \left\langle \sum_{k \in \mathbb{Z}^3} e^{2\mathrm{i}\pi\langle k, \cdot\rangle}, \varphi(A\cdot) \right\rangle.$$

Moreover, for any $\psi \in C_c^\infty(\mathbb{R}^3)$ such that $\psi(x) = \psi_1(x_1)\psi_2(x_2)\psi_3(x_3)$, we have

$$\begin{aligned} \left\langle \sum_{k \in \mathbb{Z}^3} e^{2\mathrm{i}\pi\langle k, \cdot\rangle}, \psi \right\rangle_{L^2(\mathbb{R}^3)} &= \prod_{i=1}^3 \left\langle \sum_{k_i \in \mathbb{Z}} e^{2\mathrm{i}\pi k_i \cdot}, \psi_i \right\rangle_{L^2(\mathbb{R})} \\ &= \prod_{i=1}^3 \left\langle \sum_{\ell_i \in \mathbb{Z}} \delta_{\ell_i}, \psi_i \right\rangle_{L^2(\mathbb{R})} = \left\langle \sum_{\ell \in \mathbb{Z}^3} \delta_\ell, \psi \right\rangle_{L^2(\mathbb{R}^3)} = \sum_{\ell \in \mathbb{Z}^3} \psi(\ell), \end{aligned}$$

where we have used the Fourier series of the Dirac comb. The above computation holds on $\mathscr{D}'(\mathbb{R}^3)$ by density of the functions that can be decomposed like ψ. We then deduce that

$$\left\langle \frac{1}{|\mathbb{K}|} \sum_{k \in \mathscr{L}_{\mathbb{K}}^*} e^{2i\pi\langle k,\cdot\rangle}, \varphi \right\rangle = \sum_{\ell \in \mathbb{Z}^3} \varphi(A\ell) = \sum_{\ell \in \mathscr{L}_{\mathbb{K}}} \varphi(\ell) = \left\langle \sum_{\ell \in \mathscr{L}_{\mathbb{K}}} \delta_\ell, \varphi \right\rangle.$$

□

4.1. Existence of minimizers to $E_{\mathbb{K},\lambda}(c)$. In order to prove Theorem 2.1, we need the existence of minimizers to $E_{\mathbb{K},\lambda}(c)$, for any $c \geqslant 0$, which is done in this section.

PROPOSITION 2.21 (Existence of minimizers to $E_{\mathbb{K},\lambda}(c)$). *Let $\mathbb{K}$ be the unit cube and, $c_{TF} > 0$, $\lambda > 0$ and $c \geqslant 0$ 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 $H^1_{per}(\mathbb{K})$ to a minimizer, up to extraction of a subsequence.

ii. Any minimizer w_c is in $H^2_{per}(\mathbb{K})$, is non-constant and solves the E–L equation

$$\Big(-\Delta + c_{TF}|w_c|^{\frac{4}{3}} - c|w_c|^{\frac{2}{3}} - G_{\mathbb{K}} + (|w_c|^2 \star G_{\mathbb{K}})\Big)\, w_c = -\mu_{w_c} w_c, \tag{2.37}$$

with

$$\mu_{w_c} = -\frac{\|\nabla w_c\|_2^2 + c_{TF}\,\|w_c\|_{10/3}^{10/3} - c\,\|w_c\|_{8/3}^{8/3} + D_{\mathbb{K}}(|w_c|^2, |w_c|^2) - \langle G_{\mathbb{K}}, |w_c|^2\rangle_{L^2(\mathbb{K})}}{\lambda}. \tag{2.38}$$

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 $H^2_{per}(\mathbb{K})$,

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

Note that for shortness, we have denoted $\|\cdot\|_p = \|\cdot\|_{L^p(\mathbb{K})}$.

PROOF OF PROPOSITION 2.21. In order to prove *i.*, we need the following result that will be useful all along the rest of this second part of the thesis, and is somewhat similar to Lemma 2.10.

LEMMA 2.22. *For any $c \geqslant 0$, $c_{TF}, \lambda > 0$, there exist positive constants $a < 1$ and C such that, for any $u \in H^1_{per}(\mathbb{K})$ such that $\|u\|_2^2 = \lambda$, we have*

$$\mathscr{E}_{\mathbb{K},c}(u) \geqslant a\,\|\nabla u\|^2_{L^2(\mathbb{K})} - \frac{15}{64}\frac{\lambda}{c_{TF}}c^2 - \lambda C. \tag{2.39}$$

PROOF OF LEMMA 2.22. As in Lemma 2.10, Hölder's inequality (but on $\mathbb{K}$) gives us that

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

Moreover, we have

$$\left|\int_{\mathbb{K}} G_{\mathbb{K}}|u|^2\right| \leqslant \varepsilon \|u\|^2_{L^q(\mathbb{K})} + \lambda C_\varepsilon, \qquad \forall\, q \in (3;6],\ \varepsilon > 0. \tag{2.40}$$

Indeed, suppose $q \in (3;6]$, $\varepsilon > 0$ and define q' such that $1/q' + 2/q = 1$, thus $q' \in [\frac{3}{2};3)$. By the upper bound in (2.35), the function $G_{\mathbb{K}}$ can be written $G_{\mathbb{K}} = G_{q'} + G_\infty$ where $G_{q'} = \mathbb{1}_{\{|\cdot|<r\}}G_{\mathbb{K}} \in L^{q'}(\mathbb{K})$ and $G_\infty = \mathbb{1}_{\mathbb{K}\setminus\{|\cdot|<r\}}G_{\mathbb{K}} \in L^\infty(\mathbb{K})$. Then choosing r small enough such that $\|G_{q'}\|_{L^{q'}(\mathbb{K})} \leqslant \varepsilon$, we obtain (2.40). The above results (for $q = 6$), together with Sobolev embeddings and $D_{\mathbb{K}}(u^2,u^2) \geqslant 0$, gives

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

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

Let c be fixed and let $(w_n)_n$ be a minimizing sequence. The above result gives that $(w_n)_n$ is uniformly bounded in $H^1(\mathbb{K})$ and, together with Sobolev embeddings, it implies that there exists w_c such that, up to a subsequence (denoted the same for shortness),

$$\begin{aligned}
\nabla w_n &\underset{n\to\infty}{\rightharpoonup} \nabla w_c, && \text{weakly in } L^2(\mathbb{K}); \\
w_n &\underset{n\to\infty}{\rightharpoonup} w_c, && \text{weakly in } L^p(\mathbb{K}) \text{ for all } 2 \leqslant p \leqslant 6.
\end{aligned}$$

Moreover, the cube $\mathbb{K}$ being bounded, $H^1(\mathbb{K})$ is compactly embedded in $L^p(\mathbb{K})$ for $1 \leqslant p < 6$. Consequently, up to another subsequence (still denoted the same), we have

$$\begin{aligned}
\nabla w_n &\rightharpoonup \nabla w_c, && \text{weakly in } L^2(\mathbb{K}); \\
w_n &\rightharpoonup w_c, && \text{weakly in } L^6(\mathbb{K}); \\
w_n &\to w_c, && \text{a.e. and strongly in } L^p(\mathbb{K}) \text{ for all } 2 \leqslant p < 6.
\end{aligned}$$

It follows that

$$\int_{\mathbb{K}} |w_n|^{\frac{10}{3}} \to \int_{\mathbb{K}} |w_c|^{\frac{10}{3}},\ \int_{\mathbb{K}} |w_n|^{\frac{8}{3}} \to \int_{\mathbb{K}} |w_c|^{\frac{8}{3}} \ \text{ and } \ \liminf_{n\to\infty}\int_{\mathbb{K}} |\nabla w_n|^2 \geqslant \int_{\mathbb{K}} |\nabla w_c|^2.$$

Moreover, by Fatou's Lemma, we have

$$\liminf_{n\to\infty} D_{\mathbb{K}}(|w_n|^2,|w_n|^2) \geqslant D_{\mathbb{K}}(|w_c|^2,|w_c|^2),$$

and, by the convergence in $L^3(\mathbb{K})$ for example, we have

$$\int_{\mathbb{K}} G_{\mathbb{K}}|w_n|^2 \to \int_{\mathbb{K}} G_{\mathbb{K}}|w_c|^2.$$

This leads to

$$E_{\mathbb{K},\lambda}(c) = \liminf \mathscr{E}_{\mathbb{K},c}(w_n) \geqslant \mathscr{E}_{\mathbb{K},c}(w_c)$$

thus w_c is a minimizer since it verifies $\|w_c\|^2_{L^2(\mathbb{K})} = \lambda$ and belongs to $H^1_{\mathrm{per}}(\mathbb{K})$. We then, in fact, obtain up to a subsequence that $D_{\mathbb{K}}({w_n}^2, {w_n}^2) \to D_{\mathbb{K}}(|w_c|^2, |w_c|^2)$ and $\int_{\mathbb{K}} |\nabla w_n|^2 \to \int_{\mathbb{K}} |\nabla w_c|^2$. This last convergence gives us that any minimizing sequence of $E_{\mathbb{K},\lambda}(c)$ strongly converges in $H^1_{\mathrm{per}}(\mathbb{K})$ to a minimizer up to a subsequence.

Moreover, by the convexity inequality for gradients (see [**LL01**, Theorem 7.8])

$$\|\nabla |f|\|_{L^2(\mathbb{K})} \leqslant \|\nabla f\|_{L^2(\mathbb{K})}, \qquad \forall\, f \in H^1_{\mathrm{per}}(\mathbb{K}, \mathbb{C}),$$

we obtain that $|w_c| \in H^1_{\mathrm{per}}(\mathbb{K}, \mathbb{R}_+)$ and that it is a minimizer since w_c is a minimizer. This concludes the proof of *i.*

We now prove that any minimizer w_c solves an Euler–Lagrange equation. For any $f \in H^1_{\mathrm{per}}(\mathbb{K})$, we define

$$w_\varepsilon = \frac{\sqrt{\lambda}}{\|w_c + \varepsilon f\|_{L^2(\mathbb{K})}}(w_c + \varepsilon f).$$

We obviously have that $w_\varepsilon \in H^1_{\mathrm{per}}(\mathbb{K})$ and $\|w_\varepsilon\|^2_{L^2(\mathbb{K})} = \lambda$. Moreover, w_c being a minimizer, we have $\frac{\mathrm{d}\mathscr{E}_{\mathbb{K},c}}{\mathrm{d}\varepsilon}_{|w_c} = 0$. Thus, computing $\mathscr{E}_{\mathbb{K},c}(w_\varepsilon)$ for f and $\mathrm{i}f$, we obtain

$$\left\langle \left(-\Delta + c_{TF}|w_c|^{4/3} - c|w_c|^{2/3} + (G_{\mathbb{K}} \star |w_c|^2) - G_{\mathbb{K}} + \mu_{w_c}\right) w_c, f \right\rangle_{L^2(\mathbb{K})} = 0,$$

with μ_{w_c} defined as in (2.38).

To prove that any minimizer w_c is in $H^2_{\mathrm{per}}(\mathbb{K})$, using (2.37) in $H^{-1}_{\mathrm{per}}(\mathbb{K})$ and (2.38) which are classical computations, 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 $w_c \in H^2_{\mathrm{per}}(\mathbb{K})$ 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 $w_c \in H^1_{\mathrm{per}}(\mathbb{K})$ which also gives, together with $G_{\mathbb{K}} \in L^2(\mathbb{K})$ by Lemma 2.20, 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 (2.35) and the periodic Hardy inequality on $\mathbb{K}$ (see Section 6.5 in the Appendix) give

$$\|G_{\mathbb{K}} w_c\|_{L^2(\mathbb{K})} \leqslant C \left\| |\cdot|^{-1} w_c \right\|_{L^2(\mathbb{K})} \leqslant C' \|w_c\|_{H^1_{\mathrm{per}}(\mathbb{K})}.$$

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 $0 \not\equiv w_c \geqslant 0$ 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 $(-\Delta + C)\, w_c \geqslant 0$ for $C \gg 1$. Hence, $w_c > 0$ on $\mathbb{K}$ since the periodic Laplacian is positive improving [**LL01**, Theorem 9.10]. Therefore $0 < {w_c}^{-1} \in L^\infty(\mathbb{K})$ and, for any $u \in H^1_{\mathrm{per}}(\mathbb{K})$, it holds that uw_c and $u{w_c}^{-1}$ are in $H^1(\mathbb{K})$. Indeed, we of course have that $u{w_c}^{-1} \in L^2(\mathbb{K})$ and $uw_c \in L^2(\mathbb{K})$ but also

$$\left\|\nabla(u{w_c}^{-1})\right\|_{L^2(\mathbb{K})} \leqslant \left\|{w_c}^{-1}\right\|_{L^\infty(\mathbb{K})} \left\|\nabla u\right\|_{L^2(\mathbb{K})} + \left\|{w_c}^{-1}\right\|^2_{L^\infty(\mathbb{K})} \left\|\nabla w_c\right\|_{L^4(\mathbb{K})} \left\|u\right\|_{L^4(\mathbb{K})}$$

and

$$\left\|\nabla(uw_c)\right\|_{L^2(\mathbb{K})} \leqslant \left\|u\right\|_{L^4(\mathbb{K})} \left\|\nabla w_c\right\|_{L^4(\mathbb{K})} + \left\|w_c\right\|_{L^\infty(\mathbb{K})} \left\|\nabla u\right\|_{L^2(\mathbb{K})},$$

which are both bounded since $w_c \in H^2(\mathbb{K})$ and $u \in H^1(\mathbb{K})$. We obtain

$$\begin{aligned} \langle u, -\Delta u\rangle &= \left\langle \nabla(uw_c), \nabla(u{w_c}^{-1})\right\rangle - 2\left\langle u\nabla w_c, \nabla(u{w_c}^{-1})\right\rangle + \left\langle |u|^2{w_c}^{-1}, -\Delta w_c\right\rangle \\ &= \left\langle {w_c}^2, \left|\nabla(u{w_c}^{-1})\right|^2\right\rangle + \left\langle |u|^2{w_c}^{-1}, -\Delta w_c\right\rangle, \end{aligned}$$

where $\langle\cdot,\cdot\rangle$ stands for $\langle\cdot,\cdot\rangle_{L^2(\mathbb{K})}$ and since w_c is real valued. Consequently, $w_c > 0$ verifies $H_{w_c}w_c = -\mu_{w_c}w_c$ and this implies that for any $u \in H^1_{\mathrm{per}}(\mathbb{K})$ it holds

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

This vanishes only if there exists $\alpha \in \mathbb{C}$ such that $u = \alpha w_c$ ae.

Let now w_c be a minimizer. The convexity inequality for gradients gives that $|w_c|$ is a nonnegative minimizer and that $-\mu_{w_c} \leqslant -\mu_{|w_c|}$. But we just proved that $-\mu_{|w_c|}$ is the lowest eigenvalue of $H_{w_c} = H_{|w_c|}$ and is simple, hence $-\mu_{w_c} = -\mu_{|w_c|}$ and, w_c and $|w_c|$ are equal up to a constant phase factor. This concludes the proof of Proposition 2.21. □

From this existence result, we deduce two useful corollaries.

Corollary 2.23. *On $[0, +\infty)$, $c \mapsto E_{\mathbb{K},\lambda}(c)$ is continuous and strictly decreasing.*

PROOF OF COROLLARY 2.23. Let $0 \leqslant c_1 < c_2$ and, let w_1 and w_2 be corresponding minimizers, which exist by Proposition 2.21. On one hand, we have

$$\begin{aligned} E_{\mathbb{K},\lambda}(c_2) \leqslant \mathscr{E}_{\mathbb{K},c_2}(w_1) &= \mathscr{E}_{\mathbb{K},c_1}(w_1) - \frac{3}{4}(c_2 - c_1)\int_{\mathbb{K}} |w_1|^{\frac{8}{3}} \\ &= E_{\mathbb{K},\lambda}(c_1) - \frac{3}{4}(c_2 - c_1)\int_{\mathbb{K}} |w_1|^{\frac{8}{3}} < E_{\mathbb{K},\lambda}(c_1), \end{aligned}$$

with the second inequality being strict since, for $c \geqslant 0$, any corresponding minimizer is nonnegative with positive $L^2(\mathbb{K})$-norm thus $\int_{\mathbb{K}} |w_1|^{\frac{8}{3}} > 0$. This gives that $E_{\mathbb{K},\lambda}(c)$ is strictly decreasing on $[0, +\infty)$ but also, fixing c_2 and sending c_1 to c_2 by below, 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

$$E_{\mathbb{K},\lambda}(0) \geqslant E_{\mathbb{K},\lambda}(c_2) = \mathscr{E}_{\mathbb{K},c_2}(w_2) \geqslant a\,\|\nabla w_2\|^2_{L^2(\mathbb{K})} - \frac{15}{64}\frac{\lambda}{c_{TF}}{c_2}^2 - \lambda C \tag{2.41}$$

by Lemma 2.22. Hence, by the Sobolev embedding, we have

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

which gives the right-continuity and concludes the proof of Corollary 2.23. □

COROLLARY 2.24. *If w_c is a minimizer of $E_{\mathbb{K},\lambda}(c)$, then*

$$\min_{\mathbb{K}} |w_c|^2 < \frac{\lambda}{|\mathbb{K}|} < \max_{\mathbb{K}} |w_c|^2.$$

PROOF OF LEMMA 2.24. This is a direct consequence of $w_c \in H^2(\mathbb{K}) \subset C^0(\mathbb{K})$ being non-constant and verifying $\|w_c\|^2_{L^2(\mathbb{K})} = \lambda$. □

4.2. Limit case $c = 0$: the TFW model. In order to prove Theorem 2.1, we need some results on the TFW model which corresponds to the TFDW model for $c = 0$. For clarity, we denote

$$\mathscr{E}^{TFW}_{\mathbb{K}}(w) := \mathscr{E}_{\mathbb{K},0}(w) = \int_{\mathbb{K}} |\nabla w|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{K}} |w|^{\frac{10}{3}} + \frac{1}{2}D_{\mathbb{K}}(|w|^2, |w|^2) - \int_{\mathbb{K}} G_{\mathbb{K}}|w|^2, \tag{2.42}$$

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

By Proposition 2.21, there exist minimizers to $E^{TFW}_{\mathbb{K},\lambda}$.

LEMMA 2.25.

$$E_{\mathbb{K},\lambda}(c) \underset{c\to 0^+}{\longrightarrow} E^{TFW}_{\mathbb{K},\lambda}.$$

PROOF OF LEMMA 2.25. This is a particular case of Corollary 2.23. □

We now prove the uniqueness of minimizer for the TFW model.

PROPOSITION 2.26. *The minimization problem $E^{TFW}_{\mathbb{K},\lambda}$ 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 $H^2_{per}(\mathbb{K})$, acting on $L^2_{per}(\mathbb{K})$, and with ground-state eigenvalue

$$-\mu_0 = \frac{\|\nabla w_0\|_2^2 + c_{TF}\,\|w_0\|_{10/3}^{10/3} + D_{\mathbb{K}}(w_0^2, w_0^2) - \langle G_{\mathbb{K}}, w_0^2\rangle_{L^2(\mathbb{K})}}{\lambda}. \tag{2.43}$$

PROOF OF PROPOSITION 2.26. By Proposition 2.21, we only have to prove the uniqueness. Since $\rho \mapsto G_{\mathbb{K}}\rho$ is linear, thus convex, and $\rho \mapsto \rho^{5/3}$ is strictly convex on $\mathbb{R}_+$, then their integrals over $\mathbb{K}$ are respectively convex and strictly convex. Therefore, the uniqueness of nonnegative $H^1(\mathbb{K})$ minimizers, of unitary $L^1(\mathbb{K})$-norm, to

$$\rho \mapsto \int_{\mathbb{K}} |\nabla\sqrt{\rho}|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{K}}\rho^{\frac{5}{3}} + \frac{1}{2}D_{\mathbb{K}}(\rho,\rho) - \int_{\mathbb{K}} G_{\mathbb{K}}\rho,$$

is obtained by the convexity of the $\rho \mapsto |\nabla\sqrt{\rho}|^2$ (see [**Lie81**, Proposition 7.1]) and by the (strict) convexity of $\rho \mapsto D_{\mathbb{K}}(\rho,\rho)$. The later being due to $D_{\mathbb{K}}(\rho,\rho) > 0$ for $\rho \not\equiv 0$, by Lemma 2.20, and to $2|D_{\mathbb{K}}(\rho_1,\rho_2)| < D_{\mathbb{K}}(\rho_1,\rho_1) + D_{\mathbb{K}}(\rho_2,\rho_2)$, for $\rho_1, \rho_2 \not\equiv 0$, when the expressions are well defined. This concludes the proof since any minimizer w_0 to $E^{TFW}_{\mathbb{K},\lambda}$ is equal to $|w_0|$ up to a phrase factor by Proposition 2.21. □

4.3. Proof of Theorem 2.1: 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 2.27. *Let $\{c_n\}_n \subset \mathbb{R}_+$ be such that $c_n \to \bar{c}$. 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*

$$\left(w_{c_{n_k}}, \mu_{w_{c_{n_k}}}\right) \underset{k\to\infty}{\longrightarrow} (\bar{w}, \mu_{\bar{w}})$$

holds strongly in $H^2_{per}(\mathbb{K}) \times \mathbb{R}$, 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 $c_n \to \bar{c}$:

$$\left(w_{c_n}, \mu_{w_{c_n}}\right) \underset{n\to\infty}{\longrightarrow} (\bar{w}, \mu_{\bar{c}})\,.$$

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 $\bar{c} \geqslant 0$.

Proof of Lemma 2.27. We first prove the convergence in $H^1_{\mathrm{per}}(\mathbb{K}) \times \mathbb{R}$. By the continuity of $c \mapsto E_{\mathbb{K},\lambda}(c)$ proved in Corollary 2.23, $\{w_{c_n}\}_{n\to\infty}$ is a positive minimizing sequence of $E_{\mathbb{K},\lambda}(\bar{c})$. Thus, by Proposition 2.21, up to a subsequence (denoted the same for shortness), w_{c_n} converges strongly in $H^1_{\mathrm{per}}(\mathbb{K})$ 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 $H^1_{\mathrm{per}}(\mathbb{K}) \times \mathbb{R}$:

$$\left(w_{c_n}, \mu_{w_{c_n}}\right) \underset{n\to\infty}{\longrightarrow} \left(\bar{w}, \mu_{\bar{w}}\right).$$

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

We turn to the proof of the convergence in $H^2_{\mathrm{per}}(\mathbb{K})$. For any $c_n \geqslant 0$, by Proposition 2.21, w_{c_n} is in $H^2_{\mathrm{per}}(\mathbb{K})$ thus we have

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

Moreover,

$$\begin{aligned}&\|\varepsilon_n\|_{L^2(\mathbb{K})} \\ &\leqslant c_{TF} \left\| |w_{c_n} - \bar{w}| |w_{c_n} + \bar{w}|^{\frac{4}{3}} \right\|_{L^2(\mathbb{K})} + |c_n - \bar{c}| \left\|w_{c_n}\right\|^{\frac{5}{3}}_{L^{\frac{10}{3}}(\mathbb{K})} \\ &\quad + \bar{c} C \left\| |w_{c_n} - \bar{w}| |w_{c_n} + \bar{w}|^{\frac{2}{3}} \right\|_{L^2(\mathbb{K})} + \left\|{w_{c_n}}^2 - \bar{w}^2\right\|_{L^2(\mathbb{K})} \|G_{\mathbb{K}}\|_{L^2(\mathbb{K})} \|w_{c_n}\|_{L^2(\mathbb{K})} \\ &\quad + \|w_{c_n} - \bar{w}\|_{L^2(\mathbb{K})} \left(\|\bar{w}\|^2_{L^4(\mathbb{K})} \|G_{\mathbb{K}}\|_{L^2(\mathbb{K})} + |\beta - \mu_{\bar{w}}|\right) + |\mu_{w_{c_n}} - \mu_{\bar{w}}| \|w_{c_n}\|_{L^2(\mathbb{K})} \\ &\leqslant |c_n - \bar{c}| \|w_{c_n}\|^{\frac{5}{3}}_{L^{\frac{10}{3}}(\mathbb{K})} + \|w_{c_n} - \bar{w}\|_{L^2(\mathbb{K})} \left(\|\bar{w}\|^2_{L^4(\mathbb{K})} \|G_{\mathbb{K}}\|_{L^2(\mathbb{K})} + |\beta - \mu_{\bar{w}}|\right) \\ &\quad + |\mu_{w_{c_n}} - \mu_{\bar{w}}| \|w_{c_n}\|_{L^2(\mathbb{K})} + \|w_{c_n} - \bar{w}\|_{L^4(\mathbb{K})} \left(c_{TF} \|w_{c_n} + \bar{w}\|^{\frac{4}{3}}_{L^{\frac{16}{3}}(\mathbb{K})} + \right. \\ &\qquad \left. + \bar{c} C \|w_{c_n} + \bar{w}\|^{\frac{2}{3}}_{L^{\frac{8}{3}}(\mathbb{K})} + \|w_{c_n} + \bar{w}\|_{L^4(\mathbb{K})} \|G_{\mathbb{K}}\|_{L^2(\mathbb{K})} \|w_{c_n}\|_{L^2(\mathbb{K})}\right),\end{aligned}$$

where we wrote $\|\cdot\|_p$ instead of $\|\cdot\|_{L^p(\mathbb{K})}$ and used the two technical inequalities which are the object of Lemma 2.78 in the Appendix. Since $\left(w_{c_n}, \mu_{w_{c_n}}\right)$ strongly converges in $H^1_{\rm per}(\mathbb{K})\times\mathbb{R}$, we have $\|\varepsilon_n\|_2 \longrightarrow 0$. Now, by the Rellich-Kato theorem (see the Appendix 6.9 for details), we have for β's large enough that

$$(-\Delta_{\rm per} - G_{\mathbb{K}} + \beta)^{-1} : L^2(\mathbb{K}) \to H^2_{\rm per}(\mathbb{K})$$

is a bounded operator, hence $\{w_{c_n}\}$ converges in $H^2_{\rm per}(\mathbb{K})$ since

$$w_{c_n} - \bar{w} = (-\Delta_{\rm per} - G_{\mathbb{K}} + \beta)^{-1}\,\varepsilon_n.$$

This concludes the proof of Lemma 2.27. □

PROPOSITION 2.28 (Conditional uniqueness). *Let $\mathbb{K}$ be the unit cube, $N \geqslant 1$ be an integer, $c_{TF} > 0$, $c \geqslant 0$ 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*

$$\left(-\Delta + c_{TF}w^{\frac{4}{3}} - cw^{\frac{2}{3}} + (w^2 \star G_{\mathbb{K}}) - G_{\mathbb{K}}\right) w = -\mu w. \tag{2.44}$$

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

PROOF OF PROPOSITION 2.28. First, the hypothesis give $w \in H^2_{\rm per}(N\cdot\mathbb{K})$, by the same proof as in Proposition 2.21. Moreover, we have the following lemma.

LEMMA 2.29. *Let $\rho > 0$ and $\rho' \geqslant 0$ such that $\sqrt{\rho} \in H^2_{per}(\mathbb{K})$ and $\sqrt{\rho'} \in H^1_{per}(\mathbb{K})$. Then*

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

PROOF OF LEMMA 2.29. First, we notice that

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

Defining $h = \rho' - \rho$, and using the Cauchy–Schwarz inequality, we have

$$\begin{aligned}
&\int_{N\cdot\mathbb{K}} \left|\nabla\sqrt{\rho+h}\right|^2 - \int_{N\cdot\mathbb{K}} |\nabla\sqrt{\rho}|^2 + \int_{N\cdot\mathbb{K}} \frac{\Delta\sqrt{\rho}}{\sqrt{\rho}}h \\
&= \frac{1}{4}\int_{N\cdot\mathbb{K}} \frac{|\nabla(\rho+h)|^2}{\rho+h} - \frac{1}{4}\int_{N\cdot\mathbb{K}} \frac{|\nabla\rho|^2}{\rho} + \frac{1}{2}\int_{N\cdot\mathbb{K}} h\Delta(\ln\rho) + \frac{1}{4}\int_{N\cdot\mathbb{K}} \left|\nabla(\ln\rho)\right|^2 h \\
&= -\frac{1}{4}\int_{N\cdot\mathbb{K}} \frac{|\nabla\rho|^2 h}{\rho(\rho+h)} - \frac{1}{2}\int_{N\cdot\mathbb{K}} \frac{h\nabla\rho\nabla h}{\rho(\rho+h)} + \frac{1}{4}\int_{N\cdot\mathbb{K}} \left|\nabla(\ln\rho)\right|^2 h + \frac{1}{4}\int_{N\cdot\mathbb{K}} \frac{|\nabla h|^2}{\rho+h} \\
&= \frac{1}{4}\int_{N\cdot\mathbb{K}} \frac{h^2|\nabla\rho|^2}{\rho^2(\rho+h)} - \frac{1}{2}\int_{N\cdot\mathbb{K}} \left(\frac{h\nabla\rho}{\rho\sqrt{\rho+h}}\right)\cdot\left(\frac{\nabla h}{\sqrt{\rho+h}}\right) + \frac{1}{4}\int_{N\cdot\mathbb{K}} \frac{|\nabla h|^2}{\rho+h} \\
&= \frac{1}{4}\int_{N\cdot\mathbb{K}} \left|\frac{h\nabla\rho}{\rho\sqrt{\rho+h}} - \frac{\nabla h}{\sqrt{\rho+h}}\right|^2 \geqslant 0.
\end{aligned}$$

□

Let w' be in $H^1_{\rm per}(N\cdot\mathbb{K})$ such that $\int_{N\cdot\mathbb{K}} w^2 = \int_{N\cdot\mathbb{K}} |w'|^2$ and $|w'| \not\equiv w$. Defining $\rho = w^2$ and $\rho' = |w'|^2$, this means that $\int_{N\cdot\mathbb{K}} h = 0$ where $h := \rho' - \rho \not\equiv 0$. We have

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

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 (2.44) together with Lemma 2.29 and with $D_{\mathbb{K}}(h,h) > 0$ for $h \not\equiv 0$. Defining now

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

one can check, as soon as $X \geqslant \sqrt[3]{\frac{c}{c_{TF}}}$, 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 $\min\limits_{N\cdot\mathbb{K}} w \geqslant \left(\frac{c}{c_{TF}}\right)^{3/2}$, then $\mathscr{E}_{\mathbb{K},c}(w') \geqslant \mathscr{E}_{\mathbb{K},c}(|w'|) > \mathscr{E}_{\mathbb{K},c}(w)$ for any $w' \in H^1_{\rm per}(N\cdot\mathbb{K})$ such that $|w'| \not\equiv w$ and $\int_{N\cdot\mathbb{K}} |w'|^2 = \int_{N\cdot\mathbb{K}} w^2$. This ends the proof of Proposition 2.28. ☐

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

PROOF OF THEOREM 2.1. We have already proved all the results of *i.* of Theorem 2.1 in Proposition 2.21 except for the uniqueness that we prove now. Let $(w_c)_{c\to 0^+}$ be a sequence of respective positive minimizers to $E_{\mathbb{K},\lambda}(c)$. By Proposition 2.26, $E_{\mathbb{K},\lambda}(0)$ has a unique minimizer thus, by Proposition 2.27, 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

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

and we can apply Proposition 2.28 (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 2.1. 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 $N \geqslant 1$ and verifies all the hypothesis of Proposition 2.28 hence it is also the unique minimizer of $E_{N\cdot\mathbb{K},\int_{N\cdot\mathbb{K}}|w_c|^2}(c) = E_{N\cdot\mathbb{K},N^3\lambda}(c)$. □

5. Regime of large c: symmetry breaking

This section is dedicated to the proof of the main result of the paper, namely Theorem 2.2. We introduce for clarity some notations for the rest of this section. We will denote the minimization problem for the effective model on the unit cell $\mathbb{K}$ by

$$\boxed{J_{\mathbb{K},\lambda}(c) = \inf_{\substack{v\in H^1_{\rm per}(\mathbb{K})\\ \|v\|^2_{L^2(\mathbb{K})}=\lambda}} \mathscr{J}_{\mathbb{K},c}(v),} \tag{2.45}$$

where

$$\mathscr{J}_{\mathbb{K},c}(v) = \int_{\mathbb{K}}|\nabla v|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{K}}|v|^{\frac{10}{3}} - \frac{3}{4}c\int_{\mathbb{K}}|v|^{\frac{8}{3}}. \tag{2.46}$$

We recall that the two other minimizing problems we consider are

$$\boxed{E_{\mathbb{K},\lambda}(c) = \inf_{\substack{w\in H^1_{\rm per}(\mathbb{K})\\ \|w\|^2_{L^2(\mathbb{K})}=\lambda}} \mathscr{E}_{\mathbb{K},c}(w)} \tag{2.5}$$

for the complete model on $\mathbb{K}$, where

$$\mathscr{E}_{\mathbb{K},c}(w) = \mathscr{J}_{\mathbb{K},c}(w) + \frac{1}{2}D_{\mathbb{K}}(|w|^2,|w|^2) - \int\limits_{\mathbb{K}} G_{\mathbb{K}}|w|^2, \tag{2.3}$$

and

$$\boxed{J_{\mathbb{R}^3,\lambda} = \inf_{\substack{u\in H^1(\mathbb{R}^3)\\ \|u\|^2_{L^2(\mathbb{R}^3)}=\lambda}} \mathscr{J}_{\mathbb{R}^3}(u)} \tag{2.11}$$

for the effective model on $\mathbb{R}^3$, where

$$\mathscr{J}_{\mathbb{R}^3}(u) = \int_{\mathbb{R}^3}|\nabla u|^2 + \frac{3}{5}c_{TF}\int_{\mathbb{R}^3}|u|^{\frac{10}{3}} - \frac{3}{4}\int_{\mathbb{R}^3}|u|^{\frac{8}{3}}. \tag{2.10}$$

The first but important result is the existence of minimizers for $J_{\mathbb{K},\lambda}$ which is equivalent to Proposition 2.21 but for $J_{\mathbb{K},\lambda}$.

PROPOSITION 2.30 (Existence of minimizers to $J_{\mathbb{K},\lambda}(c)$). *Let $\mathbb{K}$ be the unit cube and, $c_{TF} > 0$, $\lambda > 0$ and $c \geqslant 0$ be real constants.*

i. *There exists a nonnegative minimizer to $J_{\mathbb{K},\lambda}(c)$ and any minimizing sequence $(v_n)_n$ strongly converges in $H^1_{per}(\mathbb{K})$ to a minimizer, up to extraction of a subsequence.*

ii. *Any minimizer v_c is in $H^2_{per}(\mathbb{K})$, is non-constant and solves the Euler–Lagrange equation*
$$\left(-\Delta + c_{TF}|v_c|^{\frac{4}{3}} - c|v_c|^{\frac{2}{3}}\right) v_c = -\mu_{v_c} v_c,$$
with
$$\mu_{v_c} = -\frac{\|\nabla v_c\|_2^2 + c_{TF}\,\|v_c\|_{10/3}^{10/3} - c\,\|v_c\|_{8/3}^{8/3}}{\lambda}.$$

iii. *Up to a phase factor, a minimizer v_c is positive and the unique ground-state eigenfunction of the self-adjoint operator, with domain $H^2_{per}(\mathbb{K})$,*
$$H_{v_c} := -\Delta + c_{TF}|v_c|^{\frac{4}{3}} - c|v_c|^{\frac{2}{3}}.$$

COROLLARY 2.31. *On $[0, +\infty)$, $c \mapsto J_{\mathbb{K},\lambda}(c)$ is continuous and strictly decreasing.*

COROLLARY 2.32. *If v_c is a minimizer of $J_{\mathbb{K},\lambda}(c)$, then $\min_{\mathbb{K}} |v_c|^2 < \frac{\lambda}{|\mathbb{K}|} < \max_{\mathbb{K}} |v_c|^2$.*

The proofs are the same as the proofs of Proposition 2.21, Corollary 2.23 and Corollary 2.24, and will therefore be omitted.

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 2.33 (A priori estimates on minimal energy). *Let $\mathbb{K}$ be the unit cube and c_{TF} and c be two positive constant. Then $E_{\mathbb{K},\lambda}(c)$ verifies*
$$-\lambda C - \frac{15}{64}\frac{\lambda}{c_{TF}}c^2 \leqslant E_{\mathbb{K},\lambda}(c) \leqslant -\frac{3}{4}\frac{\lambda^{\frac{4}{3}}}{|\mathbb{K}|^{\frac{1}{3}}}c + \frac{3}{5}c_{TF}\frac{\lambda^{\frac{5}{3}}}{|\mathbb{K}|^{\frac{2}{3}}} + \frac{\lambda}{|\mathbb{K}|}\left(\frac{\lambda}{2} - 1\right)\|G_{\mathbb{K}}\|_{L^1(\mathbb{K})}, \tag{2.47}$$
for some constant $C > 0$, and $J_{\mathbb{K},\lambda}(c)$ verifies $J_{\mathbb{K},\lambda}(c) = c^2 J_{\mathbb{K},\lambda}(1)$ and
$$-\frac{15}{64}\frac{\lambda}{c_{TF}}c^2 \leqslant J_{\mathbb{K},\lambda}(c) \leqslant -\frac{3}{4}\frac{\lambda^{\frac{4}{3}}}{|\mathbb{K}|^{\frac{1}{3}}}c + \frac{3}{5}c_{TF}\frac{\lambda^{\frac{5}{3}}}{|\mathbb{K}|^{\frac{2}{3}}}. \tag{2.48}$$
Moreover, for all K such that $0 < K < -J_{\mathbb{R}^3,\lambda}$, there exists $c_* > 0$ such that for all $c \geqslant c_*$ we have
$$-\frac{15}{64}\frac{\lambda}{c_{TF}}c^2 \leqslant J_{\mathbb{K},\lambda}(c) \leqslant -c^2 K < 0. \tag{2.49}$$

REMARK 2.34. The upper bound in (2.47) implies, in particular, that there exists $c_0 := c_0(\lambda, \mathbb{K}, c_{TF}) > 0$ such that $E_{\mathbb{K},\lambda}(c) < 0$ for all $c > c_0$.

PROOF OF LEMMA 2.33. The lower bound in (2.47) has been proved in Lemma 2.22, the proof of which also leads to the inequality

$$\mathscr{J}_{\mathbb{K},c}(v) \geqslant \|\nabla v\|^2_{L^2(\mathbb{K})} - \frac{15}{64}\frac{\lambda}{c_{TF}}c^2, \tag{2.50}$$

hence the lower bound in (2.48).

REMARK 2.35. One can obtain a bound independent of c_{TF}: for any $a < 1$,

$$\mathscr{J}_{\mathbb{K},c}(v) \geqslant a\,\|\nabla v\|^2_{L^2(\mathbb{K})} - \frac{9\lambda^{\frac{5}{3}}{S_{\mathbb{K}}}^2}{64(1-a)}c^2 - \frac{3}{4}S_{\mathbb{K}}\lambda^{\frac{4}{3}}c$$

where $S_{\mathbb{K}}$ is the Sobolev constant $\|v\|_{L^6(\mathbb{K})} \leqslant S_{\mathbb{K}}\,\|v\|_{H^1(\mathbb{K})}$. See the proof in Section 6.3.

The upper bounds in (2.48) and (2.47) are simple computations of $\mathscr{J}_{\mathbb{K},c}(\bar{v})$ and $\mathscr{E}_{\mathbb{K},c}(\bar{v})$ for the constant function $\bar{v} = \sqrt{\frac{\lambda}{|\mathbb{K}|}}$, defined on $\mathbb{K}$, which belongs to the minimizing domain.

To prove (2.49), let K be such that $0 < K < -J_{\mathbb{R}^3,\lambda}$. Fix $f \in C_c^\infty(\mathbb{R}^3)$ such that $K = -\mathscr{J}_{\mathbb{R}^3}(f) > 0$. 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 $c \geqslant c_*$, the support of $f_c := c^{3/2}f(c\cdot)$ is strictly included in $\mathbb{K}$. This implies, for any $c \geqslant c_*$, that

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

and this concludes the proof of Lemma 2.33. □

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

$$\mathbb{K}_c := c\cdot\mathbb{K} := \left[-\frac{c}{2};\frac{c}{2}\right)^3. \tag{2.51}$$

Moreover, we use the notations $\breve{u}$ and $\mathring{u}$ to denote the following dilations of u:

- for any v defined on $\mathbb{K}$, $\breve{v}$ is defined on $\mathbb{K}_c$ by $\breve{v}(x) := c^{-3/2}v(c^{-1}x)$;
- for any v defined on $\mathbb{K}_c$, $\mathring{v}$ is defined on $\mathbb{K}$ by $\mathring{v}(x) := c^{+3/2}v(cx)$.

A direct computation gives $\mathscr{J}_{\mathbb{K},c}(v) = c^2\,\mathscr{J}_{\mathbb{K}_c,1}(\breve{v})$, for any $v \in H^1_{\rm per}(\mathbb{K})$. Consequently,

$$J_{\mathbb{K},\lambda}(c) = c^2 J_{\mathbb{K}_c,\lambda}(1) \tag{2.52}$$

and v is a minimizer of $J_{\mathbb{K},\lambda}(c)$ if and only if $\breve{v}$ 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 $\breve{v}$ which are given in the following corollary of Lemma 2.33.

COROLLARY 2.36 (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 $c \geqslant c_*$, a minimizer $\breve{v}_c$ of $J_{\mathbb{K}_c,\lambda}(1)$ verifies*

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

PROOF OF COROLLARY 2.36. By (2.48) and (2.50), we have that there exists $0 < c_* \leqslant \frac{4}{5} c_{TF} \left(\frac{\lambda}{|\mathbb{K}|}\right)^{\frac{1}{3}}$ such that, for all $c \geqslant c_*$, it holds that

$$0 \geqslant J_{\mathbb{K},\lambda}(c) \geqslant \|\nabla v_c\|^2_{L^2(\mathbb{K})} - \frac{15}{64} \frac{\lambda}{c_{TF}} c^2,$$

for any minimizer v_c of $J_{\mathbb{K},\lambda}(c)$. This leads to

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

REMARK. One can obtain an upper bound independent of c_{TF} (see Section 6.4).

Applying, on $\mathbb{K}$, Hölder's inequality and Sobolev embeddings to v_c, we obtain

$$\begin{cases} \|v_c\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{K})} \leqslant S(\mathbb{K}) \lambda^{\frac{5}{6}} \left(\lambda^{\frac{1}{2}} + \|\nabla v_c\|_{L^2(\mathbb{K})}\right), \\ \|v_c\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{K})} \leqslant [S(\mathbb{K})]^2 \lambda^{\frac{2}{3}} \left(\lambda + \|\nabla v_c\|^2_{L^2(\mathbb{K})}\right), \end{cases}$$

where $S(\mathbb{K})$ is the Sobolev constant on $\mathbb{K}$, and it implies that

$$\begin{cases} \|\breve{v}_c\|^{8/3}_{L^{8/3}(\mathbb{K}_c)} \leqslant S(\mathbb{K}) \lambda^{\frac{5}{6}} \left(\|\nabla \breve{v}_c\|_{L^2(\mathbb{K}_c)} + \dfrac{\lambda^{\frac{1}{2}}}{c}\right), \\ \|\breve{v}_c\|^{10/3}_{L^{10/3}(\mathbb{K}_c)} \leqslant [S(\mathbb{K})]^2 \lambda^{\frac{2}{3}} \left(\|\nabla \breve{v}_c\|^2_{L^2(\mathbb{K}_c)} + \dfrac{\lambda}{c^2}\right). \end{cases} \tag{2.53}$$

Thus there exists C such that

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

By (2.49), for any K such that $0 < K < -J_{\mathbb{R}^3,\lambda}$, there exists $c_\star > 0$ such that

$$\forall c \geqslant c_\star, \ \ 0 < \frac{4}{3} K \leqslant -\frac{4}{3} J_{\mathbb{K}_c,\lambda}(1) \leqslant \|\breve{v}_c\|^{8/3}_{L^{8/3}(\mathbb{K}_c)}$$

and, consequently, such that

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

Finally, by (2.53) and for any fixed $\widehat{c_*} > \frac{3}{4}S(\mathbb{K})\lambda^{\frac{4}{3}}K$, we have

$$\begin{aligned}
\inf_{c \geqslant \max\{c_*, c_\star, \widehat{c_*}\}} & \|\nabla \breve{v}_c\|_{L^2(\mathbb{K}_c)} \\
& \geqslant \max\left\{\frac{4K\lambda^{-\frac{5}{6}}}{3S(\mathbb{K})} - \frac{\lambda^{\frac{1}{2}}}{c}; \left(\frac{4K\lambda^{-\frac{5}{6}}}{3S(\mathbb{K})}\right)^2 - \left(\frac{\lambda^{\frac{1}{2}}}{c}\right)^2\right\} \\
& \qquad \geqslant \max\left\{\frac{4K\lambda^{-\frac{5}{6}}}{3S(\mathbb{K})} - \frac{\lambda^{\frac{1}{2}}}{\widehat{c_*}}; \left(\frac{4K\lambda^{-\frac{5}{6}}}{3S(\mathbb{K})}\right)^2 - \left(\frac{\lambda^{\frac{1}{2}}}{\widehat{c_*}}\right)^2\right\} > 0.
\end{aligned}$$

This concludes the proof of Corollary 2.36. $\square$

5.1. Concentration-compactness. In order to prove the symmetry breaking stated in Theorem 2.2, we prove the following result using the concentration-compactness method as a key ingredient.

PROPOSITION 2.37. *Let $\mathbb{K}$ be the unit cube and λ be positive. Then*

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

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

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

ii. $\mathbb{1}_{\mathbb{K}_{c_n}}\nabla\breve{w}_n(\cdot + x_n) \to \nabla u$ *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 2.37, 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 2.38. *Let $\lambda > 0$. Then*

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

PROOF OF LEMMA 2.38. 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 2.21 and Proposition 2.30. Thus

$$\mathscr{E}_{\mathbb{K},c}(w_c) - \mathscr{J}_{\mathbb{K},c}(w_c) \leqslant E_{\mathbb{K},\lambda}(c) - J_{\mathbb{K},\lambda}(c) \leqslant \mathscr{E}_{\mathbb{K},c}(v_c) - \mathscr{J}_{\mathbb{K},c}(v_c)$$

which can be rewrite as

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

By the Hardy inequality on $\mathbb{K}$ (see Section 6.5 in the Appendix) and the upper bound in (2.35), we have

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

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

$$D_{\mathbb{K}}({v_c}^2, {v_c}^2) \lesssim \|v_c\|_{H^1(\mathbb{K})}\,. \tag{2.54}$$

To prove (2.54) 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

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

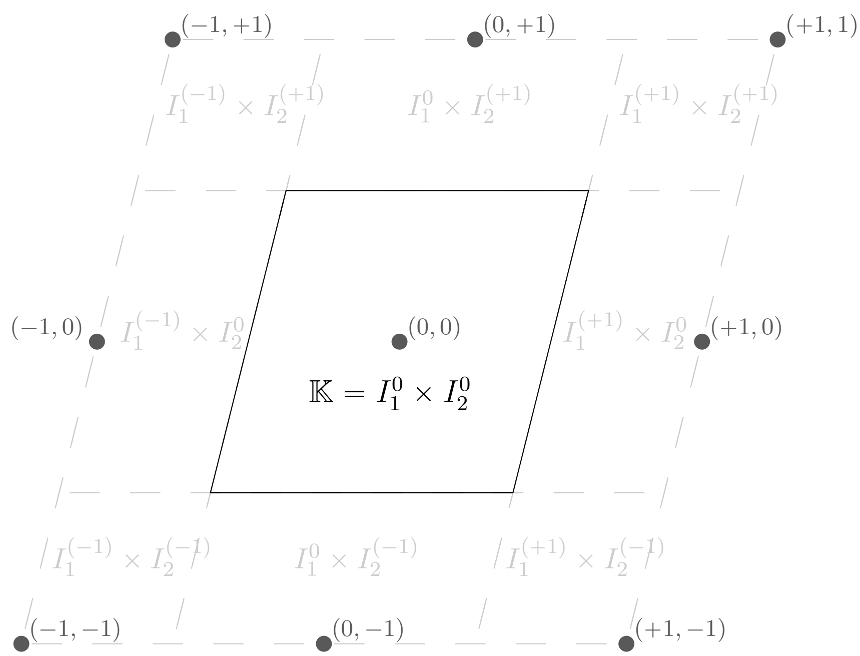


FIGURE 7. Representation, in the 2D case, of the splitting of $\mathbb{K}_2$ into subsets.

We thus have by the upper bound in (2.35) and the Hardy–Littlewood–Sobolev inequality that

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

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

$$\left|D_{\mathbb{K}}({v_c}^2,{v_c}^2)\right| = \Big|\sum_{\boldsymbol{\sigma}\in\{-1;0;+1\}^3} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K}\\ x-y\in\mathbb{K}^{\boldsymbol{\sigma}}}} {v_c}^2(x)G_{\mathbb{K}}(x-y){v_c}^2(y)\,\mathrm{d}x\,\mathrm{d}y\Big|$$
$$\lesssim \|v_c\|^4_{L^{\frac{12}{5}}(\mathbb{K})} \lesssim \|v_c\|_{H^1(\mathbb{K})}\|v_c\|^3_{L^2(\mathbb{K})}. \quad (2.55)$$

This proves (2.54) which also holds for w_c.

Then, on one hand, by (2.41) applied to $c_1 = 0 \leqslant c_2 = c$, there exist positive constants $a < 1$ and C such that for any $c > 0$ we have

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

On the other hand, the upper bound in (2.49) together with the (2.50) applied to v_c, give that there exists $c_* > 0$ such that

$$\exists\, K > 0, \forall\, c \geqslant c_*, \qquad \|\nabla v_c\|^2_{L^2(\mathbb{K})} \leqslant \left(\frac{15}{64}\frac{\lambda}{c_{TF}} - K\right)c^2. \quad (2.56)$$

Consequently, for c large enough, $\|v_c\|_{H^1(\mathbb{K})} \lesssim c$ hence $|J_{\mathbb{K},\lambda}(c) - E_{\mathbb{K},\lambda}(c)| \lesssim c$. Using (2.49), 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 2.38. □

Remark 2.39. One can deduce directly from Lemma 2.38 the symmetry breaking $E_{N\cdot\mathbb{K},N^3\lambda}(c) < N^3E_{\mathbb{K},\lambda}(c)$, see Section 6.6 in Appendix. However, since it will be also a consequence of the results in Theorem 2.2 proved below, we do not write here the direct proof of symmetry breaking for shortness.

We now prove that the periodic effective model converges,

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

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 2.37 will be a by-product of the method.

Lemma 2.40 (Upper bound). *Let $\mathbb{K}$ be the unit cube and λ be positive. Then there exists $\beta > 0$ such that*

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

In particular,

$$J_{\mathbb{R}^3,\lambda} \geqslant \limsup_{c\to\infty} c^{-2} J_{\mathbb{K},\lambda}(c). \tag{2.57}$$

Proof of Lemma 2.40. Let Q be a minimizer of $J_{\mathbb{R}^3,\lambda}$ which is, up to a phase factor and a space translation, a positive radial strictly decreasing $H^2(\mathbb{R}^3)$-solution — hence, it vanishes as $|x|$ goes to infinity — to the Euler–Lagrange equation (2.12), by Theorem 2.3. Therefore, Proposition 2.19 gives the exponential decay when r goes to infinity of the norm $\|\nabla Q\|_{L^2(^{\complement}B(0,r))}$ and the norms $\|Q\|_{L^p(^{\complement}B(0,r))}$ for $p > 0$.

We define $\mathscr{C}_c^-$ the inner $\mathbb{K}$-thick border of $\mathbb{K}_c$: $\mathscr{C}_c^- = \mathbb{K}_c\backslash\mathbb{K}_{c-1}$, and $Q_c = \frac{\sqrt{\lambda}\chi_c Q}{\|\chi_c Q\|_{L^2(\mathbb{R}^3)}}$ where $\chi_c \in C_c^\infty(\mathbb{R}^3)$, $0 \leqslant \chi_c \leqslant 1$, $\chi_c \equiv 0$ on $\mathbb{R}^3\backslash\mathbb{K}_c$, $\chi_c \equiv 1$ on $\mathbb{K}_{c-1}$ and $\|\nabla\chi_c\|_{L^\infty(\mathbb{R}^3)}$ bounded. Thus there exist $\beta > 0$ such that, for $p \in [2;6]$, we have $\|\chi_c Q\|^p_{L^p(\mathbb{R}^3)} = \|Q\|^p_{L^p(\mathbb{R}^3)} + \underset{c\to\infty}{o}(e^{-\beta c})$ and, in particular, that

$$\frac{\lambda}{\|\chi_c Q\|^2_{L^2(\mathbb{R}^3)}} = 1 + o(e^{-\beta c}).$$

Moreover the following estimates hold

$$\begin{cases} \|\chi_c \nabla Q\|^2_{L^2(\mathbb{R}^3)} = \|\nabla Q\|^2_{L^2(\mathbb{R}^3)} + o(e^{-\beta c}), \\ \|Q\nabla\chi_c\|^2_{L^2(\mathbb{R}^3)} = \|Q\nabla\chi_c\|^2_{L^2(\mathscr{C}_c^-)} \leqslant \|\nabla\chi_c\|^2_\infty \|Q\|^2_{L^2(\mathscr{C}_c^-)} = o(e^{-\beta c}), \\ \left|\int_{\mathbb{R}^3} Q\chi_c\nabla\chi_c\cdot\nabla Q\right| \leqslant \|\nabla\chi_c\|_{L^\infty(\mathbb{R}^3)} \|Q\|_{L^2(\mathscr{C}_c^-)} \|\nabla Q\|_{L^2(\mathscr{C}_c^-)} = o(e^{-\beta c}), \end{cases}$$

and they lead to $\|\nabla(\chi_c Q)\|^2_{L^2(\mathbb{R}^3)} = \|\nabla Q\|^2_{L^2(\mathbb{R}^3)} + o(e^{-\beta c})$. Consequently,

$$\begin{aligned} &\mathscr{J}_{\mathbb{R}^3}(Q_c) \\ &= \frac{\lambda}{\|\chi_c Q\|_2^2}\|\nabla(\chi_c Q)\|_2^2 + \frac{3}{5}\frac{c_{TF}\lambda^{\frac{5}{3}}}{\|\chi_c Q\|_2^{\frac{10}{3}}}\|\chi_c Q\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{R}^3)} - \frac{3}{4}\frac{\lambda^{\frac{4}{3}}}{\|\chi_c Q\|_2^{\frac{8}{3}}}\|\chi_c Q\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)} \\ &= \left(1 + o(e^{-\beta c})\right)\left(\|\nabla Q\|_2^2 + o(e^{-\beta c})\right) \\ &\quad + \frac{3}{5}c_{TF}(1 + o(e^{-\beta c}))^{\frac{5}{3}}\left(\|Q\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{R}^3)} + o(e^{-\beta c})\right) \\ &\qquad - \frac{3}{4}(1 + o(e^{-\beta c}))^{\frac{4}{3}}\left(\|Q\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)} + o(e^{-\beta c})\right) \\ &= \mathscr{J}_{\mathbb{R}^3}(Q) + o(e^{-\beta c}) \end{aligned}$$

and we finally have

$$J_{\mathbb{K}_c,\lambda}(1) \leqslant \mathscr{J}_{\mathbb{K}_c,1}(Q_c) = \mathscr{J}_{\mathbb{R}^3}(Q_c) = \mathscr{J}_{\mathbb{R}^3}(Q) + \underset{c\to\infty}{o}(e^{-\beta c}) = J_{\mathbb{R}^3,\lambda} + \underset{c\to\infty}{o}(e^{-\beta c}).$$

This concludes the proof of Lemma 2.40. $\square$

We now prove the converse inequality to (2.57).

LEMMA 2.41 (Lower bound). *Let $\mathbb{K}$ be the unit cube and λ be positive. Then*

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

See Section 6.7 in the Appendix for a detailed proof.

SKETCH OF PROOF OF LEMMA 2.41. 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 [**Gér98, BG99, HK05, KV08, Lew10**].

LEMMA 2.42 (Splitting in localized bubbles). *Let $\mathbb{K}$ be the unit cube, $\{\varphi_c\}_{c\geqslant 1}$ be a sequence of functions such that $\varphi_c \in H^1_{per}(\mathbb{K}_c)$ for all c, with $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ uniformly bounded. Then there exists a sequence of functions $\{\varphi^{(1)}, \varphi^{(2)}, \cdots\}$ in $H^1(\mathbb{R}^3)$ such that the following holds: for any $\varepsilon > 0$ and any fixed sequence $0 \leqslant R_k \to \infty$, there exist:*

- *$J \geqslant 0$,*
- *a subsequence $\{\varphi_{c_k}\}$,*
- *sequences $\{\xi_k^{(1)}\}, \cdots, \{\xi_k^{(J)}\}, \{\psi_k\}$ in $H^1_{per}(\mathbb{K}_{c_k})$,*
- *sequences of space translations $\{x_k^{(1)}\}, \cdots, \{x_k^{(J)}\}$ in $\mathbb{R}^3$*

such that

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

where

- *$\{\xi_k^{(1)}\}, \cdots, \{\xi_k^{(J)}\}, \{\psi_k\}$ 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 $2 \leqslant p < 6$,*
- *$supp(\mathbb{1}_{\mathbb{K}_{c_k}} \xi_k^{(j)}) \subset B(0, R_k)$ for all $j = 1, \cdots, J$ and all k,*
- *$supp(\mathbb{1}_{\mathbb{K}_{c_k}} \psi_k) \subset \mathbb{K}_{c_k} \setminus \bigcup_{j=1}^{J} B(x_k^{(j)}, 2R_k)$ for all k,*
- *$|x_k^{(i)} - x_k^{(j)}| \geqslant 5R_k$ for all $i \neq j$ and all k,*
- *$\int_{\mathbb{K}_{c_k}} |\psi_k|^{\frac{8}{3}} \leqslant \varepsilon$.*

REMARK. In the proof of Lemma 2.41, we really need to use all the bubbles because we do not know well enough the energy of ψ_k. In similar proofs, it is often possible to conclude after extracting few bubbles, using that $\mathscr{J}(\psi_k) \geqslant J(\int |\psi_k|^2)$ which allows to conclude. However, in our case, $J_{\mathbb{K}_c}(\int |\psi_k|^2)$ depends on c hence the same inequality of course holds but does not allow us to conclude. We therefore need to extract all the bubbles (up to ε).

We apply Lemma 2.42 to the sequence $(\breve{v}_c)_{c\geqslant 1}$ of minimizers to $J_{\mathbb{K}_c,\lambda}(1)$ which verifies the hypothesis by the upper bound proved in Corollary 2.36. The lower bound in that corollary excludes the case $J=0$. Indeed, in that case we would have $\lim\limits_{k\to\infty}\|\varphi_{c_k}-\psi_k\|_{H^1(\mathbb{K}_{c_k})}=0$ and $\int_{\mathbb{K}_{c_k}}|\psi_k|^{\frac{8}{3}}\leqslant\varepsilon$ hence $\int_{\mathbb{K}_{c_k}}|\varphi_k|^{\frac{8}{3}}\leqslant 2\varepsilon$, for k large enough, contradicting the mentioned lower bound. Consequently, there exists $J\geqslant 1$ such that

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

where $\|\varepsilon_k\|_{H^1(\mathbb{K}_{c_k})}\to 0$ and, for a each k, the supports of the $\breve{v}_k^{(j)}(\cdot-x_k^{(j)})$'s and ψ_k are pairwise disjoint. The support properties, the Minkowski inequality, Sobolev embeddings and the fact that $\operatorname{supp}(\mathbb{1}_{\mathbb{K}_{c_k}}\breve{v}_k^{(j)})\subset B(0,R_k)\subset\mathbb{K}_{c_k}$, give that

$$\begin{aligned}J_{\mathbb{K}_{c_k}}(\lambda)=\mathscr{J}_{\mathbb{K}_{c_k}}(\breve{v}_{c_k})&=\mathscr{J}_{\mathbb{K}_{c_k}}(\psi_k)+\sum_{j=1}^{J}\mathscr{J}_{\mathbb{R}^3}(\mathbb{1}_{\mathbb{K}_{c_k}}\breve{v}_k^{(j)})+o(1)_{c_k\to\infty}\\&\geqslant-\frac{3}{4}\varepsilon+\sum_{j=1}^{J}\mathscr{J}_{\mathbb{R}^3}(\mathbb{1}_{\mathbb{K}_{c_k}}\breve{v}_k^{(j)})+o(1)_{c_k\to\infty}.\end{aligned}$$

Moreover, the strong convergence of $\mathbb{1}_{\mathbb{K}_{c_k}}\breve{v}_k^{(j)}$ in L^2 and the continuity of $\lambda\mapsto J_{\mathbb{R}^3,\lambda}$, proved in Lemma 2.12, imply, for all $j=1,\cdots,J$, that

$$\mathscr{J}_{\mathbb{R}^3}(\mathbb{1}_{\mathbb{K}_{c_k}}\breve{v}_k^{(j)})\geqslant J_{\mathbb{R}^3}\Big(\|\breve{v}_k^{(j)}\|^2_{L^2(\mathbb{K}_{c_k})}\Big)\underset{k\to\infty}{\longrightarrow}J_{\mathbb{R}^3}(\lambda^{(j)}),$$

where, for any j, $\lambda^{(j)}:=\|\breve{v}^{(j)}\|_{L^2(\mathbb{R}^3)}$ is the mass of the limit of $\mathbb{1}_{\mathbb{K}_{c_k}}\breve{v}_k^{(j)}$. 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 2.16 lead to

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

The last inequality comes from the fact that

$$0\leqslant\|\psi_k\|^2_{L^2(\mathbb{K}_{c_k})}=\lambda-\sum_{j=1}^{J}\lambda^{(j)}+o(1)$$

thus $\lambda-\sum\limits_{j=1}^{J}\lambda^{(j)}\geqslant 0$ and this implies that $J_{\mathbb{R}^3}\Big(\lambda-\sum\limits_{j=1}^{J}\lambda^{(j)}\Big)\leqslant 0$. This concludes the proof of Lemma 2.41. $\square$

We can now compute the main term of $E_{\mathbb{K},\lambda}(c)$ stated in Proposition 2.37.

Proof of Proposition 2.37. From Propositions 2.40 and 2.41, we obtain for all $\lambda > 0$ that

$$\liminf_{c\to\infty} c^{-2} J_{\mathbb{K},\lambda}(c) \geqslant J_{\mathbb{R}^3,\lambda} \geqslant \limsup_{c\to\infty} c^{-2} J_{\mathbb{K},\lambda}(c)$$

hence $\lim\limits_{c\to\infty} c^{-2} J_{\mathbb{K},\lambda}(c) = J_{\mathbb{R}^3,\lambda}$ and Lemma 2.38 gives then the same limit for $E_{\mathbb{K},\lambda}(c)$. Proposition 2.41 also gives that $(\breve{v}_c)_{c\geqslant 1}$ has at least a first extracted bubble $0 \not\equiv \breve{v} \in H^1(\mathbb{R}^3)$ to which $\mathbb{1}_{\mathbb{K}_{c_k}} \breve{v}_{c_k}(\cdot + x_k)$ converges weakly in $L^2(\mathbb{R}^3)$. This leads to

$$J_{\mathbb{K}_{c_k},\lambda}(1) = \mathscr{J}_{\mathbb{K}_{c_k},1}(\breve{v}_{c_k}(\cdot + x_k)) = \mathscr{J}_{\mathbb{R}^3}(\breve{v}) + \mathscr{J}_{\mathbb{K}_{c_k},1}(\breve{v}_{c_k}(\cdot + x_k) - \breve{v}) + o(1) \quad (2.58)$$

by the following lemma.

Lemma 2.43. *Let $\mathbb{K}$ be the unit cube and $\{\varphi_c\}_{c\geqslant 1}$ be a sequence of functions on $\mathbb{R}^3$ with $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ uniformly bounded such that $\mathbb{1}_{\mathbb{K}_c}\varphi_c \underset{c\to\infty}{\rightharpoonup} \varphi$ weakly in $L^2(\mathbb{R}^3)$. Then $\varphi \in H^1(\mathbb{R}^3)$ and, up to the extraction of a subsequence, we have*

(1) $\mathbb{1}_{\mathbb{K}_c}\nabla\varphi_c \rightharpoonup \nabla\varphi$ *weakly in* $L^2(\mathbb{R}^3)$,

(2) $\|\nabla(\varphi_c - \varphi)\|^2_{L^2(\mathbb{K}_c)} = \|\nabla\varphi_c\|^2_{L^2(\mathbb{K}_c)} - \|\nabla\varphi\|^2_{L^2(\mathbb{R}^3)} + \underset{c\to\infty}{o}(1)$,

(3) $\|\varphi_c - \varphi\|^p_{L^p(\mathbb{K}_c)} = \|\varphi_c\|^p_{L^p(\mathbb{K}_c)} - \|\varphi\|^p_{L^p(\mathbb{R}^3)} + \underset{c\to\infty}{o}(1)$, *for* $p \in \left\{\frac{8}{3}, \frac{10}{3}\right\}$.

Proof of Lemma 2.43. By the uniform boundedness in $L^2(\mathbb{R}^3)$ of $\mathbb{1}_{\mathbb{K}_c}\varphi_c$, there exists such $L^2(\mathbb{R}^3)$-weak limit φ as stated in this lemma. Moreover, defining χ_c as in Lemma 2.40, we have that $\chi_c\varphi_c$ is bounded in $H^1(\mathbb{R}^3)$ since $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ is uniformly bounded. Thus there exists $\psi \in H^1(\mathbb{R}^3)$ such that $\chi_c\varphi_c \underset{c\to\infty}{\rightharpoonup} \psi$ weakly in $H^1(\mathbb{R}^3)$ and

$$\mathbb{1}_{\mathbb{K}_c}\varphi_c = (\mathbb{1}_{\mathbb{K}_c} - \chi_c)\varphi_c + \chi_c\varphi_c \underset{c\to\infty}{\rightharpoonup} \psi$$

weakly in $H^1(\mathbb{R}^3)$. Thus $\varphi = \psi \in H^1(\mathbb{R}^3)$ by uniqueness of the limit.

Let f be in $C_c^\infty(\mathbb{R}^3)$ and c^* be such that $\operatorname{supp} f \subset \mathbb{K}_{c^*}$. For $c \geqslant c^*$, we have

$$\int_{\mathbb{R}^3} f\mathbb{1}_{\mathbb{K}_c}\nabla\varphi_c = -\int_{\mathbb{K}_c} \varphi_c\nabla f \underset{\substack{c\to+\infty\\ c\geqslant c^*}}{\longrightarrow} -\int_{\mathbb{R}^3} \varphi\nabla f = \int_{\mathbb{R}^3} f\nabla\varphi$$

by the weak convergence of $\varphi_c\mathbb{1}_{\mathbb{K}_c}$ in $L^2(\mathbb{R}^3)$. Moreover, $\mathbb{1}_{\mathbb{K}_c}\nabla\varphi_c$ is bounded in $L^2(\mathbb{R}^3)$ thus, up to the extraction of a subsequence, $\mathbb{1}_{\mathbb{K}_c}\nabla\varphi_c$ converges weakly in $L^2(\mathbb{R}^3)$ and its limit is $\nabla\varphi$ by uniqueness of the limit. Claim *(1)* is therefore proved.

Claim *(2)*, comes from the weak convergence of $\mathbb{1}_{\mathbb{K}_c}\nabla\varphi_c$ and using

$$\int_{\mathbb{K}_c} |\nabla(\varphi_c - \varphi)|^2 = \int_{\mathbb{K}_c} |\nabla\varphi_c|^2 - 2\int_{\mathbb{R}^3} \mathbb{1}_{\mathbb{K}_c}\nabla\varphi_c \cdot \nabla\varphi + \int_{\mathbb{K}_c} |\nabla\varphi|^2$$

together with $\|\nabla\varphi\|_{L^2(\mathbb{K}_c)} \to \|\nabla\varphi\|_{L^2(\mathbb{R}^3)}$.

We now prove *(3)*. First we claim that $|\varphi_c - \varphi| \rightharpoonup 0$ weakly in $L^2(\mathbb{R}^3)\cap L^6(\mathbb{R}^3)$. Indeed,

$$\||\varphi_c\chi_c - \varphi|\|_{L^p(\mathbb{R}^3)} \leqslant \|\varphi_c\chi_c\|_{L^p(\mathbb{K}_c)} + \|\varphi\|_{L^p(\mathbb{R}^3)} \leqslant \|\varphi_c\|_{L^p(\mathbb{K}_c)} + \|\varphi\|_{L^p(\mathbb{R}^3)}\,,$$

for $2 \leqslant p \leqslant 6$, which is bounded since $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ is uniformly bounded by hypothesis. Therefore, there exists $\xi \geqslant 0$ such that, up to a subsequence, $|\varphi_c\chi_c - \varphi| \rightharpoonup \xi$ weakly in $L^p(\mathbb{R}^3)$. Thus for any bounded domain Ω, by Rellich-Kondrachov Theorem applied to $\chi_c\varphi_c$, which weakly converges to φ in $H^1(\mathbb{R}^3)$, we have that

$$\int_\Omega \xi^2 \leqslant \liminf_{c\to\infty} \int_\Omega |\varphi_c\chi_c - \varphi|^2 = 0.$$

Thus $\xi \equiv 0$ and $|\chi_c\varphi_c - \varphi| \rightharpoonup 0$ weakly in $L^p(\mathbb{R}^3)$ for $2 \leqslant p \leqslant 6$. Consequently $|\varphi_c - \varphi| \rightharpoonup 0$ weakly in $L^p(\mathbb{R}^3)$ for $2 \leqslant p \leqslant 6$.

Second, we claim that we have the bound

$$||x-1|^p - |x|^p + 1| < \sum_{k=1}^{\lfloor p\rfloor} \binom{\frac{q}{2}}{k} |x-1|^k, \tag{2.59}$$

for all $p > 2$ and $x \in \mathbb{R}\backslash\{1\}$. Indeed, for $0 \leqslant x \neq 1$, we in fact have

$$-\sum_{k=1}^{\lfloor p\rfloor} \binom{\frac{q}{2}}{k} (x-1)^k < |x-1|^p - x^p + 1 < -p(x-1),$$

where the right inequality can be proved by $\lfloor p\rfloor$ derivations and using that $x \mapsto x^{p-\lfloor p\rfloor}$ is increasing on $\mathbb{R}_+$, and the left inequality can be proved using the sub-additive (concavity and $f(0) = 0$) of the previous power function when $x > 1$ while the case $x < 1$ is direct (separating $\lfloor p\rfloor$ odd or even). So, for $x \geqslant 0$, the claimed bound is a rough consequence of the above. For $x < 0$, we have $|x-1|^p - |x|^p + 1 > 0$ and the upper bound on $|x-1|^p - |x|^p + 1$ is a simple computation. For a more detailed proof of (2.59), see Lemma 2.75 in Appendix 6.7.

We can now conclude. Indeed, defining $\mathbb{K}_c^* = \mathbb{K}_c\backslash\{\varphi = 0\}$ and noting that

$$\int_{\mathbb{K}_c} |\varphi_c - \varphi|^p - |\varphi_c|^p + |\varphi|^p = \int_{\mathbb{K}_c^*} \varphi^p \left(\left|\frac{\varphi_c}{\varphi} - 1\right|^p - \left|\frac{\varphi_c}{\varphi}\right|^p + 1\right),$$

the bound (2.59) then reduces the end of the proof to the demonstration that

$$\int_{\mathbb{K}_c^*} \varphi^p \left|\frac{\varphi_c}{\varphi} - 1\right|^k = \int_{\mathbb{K}_c} \varphi^{p-k}\,|\varphi_c - \varphi|^k$$

convergences to 0 for $k = 1, 2$ and $p \in \{\frac{8}{3}, \frac{10}{3}\}$, and for $k = 3$ and $p = \frac{10}{3}$. This is obtained from the weak convergence of $|\varphi - \varphi_c| \rightharpoonup 0$ in $L^2(\mathbb{R}^3)$ together with

- the fact, for $k = 1$ and $p \in \{\frac{8}{3}, \frac{10}{3}\}$, that $\varphi^{p-1} \in L^2(\mathbb{R}^3)$;
- the fact, for $k = 2$ and $p \in \{\frac{8}{3}, \frac{10}{3}\}$, that $\varphi^{2p-4} \in L^2(\mathbb{R}^3)$ and that

$$0 \leqslant \int_{\mathbb{K}_c} \varphi^{p-2} |\varphi_c - \varphi|^2 \leqslant \left(\int_{\mathbb{K}_c} \varphi^{2p-4} |\varphi_c - \varphi|\right)^{\frac{1}{2}} \|\varphi_c - \varphi\|^{\frac{3}{2}}_{L^3(\mathbb{K}_c)} \underset{c \to +\infty}{\longrightarrow} 0;$$

- the fact, for $k = 3$ and $p = \frac{10}{3}$, that

$$0 \leqslant \int_{\mathbb{K}_c} \varphi^{\frac{1}{3}} |\varphi_c - \varphi|^3 \leqslant \left(\int_{\mathbb{K}_c} \varphi |\varphi_c - \varphi|\right)^{\frac{1}{3}} \|\varphi_c - \varphi\|^{\frac{8}{3}}_{L^4(\mathbb{K}_c)} \underset{c \to +\infty}{\longrightarrow} 0.$$

This concludes the proof of Lemma 2.43. ☐

To obtain for $E_{\mathbb{K},\lambda}(c)$ an expansion similar to (2.58), we proceed the same way. We first show that the sequence of minimizers $\breve{w}_c$ is uniformly bounded in $H^1_{\mathrm{per}}(\mathbb{K}_c)$ using the upper bound in the following lemma, which is equivalent to Corollary 2.36 for $\breve{v}_c$.

Lemma 2.44 (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 $c \geqslant c_*$, the dilation $\breve{w}_c(x) := c^{-3/2} w_c(c^{-1}x)$ of a minimizer w_c to $E_{\mathbb{K},\lambda}(c)$ verifies*

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

Proof of Lemma 2.44. As seen in the proof of Lemma 2.38, $\|\nabla w_c\|_{L^2(\mathbb{K})} = O(c)$ hence

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

and, using (2.53) for the two other norms, we have

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

Let K be such that $0 < K < -J_{\mathbb{R}^3,\lambda}$ and $\varepsilon > 0$, then by (2.49) and Lemma 2.38, there exists $C > 0$ such that

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

for c's large enough and, consequently that

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

We conclude this proof of Lemma 2.44 as we did in the proof of Corollary 2.36. ☐

We now come back to the proof of Proposition 2.37. We apply Lemma 2.42 to $\{\breve{w}_c\}$ and, as for $\breve{v}_c$, the lower bound in Lemma 2.44 implies that $J \geqslant 1$, namely that there exist at least a first extracted bubble $0 \not\equiv \breve{w} \in H^1(\mathbb{R}^3)$ such that $\mathbb{1}_{\mathbb{K}_{c_k}} \breve{w}_{c_k}(\cdot + y_k) \rightharpoonup \breve{w}$ weakly in $L^2(\mathbb{R}^3)$. Lemma 2.43 then leads to

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

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 2.38.

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 $\lambda_1 := \|\breve{w}\|^2_{L^2(\mathbb{R}^3)}$, which is positive since $\breve{w} \not\equiv 0$, we thus have

$$\begin{aligned} {c_k}^{-2} E_{\mathbb{K},\lambda}(c_k) &= \mathscr{I}_{\mathbb{R}^3}(\breve{w}) + \mathscr{I}_{\mathbb{K}_{c_k},1}(\breve{w}_{c_k}(\cdot + y_k) - \breve{w}) + o(1) \\ &\geqslant J_{\mathbb{R}^3}(\lambda_1) + J_{\mathbb{K}_{c_k}}\left(\|\breve{w}_{c_k}(\cdot + y_k) - \breve{w}\|^2_{L^2(\mathbb{K}_{c_k})}\right) + o(1). \end{aligned}$$

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

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

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

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

and, sending ε to 0, the continuity of $\lambda \mapsto J_{\mathbb{R}^3}(\lambda)$, proved in Lemma 2.12, gives

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

We recall that $\lambda_1 > 0$ hence, if $\lambda_1 < \lambda$ then the above large inequality would contradict the strict binding proved in Proposition 2.16, 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 $\mathbb{1}_{\mathbb{K}_c} \breve{w}_c(\cdot + y_k)$ to $\breve{w}$ hence in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$ by Hölder's inequality, Sobolev embeddings and the facts that $\breve{w}_c$ is uniformly bounded in $H^1_{\mathrm{per}}(\mathbb{K}_c)$ and that $\breve{w} \in H^1(\mathbb{R}^3)$. The strong convergence holds in particular in $L^{\frac{8}{3}}(\mathbb{R}^3)$ thus we have proved that $\breve{w}$ is the first and only bubble.

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

$$\begin{aligned} {c_k}^{-2} E_{\mathbb{K},\lambda}(c_k) &= \mathscr{I}_{\mathbb{R}^3}(\breve{w}) + \mathscr{I}_{\mathbb{K}_{c_k},1}(\breve{w}_{c_k}(\cdot + y_k) - \breve{w}) + o(1) \\ &\geqslant \mathscr{I}_{\mathbb{R}^3}(\breve{w}) + J_{\mathbb{K}_{c_k}}\left(\|\breve{w}_{c_k}(\cdot + y_k) - \breve{w}\|^2_{L^2(\mathbb{K}_{c_k})}\right) + o(1) \\ &\geqslant \mathscr{I}_{\mathbb{R}^3}(\breve{w}) + J_{\mathbb{K}_{c_k}}(\varepsilon) + o(1). \end{aligned}$$

This leads to $J_{\mathbb{R}^3}(\lambda) \geqslant \mathscr{J}_{\mathbb{R}^3}(\breve{w}) + J_{\mathbb{R}^3}(\varepsilon)$, then to $J_{\mathbb{R}^3}(\lambda) \geqslant \mathscr{J}_{\mathbb{R}^3}(\breve{w})$ by the continuity of $J_{\mathbb{R}^3}(\lambda)$ proved in Lemma 2.12. Since $\|\breve{w}\|^2_{L^2(\mathbb{R}^3)} = \lambda$, this concludes the proof of Proposition 2.37 up to the convergence of $\mathbb{1}_{\mathbb{K}_{c_n}} \nabla \breve{w}_n(\cdot + x_n)$ and $\mathbb{1}_{\mathbb{K}_{c_n}} \nabla \breve{v}_n(\cdot + x_n)$ that we deduce now from the above results.

We first prove the convergence in $L^2(\mathbb{R}^3)$-norm. As obtained during the proof of Lemma 2.44, we have

$$\left| \int_{\mathbb{K}} G_{\mathbb{K}} {w_c}^2 \right| + \left| D_{\mathbb{K}}({w_c}^2, {w_c}^2) \right| = o(c^2).$$

Moreover, we have

$$\begin{aligned} {c_n}^{-1} \|\mathring{w}_n\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{K})} &= \|\breve{w}_n(\cdot + x_n)\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{K}_{c_n})} \to \|u\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)} \\ {c_n}^{-2} \|\mathring{w}_n\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{K})} &= \|\breve{w}_n(\cdot + x_n)\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{K}_{c_n})} \to \|u\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{R}^3)} \end{aligned}$$

and ${c_n}^{-2} E_{\mathbb{K},\lambda}(c_n)$ convergences to $J_{\mathbb{R}^3}(\lambda)$ hence

$$\|\nabla \breve{w}_n\|^2_{L^2(\mathbb{K}_c)} \underset{c\to\infty}{\longrightarrow} J_{\mathbb{R}^3}(\lambda) - \frac{3}{5} c_{TF} \|u\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{R}^3)} + \frac{3}{4} \|u\|^{\frac{8}{3}}_{L^{\frac{8}{3}}(\mathbb{R}^3)} = \|\nabla u\|^2_{L^2(\mathbb{R}^3)}$$

since u is a minimizer of $J_{\mathbb{R}^3}(\lambda)$ and $\mathring{w}_n$ of $E_{\mathbb{K},\lambda}(c_n)$.

For $\mathbb{1}_{\mathbb{K}_{c_n}} \nabla \breve{v}_n(\cdot + x_n)$ it is even simplier since it only comes from the convergence in $L^p(\mathbb{R}^3)$ of $\breve{v}_n(\cdot + x_n)$ together with the convergence of ${c_n}^{-2} J_{\mathbb{K},\lambda}(c_n)$.

Then we apply Lemma 2.43 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. Indeed, most of those results deal with the effective model and are therefore not impacted by the presence of several charges in the unit cell. For the other results, the modifications only come from the factor $\int_{\mathbb{K}} G_{\mathbb{K}} {w_c}^2$ being replaced by $\int_{\mathbb{K}} \sum_{i=1}^{N_q} z_i G_{\mathbb{K}}(\cdot - R_i) |w_c|^2$ — see (2.60) — therefore the statements of Proposition 2.37, Lemma 2.38 and Lemma 2.44 are unchanged and the only slight changes are:

- a factor N_q in the bounds of the modified term, in the proofs of those three results;
- the upper bound in (2.47) is modified by some constants but is anyway not used in any proof.

Consequently, as mentioned in Section 2.1, the results

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

from Proposition 2.37 and the result

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

from Proposition 2.16 imply together the symmetry breaking

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

We now give a corollary of Proposition 2.37.

Corollary 2.45 (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 2.21. Then there exists a subsequence $c_n \to \infty$ such that*

$$c_n{}^{-2}\mu_{c_n} \underset{n\to\infty}{\longrightarrow} \mu_{\mathbb{R}^3,\{w_{c_n}\}}$$

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 $\mathbb{1}_{\mathbb{K}_{c_n}}\breve{w}_{c_n}(\cdot + x_n)$ 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 2.45. Let u be the minimizer of $J_{\mathbb{R}^3}(\lambda)$ to which $\mathbb{1}_{\mathbb{K}_{c_n}}\breve{w}_{c_n}(\cdot + x_n)$ converges strongly in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$, by Proposition 2.37 which also gives that $\mathbb{1}_{\mathbb{K}_{c_n}}\nabla\breve{w}_{c_n}(\cdot + x_n) \to \nabla u$ strongly in $L^2(\mathbb{R}^3)$, and $\mu_{\mathbb{R}^3,u}$ the Euler–Lagrange multiplier associated with this u by Theorem 2.3.

By Lemma 2.44 and the formula (2.38) giving an expression of μ_c, we then obtain

$$\begin{aligned}- c_n{}^{-2}\mu_{c_n}\lambda &= \|\nabla\breve{w}_{c_n}\|_2^2 + c_{TF}\,\|\breve{w}_{c_n}\|_{10/3}^{10/3} - \|\breve{w}_{c_n}\|_{8/3}^{8/3} \\ &\quad + c_n{}^{-2}\left[D_{\mathbb{K}}(|w_{c_n}|^2, |w_{c_n}|^2) - \left\langle G_{\mathbb{K}}, |w_{c_n}|^2\right\rangle_{L^2(\mathbb{K})}\right] \\ &\qquad \to \|\nabla u\|_{L^2(\mathbb{R}^3)}^2 + c_{TF}\,\|u\|_{L^{10/3}(\mathbb{R}^3)}^{10/3} - \|u\|_{L^{8/3}(\mathbb{R}^3)}^{8/3}\end{aligned}$$

since, as obtained during the proof of Lemma 2.44, we have

$$\left|\int_{\mathbb{K}} G_{\mathbb{K}} w_c{}^2\right| + \left|D_{\mathbb{K}}(w_c{}^2, w_c{}^2)\right| = o(c^2).$$

Therefore, by (2.26) which gives an expression of the Euler–Lagrange parameter $\mu_{\mathbb{R}^3,u}$ associated with this u, we have

$$c_n{}^{-2}\mu_{c_n} \underset{c\to\infty}{\longrightarrow} \mu_{\mathbb{R}^3,u}.$$

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. $\square$

5.2. Location of the concentration points. In this section we consider the union of N^3 cubes $\mathbb{K}$, each containing N_q charges — not necessarily with the same charge values z_i — forming together the cube $\mathbb{K}_N := N \cdot \mathbb{K}$. The energy of the unit cell $\mathbb{K}_N$ is then

$$\mathscr{E}_{\mathbb{K}_N,c}(w) = \mathscr{J}_{\mathbb{K}_N,c}(w) + \frac{1}{2} D_{\mathbb{K}_N}(|w|^2, |w|^2) - \int_{\mathbb{K}_N} \mathscr{G}|w|^2, \tag{2.60}$$

where

$$\mathscr{G} := \sum_{m=1}^{N_q} \sum_{i=1}^{N^3} z_m G_{\mathbb{K}_N}(\cdot - R_{m,i}) \tag{2.61}$$

and $\{R_{m,i}\}_{1\leqslant m\leqslant N_q, 1\leqslant i\leqslant N^3}$ denote the positions of the $N^3 N_q$ charges in the N^3 copies of $\mathbb{K}$ which one contains N_q charges. We recall that

$$D_{\mathbb{K}_N}(f,g) = \int_{\mathbb{K}_N} \int_{\mathbb{K}_N} f(x) G_{\mathbb{K}_N}(x-y) g(y) \,\mathrm{d}y \,\mathrm{d}x.$$

In this section, we prove a localization type result (Proposition 2.47) — that any minimizer concentrates around the position of a charge of the lattice — and a lower bound on the number of distinct minimizers (Proposition 2.49). We first state the following lemma, which is a consequence of Proposition 2.37.

LEMMA 2.46 (L^∞-convergence). *Let $1 \leqslant N \in \mathbb{N}$ and $\{w_c\}_{c\to+\infty}$ be a sequence of minimizers to $E_{\mathbb{K}_N,N^3\lambda}(c)$ and u be the minimizer to $J_{\mathbb{R}^3}(N^3\lambda)$ to which the subsequence of rescaled functions $\mathbb{1}_{\mathbb{K}_{c_n N}} \breve{w}_{c_n}(\cdot + x_n)$ converges. Then*

$$\|\breve{w}_{c_n}(\cdot + x_n) - u\|_{H^2(\mathbb{K}_{c_n N})} \underset{n\to+\infty}{\longrightarrow} 0$$

and, consequently,

$$\left\|\mathbb{1}_{\mathbb{K}_{c_n N}} \breve{w}_{c_n}(\cdot + x_n) - u\right\|_{L^\infty(\mathbb{K}_{c_n N})} \underset{n\to+\infty}{\longrightarrow} 0.$$

Similarly, let $\{v_c\}_{c\to+\infty}$ be a sequence of minimizers to $J_{\mathbb{K}_N,N^3\lambda}(c)$ and u be the minimizer to $J_{\mathbb{R}^3}(N^3\lambda)$ to which the subsequence of rescaled functions $\mathbb{1}_{\mathbb{K}_{c_n N}} \breve{v}_{c_n}(\cdot + x_n)$ converges. Then

$$\|\breve{v}_{c_n}(\cdot + x_n) - u\|_{H^2(\mathbb{K}_{c_n N})} \underset{n\to+\infty}{\longrightarrow} 0$$

and, consequently,

$$\left\|\mathbb{1}_{\mathbb{K}_{c_n N}} \breve{v}_{c_n}(\cdot + x_n) - u\right\|_{L^\infty(\mathbb{R}^3)} \underset{n\to+\infty}{\longrightarrow} 0.$$

PROOF OF LEMMA 2.46. For shortness, we will omit the spatial translations $\{x_n\}$ in the rest of this proof. By Proposition 2.37, the convergence $\mathbb{1}_{c_n\cdot\mathbb{K}_N} \breve{w}_{c_n} \to u$ is strong in $L^p(\mathbb{R}^3)$, $2 \leqslant p < 6$. For any c, we define $u_c = \zeta_c u$ where ζ_c is a smooth function such that $0 \leqslant \zeta_c \leqslant 1$, $\zeta_c \equiv 0$ on $\mathbb{R}^3 \backslash \mathbb{K}_{cN}$ and $\zeta_c \equiv 1$ on $\mathbb{K}_{cN-1}$. Since

$u \in L^2(\mathbb{R}^3)$, it vanishes as $|x| \to \infty$, thus $\|u_{c_n} - u\|_{L^\infty(\mathbb{K}_{c_n N})} \underset{n\to+\infty}{\longrightarrow} 0$ and proving the stated result is equivalent to prove that $\|\breve{w}_{c_n} - u_{c_n}\|_{L^\infty(\mathbb{K}_{c_n N})} \underset{n\to+\infty}{\longrightarrow} 0$.

Applying Lemma 2.80 (in the Appendix) to $\nu = c^{-1} \leqslant 1$ and using Lemma 2.81, we obtain that there exists $0 < C < 1$ such that, for any β large enough and any $c \geqslant 1$, we have

$$\|\breve{w}_c - u_c\|_{L^\infty(\mathbb{K}_{cN})} \leqslant C \left\| \left(-\Delta_{\text{per}} - c^{-2}\mathscr{G}(c^{-1}\cdot) + \beta\right)(\breve{w}_c - u_c)\right\|_{L^2(\mathbb{K}_{cN})}.$$

Let us emphasize that the power in front of $\mathscr{G}$ is c^{-2} while the scaling inside it is c^{-1}. Moreover, by the Euler–Lagrange equations (2.12) and (2.37), we have for any $c > 0$

$$\begin{aligned}
&\left(-\Delta - c^{-2}\mathscr{G}(c^{-1}\cdot)\right)(\breve{w}_c - u_c)\\
&\quad = c_{TF}\left(\zeta_c|u|^{\frac{4}{3}}u - |\breve{w}_c|^{\frac{4}{3}}\breve{w}_c\right) + \left(|\breve{w}_c|^{\frac{2}{3}}\breve{w}_c - \zeta_c|u|^{\frac{2}{3}}u\right) + \mu_{\mathbb{R}^3}u_c - c^{-2}\mu_c\breve{w}_c\\
&\qquad\qquad + c^{-2}\mathscr{G}(c^{-1}\cdot)u_c - c^{-2}\left(|w_c|^2 \star G_{\mathbb{K}}\right)(c^{-1}\cdot)\breve{w}_c + 2\nabla\zeta_c\nabla u + u\Delta\zeta_c,
\end{aligned}$$

where $\mu_{\mathbb{R}^3}$ is the Euler–Lagrange parameter associated with u. Therefore, the fact that

- $L^\infty(\mathbb{K}_{cN})$ norms of ζ_c and of it derivatives are finite,
- $u \in H^2(\mathbb{R}^3) \subset L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$,
- $\|\nabla u\|_{L^2(\mathbb{K}_{cN}\setminus\mathbb{K}_{cN-1})} + \|u\|_{L^2(\mathbb{K}_{cN}\setminus\mathbb{K}_{cN-1})} \to 0$ (which is even an exponential decay by Proposition 2.19),
- $\|c^{-1}\mathscr{G}(c^{-1}\cdot)\|_{L^{5/2}(\mathbb{K}_{cN})} = c^{1/5}\|\mathscr{G}\|_{L^{5/2}(\mathbb{K}_N)}$,
- $\|{\zeta_{c_n}}^\alpha u - \breve{w}_{c_n}\|_{L^p(\mathbb{K}_{c_n})} = \|(1 - {\zeta_{c_n}}^\alpha)u\|_{L^p(\mathbb{K}_{c_n})} + \|u - \breve{w}_{c_n}\|_{L^p(\mathbb{K}_{c_n})} \to 0$ for any $\alpha > 0$ and $2 \leqslant p \leqslant 6$,

leads, by Corollary 2.45 and both inequalities (2.100) and (2.101) detailed in the Appendix, to $\|\breve{w}_{c_n} - u_{c_n}\|_{L^\infty(\mathbb{K}_{c_n N})} \underset{n\to+\infty}{\longrightarrow} 0$ since

$$\begin{aligned}
&\|\breve{w}_{c_n} - u_{c_n}\|_{L^\infty(\mathbb{K}_{c_n N})}\\
&\quad \leqslant Cc_{TF}\left\|{\zeta_{c_n}}^{\frac{3}{7}}u - \breve{w}_{c_n}\right\|_{L^4(\mathbb{K}_{c_n N})}\left\|{\zeta_{c_n}}^{\frac{4}{7}}|u|^{\frac{4}{3}} + |\breve{w}_{c_n}|^{\frac{4}{3}}\right\|_{L^4(\mathbb{K}_{c_n N})}\\
&\quad + C\left\|{\zeta_{c_n}}^{\frac{3}{5}}u - \breve{w}_{c_n}\right\|_{L^4(\mathbb{K}_{c_n N})}\left\|{\zeta_{c_n}}^{\frac{2}{5}}|u|^{\frac{2}{3}} + |\breve{w}_{c_n}|^{\frac{2}{3}}\right\|_{L^4(\mathbb{K}_{c_n N})}\\
&\quad + C|\mu_{\mathbb{R}^3} - {c_n}^{-2}\mu_c|\,\|\breve{w}_{c_n}\|_{L^2(\mathbb{K}_{c_n N})} + C(\mu_{\mathbb{R}^3} + \beta)\|\zeta_{c_n}u - \breve{w}_{c_n}\|_{L^2(\mathbb{K}_{c_n N})}\\
&\quad + C{c_n}^{-\frac{4}{5}}\|\mathscr{G}\|_{L^{\frac{5}{2}}(\mathbb{K}_N)}\|u_c\|_{L^{10}(\mathbb{K}_{c_n N})} + C{c_n}^{-2}\left\||u_c|^2 \star G_{\mathbb{K}_N}\right\|_{L^\infty(\mathbb{K}_N)}\|\breve{w}_{c_n}\|_{L^2(\mathbb{K}_{c_n N})}\\
&\quad + 2\|\nabla\zeta_{c_n}\|_{L^\infty(\mathbb{K}_{c_n N})}\|\nabla u\|_{L^2(\mathbb{K}_{Nc_n}\setminus\mathbb{K}_{Nc_n-1})} + \|u\|_{L^2(\mathbb{K}_{Nc_n}\setminus\mathbb{K}_{Nc_n-1})}\|\Delta\zeta_{c_n}\|_{L^\infty(\mathbb{K}_{c_n N})}.
\end{aligned}$$

The proof for v_c is similar, but does not need Lemma 2.80, writing that

$$\begin{aligned}
\|\breve{v}_c - u_c\|_{H^2(\mathbb{K}_{c_n N})} &= \|(1-\Delta)(\breve{v}_c - u_c)\|_{L^2(\mathbb{K}_{c_n N})} \\
&\leqslant C c_{TF} \left\| \zeta_c^{\frac{3}{7}} u - \breve{v}_c \right\|_{L^4(\mathbb{K}_{c_n N})} \left\| \zeta_c^{\frac{4}{7}} |u|^{\frac{4}{3}} + |\breve{v}_c|^{\frac{4}{3}} \right\|_{L^4(\mathbb{K}_{c_n N})} \\
&+ C \left\| \zeta_c^{\frac{3}{5}} u - \breve{v}_c \right\|_{L^4(\mathbb{K}_{c_n N})} \left\| \zeta_c^{\frac{2}{5}} |u|^{\frac{2}{3}} + |\breve{v}_c|^{\frac{2}{3}} \right\|_{L^4(\mathbb{K}_{c_n N})} \\
&+ C|\mu_{\mathbb{R}^3} - {c_n}^{-2}\mu_c| \, \|\breve{v}_c\|_{L^2(\mathbb{K}_{c_n N})} + C(\mu_{\mathbb{R}^3} + 1) \, \|u_c - \breve{v}_c\|_{L^2(\mathbb{K}_{c_n N})} \\
&+ 2 \, \|\nabla \zeta_c\|_{L^\infty(\mathbb{K}_{c_n N})} \, \|\nabla u\|_{L^2(\mathbb{K}_{N c_n} \setminus \mathbb{K}_{N c_n - 1})} \\
&+ \|u\|_{L^2(\mathbb{K}_{N c_n} \setminus \mathbb{K}_{N c_n - 1})} \, \|\Delta \zeta_c\|_{L^\infty(\mathbb{K}_{c_n N})} \\
&\underset{n \to +\infty}{\longrightarrow} 0.
\end{aligned}$$

This ends the proof of Lemma 2.46. $\square$

PROPOSITION 2.47 (Minimizers' concentration point). *Let $\{R_{m,i}\}_{1 \leqslant m \leqslant N_+}^{1 \leqslant i \leqslant N^3}$ be the positions of the $N^3 N_+$ largest 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 $\mathbb{1}_{\mathbb{K}_{c_n}} \breve{w}_{c_n}(\cdot + x_n)$ converges to Q, a minimizer to $J_{\mathbb{R}^3, N^3\lambda}$, verifies*

$$x_n = c_n R_{m,i} + o(1)$$

as $n \to \infty$, for one (m,i). Consequently, for $2 \leqslant p < +\infty$,

$$\|\breve{w}_{c_n}(\cdot + c_n R_{m,i}) - Q\|_{L^p(\mathbb{K}_{c_n})} \underset{n \to +\infty}{\longrightarrow} 0.$$

As the reader will notice, the proof of Proposition 2.47 only needs (in addition to things proved up to now) a convergence result on the nuclei-electron interaction term $\int G|w|^2$ — which will be proved in Lemma 2.48 — but nothing new on the electron-electron interaction term $D(|w|^2, |w|^2)$, which will be needed to prove the expansion of the energy (Proposition 2.53).

PROOF OF PROPOSITION 2.47. Since the w_{c_n}'s are minimizers, we have

$$\mathscr{E}_{\mathbb{K}_N, c_n}(w_{c_n}) \leqslant \mathscr{E}_{\mathbb{K}_N, c_n}\Big(w_{c_n}\Big(\cdot + \frac{x_n}{c_n} - R_{m*,i*}\Big)\Big),$$

for any $R_{m*,i*}$, which leads to

$$\begin{aligned}
&-\sum_{m=1}^{N_q} \sum_{i=1}^{N^3} z_m \int_{\mathbb{K}_{N c_n}} G_{\mathbb{K}_N}\Big(\frac{x}{c_n} + \frac{x_n}{c_n} - R_{m,i}\Big) \left| \breve{w}_{c_n}\Big(x + \frac{x_n}{c_n}\Big) \right|^2 \mathrm{d}x \\
&\qquad \leqslant -\sum_{m=1}^{N_q} \sum_{i=1}^{N^3} z_m \int_{\mathbb{K}_{N c_n}} G_{\mathbb{K}_N}\Big(\frac{x}{c_n} + R_{m*,i*} - R_{m,i}\Big) \left| \breve{w}_{c_n}\Big(x + \frac{x_n}{c_n}\Big) \right|^2 \mathrm{d}x \quad (2.62)
\end{aligned}$$

since the four first terms of $\mathscr{E}_{\mathbb{K}_N,c}$ are invariant under spatial translations. Lemma 2.48 below then gives, on one hand, that the right hand side of this inequality is equal to

$$-c_n\int_{\mathbb{R}^3}\frac{Q^2(x)}{|x|}\,\mathrm{d}x+o(c_n) \tag{2.63}$$

because $c_n|R_{m_*,i_*}-R_{m,i}|\to\infty$ for $(m,i)\neq(m_*,i_*)$. On the other hand, Lemma 2.48 also gives that $|x_n-c_nR_{m,i}|$ must be bounded for one (m,i), that we denote (m_0,i_0), because otherwise the left hand side would be equal to $o(c_n)$. Therefore, still by Lemma 2.48, the terms in the left hand side due to indices $(m,i)\neq(m_0,i_0)$ are equal to $o(c_n)$ while the term for (m_0,i_0) is equal to

$$-c_n\int_{\mathbb{R}^3}\frac{Q^2(x)}{|x-\eta|}\,\mathrm{d}x+o(c_n) \tag{2.64}$$

for a given $\eta\in\mathbb{R}^3$ (and up to a subsequence). Moreover, since Q is radial strictly decreasing, for $0\neq\eta\in\mathbb{R}^3$ we have

$$\begin{aligned}\int_{\mathbb{R}^3}Q^2(|x|)\left(\frac{1}{|x|}-\frac{1}{|x-\eta|}\right)\mathrm{d}x&=\int_{\mathbb{R}^3}Q^2\left(|\frac{\eta}{2}+x|\right)\left(\frac{1}{|\frac{\eta}{2}+x|}-\frac{1}{|\frac{\eta}{2}-x|}\right)\mathrm{d}x\\ &=\int_{\langle x,\frac{\eta}{2}\rangle>0}\left(Q^2\left(|\frac{\eta}{2}-x|\right)-Q^2\left(|\frac{\eta}{2}+x|\right)\right)\left(\frac{1}{|\frac{\eta}{2}-x|}-\frac{1}{|\frac{\eta}{2}+x|}\right)\mathrm{d}x>0,\end{aligned}$$

since $Q^2(r)$ and r^{-1} have the same strict monotonicity. This last result together with (2.62), (2.63) and (2.64) imply that $\eta=0$, which means by Lemma 2.48 that $x_n=c_nR_{m_0,i_0}+o(1)$ as $n\to\infty$.

The last result of Proposition 2.47 is a direct consequence of the convergence of the $L^p(\mathbb{K}_{c_n})$-norms proved in Proposition 2.37 and Lemma 2.46 together with the fact that $x_n-c_nR_{m_0,i_0}=o(1)$.

LEMMA 2.48. *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* $\|f_{c_n}-f\|_{L^2(K_{c_n})}\underset{n\to\infty}{\to}0$ *and* $\mathbb{1}_{\mathbb{K}_{c_n}}g_{c_n}\underset{n\to\infty}{\rightharpoonup}g$ *weakly in* $L^2(\mathbb{R}^3)$. *Then,*

i. if $c_n|y_n|\to+\infty$, *then* ${c_n}^{-1}\int_{\mathbb{K}_{c_n}}G_{\mathbb{K}}({c_n}^{-1}\cdot-y_n)f_{c_n}g_{c_n}\underset{n\to\infty}{\longrightarrow}0$,

ii. if $c_n|y_n|\to0$, *then* ${c_n}^{-1}\int_{\mathbb{K}_{c_n}}G_{\mathbb{K}}({c_n}^{-1}\cdot-y_n)f_{c_n}g_{c_n}\underset{n\to\infty}{\longrightarrow}\int_{\mathbb{R}^3}\frac{f(x)g(x)}{|x|}\,dx$,

iii. otherwise, there exist $\eta\in\mathbb{R}^3\backslash\{0\}$ *and a subsequence* n_k *such that*

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

Moreover, replacing $\|f_{c_n} - f\|_{L^2(K_{c_n})} \underset{n\to\infty}{\to} 0$ *by* $\|f_{c_n} - f\|_{H^1(K_{c_n})} \underset{n\to\infty}{\to} 0$*, 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 2.47 in order for it to be also useful for the proof of Lemma 2.58.

Proof of Lemma 2.48. Using the same notation $\mathbb{K}^{\boldsymbol{\sigma}}$ as in the proof of Lemma 2.38, we notice that

$$\mathbb{K} - \boldsymbol{\tau} := \{x \in \mathbb{R}^3 | x - \boldsymbol{\tau} \in \mathbb{K}\} \subset \mathbb{K}_2 = \mathbb{K} \cup \bigcup_{(0,0,0)\neq\boldsymbol{\sigma}\in\{0;\pm1\}^3} \mathbb{K}^{\boldsymbol{\sigma}},$$

for any $\boldsymbol{\tau} \in \mathbb{K}$. Therefore, by Lemma 2.20, 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 $c > 0$,

$$\begin{aligned} c^{-1} &\left| \int_{\mathbb{K}_c} G_{\mathbb{K}}(c^{-1}x - y)\varphi_c(x)\psi_c(x)\,\mathrm{d}x \right| \\ &= c^{-1} \left| \sum_{\boldsymbol{\sigma}\in\{-1;0;+1\}^3} \int_{\substack{x\in\mathbb{K}_c \\ c^{-1}x - y \in \mathbb{K}^{\boldsymbol{\sigma}}}} G_{\mathbb{K}}(c^{-1}x - y)\varphi_c(x)\psi_c(x)\,\mathrm{d}x \right| \\ &\leqslant c^{-1} C \sum_{\boldsymbol{\sigma}\in\{-1;0;+1\}^3} \int_{\substack{x\in\mathbb{K}_c \\ c^{-1}x - y \in \mathbb{K}^{\boldsymbol{\sigma}}}} \frac{|\varphi_c(x)\psi_c(x)|}{|c^{-1}x - y - \boldsymbol{\sigma}|}\,\mathrm{d}x \\ &\leqslant C \sum_{\boldsymbol{\sigma}\in\{-1;0;+1\}^3} \left\| \frac{\varphi_c\psi_c}{|\cdot - c(y+\boldsymbol{\sigma})|} \right\|_{L^1(\mathbb{K}_c)}. \end{aligned}$$

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 $c \geqslant 1$, we obtain

$$\begin{aligned} c^{-1} &\left| \int_{\mathbb{K}_c} G_{\mathbb{K}}(c^{-1} \cdot - y)\varphi_c\psi_c \right| \\ &\leqslant C' \sum_{\boldsymbol{\sigma}\in\{-1;0;+1\}^3} \|\varphi_c\|_{L^2(\mathbb{K}_c)} \|\psi_c\|_{H^1(\mathbb{K}_c)} = 27C' \|\varphi_c\|_{L^2(\mathbb{K}_c)} \|\psi_c\|_{H^1(\mathbb{K}_c)}. \end{aligned}$$

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

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

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 $n\to\infty$ and we start with the case $c_n|y_n|\to+\infty$. For $c>0$, $y\in\mathbb{K}$ and $\boldsymbol{\sigma}\in\{-1;0;+1\}^3$, we have

$$
\begin{aligned}
c^{-1}\int_{\mathbb{K}_c}\mathbb{1}_{\mathbb{K}^{\boldsymbol{\sigma}}}(c^{-1}\cdot -y)G_{\mathbb{K}}(c^{-1}\cdot -y)|fg| &\leqslant C\int_{\mathbb{K}_c}\frac{\mathbb{1}_{\mathbb{K}^{\boldsymbol{\sigma}}}(c^{-1}\cdot -y)}{|\cdot -c(y+\boldsymbol{\sigma})|}|fg| \\
&\leqslant C\int_{\mathbb{R}^3}\frac{|fg|}{|\cdot -c(y+\boldsymbol{\sigma})|}
\end{aligned}
$$

and

$$
\begin{aligned}
\int_{\mathbb{R}^3}\frac{|fg|}{|\cdot -c(y+\boldsymbol{\sigma})|} = \int_{\mathbb{R}^3}\frac{\mathbb{1}_{B(0,\frac{c}{2}|y+\boldsymbol{\sigma}|)}}{|\cdot -c(y+\boldsymbol{\sigma})|}|fg| &+ \int_{\mathbb{R}^3}\frac{\mathbb{1}_{B(c(y+\boldsymbol{\sigma}),R)}}{|\cdot -c(y+\boldsymbol{\sigma})|}|fg| \\
&+\int_{\complement B(0,\frac{c}{2}|y+\boldsymbol{\sigma}|)}\frac{\mathbb{1}_{\complement B(c(y+\boldsymbol{\sigma}),R)}}{|\cdot -c(y+\boldsymbol{\sigma})|}|fg|,
\end{aligned}
$$

hence

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

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 $\boldsymbol{\sigma}=(0,0,0)$, the convergence to 0 (for the subsequence c_n) from $c_n|y_n|\to+\infty$ and, on the other hand, there exists $R'>0$ such that $|y+\boldsymbol{\sigma}|>R'$ for any $\{-1;0;+1\}^3\ni\boldsymbol{\sigma}\neq(0,0,0)$ and any $y\in\mathbb{K}$, ending the proof that the above tends to 0. We finally obtain that

$$
\frac{1}{c_n}\int_{\mathbb{K}_{c_n}}G_{\mathbb{K}}({c_n}^{-1}\cdot -y_n)|fg| = \sum_{\boldsymbol{\sigma}\in\{0;\pm1\}^3}\frac{1}{c_n}\int_{\mathbb{K}_{c_n}}\left[\mathbb{1}_{\mathbb{K}^{\boldsymbol{\sigma}}}G_{\mathbb{K}}\right]({c_n}^{-1}\cdot -y_n)|fg| \underset{n\to\infty}{\longrightarrow} 0,
$$

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, $y_{n_k}\to 0$. However, by Lemma 2.20, there exists $M'>0$ such that $||\cdot|^{-1}-G_{\mathbb{K}}|\leqslant M'$ on $\mathbb{K}$, thus there exists $M>0$ such that

$$\begin{aligned}
\mathbb{1}_{\mathbb{K}-\tau}(x)\left|G_{\mathbb{K}}(x)-\frac{1}{|x|}\right| &\leqslant \mathbb{1}_{\mathbb{K}-\tau}(x)\left(M'\mathbb{1}_{\mathbb{K}}(x)+\frac{\mathbb{1}_{\complement\mathbb{K}}(x)}{|x|}+C\sum_{\substack{\boldsymbol{\sigma}\in\{0;\pm1\}^3\\ \boldsymbol{\sigma}\neq(0,0,0)}}\frac{\mathbb{1}_{\mathbb{K}^{\boldsymbol{\sigma}}}(x)}{|x-\boldsymbol{\sigma}|}\right)\\
&\leqslant \mathbb{1}_{\mathbb{K}-\tau}(x)\left(M'+R^{-1}+\sum_{(0,0,0)\neq\boldsymbol{\sigma}\in\{0;\pm1\}^3}\frac{C}{|x+\tau-\boldsymbol{\sigma}|-|\tau|}\right)\\
&\leqslant \mathbb{1}_{\mathbb{K}-\tau}(x)\left(M'+R^{-1}+\sum_{(0,0,0)\neq\boldsymbol{\sigma}\in\{0;\pm1\}^3}\frac{C}{R-|\tau|}\right)\\
&\leqslant \mathbb{1}_{\mathbb{K}-\tau}(x)\left(M'+R^{-1}+52CR^{-1}\right)\leqslant M\mathbb{1}_{\mathbb{K}-\tau}(x).
\end{aligned}$$

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

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

Moreover,

$$\left|\int_{\mathbb{R}^3}(1-\mathbb{1}_{\mathbb{K}_{c_{n_k}}}(x))\frac{f(x)g(x)}{|x-c_{n_k}y_{c_{n_k}}|}\,\mathrm{d}x\right|\lesssim\|f\|_{L^2(\complement\mathbb{K}_{c_{n_k}})}\|g\|_{H^1(\mathbb{R}^3)}\to0$$

and we are left with the study of

$$\begin{aligned}
\left|\int_{\mathbb{R}^3}\frac{f(x)g(x)}{|x-c_{n_k}y_{c_{n_k}}|}-\frac{f(x)g(x)}{|x-\eta|}\,\mathrm{d}x\right| &\leqslant|\eta-c_{n_k}y_{c_{n_k}}|\int_{\mathbb{R}^3}\frac{|f(x)g(x)|}{|x-c_{n_k}y_{c_{n_k}}||x-\eta|}\,\mathrm{d}x\\
&\leqslant4|\eta-c_{n_k}y_{c_{n_k}}|\,\|f\|_{H^1(\mathbb{R}^3)}\|g\|_{H^1(\mathbb{R}^3)}
\end{aligned}$$

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 $c_ny_n\to0$ then $\eta=0$, otherwise, we can find a subsequence such that $c_{n_k}y_{n_k}\to\eta\neq0$.

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

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

This concludes the proof of Lemma 2.48. □

This concludes the proof of Proposition 2.47. □

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

PROPOSITION 2.49. *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 of the lattice $\mathscr{L}_{\mathbb{K}}$.*

PROOF OF PROPOSITION 2.49. First, in Proposition 2.47, we have seen that for any sequence $\{w_c\}_{c\to+\infty}$ 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. Namely, that the sequence of translations $\{x_n\} \subset c\cdot\mathbb{K}_N$ associated with $\{w_{c_n}\}_{n\to+\infty}$ verifies that there exists $(m_0,j_0)\in[1;N^3N_+]\times[1;N^3]$ such that ${c_n}^{-1}x_n$ converges, as $n\to\infty$, to R_{m_0,j_0}, one of the positions of the N^3N_+ charges z_+ in $\mathbb{K}_N$. Then, by Lemma 2.50 below, we have for any $1\leqslant i\leqslant N^3$ that $w_c(\cdot+R_{m_0,i}-R_{m_0,j_0})$ is also a minimizer of $E_{\mathbb{K}_N,N^3\lambda}(c)$.

LEMMA 2.50. *For any $m\in[1,N_q]$, any $1\leqslant j,k\leqslant N^3$ and any $\mathbb{K}_N$-periodic function w, we have $\mathscr{E}_{\mathbb{K}_N,c}(w(\cdot+R_{m,j}-R_{m,k}))=\mathscr{E}_{\mathbb{K}_N,c}(w)$.*

PROOF. The four first terms of $\mathscr{E}_{\mathbb{K}_N,c}$ being invariant under any translations, to prove this lemma we have to prove the invariance of the term

$$\sum_{m=1}^{N_q} z_m \sum_{i=1}^{N^3}\int_{\mathbb{K}_N} G_{\mathbb{K}_N}(\cdot-R_{m,i})|w|^2$$

under those $R_{n,j}-R_{n,k}$ translations. We recall that, by definition of the $R_{m,i}$'s, for any $m\in[1,N_q]$ and any $1\leqslant j,k\leqslant N^3$, the charge value at $R_{m,j}$ and at $R_{m,k}$ are the same and the positions $R_{m,j}$ and $R_{m,k}$ are obtained one from each other by applying translations of the lattice $\mathscr{L}_{\mathbb{K}}$. Therefore the claimed invariance is due to the fact that, for any m,

$$(R_{m,1}+R_{m,j}-R_{m,k},R_{m,2}+R_{m,j}-R_{m,k},\cdots,R_{m,N^3}+R_{m,j}-R_{m,k})$$

is a permutation modulo $\mathbb{K}_N$ of $(R_{m,1},R_{m,2},\cdots,R_{m,N^3})$ thus

$$\begin{aligned}&\sum_{i=1}^{N^3}\int_{\mathbb{K}_N} G_{\mathbb{K}_N}(\cdot-R_{m,i})|w|^2(\cdot+R_{m,j}-R_{m,k})\\&=\sum_{i=1}^{N^3}\int_{\mathbb{K}_N} G_{\mathbb{K}_N}(\cdot-(R_{m,i}+R_{m,j}-R_{m,k}))|w|^2=\sum_{i=1}^{N^3}\int_{\mathbb{K}_N} G_{\mathbb{K}_N}(\cdot-R_{m,i})|w|^2.\qquad\square\end{aligned}$$

Since, the N^3 sequences of minimizers $\{w_{c_n}(\cdot+R_{m_0,i}-R_{m_0,j_0})\}_i$ have distinct limits as $n\to\infty$, 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 (2.9). To do so, we improve the convergence rate of the first order expansion of $J_{\mathbb{K},\lambda}(c)$ proved in Proposition 2.37. Namely, we prove that there exists $\beta>0$ such that

$$J_{\mathbb{K},\lambda}(c)=c^2J_{\mathbb{R}^3}(\lambda)+o(e^{-\beta c}). \tag{2.65}$$

We recall that we have proved in Lemma 2.40 that there exists $\beta > 0$ such that

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

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

LEMMA 2.51. *There exists $\beta > 0$ such that*

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

Our proof relies on the exponential decay with c of the minimizers to $J_{\mathbb{K}_c,\lambda}(1)$ close to the border of the cube $\mathbb{K}_c$, proved in Lemma 2.52.

PROOF OF LEMMA 2.51. 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 $\mathbb{1}_{\mathbb{K}_{c_n}} \breve{v}_{c_n}(\cdot + x_n)$.

LEMMA 2.52 (Exponential decrease of minimizers to $J_{\mathbb{K}_c,\lambda}(1)$). *Let $\{v_c\}_c$ be a sequence of nonnegative minimizers to $J_{\mathbb{K},\lambda}(c)$ such that a subsequence of rescaled functions $\mathbb{1}_{\mathbb{K}_{c_n}} \breve{v}_{c_n}$ 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 $0 \leqslant \breve{v}_{c_n}(x) < Ce^{-\gamma c}$ for $x \in \mathbb{K}_c \backslash \mathbb{K}_{c-1}$.*

PROOF OF LEMMA 2.52. We denote by u the minimizer of $J_{\mathbb{R}^3}(\lambda)$ to which $\mathbb{1}_{\mathbb{K}_{c_n}} \breve{v}_{c_n}$ converges strongly and by $\mu_{\mathbb{R}^3}$ the Euler–Lagrange parameter (2.12) associated with this specific u. The Euler–Lagrange equation associated with $J_{\mathbb{K}_{c_n},\lambda}(1)$ — solved by $\breve{v}_{c_n}$ — gives

$$\begin{aligned}\left(-\Delta + \frac{\mu_{\mathbb{R}^3}}{4}\right) \breve{v}_{c_n} &= \left(-c_{TF}|\breve{v}_{c_n}|^{\frac{4}{3}} + |\breve{v}_{c_n}|^{\frac{2}{3}} + \frac{\mu_{\mathbb{R}^3}}{4} - {c_n}^{-2}\mu_{c_n}\right) \breve{v}_{c_n} \\ &\leqslant \left(|\breve{v}_{c_n}|^{\frac{2}{3}} + \frac{\mu_{\mathbb{R}^3}}{4} - {c_n}^{-2}\mu_{c_n}\right) \breve{v}_{c_n}.\end{aligned}$$

We now define $\Omega_{c_n} = (1+\varepsilon)\mathbb{K}_{c_n} \backslash B(0,\alpha)$ where α is such that $|u|^{\frac{2}{3}} \leqslant \min\{\frac{1}{2}, \frac{\mu_{\mathbb{R}^3}}{4}\}$ on $\mathbb{R}^3 \backslash B(0,\alpha)$. Such α exists by Proposition 2.19. Moreover, by Lemma 2.46, for any c_n large enough, we have

$$\left\| |\breve{v}_{c_n} - u|^{2/3} \right\|_{L^\infty(\mathbb{K}_{c_n})} \leqslant \min\left\{\frac{1}{2}, \frac{\mu_{\mathbb{R}^3}}{4}\right\}$$

and, consequently, we have

$$|\breve{v}_{c_n}|^{2/3} \leqslant |\breve{v}_{c_n} - u|^{2/3} + |u|^{2/3} \leqslant \min\left\{1, \frac{\mu_{\mathbb{R}^3}}{2}\right\}$$

on $\mathbb{K}_{c_n} \backslash B(0,\alpha)$ but also on Ω_{c_n} by periodicity of $\breve{v}_{c_n}$ and for any c_n large enough (depending on ε) in order to have

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

Moreover by Corollary 2.45, for any c_n large enough, we have

$$c_n{}^{-2}\mu_{c_n} \geqslant \frac{3}{4}\mu_{\mathbb{R}^3}.$$

Hence, for c_n large enough, it holds on Ω_{c_n} that

$$|\breve{v}_{c_n}|^{\frac{2}{3}} + \frac{\mu_{\mathbb{R}^3}}{4} - c_n{}^{-2}\mu_{c_n} \leqslant \frac{\mu_{\mathbb{R}^3}}{2} + \frac{\mu_{\mathbb{R}^3}}{4} - \frac{3}{4}\mu_{\mathbb{R}^3} = 0$$

what gives on Ω_{c_n}, for c_n large enough, that

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

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

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

which solves

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

on $\mathbb{R}^3\backslash B(0,\nu)$ and verifies $f_\nu = 1$ on the boundary $\partial B(0,\nu)$. On each $(1+\varepsilon)\mathbb{K}_{c_n}$, with $\boldsymbol{e_j}$ the vectors defining $\mathscr{L}_{\mathbb{K}}$, we define the positive function

$$f_0(x) = \sum_{j=1}^{3} \frac{\cosh\left(\frac{\sqrt{\mu_{\mathbb{R}^3}}}{2}\left\langle x, \frac{\boldsymbol{e_j}}{\|\boldsymbol{e_j}\|}\right\rangle\right)}{\cosh\left(\frac{\sqrt{\mu_{\mathbb{R}^3}}}{2}(1+\varepsilon)c_n\frac{\|\boldsymbol{e_j}\|}{2}\right)}$$

which solves

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

on $(1+\varepsilon)\mathbb{K}_{c_n}$ and verifies $1 \leqslant f_0 \leqslant 3$ on the boundary $\partial\left((1+\varepsilon)\mathbb{K}_c\right)$. Denoting by g the function

$$g = f_0 + f_\alpha,$$

we have for c_n large enough that

$$\begin{aligned} \left(-\Delta + \frac{\mu_{\mathbb{R}^3}}{4}\right)(\breve{v}_{c_n} - g) &\leqslant 0, && \text{on } \Omega_{c_n} \\ \breve{v}_{c_n} - g &\leqslant 0, && \text{on } \partial\Omega_{c_n}, \end{aligned}$$

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

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

$$0 < f_0(x) \leqslant f_0\left(\frac{c_n}{2}(\boldsymbol{e_1},\boldsymbol{e_2},\boldsymbol{e_3})\right) \leqslant 2\sum_{j=1}^{3} e^{-\varepsilon\frac{\sqrt{\mu_{\mathbb{R}^3}}}{2}\frac{\|\boldsymbol{e_j}\|}{2}c_n}.$$

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

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

on $\mathbb{K}_{c_n} \backslash \mathbb{K}_{c_n-1}$. Hence there exist $C > 0$ and

$$\gamma := \frac{\sqrt{\mu_{\mathbb{R}^3}}}{2} \min\left\{m; \frac{\varepsilon}{2} \min_{1 \leqslant j \leqslant 3} \{\|\boldsymbol{e_j}\|\}\right\} > 0$$

such that for c_n large enough and any $x \in \mathbb{K}_{c_n} \backslash \mathbb{K}_{c_n-1}$, we conclude that

$$0 \leqslant \breve{v}_{c_n}(x) \leqslant g(x) < Ce^{-\gamma c}. \qquad \square$$

We now conclude the proof of Lemma 2.51. We define $\chi_c \in C_c^\infty(\mathbb{R}^3)$, $0 \leqslant \chi_c \leqslant 1$, $\chi_c \equiv 0$ on $\mathbb{R}^3 \backslash \mathbb{K}_c$ and $\chi_c \equiv 1$ on $\mathbb{K}_{c-1}$. By Lemma 2.52, for $p \in [2; 6]$ we have

$$\begin{aligned} 0 \leqslant \|\breve{v}_{c_n}\|_{L^p(\mathbb{K}_{c_n})}^p - \|\chi_{c_n} \breve{v}_{c_n}\|_{L^p(\mathbb{R}^3)}^p &= \int_{\mathbb{K}_{c_n} \backslash \mathbb{K}_{c_n-1}} (1 - {\chi_{c_n}}^p) |\breve{v}_{c_n}|^p \\ &\leqslant C^p e^{-p\gamma c_n} \left|\mathbb{K}_{c_n} \backslash \mathbb{K}_{c_n-1}\right|. \end{aligned}$$

Given that $|\mathbb{K}_c \backslash \mathbb{K}_{c-1}| \leqslant |\mathbb{K}_c| = c^3 |\mathbb{K}|$ for any $c > 1$, there exists $0 < \alpha < \gamma$ such that

$$\|\chi_{c_n} \breve{v}_{c_n}\|_{L^p(\mathbb{R}^3)}^p = \|\breve{v}_{c_n}\|_{L^p(\mathbb{K}_{c_n})}^p + o\left(e^{-p\alpha c_n}\right)$$

for any $p \in [2; 6]$ and, in particular, that

$$\frac{\lambda}{\|\chi_{c_n} \breve{v}_{c_n}\|_{L^2(\mathbb{R}^3)}^2} = 1 + o(e^{-2\alpha c_n}).$$

Moreover,

$$\begin{aligned} \int_{\mathbb{R}^3} \chi_c \breve{v}_c \nabla \chi_c \cdot \nabla \breve{v}_c = \frac{1}{2} \int_{\mathbb{R}^3} \chi_c \nabla \chi_c \cdot \nabla\left(|\breve{v}_c|^2\right) &= -\frac{1}{2} \int_{\mathbb{R}^3} |\breve{v}_c|^2 \left(\chi_c \Delta \chi_c + |\nabla \chi_c|^2\right) \\ &= -\frac{1}{2} \int_{\mathbb{K}_c \backslash \mathbb{K}_{c-1}} |\breve{v}_c|^2 \left(\chi_c \Delta \chi_c + |\nabla \chi_c|^2\right) \end{aligned}$$

thus

$$\left|\int_{\mathbb{R}^3} \chi_{c_n} \breve{v}_{c_n} \nabla \chi_{c_n} \cdot \nabla \breve{v}_{c_n}\right| \leqslant \frac{1}{2} \int_{\mathbb{K}_{c_n} \backslash \mathbb{K}_{c_n-1}} |\breve{v}_{c_n}|^2 \left(\chi_{c_n} |\Delta \chi_{c_n}| + |\nabla \chi_{c_n}|^2\right) = o(e^{-2\alpha c_n})$$

and it leads to

$$\begin{aligned} \|\nabla(\chi_{c_n} \breve{v}_{c_n})\|_{L^2(\mathbb{R}^3)}^2 = \; & \|\chi_{c_n} \nabla \breve{v}_{c_n}\|_{L^2(\mathbb{K}_{c_n})}^2 + \|\breve{v}_{c_n} \nabla \chi_{c_n}\|_{L^2(\mathbb{K}_{c_n} \backslash \mathbb{K}_{c_n-1})}^2 \\ & + \int_{\mathbb{R}^3} \chi_{c_n} \breve{v}_{c_n} \nabla \chi_{c_n} \cdot \nabla \breve{v}_{c_n} \\ = \; & \|\chi_{c_n} \nabla \breve{v}_{c_n}\|_{L^2(\mathbb{K}_{c_n})}^2 + o(e^{-2\alpha c_n}) \leqslant \|\nabla \breve{v}_{c_n}\|_{L^2(\mathbb{K}_{c_n})}^2 + o(e^{-2\alpha c_n}). \end{aligned}$$

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

$$\begin{aligned}
J_{\mathbb{R}^3}(\lambda) &\leqslant \mathscr{J}_{\mathbb{R}^3}\left(\frac{\sqrt{\lambda}\chi_{c_n}u}{\|\chi_{c_n}u\|_{L^2(\mathbb{R}^3)}}\right) \\
&\leqslant \frac{\lambda}{\|\chi_{c_n}\breve{v}_{c_n}\|^2_{L^2(\mathbb{R}^3)}}\|\nabla(\chi_{c_n}\breve{v}_{c_n})\|^2_{L^2(\mathbb{R}^3)} + \frac{3}{5}\frac{c_{TF}\lambda^{5/3}}{\|\chi_{c_n}\breve{v}_{c_n}\|^{10/3}_{L^2(\mathbb{R}^3)}}\|\chi_{c_n}\breve{v}_{c_n}\|^{10/3}_{L^{\frac{10}{3}}(\mathbb{R}^3)} \\
&\qquad\qquad - \frac{3}{4}\frac{\lambda^{4/3}}{\|\chi_{c_n}u\|^{8/3}_{L^2(\mathbb{R}^3)}}\|\chi_{c_n}\breve{v}_{c_n}\|^{8/3}_{L^{\frac{8}{3}}(\mathbb{R}^3)} \\
&\leqslant \mathscr{J}_{\mathbb{K}_{c_n}}(\breve{v}_{c_n}) + o(e^{-\beta c_n}) = J_{\mathbb{K}_{c_n}}(\lambda) + o(e^{-\beta c_n}).
\end{aligned}$$

This concludes the proof of Lemma 2.51. □

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

PROPOSITION 2.53 (Second order expansion of the energy). *We have the expansion*

$$\begin{aligned}
E_{\mathbb{K}_N,N^3\lambda}(c) &= c^2 J_{\mathbb{R}^3,N^3\lambda} \\
&\quad + c \inf_{\left\{u\middle|\mathscr{J}_{\mathbb{R}^3}(u)=J_{\mathbb{R}^3,N^3\lambda}\right\}}\left\{\frac{1}{2}D_{\mathbb{R}^3}(|u|^2,|u|^2) - z_+\int_{\mathbb{R}^3}\frac{|u(x)|^2}{|x|}\,dx\right\} + o(c). \quad (2.66)
\end{aligned}$$

The infimum is performed over all the minimizers of $J_{\mathbb{R}^3,N^3\lambda}$ and we recall that, as defined in Lemma 2.54,

$$D_{\mathbb{R}^3}(f,g) := \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{f(x)g(y)}{|x-y|}\,\mathrm{d}y\,\mathrm{d}x.$$

PROOF OF PROPOSITION 2.53. In order to deal with the term $D_{\mathbb{K}}$, we first prove a convergence result similar to what we did in Lemma 2.48 for term $\int G|w|^2$.

LEMMA 2.54. *Let v_c be such that the rescaled function $\breve{v}_c = c^{-3/2}v_c(c^{-1}x)$ verifies*

$$\mathbb{1}_{\mathbb{K}_c}\breve{v}_c \underset{c\to\infty}{\longrightarrow} v$$

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

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

Proof of Lemma 2.54. We have

$$\begin{aligned}
&D_{\mathbb{R}^3}(v^2, v^2) - c^{-1} D_{\mathbb{K}}(v_c^2, v_c^2) \\
&\qquad = D_{\mathbb{R}^3}(v^2, v^2 - \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2) + D_{\mathbb{R}^3}(v^2 - \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2, \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2) \\
&\qquad\qquad + c^{-1} \int_{\mathbb{K}} \int_{\mathbb{K}} v_c^2(x) \left(|x-y|^{-1} - G_{\mathbb{K}}(x-y) \right) v_c^2(y) \, \mathrm{d}y \, \mathrm{d}x.
\end{aligned}$$

Moreover, by the Hardy–Littlewood–Sobolev inequality, it holds that

$$\left| D_{\mathbb{R}^3}(v^2, v^2 - \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2) \right| \leqslant C \left\| v \right\|_{L^{12/5}(\mathbb{R}^3)}^2 \left\| v^2 - \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2 \right\|_{L^{6/5}(\mathbb{R}^3)}$$

and that

$$\left| D_{\mathbb{R}^3}(v^2 - \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2, \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2) \right| \leqslant C \left\| \breve{v}_c \right\|_{L^{12/5}(\mathbb{K}_c)}^2 \left\| v^2 - \mathbb{1}_{\mathbb{K}_c} \breve{v}_c^2 \right\|_{L^{6/5}(\mathbb{R}^3)}$$

which both vanish by the strong convergence of $\mathbb{1}_{\mathbb{K}_c} \breve{v}_c$ in $L^{12/5}(\mathbb{R}^3)$. Thus we are left with the proof of the vanishing of

$$c^{-1} \int_{\mathbb{K}} \int_{\mathbb{K}} v_c^2(x) \left(|x-y|^{-1} - G_{\mathbb{K}}(x-y) \right) v_c^2(y) \, \mathrm{d}y \, \mathrm{d}x.$$

To prove that, 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 2.20,

$$\begin{aligned}
&c^{-1} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K} \\ x-y\in\mathbb{K}}} v_c^2(x) \left| |x-y|^{-1} - G_{\mathbb{K}}(x-y) \right| v_c^2(y) \, \mathrm{d}y \, \mathrm{d}x \\
&\qquad \leqslant \frac{M}{c} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K} \\ x-y\in\mathbb{K}}} v_c^2(x) v_c^2(y) \, \mathrm{d}x \, \mathrm{d}y \leqslant \frac{M}{c} \left\| v_c \right\|_{L^2(\mathbb{K})}^4 = \frac{M}{c} \left\| \breve{v}_c \right\|_{L^2(\mathbb{K}_c)}^4 \xrightarrow[c\to\infty]{} 0.
\end{aligned}$$

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

$$\begin{aligned}
&c^{-1} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K} \\ x-y\in 2\mathbb{K}\setminus\mathbb{K}}} \frac{v_c^2(x) v_c^2(y)}{|x-y|} \, \mathrm{d}y \, \mathrm{d}x \\
&\qquad \leqslant \frac{2}{\min\limits_i |\boldsymbol{e_i}|} c^{-1} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K} \\ x-y\in 2\mathbb{K}\setminus\mathbb{K}}} v_c^2(x) v_c^2(y) \, \mathrm{d}y \, \mathrm{d}x \leqslant \frac{2}{\min\limits_i |\boldsymbol{e_i}|} c^{-1} \left\| v_c \right\|_{L^2(\mathbb{K})}^4 \xrightarrow[c\to\infty]{} 0,
\end{aligned}$$

with $\boldsymbol{e_j}$ the vectors defining $\mathscr{L}_{\mathbb{K}}$.

To deal with the remaining terms due to $G_{\mathbb{K}}$ when $x - y \notin \mathbb{K}$, we will use the same notation $\mathbb{K}^{\boldsymbol{\sigma}}$ as in the proof of Lemma 2.38. By (2.35), we therefore have to prove, for $\boldsymbol{\sigma} \in \{-1,0,+1\}^3 \backslash (0,0,0)$, the vanishing of

$$\left| c^{-1} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K} \\ x-y\in\mathbb{K}^{\boldsymbol{\sigma}}}} v_c^2(x) G_{\mathbb{K}}(x-y) v_c^2(y)\,\mathrm{d}y\,\mathrm{d}x \right| \lesssim c^{-1} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K} \\ x-y\in\mathbb{K}^{\boldsymbol{\sigma}}}} \frac{v_c^2(x)v_c^2(y)}{|x-y-\boldsymbol{\sigma}|}\,\mathrm{d}y\,\mathrm{d}x = \iint\limits_{\substack{\mathbb{K}_c\times\mathbb{K}_c \\ x-y\in c\cdot\mathbb{K}^{\boldsymbol{\sigma}}}} \frac{\breve{v}_c^2(x)\breve{v}_c^2(y)}{|x-y-c\boldsymbol{\sigma}|}\,\mathrm{d}y\,\mathrm{d}x.$$

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

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

Thus, for any integrand f positive, we have

$$\begin{aligned}
\iint\limits_{\substack{\mathbb{K}_c\times\mathbb{K}_c \\ x-y\in c\cdot\mathbb{K}^{\boldsymbol{\sigma}}}} f(x,y)\,\mathrm{d}y\,\mathrm{d}x &= \iint\limits_{\substack{\mathbb{K}_c\times\mathbb{K}_c\backslash B(0,c\nu)\times B(0,c\nu) \\ x-y\in c\cdot\mathbb{K}^{\boldsymbol{\sigma}}}} f(x,y)\,\mathrm{d}y\,\mathrm{d}x \\
&\leqslant \iint\limits_{\substack{(\mathbb{K}_c\backslash B(0,c\nu))\times\mathbb{K}_c \\ x-y\in c\cdot\mathbb{K}^{\boldsymbol{\sigma}}}} f(x,y)\,\mathrm{d}y\,\mathrm{d}x + \iint\limits_{\substack{\mathbb{K}_c\times(\mathbb{K}_c\backslash B(0,c\nu)) \\ x-y\in c\cdot\mathbb{K}^{\boldsymbol{\sigma}}}} f(x,y)\,\mathrm{d}y\,\mathrm{d}x \\
&\leqslant \iint\limits_{(\mathbb{K}_c\backslash B(0,c\nu))\times\mathbb{K}_c} f(x,y)\,\mathrm{d}y\,\mathrm{d}x + \iint\limits_{\mathbb{K}_c\times(\mathbb{K}_c\backslash B(0,c\nu))} f(x,y)\,\mathrm{d}y\,\mathrm{d}x.
\end{aligned}$$

Hence, using aditionnaly the Hardy–Littlewood–Sobolev inequality, we obtain

$$c^{-1} \iint\limits_{\substack{\mathbb{K}\times\mathbb{K} \\ x-y\in\mathbb{K}^{\boldsymbol{\sigma}}}} v_c^2(x) G_{\mathbb{K}}(x-y) v_c^2(y)\,\mathrm{d}y\,\mathrm{d}x \lesssim 2\,\|\breve{v}_c\|^2_{L^{12/5}(\mathbb{K}_c\backslash B(0,c\nu))}\,\|\breve{v}_c\|^2_{L^{12/5}(\mathbb{K}_c)}$$

and the right hand side vanishes when $c \to 0$ since $\|\breve{v}_c\|^2_{L^{12/5}(\mathbb{K}_c\backslash B(0,c\nu))}$ vanishes and $\|\breve{v}_c\|^2_{L^{12/5}(\mathbb{K}_c)}$ is bounded, both by the $L^{12/5}(\mathbb{R}^3)$-convergence of $\mathbb{1}_{\mathbb{K}_c}\breve{v}_c$. This concludes the proof of Lemma 2.54. □

Let w_c be a sequence of minimizers to $E_{\mathbb{K}_N,N^3\lambda}(c)$. By Propositions 2.37 and 2.47, the convergence rate (2.65), and Lemmas 2.51 and 2.54, we obtain

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

where Q is the minimizer of $J_{\mathbb{R}^3,N^3\lambda}$ to which $\mathbb{1}_{c_n\cdot\mathbb{K}_N}\breve{w}_{c_n}(\cdot+x_n)$ 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 $\mathscr{S}(u) < \mathscr{S}(Q)$, where

$$\mathscr{S}(f) := \frac{1}{2}D_{\mathbb{R}^3}(|f|^2,|f|^2) - z_+\int_{\mathbb{R}^3}\frac{|f(x)|^2}{|x|}\,\mathrm{d}x.$$

Since $|u|$ is positive by Theorem 2.3 and also a minimizer, and that $\mathscr{S}(|u|) = \mathscr{S}(u)$, we will suppose $u > 0$ and that u is radial. Let $\mathbb{K}_N^-$ be defined as $\mathbb{K}_N^- = (1-\eta)\mathbb{K}_N$ for a fixed small $\eta \in (0;1)$ and $\chi \in C_0^\infty(\mathbb{K}_N)$ be such that $0 \leqslant \chi \leqslant 1$, $\chi_{|\mathbb{K}_N^-} \equiv 1$, $\chi_{|\mathbb{R}^3\setminus\mathbb{K}_N} \equiv 0$ and $\|\nabla\chi\|_{L^\infty(\mathbb{R}^3)}$ bounded. By the exponential decay of u proved in Proposition 2.19, fixing $R > 0$ such that the ball $B(0,R)$ is included in $\mathbb{K}_N^-$, denoting $\mathring{u}_c := c^{3/2}u(c\cdot)$, we have

$$\begin{aligned}\left|\int_{\mathbb{K}_N}\chi\mathring{u}_c\nabla\chi\cdot\nabla\mathring{u}_c\right| &= \left|\int_{\complement\mathbb{K}_N^-}\chi\mathring{u}_c\nabla\chi\cdot\nabla\mathring{u}_c\right|\\ &\leqslant \|\nabla\chi\|_\infty\|\mathring{u}_c\|_{L^2(\complement\mathbb{K}_N^-)}\|\nabla\mathring{u}_c\|_{L^2(\complement\mathbb{K}_N^-)}\\ &\leqslant \|\nabla\chi\|_\infty\|\mathring{u}_c\|_{L^2(\complement B(0,R))}\|\nabla\mathring{u}_c\|_{L^2(\complement B(0,R))}\\ &\leqslant c^2\|\nabla\chi\|_\infty\|u\|_{L^2(\complement B(0,cR))}\|\nabla u\|_{L^2(\complement B(0,cR))} = o(e^{-\nu c})_{c\to\infty},\end{aligned}$$

$$\int_{\mathbb{K}_N}|\nabla\chi|^2|\mathring{u}_c|^2 = \int_{\complement\mathbb{K}_N^-}|\nabla\chi|^2|\mathring{u}_c|^2 \leqslant \|\nabla\chi\|_\infty^2\|u\|_{L^2(\complement B(0,cR))} = o(e^{-\nu c})_{c\to\infty},$$

$$0 \leqslant \int_{\mathbb{R}^3}(1-|\chi|^2)|\nabla\mathring{u}_c|^2 \leqslant \|\nabla\mathring{u}_c\|_{L^2(\complement\mathbb{K}_N^-)}^2 \leqslant c^2\|\nabla u\|_{L^2(\complement B(0,cR))}^2 = o(e^{-\nu c})_{c\to\infty}$$

and, for $p > 0$,

$$0 \leqslant \int_{\mathbb{R}^3}(1-|\chi|^p)|\mathring{u}_c|^p \leqslant \|\mathring{u}_c\|_{L^p(\complement\mathbb{K}_N^-)}^p \leqslant c^{3(\frac{p}{2}-1)}\|u\|_{L^p(\complement B(0,cR))}^p = o(e^{-\nu c})_{c\to\infty},$$

for a given $\nu > 0$. This leads to

$$\begin{aligned}\int_{\mathbb{K}_N}|\chi\mathring{u}_c|^{\frac{10}{3}} &= \int_{\mathbb{R}^3}|\mathring{u}_c|^{\frac{10}{3}} - \int_{\mathbb{R}^3}(1-|\chi|^{\frac{10}{3}})|\mathring{u}_c|^{\frac{10}{3}} = c^2\int_{\mathbb{R}^3}|u|^{\frac{10}{3}} + o(e^{-\nu c})_{c\to\infty},\\ \int_{\mathbb{K}_N}|\chi\mathring{u}_c|^{\frac{8}{3}} &= \int_{\mathbb{R}^3}|\mathring{u}_c|^{\frac{8}{3}} - \int_{\mathbb{R}^3}(1-|\chi|^{\frac{8}{3}})|\mathring{u}_c|^{\frac{8}{3}} = c\int_{\mathbb{R}^3}|u|^{\frac{8}{3}} + o(e^{-\nu c})_{c\to\infty},\\ \frac{N^3\lambda}{\|\chi\mathring{u}_c\|_{L^2(\mathbb{K}_N)}^2} &= \frac{\|u\|_{L^2(\mathbb{R}^3)}^2}{\|\chi\mathring{u}_c\|_{L^2(\mathbb{K}_N)}^2} = 1 + o(e^{-\nu c})_{c\to\infty}\end{aligned}$$

and

$$\begin{aligned}\int_{\mathbb{K}_N} |\nabla(\chi \mathring{u}_c)|^2 &= \int_{\mathbb{K}_N} |\chi|^2 |\nabla \mathring{u}_c|^2 + 2\Re\left(\int_{\mathbb{K}_N} \chi \mathring{u}_c \nabla\chi \cdot \nabla \mathring{u}_c\right) + \int_{\mathbb{K}_N} |\nabla\chi|^2 |\mathring{u}_c|^2 \\ &= \int_{\mathbb{R}^3} |\nabla \mathring{u}_c|^2 - \int_{\mathbb{R}^3} (1-|\chi|^2)|\nabla \mathring{u}_c|^2 + o(e^{-\nu c})_{c\to\infty} \\ &= c^2 \int_{\mathbb{R}^3} |\nabla u|^2 + o(e^{-\nu c})_{c\to\infty},\end{aligned}$$

and consequently to

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

On the other hand, since $\mathbb{1}_{c\cdot\mathbb{K}_N}\frac{\sqrt{N^3\lambda}}{\|\chi\mathring{u}_c\|_{L^2(\mathbb{K}_N)}}\chi(c^{-1}\cdot)u \to u$ strongly in $L^2(\mathbb{R}^3)\cap L^4(\mathbb{R}^3)$, we can apply Lemmas 2.48 and 2.54 to $f_c := \frac{\sqrt{N^3\lambda}}{\|\chi\mathring{u}_c\|_{L^2(\mathbb{K}_N)}}[\chi\mathring{u}_c](\cdot - R_{n_0,j_0})$, with n_0 such that $z_{n_0} = z_+$, and obtain

$$\frac{1}{2}D_{\mathbb{K}_N}(|f_c|^2,|f_c|^2) - \int\limits_{\mathbb{K}_N} \mathscr{G}|f_c|^2 = c\mathscr{S}(u) + o(c),$$

where we recall that $\mathscr{G}$ has been defined for shortness in (2.61). We therefore have

$$\begin{aligned}\mathscr{E}_{\mathbb{K}_N,c}\left(\sqrt{N^3\lambda}\frac{[u(c\cdot)\chi](\cdot - R_{n_0,j_0})}{\|u(c\cdot)\chi\|_{L^2(\mathbb{K}_N)}}\right) &= c^2 J_{\mathbb{R}^3,N^3\lambda} + c\mathscr{S}(u) + o(c) \\ &< c^2 J_{\mathbb{R}^3,N^3\lambda} + c\mathscr{S}(Q) + o(c) = E_{\mathbb{K}_N,N^3\lambda}(c),\end{aligned}$$

leading to a contradiction which finally proves that we in fact have

$$\mathscr{S}(Q) = \min_{\left\{u \middle| \mathscr{J}_{\mathbb{R}^3}(u) = J_{\mathbb{R}^3,N^3\lambda}\right\}} \mathscr{S}(u)$$

and thus concludes the proof of Proposition 2.53. □

Theorem 2.2 is therefore proved combining the results of Proposition 2.37, Proposition 2.47, Proposition 2.49 and Proposition 2.53.

5.4. Proof of Theorem 2.8 on the number of minimizers. The arguments developed in this section do not rely on what we have done in Section 5.3. We also recall that Theorem 2.8 only holds in the case of one unique charge per unit cell $\mathbb{K}$, i.e. $N_q = 1$.

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

$$\mathscr{E}_{\mathbb{K},c}(w_c + f) = E_{\mathbb{K},\lambda}(c) + \langle \mathring{L}_c^+ f_1, f_1\rangle_{L^2(\mathbb{K})} + \langle \mathring{L}_c^- f_2, f_2\rangle_{L^2(\mathbb{K})} - 2\mu_c \langle w_c, f_1\rangle_{L^2(\mathbb{K})} \\ - \mu_c \|f\|^2_{L^2(\mathbb{K})} + 2D_{\mathbb{K}}(\Re(w_c\bar{f}), \Re(w_c\bar{f})) + o(\|f\|^2_{H^1(\mathbb{K})}), \quad (2.67)$$

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

$$\mathring{L}_c^- := -\Delta + c_{TF}|w_c|^{\frac{4}{3}} - c|w_c|^{\frac{2}{3}} + \mu_c - \mathscr{G} + |w_c|^2 \star G_{\mathbb{K}} \quad (2.68)$$

and

$$\mathring{L}_c^+ = -\Delta + \frac{7}{3}c_{TF}|w_c|^{\frac{4}{3}} - \frac{5}{3}c|w_c|^{\frac{2}{3}} + \mu_c - \mathscr{G} + |w_c|^2 \star G_{\mathbb{K}}, \quad (2.69)$$

where we recall that $\mathscr{G}$ is defined by

$$\mathscr{G} := \sum_{n=1}^{N_q}\sum_{i=1}^{N^3} z_n G_{\mathbb{K}_N}(\cdot - R_{n,i}). \quad (2.61)$$

The only terms of the expansion that are not one line computations, and that we therefore explicitly prove in Lemma 2.55, are those with the powers 8/3 and 10/3.

Lemma 2.55. *If $2 \leqslant p < 4$, for any complex-valued $w, h \in H^1$, we have*

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

Proof of Lemma 2.55. Since, $|w(x)+h(x)| = ||w(x)| + \frac{w(x)}{|w(x)|}h(x)|$ if $w(x) \neq 0$, proving

$$R_w(f) := \int |w+f|^p - \int |w|^p - p\int |w|^{p-2}wf_1 \\ - \frac{p(p-1)}{2}\int |w|^{p-2}|f_1|^2 - \frac{p}{2}\int |w|^{p-2}|f_2|^2 = o\left(\|f\|^2_{H^1}\right),$$

for $w \geqslant 0$ and $f \in H^1$, is equivalent to prove Lemma 2.55.

If $3 \leqslant p < 4$, for any $(x, y) \in \mathbb{R}\backslash\{0\} \times (0; +\infty)$ we have

$$\left||y+x|^p - \sum_{k=0}^{\lfloor p\rfloor - 1}\binom{\frac{q}{2}}{k} y^{p-k}x^k\right| < |x|^p + \binom{p}{3}y^{p-3}|x|^3 \quad (2.70)$$

hence $|R_w(f_1)| \leqslant \|f\|_p^p + \binom{p}{3} \|w\|_2^{p-3} \|f\|_{\frac{6}{5-p}}^3$ and

$$\int \left||w+f_1|^{p-2} - |w|^{p-2}\right| |f_2|^2 \leqslant \left\||f_1|^{p-2}|f_2|^2\right\|_1 + (p-2)\left\||w|^{p-3}|f_1||f_2|^2\right\|_1$$
$$\leqslant \|f\|_p^p + (p-2)\|w\|_2^{p-3}\|f\|_{\frac{6}{5-p}}^3 ,$$

while, if $2 \leqslant p < 3$, for any $(x,y) \in \mathbb{R}\backslash\{0\} \times (0;+\infty)$ we have

$$\left||y+x|^p - \sum_{k=0}^{2} \binom{\frac{q}{2}}{k} y^{p-k}x^k\right| < |x|^p \tag{2.71}$$

hence $|R_w(f_1)| \leqslant \|f\|_p^p$ and

$$\int \left||w+f_1|^{p-2} - |w|^{p-2}\right| |f_2|^2 \leqslant \left\||f_1|^{p-2}|f_2|^2\right\|_1 \leqslant \|f\|_p^p .$$

Moreover, for any $(z,p) \in \mathbb{C}\backslash\{\mathbb{R}\times\{0\} \cup \{0\}\times\mathbb{R}\} \times [0;+\infty)$, we have

$$\left||z|^p - \sum_{k=0}^{\lfloor\frac{p}{2}\rfloor} \binom{\frac{p}{2}}{k} |\Re(z)|^{p-2k}|\Im(z)|^{2k}\right| < |\Im(z)|^p \tag{2.72}$$

and identically exchanging the roles of the real part $\Re$ and the imaginary part $\Im$. Thus, we have

$$\int \left||w+f|^p - |w+f_1|^p - \frac{p}{2}|w+f_1|^{p-2}|f_2|^2\right| \leqslant \|f_2\|_p^p \leqslant \|f\|_p^p .$$

We finally have that $R_w(f) = 0$ for $p = 2$, that

$$|R_w(f)| \leqslant \frac{p+4}{2}\|f\|_p^p + \left[\binom{\frac{p}{2}}{k} + \frac{p}{2}(p-2)\right]\|w\|_2^{p-3}\|f\|_{\frac{6}{5-p}}^3 = O\big(\|f\|_{H^1}^3\big)$$

hence $|R_w(f)| = o\big(\|f\|_{H^1}^2\big)$ if $3 \leqslant p < 4$ and, if $2 < p < 3$, that

$$|R_w(f)| \leqslant \frac{p+4}{2}\|f\|_p^p = O\big(\|f\|_{H^1}^p\big) = o\big(\|f\|_{H^1}^2\big).$$

Proofs of inequalities (2.70), (2.71) and (2.72) can be found in the Appendix. $\square$

Let us suppose that Conjecture 2.6 holds and that there exist two sequences w_c and ω_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 2.47, we have for $2 \leqslant p < +\infty$ that

$$\|\breve{w}_{c_n}(\cdot + c_nR) - Q\|_{L^p(\mathbb{K}_{c_n})} + \|\breve{\omega}_{c_n}(\cdot + c_nR) - Q\|_{L^p(\mathbb{K}_{c_n})} \underset{n\to+\infty}{\longrightarrow} 0$$

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

$$\langle w_{c_n} + \omega_{c_n}, f_n\rangle_{L^2_{\text{per}}(\mathbb{K})} = \langle \breve{w}_{c_n} + \breve{\omega}_{c_n}, \breve{f}_n\rangle_{L^2_{\text{per}}(\mathbb{K}_{c_n})} = 0 \tag{2.73}$$

and

$$\langle \mathscr{G}({c_n}^{-1}\cdot), \nabla((\breve{w}_{c_n} + \breve{\omega}_{c_n})\breve{f}_n)\rangle_{L^2_{\mathrm{per}}(\mathbb{K}_{c_n})} = 0 \tag{2.74}$$

Indeed, on one hand,

$$\langle w_c + \omega_c, f_c\rangle_{\mathbb{K}} = 2\Im\left(\langle \omega_c, w_c\rangle_{\mathbb{K}}\right)$$

which vanishes since ω_c and w_c are real-valued. On the other hand, the orthogonality property stated in the following lemma leads to (2.74).

LEMMA 2.56. *If w_c is a real-valued minimizer to $E_{\mathbb{K},\lambda}(c)$, then w_c is orthogonal to $\mathscr{G}\nabla w_c$.*

PROOF OF LEMMA 2.56. As mentioned in Proposition 2.49, the four first terms of $\mathscr{E}_{\mathbb{K},c}$ are invariant under any space translations thus we have

$$\begin{aligned}\mathscr{E}_{\mathbb{K},c}(w_c(\cdot+\tau)) &= \mathscr{E}_{\mathbb{K},c}(w_c) - \left\langle \mathscr{G}, |w_c(\cdot+\tau)|^2 - |w_c|^2\right\rangle_{L^2(\mathbb{K})}\\ &= E_{\mathbb{K},\lambda}(c) - 2\tau\cdot\int_{\mathbb{K}} \mathscr{G}\Re(w_c\nabla\bar{w}_c) + O(|\tau|^2).\end{aligned}$$

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

By property (2.74) together with $D_{\mathbb{K}}(h,h) \geqslant 0$ (Lemma 2.20) and

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

we obtain from (2.67) that

$$E_{\mathbb{K},\lambda}(c_n) = \mathscr{E}_{\mathbb{K},c_n}(\omega_{c_n}) \geqslant E_{\mathbb{K},\lambda}(c_n) + {c_n}^2\langle L_n^+\breve{f}_n, \breve{f}_n\rangle_{\mathbb{K}_{c_n}} + o(\|f_n\|^2_{H^1(\mathbb{K})})$$

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

$$L_n^+ = -\Delta + \frac{7}{3}c_{TF}|\breve{w}_c|^{\frac{4}{3}} - \frac{5}{3}|\breve{w}_c|^{\frac{2}{3}} + \frac{\mu_{c_n}}{{c_n}^2} + {c_n}^{-2}[-\mathscr{G} + |w_{c_n}|^2 \star G_{\mathbb{K}}]({c_n}^{-1}\cdot). \tag{2.75}$$

Therefore, by the ellipticity result $\langle L_n^+\breve{f}_n, \breve{f}_n\rangle_{L^2(\mathbb{K}_{c_n})} \geqslant C\|\breve{f}_n\|^2_{H^1(\mathbb{K}_{c_n})} \geqslant 0$ of the next proposition, which rely on Conjecture 2.6, we obtain (for c_n large enough) that

$$0 \geqslant C{c_n}^2\|\breve{f}_n\|^2_{H^1(\mathbb{K}_{c_n})} + o(\|f_n\|^2_{H^1(\mathbb{K})}) = C{c_n}^2\|\breve{f}_n\|^2_{H^1(\mathbb{K}_{c_n})} + o({c_n}^2\|\breve{f}_n\|^2_{H^1(\mathbb{K}_{c_n})})$$

hence that $f_n \equiv 0$ for c large enough, i.e. $w_{c_n} \equiv \omega_{c_n}$. This means that if Conjecture 2.6 holds then there cannot be more than N^3 nonnegative minimizers for c large enough and, together with Proposition 2.49, this concludes the proof of Theorem 2.8. We are thus left with the proof of the following non-degeneracy result.

PROPOSITION 2.57. *Let $(w_c)_c$ be a sequence of minimizer to $E_{\mathbb{K},\lambda}(c)$ and L_n^+ the associated operator as in* (2.75)*. 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* (2.73) *and* (2.74)*, we have*

$$\left\langle L_n^+ f_n, f_n \right\rangle_{L^2(\mathbb{K}_{c_n})} \geqslant C \left\| f_n \right\|_{H^1(\mathbb{K}_{c_n})}^2 . \tag{2.76}$$

PROOF OF PROPOSITION 2.57. Following ideas in [**Wei85**], we define

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

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

LEMMA 2.58. *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 $\mathbb{1}_{\mathbb{K}_{c_n}} \breve{w}_{c_n}(\cdot + c_n R)$. Define as in* (2.14) *the operator L_μ^+ associated with Q and, as in* (2.75)*, L_n^+ associated with w_{c_n}. Let $(f_n)_n$ be a uniformly bounded sequence of $H^1_{per}(\mathbb{K}_{c_n})$ then*

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

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 2.58. 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 2.43,

$$\left\| \nabla f_n \right\|_{L^2(\mathbb{K}_{c_n})}^2 = \left\| \nabla f \right\|_{L^2(\mathbb{R}^3)}^2 + \left\| \nabla (f_n - f) \right\|_{L^2(\mathbb{K}_{c_n})}^2 + \underset{c \to \infty}{o}(1)$$

hence

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

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

$${c_n}^{-2} \langle \mathscr{G}({c_n}^{-1} \cdot) f_n, f_n \rangle \leqslant {c_n}^{-\frac{1}{2}} \left\| \mathscr{G} \right\|_{L^2(\mathbb{K})} \left\| f_n \right\|_{L^4(\mathbb{K}_{c_n})}^2 \underset{c \to +\infty}{\longrightarrow} 0$$

and, by the same argument as the one to obtain (2.55), we have

$${c_n}^{-2} \langle |w_{c_n}|^2 \star G_{\mathbb{K}}({c_n}^{-1} \cdot) f_n, f_n \rangle \lesssim {c_n}^{-1} \left\| \breve{w}_{c_n} \right\|_{L^{\frac{12}{5}}(\mathbb{K}_{c_n})}^2 \left\| f_n \right\|_{L^{\frac{12}{5}}(\mathbb{K}_{c_n})}^2 \underset{c \to +\infty}{\longrightarrow} 0.$$

Moreover, by Proposition 2.37, $\mathbb{1}_{\mathbb{K}_{c_n}} \breve{w}_n(\cdot + c_n R)$ strongly converges in $L^q(\mathbb{R}^3)$ for $2 \leqslant q < 6$ hence for $p = \frac{2}{3}$ and $p = \frac{4}{3}$ we have

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

Indeed, $\|f_n\|_{L^p(\mathbb{K}_{c_n})}$ is uniformly bounded for $2 \leqslant p < 6$, since $\|f_n\|_{H^1(\mathbb{K}_{c_n})}$ is uniformly bounded, hence $|\mathbb{1}_{\mathbb{K}_{c_n}} f_n|^2 \rightharpoonup |f|^2$ converges weakly (up to an omitted subsequence) in $L^p(\mathbb{R}^3)$ for any $1 \leqslant p < 3$. Consequently $\langle |Q|^p f_n, f_n\rangle_{L^2(\mathbb{K}_{c_n})} \to \langle |Q|^p f, f\rangle_{L^2(\mathbb{R}^3)}$ for $p = \frac{2}{3}$ and $p = \frac{4}{3}$ and we then obtain $\langle |\breve{w}_{c_n}|^p f_n, f_n\rangle_{L^2(\mathbb{K}_{c_n})} \to \langle |Q|^p f, f\rangle_{L^2(\mathbb{R}^3)}$ for $p = \frac{2}{3}$ and $p = \frac{4}{3}$ by the strong convergence of $\mathbb{1}_{\mathbb{K}_{c_n}} \breve{w}_n(\cdot + c_n R)$.

Finally, by Corollary 2.45 and weak convergence in $L^2(\mathbb{R}^3)$ of $\mathbb{1}_{\mathbb{K}_{c_n}} f_n(\cdot + c_n R)$,

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

This concludes the proof of Lemma 2.58. □

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 $\|f_n\|_{H^1(\mathbb{K}_{c_n})} = 1$,

$$\langle \breve{w}_{c_n} + \breve{\omega}_{c_n}, f_n\rangle_{L^2_{\rm per}(\mathbb{K}_{c_n})} = 0$$

and

$$\langle \mathscr{G}({c_n}^{-1}\cdot), \nabla((\breve{w}_{c_n} + \breve{\omega}_{c_n})\breve{f}_n)\rangle_{L^2_{\rm per}(\mathbb{K}_{c_n})} = 0,$$

with $\langle L_n^+ f_n, f_n\rangle_{L^2(\mathbb{K}_{c_n})} \to 0$.

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 $\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)} \leqslant 0$, by Lemma 2.58, and $\|f\|_{H^1(\mathbb{K}_{c_n})} \leqslant 1$. 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 $Q \geqslant 0$ (given by the conjecture), that $\mathbb{1}_{\mathbb{K}_{c_n}}(\breve{w}_{c_n}(\cdot + c_n R) + \breve{\omega}_{c_n}(\cdot + c_n R)) \to 2Q$ in $L^2(\mathbb{R}^3) \cap L^{6-}(\mathbb{R}^3)$. This, together with (2.73) and the weak convergence of the subsequence f_n in $L^2(\mathbb{R}^3) \cap L^6(\mathbb{R}^3)$ 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

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

Thus, applying Lemma 2.48 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 2.48 and, on the other hand, to $\mathbb{1}_{\mathbb{K}_{c_n}}(\breve{w}_{c_n}(\cdot + c_n R) + \breve{\omega}_{c_n}(\cdot + c_n R)) \to 2Q$ 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 2.43 — with the second set of conditions, we obtain

$$\langle \mathscr{G}({c_n}^{-1}\cdot + R), \nabla[(\breve{w}_{c_n}(\cdot + c_n R) + \breve{\omega}_{c_n}(\cdot + c_n R))\breve{f}_n(\cdot + c_n R)]\rangle_{L^2_{\rm per}(\mathbb{K}_{c_n})} \to 2\int_{\mathbb{R}^3} \frac{\nabla(fQ)}{|\cdot|}.$$

Finally, (2.74) 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 2.59, if Conjecture 2.6 holds then these two orthogonality properties imply that there exists $\alpha > 0$ such that

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

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

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

hence both norms vanish, since $\mu > 0$, which means that $\|f_n\|_{H^1(\mathbb{K}_{c_n})} \to 0$. This contradicts $\|f_n\|_{H^1(\mathbb{K}_{c_n})} = 1$ and concludes the proof that α_n cannot vanish, hence that of Proposition 2.57. $\square$

We are left with the proof of Proposition 2.59.

PROPOSITION 2.59. *If Conjecture 2.6 holds then there exists* $\alpha > 0$ *such that*

$$\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)} \geqslant \alpha \|f\|_{H^1(\mathbb{R}^3)}^2, \tag{2.77}$$

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 [**Wei85**] and Grillakis–Shatah–Strauss [**GSS87**]. The idea is the following. Using a Perron-Frobenius argument in each spherical harmonics sector as in [**Wei85, Len09, LRN15**], 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 [**Wei85**], 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 2.6.

PROOF OF PROPOSITION 2.59. First we note that it is obviously enough to prove it for f real valued but also that it is enough to prove

$$\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)} \geqslant \alpha \|f\|_{L^2(\mathbb{R}^3)}^2 \tag{2.78}$$

with $\alpha > 0$. Indeed, if f verifies (2.78) then, for any $\varepsilon > 0$, we have

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

hence f verifies (2.77) 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

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

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 $L^2(\mathbb{R}_+, r^2\, \mathrm{d}r)$ given by

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

We thus prove inequality (2.78) 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 $\langle f, Q\nabla|\cdot|^{-1}\rangle_{L^2(\mathbb{R}^3)} = 0$.

We first prove a Perron–Frobenius type result.

Lemma 2.60 (Perron–Frobenius property of the $L_{\mu,\ell}^+$). *For $\ell \geqslant 1$, $L_{\mu,\ell}^+$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}_+) \subset L^2(\mathbb{R}_+, r^2\, dr)$ and bounded below.*

Moreover, 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 of Lemma 2.60. We follow the structure of the proof of [**Len09**, Lemma 8].

Self-adjointness. Since $Q(r)$ decays exponentially, $|Q|^{\frac{4}{3}}$ and $|Q|^{\frac{2}{3}}$ are bounded multiplication operators on $L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)$. Moreover, the multiplication operator μ is also bounded and

$$-\Delta_{(\ell)} := -\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{2}{r}\frac{\mathrm{d}}{\mathrm{d}r} + \frac{\ell(\ell+1)}{r^2}$$

is bounded below hence $L^+_{\mu,\ell}$ is bounded below for $\ell \geqslant 0$. On another hand, it is known that $-\Delta_{(\ell)}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}_+)$ provided that $\ell \geqslant 1$. Thus, given that $\frac{7}{3}c_{TF}|Q_\mu|^{\frac{4}{3}} - \frac{5}{3}|Q_\mu|^{\frac{2}{3}} + \mu$ is bounded (so $-\Delta_{(\ell)}$-bounded of relative bound zero), symmetric (moreover self-adjoint) and that its domain contains the domain of $-\Delta_{(\ell)}$, we obtain by the Rellich–Kato theorem the essential self-adjointness of $L^+_{\mu,\ell}$ on $C_0^\infty(\mathbb{R}_+)$.

Positivity improving. We know (see [**Len09**]) that $(-\Delta_{(\ell)} + \beta)^{-1}$ is positivity improving on $L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)$ for all $\beta > 0$. Moreover, denoting by A_β the bounded self-adjoint operator

$$A_\beta := \frac{7}{3}c_{TF}|Q_\mu|^{\frac{4}{3}} - (\beta - \mu) - \frac{5}{3}|Q_\mu|^{\frac{2}{3}},$$

we have that $-A_\beta$ is positivity preserving on $L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)$ for all $\beta \geqslant \mu + \frac{7}{3}c_{TF}|Q(0)|^{\frac{4}{3}}$ since Q is radial decreasing and, for β large enough, that

$$\left\|\left| A_\beta(-\Delta_{(\ell)} + \beta)^{-1} \right\|\right|_{L^2 \to L^2} < 1$$

since A_β is bounded. Consequently, a Neumann expansion on

$$(L^+_{\mu,\ell} + \beta)^{-1} = (-\Delta_{(\ell)} + \beta)^{-1}\left(1 + A_\beta(-\Delta_{(\ell)} + \beta)^{-1}\right)^{-1},$$

which holds for β large enough, yields

$$(L^+_{\mu,\ell} + \beta)^{-1} = (-\Delta_{(\ell)} + \beta)^{-1}\sum_{\nu=0}^{\infty}\left(-A_\beta(-\Delta_{(\ell)} + \beta)^{-1}\right)^{\nu}.$$

Finally, $(-\Delta_{(\ell)} + \beta)^{-1}$ and $-A_\beta$ being respectively positivity improving and preserving, we conclude that the resolvent $(L^+_{\mu,\ell} + \beta)^{-1}$ is positivity improving for β large enough.

Conclusion. We choose $\beta \gg 1$ such that $(L^+_{\mu,\ell} + \beta)^{-1}$ is positivity improving and bounded. Then, by [**RS78**, Thm XIII.43], the largest eigenvalue $\sup \sigma((L^+_{\mu,\ell} + \beta)^{-1})$ is simple and the associated eigenfunction $\varphi_\ell \in L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)$ is positive. Since, for any $\psi \in L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)$, having ψ being an eigenfunction of $L^+_{\mu,\ell}$ for the eigenvalue λ is equivalent to having ψ being an eigenfunction of $(L^+_{\mu,\ell} + \beta)^{-1}$ for the eigenvalue $(\lambda + \beta)^{-1}$, we have proved Lemma 2.60. $\square$

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

$$\alpha_1 := \inf_{\substack{f \in \mathcal{H}_{(1)} \cap H^1(\mathbb{R}^3) \\ \langle f, Q\nabla|\cdot|^{-1}\rangle_{L^2(\mathbb{R}^3)}=0}} \frac{\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)}}{\|f\|^2_{L^2(\mathbb{R}^3)}} > 0. \tag{2.79}$$

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 2.4, we know that $\partial_{x_i} Q$ is an eigenfunction of L_μ^+ associated with the eigenvalue 0 hence $Q'(r)$ is an eigenfunction of $L^+_{(1)}$ associated with the eigenvalue $e_{\mu,1} = 0$. Therefore, the fact that $Q'(r) < 0$ (as proved in Theorem 2.3) implies, using the Perron-Frobenius property verified by $L^+_{(1)}$, that $e_{\mu,1} = 0$ is the lowest eigenvalue of $L^+_{(1)}$ and is simple with $-Q' > 0$ the associated eigenfunction. Consequently, we have for any $f \in \mathcal{H}_{(1)}$ that

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

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

We thus suppose that $\alpha_1 = 0$ and prove it is impossible. Let f_n be a minimizing sequence to (2.79) with $\|f_n\|_{L^2(\mathbb{R}^3)} = 1$. One has

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

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

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

where the second inequality is due to

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

$\mu > 0$ and to $\langle |Q|^p f_n, f_n\rangle_{L^2(\mathbb{R}^3)} \to \langle |Q|^p f, f\rangle_{L^2(\mathbb{R}^3)}$, for $p = \frac{2}{3}$ and $p = \frac{4}{3}$, obtained by a similar argument to the one in proof of Lemma 2.58. 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 $\mathrm{span}\{Y_1^{-1}, Y_1^0, Y_1^1\}$. However, for any $i = 1, 2, 3$, we have after passing to the weak limit that

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

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

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

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

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

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 (2.79) converges weakly to 0 in $H^1(\mathbb{R}^3)$. This gives $\langle |Q|^p f_n, f_n\rangle_{L^2(\mathbb{R}^3)} \to 0$ and

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

therefore $f_n \to 0$ 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 $\ell \geqslant 2$. We now deal with the cases $\ell \geqslant 2$ and prove that there exists $\alpha > 0$ such that

$$\langle L^+_{\mu,\ell}\varphi, \varphi\rangle_{L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)} \geqslant \alpha \|\varphi\|^2_{L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)} \tag{2.80}$$

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

$$\langle L^+_{\mu,\ell}\varphi, \varphi\rangle_{L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)} = \langle L^+_{(\ell-1)}\varphi, \varphi\rangle_{L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)} + 2(\ell-1)\|\varphi/r\|^2_{L^2(\mathbb{R}_+, r^2\,\mathrm{d}r)}, \tag{2.81}$$

it is then sufficient to prove (2.80) in the case $\ell = 2$ in order to prove it for all $\ell \geqslant 2$.

For $\ell = 2$, we can assume that $\inf \sigma(L^+_{(2)})$ 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 $r \to \infty$, it is well-known (see e.g. [**Tes09**]) that $\sigma_{\mathrm{ess}}(L^+_{(2)}) = [\mu; +\infty)$ and (2.80) follows. We thus have, by (2.81) and $L^+_{(1)} \geqslant 0$, that the eigenvalue $e_{\mu,2} = \inf \sigma(L^+_{(2)})$ and its associated eigenfunction $\varphi_2 \not\equiv 0$ verify that

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

and (2.80) is therefore proved. It concludes the case $\ell \geqslant 2$.

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

$$\alpha_0 := \inf_{\substack{f \in \mathcal{H}_{(0)} \cap H^1(\mathbb{R}^3) \\ \langle f, Q\rangle_{L^2(\mathbb{R}^3)} = 0}} \frac{\langle L^+_\mu f, f\rangle_{L^2(\mathbb{R}^3)}}{\|f\|^2_{L^2(\mathbb{R}^3)}} > 0. \tag{2.82}$$

We already know that $\alpha_0 \geqslant 0$ 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 (2.67) and using (2.12), (2.26), Lemma 2.55 and that Q is a minimizer of $J_{\mathbb{R}^3}(\lambda)$, we obtain

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

which implies in particular that $\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)} \geqslant 0$ 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 (2.82) with $\|f_n\|_{L^2(\mathbb{R}^3)} = 1$. As in the proof of case $\ell = 1$ above, f_n is in fact bounded in $H^1(\mathbb{R}^3)$ and denoting by $f \in \mathcal{H}_{(0)}$ its weak limit in $H^1(\mathbb{R}^3)$, up to a subsequence, we have $\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)} = 0$. This leads, to $L_\mu^+ f = \beta Q$ thus, using that L_μ^+ is inversible, to $f = \beta(L_\mu^+)^{-1}Q$. Indeed, for any $\eta \in \mathcal{H}_{(0)}$ orthogonal to Q and any τ, $f + \tau\eta$ verifies

$$0 = \frac{\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)}}{\|f\|^2_{L^2(\mathbb{R}^3)}} \leqslant \frac{\langle L_\mu^+(f+\tau), f+\tau\rangle_{L^2(\mathbb{R}^3)}}{\|f+\tau\|^2_{L^2(\mathbb{R}^3)}} = 2\tau\frac{\langle L_\mu^+ f, \eta\rangle_{L^2(\mathbb{R}^3)}}{\|f\|^2_{L^2(\mathbb{R}^3)}} + o(\tau^2),$$

due to f minimizing (2.82) and to $\langle L_\mu^+ f, f\rangle_{L^2(\mathbb{R}^3)} = 0$, hence $\langle L_\mu^+ f, \eta\rangle_{L^2(\mathbb{R}^3)} = 0$ for any $\eta \in \operatorname{span}\{Q\}^\perp$ which implies that $L_\mu^+ f$ is proportional to 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 2.6. We have obtained $f \equiv 0$ which is absurd as before. Indeed, we then have $\langle |Q|^p f_n, f_n\rangle_{L^2(\mathbb{R}^3)} \to 0$, thus

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

hence both norms would vanish (since $\mu > 0$), which would imply $\|f_n\|_{H^1(\mathbb{R}^3)} \to 0$, contradicting $\|f_n\|_{L^2(\mathbb{R}^3)} = 1$ and concluding the case $\ell = 0$. □

This concludes the proof of Theorem 2.8. □

6. Appendix: Complementary proofs and results

6.1. Details of Step 9 of the proof of Theorem 2.3: Minimizing sequences are precompact up to a translations. Let $\{Q_n\}_n \subset H^1(\mathbb{R}^3)$ be a minimizing sequence of $J_{\mathbb{R}^3,c}(\lambda)$. We claim that there exist a subsequence and translations $\{x_k\}_k \subset \mathbb{R}^3$ such that $Q_{n_k}(\cdot - x_k) \rightharpoonup Q^{(1)} \not\equiv 0$ weakly in $H^1(\mathbb{R}^3)$. This result rely on the number

$$\mathbf{m}(\{\varphi_n\}) = \sup\left\{\int_{\mathbb{R}^3} |\varphi|^2 \;\Big|\; \exists\{x_n\} \subset \mathbb{R}^3, \varphi_{n_k}(\cdot - x_k) \rightharpoonup \varphi \text{ weakly in } H^1(\mathbb{R}^3)\right\},$$

defined for any sequence $\{\varphi_n\}$ bounded in $H^1(\mathbb{R}^3)$, and on Lemma 1.26 that we recall here for clarity.

Lemma. *For any sequence $\{\varphi_n\}$ bounded in $H^1(\mathbb{R}^3)$, the following assertions are equivalent:*

i. $\mathbf{m}(\{\varphi_n\}) = 0$;

ii. $\displaystyle\lim_{n\to\infty} \sup_{z\in\mathbb{Z}^3} \int_{C_z} |\varphi_n|^2 = 0$;

iii. $\forall\, R > 0,\ \displaystyle\lim_{n\to\infty} \sup_{x\in\mathbb{R}^3} \textstyle\int_{B(x,R)} |\varphi_n|^2 = 0$;

iv. $\varphi_n \to 0$ *strongly in* $L^p(\mathbb{R}^3)$ *for all* $2 < p < 6$,

where the $C_z = \displaystyle\prod_{j=1}^{3} [z_j, z_j + 1)$, *for any* $z = (z_1, z_2, z_3) \in \mathbb{Z}^3$, *tile the whole space:* $\mathbb{R}^3 = \displaystyle\bigcup_{z\in\mathbb{Z}^3} C_z$.

Remark. Our definition of $\mathbf{m}$ is slightly different from our previous one in (1.45) as this new definition uses weak convergence on H^1 while the previous used weak convergence on L^2. Nevertheless, Lemma 1.26 suppose that the function is in H^1 hence its proof stay the same.

If our claim that $Q_{n_k}(\cdot - x_k) \rightharpoonup Q^{(1)} \not\equiv 0$ were not true it would mean that $\mathbf{m}(\{Q_n\}) = 0$ and, since $\{Q_n\}$ is bounded in $H^1(\mathbb{R}^3)$ due to Lemma 2.10, it would imply by Lemma 1.26 that $Q_n \to 0$ strongly in $L^p(\mathbb{R}^3)$ for all $2 < p < 6$ and $Q_n \rightharpoonup 0$ weakly in $H^1(\mathbb{R}^3)$. But this contradicts $J_{\mathbb{R}^3}(\lambda) < 0$ proved in Lemma 2.12, since it would give that

$$J_{\mathbb{R}^3,c}(\lambda) = \liminf_{n\to\infty} \mathscr{J}_{\mathbb{R}^3,c}(Q_n) = \liminf_{n\to\infty} \int_{\mathbb{R}^3} |\nabla Q_n|^2 \geqslant 0,$$

and we have hence proved that $Q_{n_k}(\cdot - x_k) \rightharpoonup Q^{(1)} \not\equiv 0$.

Since $Q_{n_k}(\cdot - x_k) \rightharpoonup Q^{(1)}$ weakly in $H^1(\mathbb{R}^3)$, using Lemma 2.61, and its corollary — that we both state and prove at the end of this Step 9, for the readability of the proof — we can write

$$Q_{n_k}(\cdot - x_k) = \xi_k + \psi_k + \varepsilon_k$$

where $\xi_k \to Q^{(1)}$ weakly in $H^1(\mathbb{R}^3)$ and strongly in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$, $\mathrm{supp}(\xi_k) \subset B(0,k)$, $\mathrm{supp}(\psi_k) \subset \mathbb{R}^3 \backslash B(0,2k)$, and $\varepsilon_k \to 0$ strongly in $H^1(\mathbb{R}^3)$.

The disjoint supports property and the strong convergence of ε_k give that

$$\mathscr{J}_{\mathbb{R}^3,c}(Q_{n_k}) = \mathscr{J}_{\mathbb{R}^3,c}(Q_{n_k}(\cdot - x_k)) = \mathscr{J}_{\mathbb{R}^3,c}(\xi_k) + \mathscr{J}_{\mathbb{R}^3,c}(\psi_k) + o(1)_{k\to\infty}. \tag{2.83}$$

On another hand, the strong and weak convergence of ξ_k give that

$$\liminf_{k\to\infty} \mathscr{J}_{\mathbb{R}^3,c}(\xi_k) \geqslant \mathscr{J}_{\mathbb{R}^3,c}(Q^{(1)}) \geqslant J_{\mathbb{R}^3,c}(\lambda_1),$$

where $\lambda_1 = \left\|Q^{(1)}\right\|^2_{L^2(\mathbb{R}^3)}$, while the respectively strong and weak convergences to $Q^{(1)}$ in $L^2(\mathbb{R}^3)$ of ξ_k and Q_{n_k}, together with the strong convergence to 0 of ε_k, give $\|\psi_k\|^2_{L^2(\mathbb{R}^3)} = \lambda - \lambda_1 + o(1)_{k\to\infty}$, hence

$$\mathscr{J}_{\mathbb{R}^3,c}(\psi_k) \geqslant J_{\mathbb{R}^3,c}(\|\psi_k\|^2_{L^2(\mathbb{R}^3)}) \to J_{\mathbb{R}^3,c}(\lambda - \lambda_1),$$

by the continuity of $\lambda \mapsto J_{\mathbb{R}^3,c}(\lambda)$ proved in Lemma 2.12. Passing to the limit in (2.83), we obtain $J_{\mathbb{R}^3,c}(\lambda) \geqslant J_{\mathbb{R}^3,c}(\lambda_1) + J_{\mathbb{R}^3,c}(\lambda-\lambda_1)$ but the strict binding (2.13) implies that either $\lambda_1 = 0$ or $\lambda_1 = \lambda$. However, we have proved that $Q^{(1)} \not\equiv 0$ hence $\lambda_1 = \lambda$.

Now that we have proved that $\|Q^{(1)}\|^2_{L^2(\mathbb{R}^3)} = \lambda$, we obtain the strong convergence $Q_{n_k}(\cdot - x_k) \to Q^{(1)}$ in $L^2(\mathbb{R}^3)$, by the weak convergence in $L^2(\mathbb{R}^3)$, and this strong convergence holds in fact in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$, by the Sobolev embedding, the fact that $Q_{n_k}(\cdot - x_k)$ is H^1-bounded and interpolation. But those strong convergences and the H^1-weak convergence give

$$J_{\mathbb{R}^3,c}(\lambda) = \liminf_{n\to\infty} \mathscr{J}_{\mathbb{R}^3,c}(Q_{n_k}(\cdot - x_k)) \geqslant \mathscr{J}_{\mathbb{R}^3,c}(Q^{(1)}) \geqslant J_{\mathbb{R}^3,c}(\lambda)$$

which proves that $Q^{(1)}$ is a minimizer but also that

$$\|\nabla Q_{n_k}\|_{L^2(\mathbb{R}^3)} = \|\nabla Q_{n_k}(\cdot - x_k)\|_{L^2(\mathbb{R}^3)} \to \left\|\nabla Q^{(1)}\right\|_{L^2(\mathbb{R}^3)},$$

using that $\|Q_{n_k}\|_{L^p(\mathbb{R}^3)} = \|Q_{n_k}(\cdot - x_k)\|_{L^p(\mathbb{R}^3)}$ and again the strong convergence of $Q_{n_k}(\cdot - x_k)$ in the L^p.

We have therefore proved that $Q_{n_k}(\cdot - x_k)$ converges strongly in $H^1(\mathbb{R}^3)$ to $Q^{(1)}$ which is a minimizer : Q_n is precompact up to translations.

We conclude this Step 9 by the statements and proofs of Lemma 2.61 and of Corollary 2.62. For both results, we will follow the proof in [**Lew10**] which itself follows Lions [**Lio82, Lio84a, Lio84b**].

LEMMA 2.61 (Extracting the locally convergent part). *Let $\{\varphi_n\}$ be a sequence bounded in $H^1(\mathbb{R}^3)$ such that $\varphi_n \rightharpoonup \varphi$ weakly in $H^1(\mathbb{R}^3)$ and let $0 \leqslant R_k \leqslant R'_k$ such that $R_k \to \infty$. Then there exists $\{\varphi_{n_k}\}$ such that, as $k \to \infty$, it holds that*

$$\int_{|x| \leqslant R_k} |\varphi_{n_k}(x)|^2 \, dx \to \int_{\mathbb{R}^3} |\varphi(x)|^2 \, dx \tag{2.84}$$

and

$$\int_{R_k \leqslant |x| \leqslant R'_k} \left(|\varphi_{n_k}(x)|^2 + |\nabla \varphi_{n_k}(x)|^2\right) \, dx \to 0. \tag{2.85}$$

In particular, it holds that $\mathbb{1}_{B(0,R_k)}\varphi_{n_k} \to \varphi$ strongly in $L^p(\mathbb{R}^3)$ for all $2 \leqslant p < 6$.

Note that this lemma will also be needed in Lemma 2.41, our concentration-compactness result for the effective model on the cube $\mathbb{K}$.

COROLLARY 2.62. *Let $0 \leqslant R_k \leqslant R'_k$ be such that $R_k \to \infty$ and $\{\varphi_n\}$ be a sequence bounded in $H^1(\mathbb{R}^3)$ such that $\varphi_n \underset{n\to\infty}{\rightharpoonup} \varphi$ weakly in $H^1(\mathbb{R}^3)$. Then there exists a subsequence $\{\varphi_{n_k}\}_{k\to\infty}$ such that*

$$\lim_{k\to\infty} \|\varphi_{n_k} - \xi_k - \psi_k\|_{H^1(\mathbb{R}^3)} = 0$$

where $\{\xi_k\}_k$ and $\{\psi_k\}_k$ are sequences bounded in $H^1(\mathbb{R}^3)$ such that

(1) $\xi_k \to \varphi$ weakly in $H^1(\mathbb{R}^3)$ and strongly in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$,

(2) $\operatorname{supp}(\xi_k) \subset B(0, R_k)$ and $\operatorname{supp}(\psi_k) \subset \mathbb{R}^3 \backslash B(0, R'_k)$,

(3) $\mathbf{m}(\{\psi_k\}) \leqslant \mathbf{m}(\{\varphi_{n_k}\}) \leqslant \mathbf{m}(\{\varphi_n\})$.

PROOF OF LEMMA 2.61. We introduce the so-called *Levy concentration functions* **[Lev54]**

$$M_n(R) = \int_{B(0,R)} |\varphi_n|^2 \quad \text{and} \quad K_n(R) = \int_{B(0,R)} |\nabla \varphi_n|^2.$$

The functions M_n and K_n are continuous nondecreasing functions on $[0, \infty)$ such that

$$\forall n \geqslant 1, \forall R > 0, M_n(R) + K_n(R) \leqslant \int_{\mathbb{R}^3} |\varphi_n|^2 + |\nabla \varphi_n|^2 \leqslant C$$

since $\{\varphi_n\}$ is bounded in $H^1(\mathbb{R}^3)$. Thus, by the Rellich-Kondrachov Theorem, we obtain that

$$M_n(R) \to \int_{B(0,R)} |\varphi|^2 =: M(R)$$

for all $R \geqslant 0$. Moreover, up to extraction of a subsequence (we do not change notation to simplify), there exists a nondecreasing function K such that, for all $R \geqslant 0$, $K_n(R) \to K(R)$ as $n \to +\infty$. We denote $\ell := \lim_{R\to\infty} K(R)$ which is finite since $K_n(R)$ is bounded uniformly in n and R.

Applying now the above limit result to our R_k and R_k', we deduce that, up to another subsequence, we have that

$$|M_{n_k}(R_k) - M(R_k)| + |M_{n_k}(R_k') - M(R_k')| \\ + |K_{n_k}(R_k) - K(R_k)| + |K_{n_k}(R_k') - K(R_k')| \leqslant \frac{1}{k}.$$

Consequently, we have that

$$\left|\int_{|x|\leqslant R_k} |\varphi_{n_k}|^2 - \int_{\mathbb{R}^3} |\varphi|^2\right| \leqslant |M_{n_k}(R_k) - M(R_k)| + \int_{|x|\geqslant R_k} |\varphi|^2 \underset{k\to+\infty}{\longrightarrow} 0,$$

$$\int_{R_k\leqslant|x|\leqslant R_k'} |\varphi_{n_k}|^2 = M_{n_k}(R_k') - M_{n_k}(R_k) \leqslant \frac{1}{k} + M(R_k') - M(R_k) \underset{k\to+\infty}{\longrightarrow} 0$$

and

$$\int_{R_k\leqslant|x|\leqslant R_k'} |\nabla\varphi_{n_k}|^2 = K_{n_k}(R_k') - K_{n_k}(R_k) \leqslant \frac{1}{k} + K(R_k') - K(R_k) \underset{k\to+\infty}{\longrightarrow} 0,$$

where the last convergence uses the fact that $K(R_k') - K(R_k) \to \ell - \ell = 0$.

Moreover, $\mathbb{1}_{B(0,R_k)}\varphi_{n_k} \rightharpoonup \varphi$ weakly in $L^2(\mathbb{R}^3)$ since $\varphi_{n_k} \rightharpoonup \varphi$. But this convergence is in fact strong given the norm convergence just proved. By the Sobolev embeddings, we obtain that φ_{n_k} and, consequently, $\mathbb{1}_{B(0,R_k)}\varphi_{n_k}$ are bounded in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$ which leads, by interpolation to the strong convergence of $\mathbb{1}_{B(0,R_k)}\varphi_{n_k} \to \varphi$ in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$. This concludes the proof of Lemma 2.61. ☐

Proof of Corollary 2.62. We can apply Lemma 2.61 to $\varphi_n \rightharpoonup \varphi$ with $R_k/2$ and $4R_k'$ and obtain a subsequence $\{\varphi_{n_k}\}$ such that

$$\int_{|x|\leqslant R_k/2} |\varphi_{n_k}|^2 \to \int_{\mathbb{R}^3} |\varphi|^2 \quad \text{and} \quad \int_{R_k/2\leqslant|x|\leqslant 4R_k'} \left(|\varphi_{n_k}|^2 + |\nabla\varphi_{n_k}|^2\right) \to 0. \tag{2.86}$$

Let $\chi : \mathbb{R}^+ \to [0,1]$ be a smooth function such that $0 \leqslant \chi' \leqslant 2$, $\chi_{|[0,1]} \equiv 1$, $\chi_{|[2,\infty)} \equiv 0$. We then denote $\tilde{\chi}_k(x) := \chi(2|x|/R_k)$ and $\tilde{\zeta}_k(x) := 1 - \chi(|x|/R_k')$ and introduce $\xi_k := \tilde{\chi}_k\varphi_{n_k}$ and $\psi_k := \tilde{\zeta}_k\varphi_{n_k}$. Since

$$\varphi_{n_k} - \xi_k - \psi_k = \varphi_{n_k}(\chi(|x|/R_k') - \chi(2|x|/R_k)),$$

we have supp $(\varphi_{n_k} - \xi_k - \psi_k) \subset \{R_k/2 \leqslant |x| \leqslant 2R_k'\}$ hence, using (2.86), we have

$$\lim_{k\to\infty} \|\varphi_{n_k} - \xi_k - \psi_k\|_{H^1(\mathbb{R}^3)} = 0.$$

Together with the disjoint support property, it implies in particular that

$$\|\xi_k\|_{H^1(\mathbb{R}^3)} + \|\psi_k\|_{H^1(\mathbb{R}^3)} = \|\xi_k + \psi_k\|_{H^1(\mathbb{R}^3)} = \|\varphi_{n_k}\|_{H^1(\mathbb{R}^3)} + o(1)$$

hence that ξ_k and ψ_k are bounded sequences in $H^1(\mathbb{R}^3)$.

By construction, $\xi_k \rightharpoonup \varphi$ weakly in $H^1(\mathbb{R}^3)$ and

$$\lim_{k\to\infty}\int_{\mathbb{R}^3}|\xi_k|^2 = \lim_{k\to\infty}\int_{B(0,R_k/2)}|\xi_k|^2 = \int_{\mathbb{R}^3}|\varphi|^2,$$

hence ξ_k strongly converges to φ in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$ by Sobolev embeddings and because $\|\varphi_n\|_{H^1(\mathbb{R}^3)}$ is uniformly bounded. In addition, it is easy to see that $\mathbb{1}_{B(0,4R'_k)}\psi_k \to 0$ strongly in $L^2(\mathbb{R}^3)$.

We now prove that $\mathbf{m}(\{\psi_k\}) \leqslant \mathbf{m}(\{\varphi_{n_k}\}) \leqslant \mathbf{m}(\{\varphi_n\})$. We suppose $\mathbf{m}(\{\psi_k\}) > 0$, otherwise there is nothing to prove. Thus, there exists k_j's, $\{x_j\} \subset \mathbb{R}^3$ and $\psi \not\equiv 0$ such that $\psi_{k_j}(\cdot - x_j) \rightharpoonup \psi$ weakly in $L^2(\mathbb{R}^3)$. We first prove that, for j large enough, we have $|x_j| \geqslant 3R'_{k_j}$. Indeed, if for a subsequence (denoted the same), we have $|x_j| < 3R'_{k_j}$ then $\psi_{k_j}(\cdot - x_j)\mathbb{1}_{B(0,R'_k)} \rightharpoonup 0 \equiv \psi$ weakly in $L^2(\mathbb{R}^3)$ — since $B(x_j, R'_k) \subset B(0, 4R'_k)$ and $\mathbb{1}_{B(0,4R'_k)}\psi_k \to 0$ strongly in $L^2(\mathbb{R}^3)$ — a contradiction. Consequently, we have that

$$\psi_{k_j}(\cdot - x_j)\mathbb{1}_{B(0,R'_{k_j})} = \varphi_{n_{k_j}}(\cdot - x_j)\mathbb{1}_{B(0,R'_{k_j})} \rightharpoonup \psi$$

since $\tilde{\zeta}_k \equiv 1$ on $B(x_j, R'_{k_j})$ which implies that $\varphi_{n_{k_j}}(\cdot - x_j) \rightharpoonup \psi$ weakly in $L^2(\mathbb{R}^3)$ hence that $\mathbf{m}(\{\psi_k\}) \leqslant \mathbf{m}(\{\varphi_{n_k}\})$. $\square$

6.2. Detailed proof of Theorem 2.4. This proof follows essentially line by line the proof of [**LRN15**, Thm. 2]. We divide the proof into several steps for clarity.

Step 1: Positivity of nonnegative $H^1(\mathbb{R}^3)$-solutions. Let $u \geqslant 0$ be a non trivial $H^1(\mathbb{R}^3)$-solution to the Euler–Lagrange equation (2.12). The equation gives us the upper bound

$$\|\Delta u\|^2_{L^2(\mathbb{R}^3)} \leqslant c_{TF}\|u\|^{\frac{14}{3}}_{L^{\frac{14}{3}}(\mathbb{R}^3)} + \|u\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{R}^3)} + \mu\|u\|^2_{L^2(\mathbb{R}^3)}$$

which is bounded since $u \in H^1(\mathbb{R}^3)$. Hence, $u \in H^2(\mathbb{R}^3) \subset C^0_0(\mathbb{R}^3)$ and we obtain that $Q > 0$ with the same end of the proof as in Step 6 of the proof of Theorem 2.3.

Step 2: Positive solution are radial decreasing, the moving plane method. Contrarily to [**LRN15**] we cannot use [**GNN81**, Thm. 2] because our function

$$F_\mu(y) = -c_{TF}y^{\frac{7}{3}} + y^{\frac{5}{3}} - \mu y \tag{2.34}$$

is not C^2 at $y = 0$ (F''_μ is not even defined at 0). However, given that we are interested in nonnegative solution and since one can prove similarly to Step 6 in the proof of Theorem 2.3 that any non trivial nonnegative solution is positive, we have in particular that their inverse are locally bounded. Hence, when we recursively differentiate the Euler–Lagrange equation, the negative powers that will appear (due to powers $7/3$ and $5/3$ of E–L equation) will not create any difficulty to obtain that such positive solutions are C^∞. Therefore, we can apply [**Li91**, Thm. 1.1] that we recall for clarity in the following lemma.

LEMMA (Positive solution are radial decreasing, [**Li91**]). *Let f be a C^1 function such that $f'(0) < 0$. Any C^2 positive solution of*

$$\begin{cases} \Delta u + f(u) = 0, & \text{in } \mathbb{R}^3 \\ u(x) \to 0 & \text{as } |x| \to \infty \end{cases}$$

is radial decreasing about some point in $\mathbb{R}^3$.

Consequently, we know at this point that any nonnegative $H^2(\mathbb{R}^3)$-solutions to the Euler–Lagrange equation (2.12) is, up to a spatial translation, a positive radial decreasing solution of

$$\begin{cases} u'' + \dfrac{2}{r}u' + F_\mu(u) = 0 & \text{on } \mathbb{R}_+ \\ u'(0) = 0 \end{cases} \tag{2.87}$$

with the condition

$$(u(r), u'(r)) \underset{r\to\infty}{\longrightarrow} (0,0). \tag{2.88}$$

We will show the uniqueness (for each admissible μ) of solutions to (2.87) that fulfill that condition (2.88), that we will call solution of the problem (RPb-μ).

Step 3: Admissible μ's. We first give some properties of F_μ together with a first condition of admissibility for the μ's.

LEMMA 2.63. *Let $\lambda, c_{TF} > 0$. Then an admissible μ verifies $4\mu c_{TF} < 1$ and, for such μ, the function $F_\mu(x) := -c_{TF}x^{\frac{7}{3}} + x^{\frac{5}{3}} - \mu x$ verifies that*

(1) F_μ is positive on (β, γ) and negative on $(0,\beta) \cup (\gamma, \infty)$;

(2) $H : x \mapsto xF_\mu'(x)/F_\mu(x)$ is strictly decreasing from 1 to $-\infty$ on $(0,\beta)$, from $+\infty$ to $-\infty$ on (β,γ) and from $+\infty$ to $7/3$ on $(\gamma,+\infty)$;

(3) for every $\lambda \geqslant 1$, the function $I(x) := xF_\mu'(x) - \lambda F_\mu(x)$ has exactly one root on $(0,\gamma)$ and this root x_* verifies $x_* \in (\beta,\gamma)$ and $I'(x_*) < 0$.

Where

$$\beta = \left(\frac{1-\sqrt{1-4c_{TF}\mu}}{2c_{TF}}\right)^{3/2} \qquad \text{and} \qquad \gamma = \left(\frac{1+\sqrt{1-4c_{TF}\mu}}{2c_{TF}}\right)^{3/2}.$$

PROOF OF LEMMA 2.63. By Theorem 2.3, a minimizer u of $J_{\mathbb{R}^3,\lambda}(1)$ is in $H^2(\mathbb{R}^3)$, positive and verifies $\Delta u + F_\mu(u) = 0$ where $F_\mu(u) = -c_{TF}u^{\frac{7}{3}} + u^{\frac{5}{3}} - \mu u$ on $[0;\infty)$. We first claim that there necessarily exist $x \in (0;\infty)$ such that $F_\mu(x) > 0$.

Indeed, if it were not the case, then we would have that $\Delta u \geqslant 0$ on $\mathbb{R}^3$ which leads, since $u \geqslant 0$, to $\|\nabla u\|_{L^2(\mathbb{R}^3)} \leqslant 0$ and thus to $u \equiv \lim_{|x|\to\infty} u(x) = 0$ hence a contradiction to Theorem 2.3. The fact that F_μ is not nonpositive together with rewriting

$$F_\mu(x) = \frac{x}{4c_{TF}}\left(1 - 4c_{TF}\mu - \left(2c_{TF}x^{\frac{2}{3}} - 1\right)^2\right), \tag{2.89}$$

gives that necessarily $4\mu c_{TF} < 1$. Moreover, (2.89) immediately gives *(1)*.

For shortness in the end of this proof, we will denote F_μ simply by F. On $(0;+\infty)\backslash\{\beta;\gamma\}$, denoting $G(x) = 2c_{TF}x^{\frac{7}{3}} - x^{\frac{5}{3}}$, we have

$$H(x) := \frac{xF'(x)}{F(x)} = 1 - \frac{2}{3}\frac{G(x)}{F(x)},$$

thus the sign of the derivative H' is the same as the sign of $F'G - FG'$ on $(0;+\infty)\backslash\{\beta;\gamma\}$. Since $4\mu c_{TF} < 1$, it holds on $(0;+\infty)$ that

$$F'(x)G(x) - F(x)G'(x) = -\frac{2}{3}c_{TF}x^{\frac{5}{3}}\left((x^{\frac{2}{3}} - 2\mu)^2 + \frac{\mu}{c_{TF}}(1 - 4\mu c_{TF})\right) < 0$$

and consequently H is strictly decreasing on each of the three intervals where it is defined. The limit values are easy to check which concludes the proof of *(2)*.

For every $\lambda \geqslant 1$, we have on $(0;\beta)$ that $H(x) = xF'(x)/F(x) < 1 \leqslant \lambda$ thus it holds that $I > 0$ on $(0;\beta)$ since $F < 0$ on this interval. Moreover, we deduce from *(2)* that I has a unique zero on $(\beta;\gamma)$ that we denote x_*. Finally, since $I' = FH' + \frac{F'}{F}I$, $F(x_*) > 0$, $H'(x_*) < 0$, $F(x_*) \neq 0$ and $I(x_*) = 0$, we obtain

$$I'(x_*) < \frac{F'(x_*)}{F(x_*)}I(x_*) = 0.$$

$\square$

To conclude about the admissible μ's (but also for the proof of uniqueness and non-degeneracy proved in the next Step), we define for any u the local energy

$$H_\alpha(r) := \frac{(u'(r))^2}{2} + \int_\alpha^{u(r)} F_\mu(x)\,\mathrm{d}x, \tag{2.90}$$

for any $\alpha \geqslant 0$ (we omit the dependency with u in the subscript for shortness). For any u solution to (2.87), we have that

$${H_\alpha}'(r) = (u''(r) + F_\mu(u(r)))\,u'(r) = \begin{cases} -\dfrac{2}{r}(u'(r))^2 \leqslant 0 & \text{if } r > 0, \\ 0 & \text{if } r = 0. \end{cases} \tag{2.91}$$

Therefore, H_α is strictly decreasing on $[0;\infty)$, for any u solution to (2.87). The decrease is strict otherwise we would have an interval on which $u'=0$ and this is impossible.

LEMMA 2.64. *The existence of a solution to* (RPb-μ) *is equivalent to* $\frac{64}{15}\mu c_{TF} < 1$*. Moreover, if u is solution, then necessarily $\omega < u(0) < \theta$ where*

$$\omega^{\frac{2}{3}} = \frac{5}{8c_{TF}}\left(1-\sqrt{1-\frac{64}{15}\mu c_{TF}}\right) \quad \text{and} \quad \theta^{\frac{2}{3}} = \frac{5}{8c_{TF}}\left(1+\sqrt{1-\frac{64}{15}\mu c_{TF}}\right)$$

which verify $0<\beta<\omega<\gamma<\theta$.

PROOF OF LEMMA 2.64. A computation gives that

$$\int_0^y F_\mu(x)\,\mathrm{d}x = -\frac{3}{10}c_{TF}y^2\left(\left(y^{\frac{2}{3}}-\frac{5}{8c_{TF}}\right)^2+\left(\frac{5}{8c_{TF}}\right)^2\left(\frac{64}{15}\mu c_{TF}-1\right)\right).$$

On one hand, [**BL83**, Theorem 1] gives that if there exists $y>0$ such that $\int_0^y F_\mu(x)\,\mathrm{d}x > 0$ then a solution to *(RPb-μ)* exists. On the other hand, let us suppose that there exists a solution u to (RPb-μ), then H_0 is strictly decreasing and $\lim_{r\to\infty} H_0(r) = 0$, hence

$$0 < H_0(0) = \int_0^{u(0)} F_\mu(x)\,\mathrm{d}x.$$

We thus have proved that the existence of a solution is equivalent to the existence of $y>0$ such that $\int_0^y F_\mu(x)\,\mathrm{d}x > 0$. In terms of μ, it says that the existence of a solution is equivalent to $\frac{64}{15}\mu c_{TF} < 1$. Then, under this condition on μ, a direct computation gives the bounds ω and θ.

One can easily find that $\beta<\omega$ by checking that $\beta<\frac{4}{5}\omega$. But we can find all the ordering by defining, on $[0;\frac{15}{64}]$, the functions

$$B(x) = \frac{1}{2}(1-\sqrt{1-4x}), \quad \Omega(x) = \frac{5}{8}(1-\sqrt{1-64x/15}),$$
$$\Gamma(x) = \frac{1}{2}(1+\sqrt{1-4x}), \quad \Theta(x) = \frac{5}{8}(1+\sqrt{1-64x/15})$$

and verifying that $\Theta' < \Gamma' < 0 < B' < \Omega'$ on $(0;15/64)$, that $B(0)=\Omega(0)$ and that $\Theta(15/64)=\Gamma(15/64)=\Omega(15/64)$. □

Before proving the uniqueness and non-degeneracy, we give a result about the exponential decay of the solutions, which will be useful in the next Step.

LEMMA 2.65 (Exponential decrease). *Let G be a continuous function on $\mathbb{R}_+$ with $G(0)=0$, and $\mu>0$. If $u \geqslant 0$, such that $u\to 0$ as $r\to\infty$, is a solution to*

$$u'' + \frac{2}{r}u' = (\mu+G(u))u \quad \text{on } \mathbb{R}_+,$$

then for any $0 < \varepsilon < \mu$, *there exists a constant* C *such that*

$$0 \leqslant u, |u'| \leqslant \frac{C}{r} e^{-r\sqrt{\mu-\varepsilon}}.$$

PROOF OF LEMMA 2.65. Since $u \to 0$ at infinity, we rewrite the equation and for any $0 < \varepsilon < \mu$ we have for r large enough

$$(ru)'' = (\mu + G(u))ru \geqslant (\mu - \varepsilon)ru.$$

Then we define $\alpha = \mu - \varepsilon$ and $f(r) := -ru(r)e^{-\sqrt{\alpha}r}$, and obtain

$$f'' \leqslant -2\sqrt{\alpha} f'$$

for r large enough. Consequently, by Grönwall's lemma, there exists R such that for any $r \geqslant r_0 \geqslant R$, it holds that

$$f'(r) \leqslant f'(r_0) e^{2\sqrt{\alpha}r_0} e^{-2\sqrt{\alpha}r}. \tag{2.92}$$

Since $f \to 0$ as $r \to \infty$, integrating on $(r;\infty)$ the above inequality for $r \geqslant r_0 \geqslant R$, we obtain

$$-f(r) \leqslant \frac{f'(r_0)}{2\sqrt{\alpha}} e^{2\sqrt{\alpha}r_0} e^{-2\sqrt{\alpha}r}$$

thus $f'(r_0) \geqslant 0$ for any $r_0 \geqslant R$, since $u \geqslant 0$, and

$$0 \leqslant u(r) \leqslant \frac{f'(r_0)}{2\sqrt{\alpha}} e^{2\sqrt{\alpha}r_0} \frac{e^{-\sqrt{\alpha}r}}{r} := C \frac{e^{-\sqrt{\alpha}r}}{r}.$$

This concludes the proof for u. The fact that $f'(r) \geqslant 0$, combined with (2.92) and the definition of f, implies for $r \geqslant r_0$ that

$$\left(\sqrt{\alpha} - \frac{1}{r}\right) u \geqslant u'(r) \geqslant \left(\sqrt{\alpha} - \frac{1}{r}\right) u - 2\sqrt{\alpha} C \frac{e^{-\sqrt{\alpha}r}}{r}.$$

Thus, for $r \geqslant \max\{r_0; \alpha^{-1/2}\}$ that

$$\sqrt{\alpha} C \frac{e^{-\sqrt{\alpha}r}}{r} \geqslant u'(r) \geqslant -2\sqrt{\alpha} C \frac{e^{-\sqrt{\alpha}r}}{r}.$$

This concludes the proof of Lemma 2.65. $\square$

Step 4: Uniqueness and non-degeneracy.

PROPOSITION 2.66 (Uniqueness and non-degeneracy of radial solutions). *Let* $c_{TF} > 0$, *fix* $\mu \in \left(0; \frac{15}{64}\frac{1}{c_{TF}}\right)$ *and define* F_μ *by* (2.34). *Then the problem* (RPb-μ) *has a unique non-trivial radial solution* u. *Moreover, it verifies*

$$0 < \omega < \|u\|_{L^\infty(\mathbb{R}^3)} = u(0) < \gamma,$$

with ω and γ defined as in Lemma 2.64, and is non-degenerate: the unique solution v to

$$\begin{cases} L(v) = v'' + \dfrac{2}{r}v' + F'_\mu(u)v = 0 \\ v(0) = 1 \\ v'(0) = 0 \end{cases}$$

diverges exponentially fast when $r \to \infty$. More precisely, $v(r) \to -\infty$ and $v'(r) \to -\infty$ exponentially fast when $r \to \infty$.

The pioneering works on uniqueness of solutions to the NLS nonlinearity [**Cof72, Kwo89**] have been followed by many results introducing conditions on F ensuring uniqueness of radial solutions to semi-linear equations of the type $(\Delta + F(u))u = 0$, see e.g. [**PS83, MS87, KZ91, McL93, ST00, LRN15**]. For our particular function F as defined in (2.34), the uniqueness is given by [**ST00**, Theorem 1'], by means of Lemma 2.63. The non-degeneracy result is not always stated in those works although sometimes present in the middle of the proof. Therefore, for clarity, we will give the detail of the proof of our Theorem, following [**LRN15**] which is mainly based on the approach of McLeod in [**McL93**] and its summary in [**Tao06**, App. B] and [**Fra13**].

Proof of Proposition 2.66. We start by proving that the solutions u to (RPb-μ) verify

$$0 < \omega < \|u\|_\infty = u(0) < \gamma.$$

To do that, we state the following Lemma that we will need several times.

Lemma 2.67. *Let u be solution of* (RPb-μ). *If $r_0 \geqslant 0$ is such that $u'(r_0) = 0$ and $u(r_0) > 0$ then $u(r) \leqslant u(r_0)$ for all $r > r_0$. In particular, $\|u\|_\infty = u(0)$.*

Proof of Lemma 2.67. Let $r_0 \geqslant 0$ be such that $u'(r_0) = 0$ and $u(r_0) > 0$ and suppose that $u(r) \leqslant u(r_0)$ for all $r > r_0$ does not hold. The function u being continuous and vanishing at infinity, there would exist $r_* > r_0$ such that $u(r_*) = u(r_0)$ with u not constant over (r_*, r_0). Then, for H defined in (2.90), we have $H_{u(r_0)}(r_0) = 0$ and $H_{u(r_0)}(r_*) \geqslant 0$ but the computation of H' made in (2.91) and the fact that u' is not identical to zero on $[r_0, r_*]$ implies that $H_{u(r_0)}(r_*) < H_{u(r_0)}(r_0)$ giving a contradiction. $\square$

By Lemma 2.64, we have $u(0) > \omega$. We now prove that $u(0) \leqslant \gamma$. Indeed, suppose that $u(0) > \gamma$ then there exists $r_0 > 0$ such that $u > \gamma$ on $[0; r_0)$ and

$u(r_0) = \gamma$. Then, since H_γ is strictly decreasing, we have

$$0 > H_\gamma(r_0) - H_\gamma(0) = \frac{(u'(r_0))^2}{2} - \int_\gamma^{u(0)} F_\mu(x)\,\mathrm{d}x$$

which is impossible since $u(0) > \gamma$ and $F_\mu < 0$ on $(\gamma;\infty)$. Finally, $r \mapsto \gamma$ being a stationary solution of (2.87), we cannot have $u(0) = \gamma$ which concludes the proof of $\omega < u(0) < \gamma$.

We now look at the unique solutions to (2.87) with $u(0) = y$, that we denote by u_y and we let y vary in $(0,\gamma)$. As in **[McL93]**, we introduce the sets

$$\begin{aligned} S_+ &= \big\{y \in (0,\gamma) |\ \min_{\mathbb{R}_+} u_y > 0\big\}, \\ S_0 &= \big\{y \in (0,\gamma) | u_y > 0 \text{ and } \lim_{\infty} u_y = 0\big\}, \\ S_- &= \big\{y \in (0,\gamma) | u_y(r_y) = 0 \text{ for some (first) } r_y > 0\big\} \end{aligned}$$

which form a partition of $(0;\gamma)$. We first remark that $(r,y) \mapsto u_y(r)$ is smooth since real-analytic given that F_μ is analytic. Therefore, S_- is open. For convenience, for $y \in S_0$, we denote $r_y := +\infty$. Since H' decreases along a solution, as we proved earlier, Lemma 2.64 gives $(0;\omega] \subset S_+$ which implies that $S_0 \cup S_- \subset (\omega;\gamma)$. Moreover, the existence of positive radial minimizers proved in Theorem 2.3 implies that $S_0 \neq \varnothing$. We state first two lemmas giving properties of elements of S_-, S_0 and S_+.

Lemma 2.68. *Let $y \in S_0 \cup S_-$. Then $u_y' < 0$ on $(0, r_y)$, that is, u_y vanishes before u_y'. In particular, u_y is strictly decreasing on $(0, r_y)$.*

Proof of Lemma 2.68. By means of $S_0 \cup S_- \subset (\omega;\gamma) \subset (\beta;\gamma)$ and (2.87), it holds that $3u_y''(0) = -F_\mu(u_y(0)) < 0$, since $u''(r) \sim_{r\to 0} \frac{u'(r)}{r}$. Hence $u_y'(r) < 0$ for $r > 0$ small enough. Moreover, by definition of r_y together with the fact that u_y cannot have double zeroes since it is solution of (2.87), we know that $u_y'(r_y) < 0$.

Let us assume that u_y' changes sign before r_y. Then u_y has a local strict minimum at $r_* \in (0, r_y)$ with $u_y(r_*) > 0$. But since $\lim_{r\to r_y} = 0$, there must be $r_\star \in (r_*; r_y)$ such that $u_y(r_\star) = u_y(r_*)$. This leads to a contradiction since we then have

$$\frac{(u_y'(r_\star))^2}{2} = H_\beta(r_\star) - H_\beta(r_*) = \int_{r_*}^{r_\star} H_\beta'(s)\,\mathrm{d}s = -2\int_{r_*}^{r_\star} \frac{(u_u'(s))^2}{s}\,\mathrm{d}s < 0.$$

$\square$

Lemma 2.69. *Let $y \in S_+$. Then u_y' vanishes at least once and, for the first positive root r_* of u_y', we have $H_0(r_*) < 0$. The set S_+ is open.*

Proof of Lemma 2.69. If $y = \beta$ then $u_y \equiv \beta$ and $H_0(r) = \int_0^\beta F_\mu(x)\,\mathrm{d}x < 0$ for all $r \geqslant 0$. Let us now suppose $y \neq \beta$.

We claim that u_y' vanishes. Otherwise, since $3u_y''(0) = -F_\mu(u_y(0))$ by means of (2.87), either $y > \beta$ and u_y is decreasing or $y < \beta$ and u_y is increasing, and in both cases u_y has a limit at infinity $u_\infty \in (0, \gamma)$. Then the equation (2.87) leads to $F_\mu(u_\infty) = 0$ hence that $u_\infty = \beta$. Now, following [**BLP81, Fra13**], we introduce $V := r(u - \beta)$ which solves

$$V'' = -\frac{F(u)}{u-\beta}V. \tag{2.93}$$

Recording that $F_\mu(u) = -c_{TF}u(u^{\frac{2}{3}} - \beta^{\frac{2}{3}})(u^{\frac{2}{3}} - \gamma^{\frac{2}{3}})$, we obtain

$$\lim_{r\to\infty} \frac{F_\mu(u(r))}{u(r)-\beta} = c_{TF}\beta(\gamma^{\frac{2}{3}} - \beta^{\frac{2}{3}}) \lim_{u\to\beta} \frac{u^{\frac{2}{3}} - \beta^{\frac{2}{3}}}{u-\beta} = \frac{2}{3}c_{TF}\beta^{\frac{2}{3}}(\gamma^{\frac{2}{3}} - \beta^{\frac{2}{3}}) > 0.$$

Therefore $V''(r) \sim_{r\to\infty} -\frac{2}{3}c_{TF}\beta^{\frac{2}{3}}(\gamma^{\frac{2}{3}} - \beta^{\frac{2}{3}})V(r)$. On one hand, if $y > \beta$ then $V > 0$ on $(0;\infty)$ thus V' is strictly decreasing for r large enough. Let suppose that $0 > \lim_{r\to\infty} V'(r) \geqslant -\infty$, then $V(r) \to -\infty$ when $r \to \infty$ which is impossible since $V > 0$. If we now suppose that $\lim_{r\to\infty} V'(r) \geqslant 0$ then there exists $r_\star > 0$ such that $V'(r) > 0$ on $(r_\star;\infty)$ — since V' is strictly decreasing for r large enough — which implies that $V(r) \geqslant V(r_\star) > 0$ for $r \geqslant r_\star$. Consequently, $V'' < 0$ on $[r_\star;\infty)$ which contradicts our hypothesis $\lim_{r\to\infty} V'(r) \geqslant 0$. On the other hand, the case $y < \beta$ leads to a contradiction following the same arguments. We have proved that u_y' vanishes and we denote by r_* its first root.

We now prove that $H_0(r_*) < 0$. On one hand, if $y < \beta$ then

$$H_0(0) = \int_0^y F_\mu(x)\,\mathrm{d}x < 0$$

and H_0 being non-increasing, we conclude that $H_0(r_*) < 0$. On the other hand, if $y > \beta$ then $u_y' < 0$ for small $r > 0$ since $3u_y''(0) = -F_\mu(u_y(0))$ by means of (2.87). However $u_y''(r_*) \neq 0$, otherwise $F_\mu(u_y(r_*)) = 0$ and then u_y is constant, thus u_y attains a local minimum at r_* which implies by (2.87) that $F_\mu(u_y(r_*)) < 0$. Since we have also $u_y(r_*) \leqslant u_y(0) < \gamma$, we can conclude that $u_y(r_*) < \beta$ and finally that $H_0(r_*) < 0$.

We conclude by the proof that S_+ is open. We know that $(0;\omega] \subset S_+$ and we recall that $0 < \beta < \omega < \gamma$. Let $y \in S_+ \cap (\beta;\gamma)$. For z in a neighborhood of y, by the smoothness of $(r,y) \mapsto u_y(r)$ and since u_y has a local minimum at $r_* > 0$, u_z has a local minimum at a point r_z close to r_*. Moreover, the local energy $H_0^{u_z}$

associated to u_z verifies

$$H_0^{u_z}(r_z) = H_0^{u_y}(r_*) + \int_{u_y(r_*)}^{u_z(r_z)} F_\mu(x)\,\mathrm{d}x$$

which is strictly negative for z close enough to y, since $H_0^{u_y}(r_*) < 0$ and by the smoothness of $(r, y) \mapsto u_y(r)$. Since u_z is solution to (2.87), $H_0^{u_z}$ is strictly decreasing on $[0; \infty)$ hence, for any $r > r_z$, we have

$$\frac{3}{10} c_{TF} (u_z(r))^2 \left((u_z(r))^{\frac{2}{3}} - \omega^{\frac{2}{3}} \right) \left(\theta^{\frac{2}{3}} - (u_z(r))^{\frac{2}{3}} \right) \leqslant H_0^{u_z}(r) < H_0^{u_z}(r_z) < 0.$$

Thus there exists $\varepsilon > 0$ such that for any $r > r_z$, we have $0 < \varepsilon < u_z(r) < \omega - \varepsilon$. In particular u_z does not vanish hence $z \in S_+$. We proved that S_+ is open. $\square$

Those two lemmas stated, we consider v_y, the unique solution to the ODE

$$\begin{cases} L(v) := v'' + \dfrac{2}{r} v' + F_\mu'(u_y) v = 0 \\ v(0) = 1 \\ v'(0) = 0. \end{cases}$$

This function is simply $v_y = \partial_y u_y$, the variation of u_y with respect to the initial condition $u_y(0) = y$. This implies the following Lemma.

Lemma 2.70. *If $y \in S_0$ and $v_y(r), v_y'(r) \to -\infty$ when $r \to \infty$, then there exists $\varepsilon > 0$ such that $(y - \varepsilon, y) \subset S_+$ and $(y, y + \varepsilon) \subset S_-$.*

Proof of Lemma 2.70. This lemma is [**McL93**, Lemma 3(b)] and we follow its proof. Let $\alpha > 0$ be such that $F_\mu' \leqslant -\frac{\mu}{2}$ on $[0; \alpha)$. Then choose R such that $u_y \leqslant \alpha$ on $[R; +\infty)$. Finally, choose $R_1 \geqslant R$ such that $v_y(R_1) < 0$ and $v_y'(R_1) < 0$. Since $v_y = \partial_y u_y$ and $u_y(R_1) > 0$ (because $y \in S_0$), then there exists $\varepsilon > 0$ such that for $z \in (y; y+\varepsilon)$ it holds that $0 < u_z(R_1) < u_y(R_1)$ and $u_z'(R_1) < u_y'(R_1) < 0$. The function $w := u_z - u_y$ is negative at R_1 with $w'(R_1) < 0$. Let suppose that $z \in S_0 \cup S_+$ then either w tend to 0 or becomes positive at some point, since $y \in S_0$. Consequently, w must have a local minimum at some point $R_2 > R_1$, and with $w(R_2) \leqslant w(r) \leqslant w(R_1) < 0$ for all $R_1 \leqslant r \leqslant R_2$. Hence, (2.87) implies that

$$0 \leqslant w''(R_2) = F_\mu(u_y(R_2)) - F_\mu(u_z(R_2)) = -F_\mu'(\eta) w(R_2)$$

for some $0 < u_z(R_2) < \eta < u_y(R_2) \leqslant \alpha$ where the strict positivity comes from the fact that $z \in S_0 \cup S_+$. But $F_\mu'(\eta) \leqslant -\frac{\mu}{2} < 0$ and $w(R_2) < 0$, leading to a contradiction. The proof is the same for $z < y$. $\square$

We now prove that for all $y \in S_0$, we have $v_y, v_y' \to -\infty$. The argument will be based on the Wronskian identity

$$(r^2(f'v_y - fv_y'))' = r^2 v_y L(f), \tag{2.94}$$

that holds for any f twice differentiable. We first compute the three functions $L(u_y)$, $L(u_y')$ and $L(ru_y')$. First, we have

$$L(u_y) = u_y'' + \frac{2}{r}u_y' + F_\mu'(u_y)u_y = F_\mu'(u_y)u_y - F_\mu(u_y). \tag{2.95}$$

Moreover, $F_\mu'(u_y)u_y' = (F_\mu(u_y))' = -u_y''' + \frac{2}{r^2}u_y' - \frac{2}{r}u_y''$, thus

$$L(u_y') = u_y''' + \frac{2}{r}u_y'' + u_y'F_\mu'(u_y) = \frac{2}{r^2}u_y'$$

and

$$\begin{aligned} L(ru_y') &= 4u_y'' + ru_y''' + \frac{2}{r}u_y' + rF_\mu'(u_y)u_y', \\ &= -F_\mu(u_y) + u_y'' + r\left(\frac{2}{r}u_y'' + u_y''' + (F_\mu(u_y))'\right) = -2F_\mu(u_y). \end{aligned}$$

Lemma 2.71. *For every $y \in S_0$, the function v_y vanishes exactly once.*

Proof of Lemma 2.71. We first prove that v_y vanishes at least once. Suppose on the contrary that v_y does not vanishes, then $v_y > 0$ on $\mathbb{R}_+$ since $v_y(0) = 1 > 0$. From (2.94), for $f = u_y'$, we deduce that

$$(r^2(u_y''v_y - u_y'v_y'))' = 2v_y u_y' < 0$$

and, consequently, $r^2(u_y''v_y - u_y'v_y') = r^2{v_y}^2(u_y'/v_y)'$ is decreasing and vanishes at $r = 0$, thus there exists ε such that $r^2(u_y''v_y - u_y'v_y') \leqslant -\varepsilon < 0$ for $r \geqslant 1$ and $(u_y'/v_y)' < 0$. The latter leads (up to taking an even smaller ε) to $u_y'/v_y \leqslant -\varepsilon < 0$ for $r \geqslant 1$, since $u_y'(0)/v_y(0) = 0$, and finally that $0 < v_y \leqslant -u_y'/\varepsilon$. However, for r large enough, $r^2|v_y(r)u_y''(r)| \leqslant \frac{r^2}{\varepsilon}|u_y'(r)||u_y''(r)|$ decays exponentially fast. Indeed, $|u_y'|$ decays exponentially fast by Lemma 2.65 and u_y'' too by (2.87) and the exponential decay of all the other terms in said equation. Hence $r^2u_y'v_y' \geqslant \varepsilon/2$ for r large enough. Using again that u_y' decays exponentially fast together with $u_y' < 0$, we obtain that v_y' diverges exponentially fast to $-\infty$, which contradicts $v_y > 0$.

We now prove that v_y can only vanish once and our proof follows [**Tao06**, pp. 357–358]. First we note that for $z = \beta$, at which the solution is stationary, the function $u_y - u_z = u_y - \beta$ vanishes exactly once since, by Lemma 2.68, u_y strictly decreases from $y > z = \beta$ to 0. Using on one hand that, for any z, $u_y - u_z$ cannot have double zeroes (because u_y and u_z solve the same second order ODE) and, on another hand, that $v_y = \partial_y u_y$, we obtain by taking $z \to y$ that v_y vanishes at most once. $\square$

This Lemma 2.71 allows us to now prove that v_y and v_y' diverges to $-\infty$.

LEMMA 2.72. *For $y \in S_0$, we have $v_y(r), v_y'(r) \to -\infty$ as $r \to \infty$.*

PROOF OF LEMMA 2.72. By Lemma 2.71, let r_* be the unique root of v_y, which verifies $v_y'(r_*) < 0$. We define

$$f(r) := u_y(r) - \frac{r u_y'(r)}{r_* u_y'(r_*)} u_y(r_*)$$

which vanishes at r_*. We first note that $c := -u_y(r_*)/(r_* u_y'(r_*)) > 0$, by means of Lemma 2.68. Then, by (2.94), we have

$$(r^2(f'v_y - fv_y'))' = r^2 v_y L(u_y + cru_y') = r^2 v_y \left(F_\mu'(u_y)u_y - (1+2c)F_\mu(u_y)\right).$$

Moreover, $r^2(f'v_y - fv_y')$ vanishes at $r = 0$ and $r = r_*$ hence $F_\mu'(u_y)u_y - (1 + 2c)F_\mu(u_y)$ vanishes at least once in $(0; r_*)$. However, by means of Lemma 2.63, $x \mapsto F_\mu'(x)x - (1+2c)F_\mu(x)$ vanishes exactly once on $(0, \gamma)$ with strictly negative derivative at the vanishing point which, together with the fact that u_y is strictly decreasing from y to 0, gives that $F_\mu'(u_y)u_y - (1 + 2c)F_\mu(u_y) > 0$ for any r strictly larger than its vanishing point, in particular for any $r \geqslant r_*$. Hence $(r^2(f'v_y - fv_y'))'$ is negative for $r > r_*$ since $r^2 v_y(r) < 0$ for $r > r_*$. Thus $r^2(f'v_y - fv_y')$ is strictly decreasing after r_* (where it vanishes) and, in particular, there exists $\varepsilon > 0$ such that $r^2(fv_y' - f'v_y) \geqslant \varepsilon > 0$ for r large enough. However, by Lemma 2.65, f and f' decay exponentially fast to 0 at infinity. Assume v_y does not diverge exponentially fast (thus it either diverges at a slower rate or is bounded), then $-r^2 f' v_y$ tends to 0 and $r^2 f v_y' \geqslant \varepsilon/2 > 0$ for r large enough. Hence v_y' diverges exponentially fast which contradicts the fact that v_y does not diverge exponentially fast. So we proved that $v_y \to -\infty$ exponentially fast as $r \to \infty$.

We now use $(r^2 v_y')' = -r^2 F_\mu'(u_y)v_y \to -\infty$ exponentially fast since $F_\mu'(u) \to -\mu < 0$ at infinity and v_y diverges to $-\infty$ exponentially fast. Consequently, $r^2 v_y'$ diverges exponentially fast to $-\infty$ which implies the same for v_y'. $\square$

This proves that u_y is non-degenerate for any $y \in S_0$.

We can now conclude the proof of Proposition 2.66. Indeed, S_- and S_+ are open therefore they are separated by points in S_0. However, by Lemma 2.72 together with Lemma 2.70, such points in S_0 are isolated points that makes transition between (part of) S_+ below and (part of) S_- above. This implies that there can be only one element in S_0 and finally the uniqueness of the solution to our problem. $\square$

This concludes the proof of Theorem 2.4. □

6.3. Proofs of Remarks 2.11 and 2.35: a priori bounds on $J_{\mathbb{R}^3,c}(\lambda)$ and $J_{\mathbb{K},c}(\lambda)$, independent of c_{TF}.

LEMMA 2.73. *For any $a < 1$, any $u \in H^1(\mathbb{R}^3)$ and $v \in H^1(\mathbb{K})$, we have*

$$\mathscr{J}_{\mathbb{R}^3,c}(u) \geqslant a \|\nabla u\|^2_{L^2(\mathbb{R}^3)} - \frac{9\lambda^{\frac{5}{3}} {S_3}^2}{64(1-a)} c^2,$$

and

$$\mathscr{J}_{\mathbb{K},c}(v) \geqslant a \|\nabla v\|^2_{L^2(\mathbb{K})} - \frac{9\lambda^{\frac{5}{3}} {S_{\mathbb{K}}}^2}{64(1-a)} c^2 - \frac{3}{4} S_{\mathbb{K}} \lambda^{\frac{4}{3}} c,$$

where $S_{\mathbb{K}}$ is the Sobolev constant $\|v\|_{L^6(\mathbb{K})} \leqslant S_{\mathbb{K}} \|v\|_{H^1(\mathbb{K})}$ and S_3 the Sobolev constant $\|u\|_{L^6(\mathbb{R}^3)} \leqslant S_3 \|\nabla u\|_{L^2(\mathbb{R}^3)}$. In particular, together with (2.23) and (2.48), this gives for any $\lambda > 0$ and $c > 0$ that

$$J_{\mathbb{R}^3,c}(\lambda) > -\frac{15}{64} \lambda c^2 \min\left\{ \frac{1}{c_{TF}}; \frac{3}{5}\left(S_3 \lambda^{\frac{1}{3}}\right)^2 \right\},$$

and

$$J_{\mathbb{K},c}(\lambda) > -\frac{15}{64} \lambda c^2 \min\left\{ \frac{1}{c_{TF}}; \frac{3}{5}\left(S_{\mathbb{K}} \lambda^{\frac{1}{3}}\right)^2 + \frac{16}{5} S_{\mathbb{K}} \lambda^{\frac{1}{3}} c^{-1} \right\}.$$

PROOF OF LEMMA 2.73. For $\Omega = \mathbb{K}$ ou $\mathbb{R}^3$, using the non-negativity of $\|u\|_{L^{\frac{10}{3}}(\Omega)}$, Hölder's inequality and Sobolev embeddings, we obtain

$$\mathscr{J}_{\Omega,c}(u) \geqslant \|\nabla u\|^2_{L^2(\Omega)} - \frac{3}{4} \|\nabla u\|_{L^2(\Omega)} K_1(\Omega) \lambda^{\frac{5}{6}} c - \frac{3}{4} K_2(\Omega) \lambda^{\frac{4}{3}} c,$$

where $K_1(\mathbb{K}) = K_2(\mathbb{K}) = S_{\mathbb{K}}$, $K_1(\mathbb{R}^3) = S_3$ and $K_2(\mathbb{R}^3) = 0$. But, for any $\nu > 0$ and $(X, \alpha) \in \mathbb{R}^2$, $-\alpha X \geqslant -\nu X^2 - \frac{\alpha^2}{4\nu}$ hence defining $a := 1 - \nu < 1$, we obtain the announced inequalities. Finally, taking $a = 0$, we obtain the two final inequality but with large inequalities while the strict inequalities are obtained from the existence of minimizer and since $\int u^{\frac{10}{3}} > 0$ for a minimizer. □

6.4. Independency from c_{TF} of the upper bound on $\|\nabla \breve{v}_c\|^2_{L^2(\mathbb{K}_c)}$ in Corollary 2.36. Using the lower bound independent of c_{TF} in Lemma 2.73 and the upper bound in (2.48), we obtain that there exists $0 < c_* \leqslant \frac{4}{5} c_{TF} \sqrt[3]{\lambda |\mathbb{K}|^{-1}}$ such that, for all $c \geqslant c_*$ and any $0 < a < 1$, we have

$$0 \geqslant J_{\mathbb{K},\lambda}(c) \geqslant a \|\nabla v_c\|^2_{L^2(\mathbb{K})} - \frac{9}{64} \frac{{S_{\mathbb{K}}}^2 \lambda^{\frac{5}{3}}}{1-a} c^2 - \frac{3}{4} S_{\mathbb{K}} \lambda^{\frac{4}{3}} c,$$

thus

$$\|\nabla\breve{v}_c\|^2_{L^2(\mathbb{K}_c)} \leqslant \frac{9}{64}\frac{{S_{\mathbb{K}}}^2\lambda^{\frac{5}{3}}}{a(1-a)} + \frac{3}{4}\frac{S_{\mathbb{K}}\lambda^{\frac{4}{3}}}{a}c^{-1} =: \frac{x}{a(1-a)} + \frac{y}{a}$$

and one can check, for x, y positive, that the right hand side attains its minimum (with respect to $a \in (0;1)$) at

$$a_0 := \frac{x+y-\sqrt{x(x+y)}}{y} \in (1/2;1)$$

and this minimum is $2x+y+2\sqrt{x(x+y)}$. This gives

$$0 \leqslant \|\nabla\breve{v}_c\|^2_{L^2(\mathbb{K}_c)} \leqslant \frac{C^2\lambda}{32}\left(1+\frac{8}{Cc}+\sqrt{1+\frac{16}{Cc}}\right),$$

for all $c \geqslant c_*$ and where $C = C(\mathbb{K},\lambda) = 3S_{\mathbb{K}}\lambda^{\frac{1}{3}}$. The right hand side is a decreasing function of c that tends to $\frac{C^2}{16}\lambda$ as c goes to $+\infty$ hence, for c large enough, we have

$$0 \leqslant \|\nabla\breve{v}_c\|^2_{L^2(\mathbb{K}_c)} \leqslant \frac{9}{8}{S_{\mathbb{K}}}^2\lambda^{\frac{5}{3}},$$

a bound independent of c_{TF} (and c).

6.5. Proof of the Hardy inequality on $\mathbb{K}$.

Lemma 2.74. *For any $c_* > 0$, there exists C such that for any $c \geqslant c_*$ we have*

$$\left\|\frac{f}{|\cdot - c\tau|}\right\|_{L^2(\mathbb{K}_c)} \leqslant C\,\|f\|_{H^1_{per}(\mathbb{K}_c)},$$

for any $f \in H^1_{per}(\mathbb{K}_c)$ and any $\tau \in \mathbb{R}^3$.

Proof of Lemma 2.74. First we can suppose that τ is in the closure of $\mathbb{K}$ otherwise, if $m := d(\tau,\mathbb{K}) > 0$, we have

$$\left\|\frac{f}{|\cdot - c\tau|}\right\|_{L^2(\mathbb{K}_c)} \leqslant (cm)^{-1}\,\|f\|_{L^2(\mathbb{K}_c)}.$$

Let χ and η be such that $\chi^2+\eta^2$ is a smooth partition of the unity with $\mathrm{supp}(\chi) \subset B(0,R')$ and $\mathrm{supp}(\eta) \subset {}^{\complement}B(0,R)$ where $R' > R > 0$ is such that $B(0,2R') \subset$

$\mathbb{K}_{c_*} \subset \mathbb{K}_c$. Thus, by the Hardy inequality on $\mathbb{R}^3$, we have

$$\begin{aligned}
\int_{\mathbb{K}_c} \frac{f^2}{|\cdot - c\tau|^2} &= \int_{-c\tau+\mathbb{K}_c} \frac{f^2(\cdot + c\tau)}{|\cdot|^2} \\
&= \int_{\mathbb{R}^3} \frac{(f(\cdot + c\tau)\chi)^2}{|\cdot|^2} + \int_{(-c\tau+\mathbb{K}_c)\cap^{\complement}B(0,R)} \frac{(f(\cdot + c\tau)\eta)^2}{|\cdot|^2} \\
&\leqslant 4\left\|\nabla(f(\cdot + c\tau)\chi)\right\|^2_{L^2_{\mathrm{per}}(\mathbb{R}^3)} + R^{-2}\left\|f\right\|^2_{L^2(\mathbb{K}_c)} \\
&\leqslant 8\left(\left\|\nabla f(\cdot + c\tau)\chi\right\|^2_{L^2_{\mathrm{per}}(\mathbb{K}_{c_*})} + \left\|f(\cdot + c\tau)\nabla\chi\right\|^2_{L^2(\mathbb{K}_{c_*})}\right) + \frac{\left\|f\right\|^2_{L^2(\mathbb{K}_c)}}{R^2} \\
&\leqslant 8\left(\left\|\nabla f(\cdot + c\tau)\right\|^2_{L^2_{\mathrm{per}}(\mathbb{K}_c)} + \left\|\nabla\chi\right\|^2_\infty \left\|f(\cdot + c\tau)\right\|^2_{L^2(\mathbb{K}_c)}\right) + \frac{\left\|f\right\|^2_{L^2(\mathbb{K}_c)}}{R^2} \\
&\leqslant C^2\left\|\nabla f\right\|^2_{H^1_{\mathrm{per}}(\mathbb{K}_c)},
\end{aligned}$$

where

$$C = 2\sqrt{2}\sqrt{\max\{1, \left\|\nabla\chi\right\|^2_\infty + R^{-2}\}}.$$

This concludes the proof of Lemma 2.74. □

6.6. Direct proof of symmetry breaking. As stated in Remark 2.39, we can deduce directly from Lemma 2.38 the symmetry breaking $E_{N\cdot\mathbb{K},N^3\lambda}(c) < N^3E_{\mathbb{K},\lambda}(c)$. Indeed, if there exists $\varepsilon > 0$ and $c_J > 0$ such that for all $c > c_J$ we have

$$\frac{J_{N\cdot\mathbb{K},N^3\lambda}(c)}{N^3J_{\mathbb{K},\lambda}(c)} > 1 + \varepsilon, \tag{2.96}$$

then, by Lemma 2.38, there exists $c_* \geqslant c_J$ such that for all $c \geqslant c_*$, we have

$$\frac{E_{N\cdot\mathbb{K},N^3\lambda}(c)}{N^3E_{\mathbb{K},\lambda}(c)} > 1 + \frac{\varepsilon}{2}.$$

We thus have to prove (2.96). For any $u \in H^1_{\mathrm{per}}(\mathbb{K})$ and $\eta > 0$, we have

$$\begin{cases}
u\left(\eta^{-1}\cdot\right) \in H^1_{\mathrm{per}}(\eta\mathbb{K}), \\
\left\|u(\eta^{-1}\cdot)\right\|^p_{L^p(\eta\mathbb{K})} = \eta^3\left\|u\right\|^p_{L^p(\mathbb{K})}, \quad \forall p \in [2;\infty) \\
\left\|\nabla u(\eta^{-1}\cdot)\right\|^2_{L^2(\eta\mathbb{K})} = \eta\left\|\nabla u\right\|^2_{L^2(\mathbb{K})}.
\end{cases}$$

Thus $\eta^3\mathscr{J}_{\mathbb{K},c}(u) = (\eta^3 - \eta)\left\|\nabla u\right\|^2_{L^2(\mathbb{K})} + \mathscr{J}_{\eta\mathbb{K},c}\left(u(\eta^{-1}\cdot)\right)$. Let v be a minimizer of $J_{\mathbb{K},\lambda}(c)$ which exists by Proposition 2.30 and $\eta > 1$, then

$$\begin{aligned}
\eta^3J_{\mathbb{K},\lambda}(c) &= (\eta^3 - \eta)\left\|\nabla v\right\|^2_{L^2(\mathbb{K})} + \mathscr{J}_{\eta\mathbb{K},c}\left(v(\eta^{-1}\cdot)\right) \\
&\geqslant (\eta^3 - \eta)\left\|\nabla v\right\|^2_{L^2(\mathbb{K})} + J_{\eta\mathbb{K},\eta^3\lambda}(c).
\end{aligned}$$

By Corollary 2.36, we know that there exists $C > 0$ such that for any c large enough, we have $\|\nabla v\|^2_{L^2(\mathbb{K})} \geqslant Cc^2$. Thus, for any $0 < \varepsilon < C\left(1-\eta^{-2}\right)\frac{64}{15}\frac{c_{TF}}{\lambda}$, we have by Lemma 2.33 that

$$\begin{aligned}\eta^3 J_{\mathbb{K},\lambda}(c) &\geqslant (\eta^3-\eta)Cc^2 + J_{\eta\mathbb{K},\eta^3\lambda}(c).\\ &> \varepsilon\frac{\eta^3-\eta}{1-\eta^{-2}}\frac{15}{64}\frac{\lambda}{c_{TF}}c^2 + J_{\eta\mathbb{K},\eta^3\lambda}(c).\\ &\geqslant \varepsilon\eta^3(-J_{\mathbb{K},\lambda}(c)) + J_{\eta\mathbb{K},\eta^3\lambda}(c).\end{aligned}$$

Consequently, for c large enough, we have

$$0 > \eta^3 J_{\mathbb{K},\lambda}(c) > \eta^3(1+\varepsilon)J_{\mathbb{K},\lambda}(c) > J_{\eta\mathbb{K},\eta^3\lambda}(c)$$

and finally, for $\eta = N$, that

$$1+\varepsilon < \frac{J_{N\cdot\mathbb{K},N^3\lambda}(c)}{N^3 J_{\mathbb{K},\lambda}(c)}.$$

The proof of the symmetry breaking is thus complete.

6.7. Details of the proof of Lemma 2.41. We start by proving the following lemma which allows us to obtain (2.59).

Lemma 2.75. *For any $(x,y,p) \in \mathbb{R}\backslash\{0\} \times (0;+\infty) \times [0;+\infty)$, we have*

$$\left||y+x|^p - \sum_{k=0}^{\lfloor p\rfloor}\binom{p}{k}y^{p-k}x^k\right| < |x|^p \qquad \textit{if } \lfloor p\rfloor \textit{ is even,}$$

$$\left||y+x|^p - \sum_{k=0}^{\lfloor p\rfloor-1}\binom{p}{k}y^{p-k}x^k\right| < |x|^p + \binom{p}{\lfloor p\rfloor}y^{p-\lfloor p\rfloor}|x|^{\lfloor p\rfloor} \qquad \textit{if } \lfloor p\rfloor \textit{ is odd.}$$

Moreover, for any $(x,y,p) \in (0;+\infty)^2 \times [0;+\infty)$, we have

$$\left||y+x|^p - \sum_{k=0}^{\lfloor p\rfloor}\binom{p}{k}y^{p-k}x^k\right| < |x|^p$$

and, consequently, for any $(z,p) \in \mathbb{C}\backslash\left\{\mathbb{R}\times\{0\}\cup\{0\}\times\mathbb{R}\right\} \times [0;+\infty)$, we have

$$\left||z|^p - \sum_{k=0}^{\lfloor \frac{p}{2}\rfloor}\binom{\frac{p}{2}}{k}|\Re(z)|^{p-2k}|\Im(z)|^{2k}\right| < |\Im(z)|^p$$

and identiquely exchanging $\Re$ — the real part — and $\Im$ — the imaginary part.

Proof of Lemma 2.75. If $p \in \mathbb{N}$ and p is even then

$$|y+x|^p - \sum_{k=0}^{\lfloor p\rfloor}\binom{p}{k}y^{p-k}x^k = 0$$

hence the first strict inequality holds for $x \neq 0$. If $p \in \mathbb{N}$ and p is odd then, on one hand we have

$$|y+x|^p - \sum_{k=0}^{\lfloor p \rfloor - 1} \binom{p}{k} y^{p-k} x^k = x^p$$

for $x \geqslant -y$, hence the second strict inequality holds for $x \neq 0$. On the other hand, for $x < -y$, we have

$$|y+x|^p - \sum_{k=0}^{\lfloor p \rfloor - 1} \binom{p}{k} y^{p-k} x^k = 2(y+x)^p - x^p$$

and one can check that $|2(y+x)^p - x^p| < |x|^p$ since $y > 0$ and p is odd. Hence the second strict inequality holds for $x < -y$ too.

We now suppose that $p \notin \mathbb{N}$, thus $0 < p - \lfloor p \rfloor < 1$, and $\lfloor p \rfloor$ is even. We define on $\mathbb{R}$ the functions

$$f_y^{\pm}(x) = |x|^p \mp |y+x|^p \pm \sum_{k=0}^{\lfloor p \rfloor} \binom{p}{k} y^{p-k} x^k,$$

which is indefinitely differentiable on $\mathbb{R}\backslash\{0, -y\}$ with its j-th derivative being

$$f_y^{\pm(j)}(x) = \frac{p!}{(p-j)!} \Bigg((\mathrm{sgn}(x))^j |x|^{p-j} \mp (\mathrm{sgn}(y+x))^j |y+x|^{p-j} \\ \pm \sum_{k=j}^{\lfloor p \rfloor} \binom{p-j}{k-j} y^{p-k} x^{k-j} \Bigg),$$

for any integer $j \in [0; \lfloor p \rfloor]$. Those derivatives can be continuously extended at 0 and at $-y$ therefore, from now on, we will call $f_y^{\pm(j)}$ the continuous extensions too. For any integer $j \in [0; \lfloor p \rfloor]$, we have $f_y^{\pm(j)}(0) = 0$. Moreover,

$$f_y^{\pm(\lfloor p \rfloor+1)}(x) = p! \frac{(p - \lfloor p \rfloor)}{(p - \lfloor p \rfloor)!} \left(\frac{\mathrm{sgn}(x)}{|x|^{\lfloor p \rfloor + 1 - p}} \mp \frac{\mathrm{sgn}(y+x)}{|y+x|^{\lfloor p \rfloor + 1 - p}} \right)$$

on $\mathbb{R}\backslash\{-y, 0\}$. Thus $f_y^{+(\lfloor p \rfloor+1)}$ is positive on $\mathbb{R}\backslash[-y; 0]$ and negative on $(-y; 0)$ while $f_y^{-(\lfloor p \rfloor+1)}$ is positive on $(-y; -y/2) \cup (0; +\infty)$ and negative on $(-\infty; -y) \cup (-y/2; 0)$. Therefore the monotonicity properties on intervals combined with the fact that $f_y^{\pm(\lfloor p \rfloor)}(0) = f_y^{-(\lfloor p \rfloor)}(-y) = 0$ and

$$\lim_{-\infty} f_y^{+(\lfloor p \rfloor)} = \frac{p!}{(p - \lfloor p \rfloor)!} y^{p - \lfloor p \rfloor} > 0$$

imply that $f_y^{\pm(\lfloor p \rfloor)} > 0$ on $\mathbb{R}\backslash\{-y, 0\}$. Finally, since $f_y^{\pm(j)}(0) = 0$ for any integer $j \in [0; \lfloor p \rfloor]$, we conclude that $f_y^{\pm(j)} < 0$ on $\mathbb{R}_-\backslash\{0\}$ for j odd, $f_y^{\pm(j)} > 0$ on $\mathbb{R}_+\backslash\{0\}$

for j odd and $f_y^{\pm(j)} > 0$ on $\mathbb{R}\backslash\{0\}$ for j even. In particular, $f_y^{\pm} > 0$ on $\mathbb{R}\backslash\{0\}$. This concludes the proof of the first inequality.

We now suppose that $p \notin \mathbb{N}$ with $\lfloor p \rfloor$ odd and define on $\mathbb{R}$ the functions

$$g_y^{\pm}(x) = |x|^p + \binom{p}{\lfloor p \rfloor} y^{p-\lfloor p \rfloor}|x|^{\lfloor p \rfloor} \mp |y+x|^p \pm \sum_{k=0}^{\lfloor p \rfloor -1} \binom{p}{k} y^{p-k} x^k,$$

which is indefinitely differentiable on $\mathbb{R}\backslash\{0,-y\}$ with its j-th derivative being

$$\begin{aligned} g_y^{\pm(j)}(x) = & \frac{p!}{(p-j)!}(\operatorname{sgn}(x))^j \left(|x|^{p-j} + \binom{p-j}{k-j} y^{p-\lfloor p \rfloor}|x|^{\lfloor p \rfloor -j} \right) \\ & \mp \frac{p!}{(p-j)!}\left((\operatorname{sgn}(y+x))^j |y+x|^{p-j} - \sum_{k=j}^{\lfloor p \rfloor -1} \binom{p-j}{k-j} y^{p-k} x^{k-j} \right), \end{aligned}$$

for any integer $j \in [0; \lfloor p \rfloor - 1]$. Those derivatives can be continuously extended at 0 and at $-y$ therefore, from now on, we will call $g_y^{\pm(j)}$ the continuous extensions too. For any integer $j \in [0; \lfloor p \rfloor - 1]$, we have $g_y^{\pm(j)}(0) = 0$. Moreover,

$$g_y^{\pm(\lfloor p \rfloor)}(x) = \frac{p!}{(p-\lfloor p \rfloor)!}\left((\operatorname{sgn}(x))^{\lfloor p \rfloor}(|x|^{p-\lfloor p \rfloor} + y^{p-\lfloor p \rfloor}) \mp (\operatorname{sgn}(y+x))^{\lfloor p \rfloor}|y+x|^{p-\lfloor p \rfloor} \right)$$

on $\mathbb{R}\backslash\{0\}$, by continuous extension at $-y$. One can check that both $g_y^{-(\lfloor p \rfloor)}$ and $g_y^{+(\lfloor p \rfloor)}$ are positive on $(0;\infty)$ and negative on $(-\infty;0)$. Finally, since $g_y^{\pm(j)}(0) = 0$ for any integer $j \in [0; \lfloor p \rfloor - 1]$ and $\lfloor p \rfloor$ is odd, we conclude that $g_y^{\pm(j)} < 0$ on $(-\infty;0)$ and $g_y^{\pm(j)} > 0$ on $(0;\infty)$ for j odd and $g_y^{\pm(j)} > 0$ on $\mathbb{R}\backslash\{0\}$ for j even. In particular, $g_y^{\pm} > 0$ on $\mathbb{R}\backslash\{0\}$. This concludes the proof of the first two inequalities.

If we now restrict the study to $x \in \mathbb{R}_+$ the study of $f_y^{\pm}$ for any p gives that

$$\left| |y+x|^p - \sum_{k=0}^{\lfloor p \rfloor} \binom{p}{k} y^{p-k} x^k \right| < |x|^p, \qquad \forall (x,y,p) \in (0;+\infty)^2 \times [0;+\infty).$$

Thus, for $(t,z) \in (\mathbb{R}\backslash\{0\})^2$, applying the above to $x = z^2 > 0$, $y = t^2 > 0$ and $p = \frac{q}{2}$ leads to

$$\left| |t + \mathrm{i}z|^q - \sum_{k=0}^{\lfloor \frac{q}{2} \rfloor} \binom{\frac{q}{2}}{k} |t|^{q-2k}|z|^{2k} \right| < |z|^q.$$

This concludes the proof of Lemma 2.75. □

We can now turn to the details of the proof of Lemma 2.41. Let $(\breve{v}_c)_{c \geqslant 1}$ be a sequence of $J_{\mathbb{K}_c,\lambda}(1)$'s minimizers thus, in particular, $\breve{v}_c \in H^1_{\mathrm{per}}(\mathbb{K}_c)$ for each c. We split the proof in several step for clarity. Note that our proof uses the number

m (defined just below) but that it could be also proved without introducing it, similarly to Lemma 2.42.

Step 1: non vanishing. We prove here that there exits a sequence of translations $\mathbf{y} := \{y_c\} \subset \mathbb{R}^3$ such that $\breve{v}_c^{\mathbf{y}} \mathbb{1}_{\mathbb{K}_c} \rightharpoonup u_y \not\equiv 0$ weakly in $L^2(\mathbb{R}^3)$, up to the extraction of a subsequence, where $\breve{v}_c^{\mathbf{y}} := \breve{v}_c(\cdot - y_c)$. First, by $\mathbb{K}_c$-periodicity, we have that $\|\breve{v}_c^{\mathbf{y}} \mathbb{1}_{\mathbb{K}_c}\|_{L^2(\mathbb{R}^3)}$ does not depend on $\mathbf{y}$ and is equal to $\sqrt{\lambda}$. Thus such $L^2(\mathbb{R}^3)$-weak limits $u_y \geqslant 0$ exist. This step consists therefore in proving that there exists $u_y \not\equiv 0$.

Similarly to the proof of Theorem 2.3, we introduce, for any sequence $\{\varphi_n\}$ bounded in $L^2_{\text{loc}}(\mathbb{R}^3)$, the number

$$\mathbf{m}(\{\varphi_n\}) = \sup\left\{ \int_{\mathbb{R}^3} |\varphi|^2 \ \middle|\ \exists \{x_n\} \subset \mathbb{R}^3, \varphi_{n_k}(\cdot - x_k) \rightharpoonup \varphi \text{ weakly in } L^2(\mathbb{R}^3) \right\}.$$

We thus have to prove that $\mathbf{m}(\{\breve{v}_c\}) > 0$.

REMARK. $\forall \mathbf{y} := \{y_n\} \subset \mathbb{R}^3, \mathbf{m}(\{\varphi_n^{\mathbf{y}}\}) = \mathbf{m}(\{\varphi_n\})$ and $\mathbf{m}(\{\varphi_{n_k}\}) \leqslant \mathbf{m}(\{\varphi_n\})$.

For any $z \in \mathbb{R}^3$, $\mathbb{K} + z$ will denote the z-translation of $\mathbb{K}$. Then, for any $c > 1$, we take a finite family $\{z_i\}_{i \in \mathbb{N}} \subset \mathscr{L}_{\mathbb{K}}$ such that $\bigcup_{\{z_i\}} (\mathbb{K} + z_i)$ forms an tiling of $\mathbb{K}_{\lceil c \rceil} := \lceil c \rceil \cdot \mathbb{K}$. We thus have that $z_i \neq z_j$ and $(\mathbb{K} + z_i) \cap (\mathbb{K} + z_j) = \varnothing$ if $i \neq j$ and that

$$\bigcup_{\{z_i\}} (\mathbb{K} + z_i) = \mathbb{K}_{\lceil c \rceil}.$$

Consequently, we have

$$\begin{aligned}
\|\breve{v}_c\|_{L^{\frac{10}{3}}(\mathbb{K}_c)}^{\frac{10}{3}} &\leqslant \sum_{\{z_i\}} \|\breve{v}_c\|_{L^{\frac{10}{3}}(\mathbb{K}+z_i)}^{\frac{10}{3}} \\
&\leqslant \sum_{\{z_i\}} \|\breve{v}_c\|_{L^2(\mathbb{K}+z_i)}^{\frac{4}{3}} \|\breve{v}_c\|_{L^6(\mathbb{K}+z_i)}^{2} \\
&\leqslant \sum_{\{z_i\}} \left(\sup_i \|\breve{v}_c\|_{L^2(\mathbb{K}+z_i)} \right)^{\frac{4}{3}} C(\mathbb{K}) \|\breve{v}_c\|_{H^1(\mathbb{K}+z_i)}^{2} \\
&\leqslant 8C(\mathbb{K}) \Big(8 \sup_{(\mathbb{K}+z) \subset \mathbb{K}_c} \|\breve{v}_c\|_{L^2(\mathbb{K}+z)} \Big)^{\frac{4}{3}} \|\breve{v}_c\|_{H^1(\mathbb{K}_c)}^{2},
\end{aligned}$$

where the factor 8 is a rough upper bound arising twice (respectively for L^2 and H^1 norms) from the fact that the $(\mathbb{K} + z_i)$'s on the edges belong at worst (when z_i is near a corner of $\mathbb{K}_c$) to 8 distinct replicas of $\mathbb{K}_c$. Passing to the limit $c \to \infty$, we deduce that there exists C depending only on $\mathbb{K}$ (not on $\mathbb{K}_c$) such that

$$\limsup_{c\to\infty} \|\breve{v}_c\|^{\frac{10}{3}}_{L^{\frac{10}{3}}(\mathbb{K}_c)} \leqslant C \left(\limsup_{c\to\infty} \sup_{(\mathbb{K}+z)\subset\mathbb{K}_c} \int_{\mathbb{K}+z} |\breve{v}_c|^2 \right)^{2/3} \limsup_{c\to\infty} \|\breve{v}_c\|^2_{H^1(\mathbb{K}_c)} .$$

Let now consider $\{y_c\} \subset \mathbb{R}^3$ such that $(\mathbb{K}+y_c) \subset \mathbb{K}_c$ and such that

$$\lim_{c\to\infty} \int_{\mathbb{K}+y_c} |\breve{v}_c|^2 = \limsup_{c\to\infty} \sup_{(\mathbb{K}+z)\subset\mathbb{K}_c} \int_{\mathbb{K}+z} |\breve{v}_c|^2$$

and let $\chi_c \in C_0^\infty(\mathbb{K}_c)$ be such that $0 \leqslant \chi_c \leqslant 1$, $\chi_{c|\mathbb{K}_{c-1}} \equiv 1$, $\chi_{c|\mathbb{R}^3\setminus\mathbb{K}_c} \equiv 0$ and $\|\nabla\chi_c\|_{L^\infty(\mathbb{R}^3)}$ bounded. The sequence $(\breve{v}_c^{\mathbf{y}}\chi_c)_c$ being bounded in $H^1(\mathbb{R}^3)$ by Corollary 2.36, there exists, up to extraction of a subsequence, $u_y \in H^1(\mathbb{R}^3)$ such that $\breve{v}_{c_k}^{\mathbf{y}}\chi_{c_k} \rightharpoonup u_y$ weakly in $H^1(\mathbb{R}^3)$ (which is the same weak limit as $\breve{v}_c^{\mathbf{y}}$'s weak limit) and, by Rellich-Kondrachov Theorem, strongly in $L^2(\mathbb{K})$. Thus

$$\lim_{c\to\infty} \int_{\mathbb{K}+y_c} |\breve{v}_c|^2 = \lim_{c\to\infty} \int_{\mathbb{K}} |\breve{v}_c^{\mathbf{y}}|^2 = \lim_{c\to\infty} \int_{\mathbb{K}} |\breve{v}_c^{\mathbf{y}}\chi_c|^2 = \int_{\mathbb{K}} |u_y|^2 \leqslant \mathbf{m}(\{\breve{v}_c\})$$

and, consequently,

$$\limsup_{c\to\infty} \|\breve{v}_c\|^{10/3}_{L^{10/3}(\mathbb{K}_c)} \leqslant C \left(\mathbf{m}(\{\breve{v}_c\})\right)^{2/3} \limsup_{c\to\infty} \|\breve{v}_c\|^2_{H^1(\mathbb{K}_c)} . \tag{2.97}$$

This concludes this step since

$$\limsup_{c\to\infty} \|\breve{v}_c\|_{H^1(\mathbb{K}_c)} \lesssim 1 \lesssim \limsup_{c\to\infty} \|\breve{v}_c\|_{L^{10/3}(\mathbb{K}_c)}$$

by Corollary 2.36 thus $\mathbf{m}(\{\breve{v}_c\}) > 0$.

Similarly to (2.97) but using $\|\breve{v}_c\|^{8/3}_{L^{8/3}(\mathbb{K}+z_i)} \leqslant \|\breve{v}_c\|^{5/3}_{L^2(\mathbb{K}+z_i)} \|\breve{v}_c\|_{L^6(\mathbb{K}+z_i)}$ in the first upper bound of this Step, one obtains

$$\limsup_{c\to\infty} \|\breve{v}_c\|^{8/3}_{L^{8/3}(\mathbb{K}_c)} \leqslant C' \left(\mathbf{m}(\{\breve{v}_c\})\right)^{5/6} \limsup_{c\to\infty} \|\breve{v}_c\|_{H^1(\mathbb{K}_c)} . \tag{2.98}$$

Step 2: bubbles' extraction. We prove here that the minimizers split into a sum of localized bubbles as c goes to ∞. Using Lemmas 2.43 and 2.61, we start by proving a H^1-convergence result in the following lemma.

LEMMA 2.76. *Let $\mathbb{K}$ be the unit cube, $0 \leqslant R_k \leqslant R'_k$ be such that $R_k \to \infty$ and $\{\varphi_c\}_{c\geqslant 1}$ be a sequence of functions such that $\varphi_c \in H^1_{per}(\mathbb{K}_c)$ for all c, $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ uniformly bounded and $\varphi_c \underset{c\to\infty}{\rightharpoonup} \varphi$ weakly in $L^2(\mathbb{R}^3)$. Then there exists a subsequence $\{\varphi_{c_k}\}_{k\to\infty}$ such that*

$$\lim_{k\to\infty} \|\varphi_{c_k} - \xi_k - \psi_k\|_{H^1(\mathbb{K}_{c_k})} = 0$$

where $B(0,4R'_k) \subset \mathbb{K}_{c_k}$, $\{\xi_k\}_k$ and $\{\psi_k\}_k$ are in $H^1_{per}(\mathbb{K}_{c_k})$ with their $H^1(\mathbb{K}_{c_k})$-norms uniformly bounded such that

(1) $\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k \rightharpoonup \varphi$ *weakly in* $H^1(\mathbb{R}^3)$ *and strongly in* $L^p(\mathbb{R}^3)$ *for* $2 \leqslant p < 6$,

(2) $\operatorname{supp}(\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k) \subset B(0, R_k)$ *and* $\operatorname{supp}(\mathbb{1}_{\mathbb{K}_{c_k}}\psi_k) \subset \mathbb{K}_{c_k}\backslash B(0, R'_k)$,

(3) $\mathbf{m}(\{\psi_k\}) \leqslant \mathbf{m}(\{\varphi_{c_k}\}) \leqslant \mathbf{m}(\{\varphi_c\})$.

Proof of Lemma 2.76. The proof is similar to the one of Corollary 2.62 but adapting it to our specific case which is periodic and the sequences are not, per se, in $H^1(\mathbb{R}^3)$.

Since $\mathbb{1}_{\mathbb{K}_c}\varphi_c \underset{c\to\infty}{\rightharpoonup} \varphi$ weakly in $L^2(\mathbb{R}^3)$ and $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ uniformly bounded we have by Lemma 2.43 that $\varphi \in H^1(\mathbb{R}^3)$ and $\varphi_c \rightharpoonup \varphi$ weakly in $H^1(\mathbb{R}^3)$.

Let $\{\eta_c\}$ be smooth functions such that, for any c, $\eta_c : \mathbb{R}^3 \to [0, 1]$, $\eta_{c|\mathbb{K}_c} \equiv 1$, $\eta_{c|\mathbb{R}^3\backslash\mathbb{K}_{c+1}} \equiv 0$ and $\|\nabla\eta_c\|_{L^\infty(\mathbb{R}^3)}$ bounded. Since $\eta_c\varphi_c$ is $H^1(\mathbb{R}^3)$-bounded and converges weakly to φ in $H^1(\mathbb{R}^3)$, we apply Lemma 2.61 to it together with $R_k/2$ and $4R'_k$ and obtain a subsequence $\{\varphi_{c_k}\}$, that can be chosen to verify $B(0, 4R'_k) \subset \mathbb{K}_{c_k}$ for all k, such that

$$\int_{|x|\leqslant R_k/2} |\varphi_{c_k}|^2 \to \int_{\mathbb{R}^3} |\varphi|^2 \quad \text{and} \quad \int_{R_k/2\leqslant|x|\leqslant 4R'_k} \left(|\varphi_{c_k}|^2 + |\nabla\varphi_{c_k}|^2\right) \to 0. \quad (2.99)$$

Let $\chi : \mathbb{R}^+ \to [0, 1]$ be a smooth function such that $0 \leqslant \chi' \leqslant 2$, $\chi_{|[0,1]} \equiv 1$, $\chi_{|[2,\infty)} \equiv 0$. We then denote $\tilde{\chi}_k(x) := \chi(2|x|/R_k)$ and $\tilde{\zeta}_k(x) := 1 - \chi(|x|/R'_k)$ and introduce ξ_k and ψ_k the two $\mathbb{K}_{c_k}$-periodic functions such that $\xi_{k|\mathbb{K}_{c_k}} := \tilde{\chi}_k\varphi_{c_k}$ and $\psi_{k|\mathbb{K}_{c_k}} := \tilde{\zeta}_k\varphi_{c_k}$. It holds, on $\mathbb{K}_{c_k}$, that

$$\varphi_{c_k} - \xi_k - \psi_k = \varphi_{c_k}(\chi(|x|/R'_k) - \chi(2|x|/R_k))$$

which leads to $\mathbb{K}_{c_k} \cap \operatorname{supp}(\varphi_{c_k} - \xi_k - \psi_k) \subset \{R_k/2 \leqslant |x| \leqslant 2R'_k\}$ and finally, using (2.99), to the fact that

$$\lim_{k\to\infty} \|\varphi_{c_k} - \xi_k - \psi_k\|_{H^1(\mathbb{K}_{c_k})} = 0.$$

Moreover, by construction, $\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k \rightharpoonup \varphi$ weakly in $H^1(\mathbb{R}^3)$ and it also holds that

$$\lim_{k\to\infty} \int_{\mathbb{R}^3} \left|\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k\right|^2 = \lim_{k\to\infty} \int_{B(0,R_k/2)} |\xi_k|^2 = \int_{\mathbb{R}^3} |\varphi|^2,$$

hence $\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k$ also strongly converges to φ in $L^p(\mathbb{R}^3)$ for $2 \leqslant p < 6$ by Sobolev embeddings and because $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ is uniformly bounded. In addition, it is easy to see that $\mathbb{1}_{B(0,4R'_k)}\psi_k \to 0$ strongly in $L^2(\mathbb{R}^3)$.

We now prove that $\mathbf{m}(\{\psi_k\}) \leqslant \mathbf{m}(\{\varphi_{c_k}\}) \leqslant \mathbf{m}(\{\varphi_c\})$. We suppose $\mathbf{m}(\{\psi_k\}) > 0$, otherwise there is nothing to prove. Thus, there exists k_j's, $\{x_j\} \subset \mathbb{R}^3$ and $\psi \not\equiv 0$ such that $\psi_{k_j}(\cdot - x_j) \rightharpoonup \psi$ weakly in $L^2(\mathbb{R}^3)$. We first prove that, for j large enough, we have $|x_j| \geqslant 3R'_{k_j}$. Indeed, if for a subsequence (denoted the same), we have $|x_j| < 3R'_{k_j}$ then $\psi_{k_j}(\cdot - x_j)\mathbb{1}_{B(0,R'_k)} \rightharpoonup 0 \equiv \psi$ weakly in $L^2(\mathbb{R}^3)$

— since $B(x_j, R'_k) \subset B(0, 4R'_k)$ and $\mathbb{1}_{B(0,4R'_k)}\psi_k \to 0$ strongly in $L^2(\mathbb{R}^3)$ — a contradiction. Consequently, we have that

$$\psi_{k_j}(\cdot - x_j)\mathbb{1}_{B(0,R'_{k_j})} = \varphi_{c_{k_j}}(\cdot - x_j)\mathbb{1}_{B(0,R'_{k_j})} \rightharpoonup \psi$$

since $\tilde{\zeta}_k \equiv 1$ on $B(x_j, R'_{k_j})$ which implies that $\varphi_{c_{k_j}}(\cdot - x_j) \rightharpoonup \psi$ weakly in $L^2(\mathbb{R}^3)$ hence that $\mathbf{m}(\{\psi_k\}) \leqslant \mathbf{m}(\{\varphi_{c_k}\})$. □

This result allows us to obtain Lemma 2.77 which concludes this Step 2.

LEMMA 2.77 (Splitting in localized bubbles). *Let $\mathbb{K}$ be the unit cube, $\{\varphi_c\}_{c\geqslant 1}$ be a sequence of functions such that $\varphi_c \in H^1_{per}(\mathbb{K}_c)$ for all c, $\|\varphi_c\|_{H^1(\mathbb{K}_c)}$ uniformly bounded and $\mathbf{m}(\{\varphi_c\}) > 0$. Then there exists a sequence of functions $\{\varphi^{(1)}, \varphi^{(2)}, \cdots\}$ in $H^1(\mathbb{R}^3)$ such that the following holds: for any $\varepsilon > 0$ and any fixed sequence $0 \leqslant R_k \to \infty$, there exist:*

- *$J \geqslant 1$,*
- *a subsequence $\{\varphi_{c_k}\}$,*
- *sequences $\{\xi_k^{(1)}\}, \cdots, \{\xi_k^{(J)}\}, \{\psi_k\}$ in $H^1_{per}(\mathbb{K}_{c_k})$,*
- *sequences of space translations $\{x_k^{(1)}\}, \cdots, \{x_k^{(J)}\}$ in $\mathbb{R}^3$,*

such that

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

where

- *$\{\xi_k^{(1)}\}, \cdots, \{\xi_k^{(J)}\}, \{\psi_k\}$ 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 $2 \leqslant p < 6$,*
- *$supp(\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k^{(j)}) \subset B(0, R_k)$ for all $j = 1, \cdots, J$ and all k,*
- *$supp(\mathbb{1}_{\mathbb{K}_{c_k}}\psi_k) \subset \mathbb{K}_{c_k} \setminus \bigcup_{j=1}^{J} B(x_k^{(j)}, 2R_k)$ for all k,*
- *$|x_k^{(i)} - x_k^{(j)}| \geqslant 5R_k$ for all $i \neq j$ and all k,*
- *$\mathbf{m}(\{\psi_k\}) \leqslant \varepsilon$.*

PROOF OF LEMMA 2.77. Let $\varepsilon > 0$ and the sequence $\{R_k\}$ be fixed.

Since $\mathbf{m}(\{\varphi_c\}) > 0$, there exist a subsequence c_{c_k}, a sequence translation $\{x_k^{(1)}\} \subset \mathbb{R}^3$ and a function $0 \not\equiv \varphi^{(1)} \in L^2(\mathbb{R}^3)$ such that $\varphi_{c_k}(\cdot + x_k^{(1)}) \rightharpoonup \varphi^{(1)}$ weakly in $L^2(\mathbb{R}^3)$. We apply Lemma 2.76 to $\varphi_{c_k}(\cdot + x_k^{(1)})$, R_k and $R'_k = 2R_k$.

Thus, up to a subsequence (we keep the same notation for simplicity), $\{\varphi_{c_k}\}_{k\to\infty}$ is such that

$$\lim_{k\to\infty}\left\|\varphi_{c_k}-\xi_k^{(1)}(\cdot-x_k^{(1)})-\psi_k^{(2)}\right\|_{H^1(\mathbb{K}_{c_k})}=0$$

where $\xi_k^{(1)}$ and $\psi_k^{(2)}$ are in $H^1_{\rm per}(\mathbb{K}_{c_k})$ for all k and $\|\xi_k^{(1)}\|_{H^1(\mathbb{K}_{c_k})}$ and $\|\psi_k^{(2)}\|_{H^1(\mathbb{K}_{c_k})}$ uniformly bounded. Moreover

(1) $\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k^{(1)}\rightharpoonup\varphi^{(1)}$ weakly in $H^1(\mathbb{R}^3)$ and strongly in $L^p(\mathbb{R}^3)$ for $2\leqslant p<6$,

(2) $\mathrm{supp}(\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k^{(1)})\subset B(0,R_k)$ and $\mathrm{supp}(\mathbb{1}_{\mathbb{K}_{c_k}}\psi_k^{(2)})\subset\mathbb{K}_{c_k}\backslash B(x_k^{(1)},2R_k)$,

(3) $\mathbf{m}(\{\psi_k^{(2)}\})\leqslant\mathbf{m}(\{\varphi_{c_k}\})\leqslant\mathbf{m}(\{\varphi_c\})$.

Remark. Unlike how things have been written in Lemma 2.76, from now on $\psi_k^{(2)}$ includes in its definition the translation sequence $x_k^{(1)}$.

If $\mathbf{m}(\{\psi_k^{(2)}\})=0$, then we can stop here. Otherwise, we apply the same to the sequence $\{\psi_k^{(2)}\}$ which verifies the same three properties as $\{\varphi_c\}$ was verifying. There exist a subsequence (same notation for simplicity), a sequence translation $\{x_k^{(2)}\}\subset\mathbb{R}^3$ and a function $0\not\equiv\varphi^{(2)}\in L^2(\mathbb{R}^3)$ such that $\psi_k^{(2)}(\cdot+x_k^{(2)})\rightharpoonup\varphi^{(2)}$ weakly in $L^2(\mathbb{R}^3)$. We claim that $|x_k^{(2)}-x_k^{(1)}|\to\infty$. Indeed, if it were not divergent, then up to another subsequence, we would have $|x_k^{(2)}-x_k^{(1)}|\to\nu$. Then the fact that $\varphi_{c_k}-\varphi^{(1)}(\cdot-x_k^{(1)})=\psi_k^{(2)}+\varepsilon_k$, where $\|\varepsilon_k\|_{H^1(\mathbb{K}_{c_k})}\to0$ thus $\varepsilon_k\rightharpoonup0$ weakly in $L^2(\mathbb{R}^3)$, would lead to the fact that $\varphi_{c_k}(\cdot+x_k^{(1)})\rightharpoonup\varphi^{(1)}+\varphi^{(2)}(\cdot+\nu)$ which contradicts the fact that $\varphi_{c_k}(\cdot+x_k^{(1)})\rightharpoonup\varphi^{(1)}$ since $+\varphi^{(2)}\not\equiv0$.

We now apply Lemma 2.76 to $\psi_k^{(2)}(\cdot+x_k^{(2)})$, R_k and $R'_k=2R_k$. Thus, up to a subsequence (same notation for simplicity), $|x_k^{(2)}-x_k^{(1)}|\geqslant5R_k$ for all k and $\{\psi_k^{(2)}\}_{k\to\infty}$ is such that

$$\lim_{k\to\infty}\left\|\psi_k^{(2)}-\xi_k^{(2)}(\cdot-x_k^{(2)})-\psi_k^{(3)}\right\|_{H^1(\mathbb{K}_{c_k})}=0$$

where $\xi_k^{(2)}$ and $\psi_k^{(3)}$ are in $H^1_{\rm per}(\mathbb{K}_{c_k})$ for all k and $\|\xi_k^{(2)}\|_{H^1(\mathbb{K}_{c_k})}$ and $\|\psi_k^{(3)}\|_{H^1(\mathbb{K}_{c_k})}$ uniformly bounded. Moreover

(1) $\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k^{(2)}\rightharpoonup\varphi^{(2)}$ weakly in $H^1(\mathbb{R}^3)$ and strongly in $L^p(\mathbb{R}^3)$ for $2\leqslant p<6$,

(2) $\mathrm{supp}(\mathbb{1}_{\mathbb{K}_{c_k}}\xi_k^{(2)})\subset B(0,R_k)$ and $\mathrm{supp}(\mathbb{1}_{\mathbb{K}_{c_k}}\psi_k^{(3)})\subset\mathbb{K}_{c_k}\backslash\bigcup_{j=1}^{2}B(x_k^{(j)},2R_k)$,

(3) $\mathbf{m}(\{\psi_k^{(3)}\})\leqslant\mathbf{m}(\{\psi_k^{(2)}\})$.

Repeating this, we obtain that for any $i\geqslant1$ such that $\mathbf{m}(\{\psi_k^{(i)}\})>0$, we have that

$$\left\|\varphi_{c_k}-\sum_{j=1}^{i}\xi_k^{(j)}(\cdot-x_k^{(j)})-\psi_k^{(i+1)}\right\|\leqslant\sum_{j=1}^{i}\left\|\psi_k^{(j)}-\xi_k^{(j)}(\cdot-x_k^{(j)})-\psi_k^{(j+1)}\right\|\to0,$$

where the norm is the $H^1(\mathbb{K}_{c_k})$-norm and $\psi_k^{(1)} := \varphi_{c_k}$ and with all the wanted properties verified, except the upper bound by ε. This last one comes from the fact that $\mathbf{m}(\{\psi_k^{(i)}\}) > 0$ for all i and their infinite sum is bounded by λ thus the sequence converges to 0. Hence, there exist $J \geqslant 1$ such that $\mathbf{m}(\{\psi_k^{(J+1)}\}) \leqslant \varepsilon$ and this concludes the proof of Lemma 2.77. $\square$

Step 3: end of the proof. We apply Lemma 2.77 to the sequence of minimizers $\{\breve{v}_c\}$ which verifies the hypothesis of the proposition by Corollary 2.36 and does not vanish (see Step 1). Thus

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

where $\|\varepsilon_k\|_{H^1(\mathbb{K}_{c_k})} \to 0$ and, for a given k, the supports of the $\breve{v}_k^{(j)}(\cdot - x_k^{(j)})$'s and ν_k are pairwise disjoint. Using the support properties of the functions, the Minkowski inequality, Sobolev embeddings and the fact that $\mathrm{supp}(\mathbb{1}_{\mathbb{K}_{c_k}} \breve{v}_k^{(j)}) \subset B(0, R_k) \subset \mathbb{K}_{c_k}$, we then have that

$$\begin{aligned} J_{\mathbb{K}_{c_k}}(\lambda) = \mathscr{J}_{\mathbb{K}_{c_k}}(\breve{v}_{c_k}) &= \mathscr{J}_{\mathbb{K}_{c_k}}(\nu_k) + \sum_{j=1}^{J} \mathscr{J}_{\mathbb{K}_{c_k}}(\breve{v}_k^{(j)}) + o(1)_{c_k \to \infty} \\ &= \mathscr{J}_{\mathbb{K}_{c_k}}(\nu_k) + \sum_{j=1}^{J} \mathscr{J}_{\mathbb{K}_{c_k}}(\mathbb{1}_{\mathbb{K}_{c_k}} \breve{v}_k^{(j)}) + o(1)_{c_k \to \infty} \\ &= \mathscr{J}_{\mathbb{K}_{c_k}}(\nu_k) + \sum_{j=1}^{J} \mathscr{J}_{\mathbb{R}^3}(\mathbb{1}_{\mathbb{K}_{c_k}} \breve{v}_k^{(j)}) + o(1)_{c_k \to \infty}. \end{aligned}$$

Moreover, the strong convergence of $\mathbb{1}_{\mathbb{K}_{c_k}} \breve{v}_k^{(j)}$ in L^2 and the continuity of $\lambda \mapsto J_{\mathbb{R}^3,\lambda}$, proved in Lemma 2.12, imply, for all $j = 1, \cdots, J$, that

$$\mathscr{J}_{\mathbb{R}^3}(\mathbb{1}_{\mathbb{K}_{c_k}} \breve{v}_k^{(j)}) \geqslant J_{\mathbb{R}^3}\left(\|\breve{v}_k^{(j)}\|^2_{L^2(\mathbb{K}_{c_k})}\right) \underset{k \to \infty}{\longrightarrow} J_{\mathbb{R}^3}(\lambda^{(j)}),$$

where, for any j, $\lambda^{(j)} := \|\breve{v}^{(j)}\|_{L^2(\mathbb{R}^3)}$ is the mass of the limit of $\mathbb{1}_{\mathbb{K}_{c_k}} \breve{v}_k^{(j)}$. We also have denoted $J_{\mathbb{R}^3}(\lambda) := J_{\mathbb{R}^3,\lambda}$ to simplify notations here. In addition, given that the $H^1(\mathbb{K}_{c_k})$-norms of $\{\nu_k\}$ are uniformly bounded, we can use (2.98) to obtain that there exist $C > 0$ such that

$$\mathscr{J}_{\mathbb{K}_{c_k}}(\nu_k) \geqslant -\frac{3}{4} \int_{\mathbb{K}_{c_k}} |\nu_k|^{8/3} \geqslant -C\left(\mathbf{m}(\{\nu_k\})\right)^{5/6} \geqslant -C\varepsilon^{5/6}.$$

Those inequalities together with the strict binding proved in Proposition 2.16 lead to

$$\begin{aligned}\liminf_{k\to\infty} J_{\mathbb{K}_{c_k}}(\lambda) &\geqslant \sum_{j=1}^{J} J_{\mathbb{R}^3}(\lambda^{(j)}) - C\varepsilon^{5/6} \\ &> J_{\mathbb{R}^3}\Big(\sum_{j=1}^{J}\lambda^{(j)}\Big) - C\varepsilon^{5/6} > J_{\mathbb{R}^3}(\lambda) - J_{\mathbb{R}^3}\Big(\lambda - \sum_{j=1}^{J}\lambda^{(j)}\Big) - C\varepsilon^{5/6}.\end{aligned}$$

By the support properties, we have

$$0 \leqslant \|\nu_k\|^2_{L^2(\mathbb{K}_{c_k})} = \lambda - \sum_{j=1}^{J}\lambda^{(j)} + o(1)$$

thus $\lambda - \sum_{j=1}^{J}\lambda^{(j)} \geqslant 0$ and this implies that $J_{\mathbb{R}^3}\Big(\lambda - \sum_{j=1}^{J}\lambda^{(j)}\Big) \leqslant 0$ which leads to

$$\liminf_{k\to\infty} J_{\mathbb{K}_{c_k}}(\lambda) > J_{\mathbb{R}^3}(\lambda) - C\varepsilon^{5/6}.$$

This concludes the detailed proof of Lemma 2.41.

6.8. Two technical inequalities.

LEMMA 2.78. *There exists $C \leqslant \frac{2}{e\ln(2)}$ such that, for all integers $p \geqslant k \geqslant 1$ and all nonnegative real numbers X and Y, we have*

$$\left|X^{2+1/p} - Y^{2+1/p}\right| \leqslant |X-Y|(X+Y)^{1+1/p} \tag{2.100}$$

and

$$\left|X^{1+k/p} - Y^{1+k/p}\right| \leqslant C|X-Y|(X+Y)^{k/p}. \tag{2.101}$$

PROOF OF LEMMA 2.78. It is enough to prove the two results for $0 \leqslant Y \leqslant X$. Moreover, the equality cases being obvious in the two inequalities, we in fact suppose that $0 < Y < X$.

We start with the proof of (2.100). Defining, on $(Y;\infty)$, the function

$$f_Y(X) = (X-Y)(X+Y)^{1+1/p} - X^{2+1/p} + Y^{2+1/p},$$

its derivative is

$$f_Y'(X) = (X+Y)^{\frac{1}{p}}\left[2X + \frac{X-Y}{p}\right] - \frac{2p+1}{p}X^{1+\frac{1}{p}} =: g_X(Y),$$

where g_X is defined on $(0;X)$. Its own derivative is

$$g_X'(Y) = \frac{1}{p}(X+Y)^{\frac{1}{p}-1}\left(1+\frac{1}{p}\right)(X-Y) > 0,$$

hence g_X is strictly increasing. Since $g_X(0) = 0$, it implies that $g_X > 0$ on $(0; X)$. Finally, for any $Y > 0$, f_Y is strictly increasing on its domain $(Y; \infty)$. It concludes the proof of (2.100) since $f_Y(Y) = 0$.

We now prove (2.101). For $p = k$, the result is obvious hence we suppose that $p > k \geqslant 1$. Defining, on $(Y; \infty)$, the function

$$f_{Y,C}(X) = C(X-Y)(X+Y)^{k/p} - X^{1+k/p} + Y^{1+k/p},$$

its derivative is

$$f'_{Y,C}(X) = C(X+Y)^{\frac{k}{p}-1}\left[X\left(1+\frac{k}{p}\right) + Y\left(1-\frac{k}{p}\right)\right] - \frac{p+k}{p}X^{\frac{k}{p}} =: g_{X,C}(Y),$$

where $g_{X,C}$ is defined on $(0; X)$. Its own derivative is

$$g'_{X,C}(Y) = -C\frac{k}{p}\left(1-\frac{k}{p}\right)(X+Y)^{\frac{k}{p}-2}(X-Y) < 0.$$

Moreover, $g_{X,C}(X) = \left(\frac{C}{2}2^{\frac{p+k}{p}} - \frac{p+k}{p}\right)X^{\frac{k}{p}}$, thus it is sufficient for $\eta_C(z) = \frac{C}{2}2^z - z$ to be positive on $(1; 2)$ to have $f_{Y,C}$ increasing and then $f_{Y,C}(X) \geqslant f_{Y,C}(Y) = 0$.

We have $\eta'_C(z) = \ln 2\frac{C}{2}2^z - 1$. Thus, for $C = \frac{2}{e\ln(2)}$, we have $\eta'_C(z) = e^{-1}2^z - 1$ thus $\eta'_C(1) < 0$ and $\eta'_C(2) > 0$. Moreover, since $\eta''_C(z) = \frac{C}{2}(\ln 2)^2 2^z > 0$, $z_0 = \frac{1}{\ln 2}$ is the unique value in $(1; 2)$ such that $\eta'_C(z_0) = 0$ and we have

$$\eta_C(z) > \eta_C(z_0) = 0, \qquad \forall z \in (1; 2)\backslash\{z_0\}.$$

This concludes the proof of Lemma 2.78. $\square$

6.9. Detailed proof of boundedness property of $(-\Delta_{\mathbf{per}} - G_{\mathbb{K}} + \beta)^{-1}$.

LEMMA 2.79. *Then the $L^2_{per}(\mathbb{K})$-operator $-\Delta_{per} - G_{\mathbb{K}}$ is self-adjoint of domain $H^2_{per}(\mathbb{K})$ and, for β large enough,*

$$(-\Delta_{per} - G_{\mathbb{K}} + \beta)^{-1} : L^2(\mathbb{K}) \to H^2(\mathbb{K})$$

is bounded uniformly in β.

PROOF OF LEMMA 2.79. Let f, defined on $\mathbb{R}^3$, be $\mathbb{K}$-periodic and in $H^2_{\mathrm{per}}(\mathbb{K})$. We define $\mathbb{K}'$ as the union of $\mathbb{K}$ with its twenty-six closest neighbors. Let $\chi \in C_c^\infty(\mathbb{R}^3)$ be such that $0 \leqslant \chi \leqslant 1$, $\chi_{|\mathbb{K}} \equiv 1$ and $\chi_{|\mathbb{R}^3\backslash\mathbb{K}'} \equiv 0$. By Sobolev inequalities, we have

$$\begin{aligned}
\|\chi f\|_{L^\infty(\mathbb{R}^3)} &\leqslant C_{\mathbb{R}^3}\|\chi f\|_{H^2(\mathbb{R}^3)} \\
&\leqslant C_{\mathbb{R}^3}\left(\|\Delta(\chi f)\|_{L^2(\mathbb{R}^3)} + \|\chi f\|_{L^2(\mathbb{R}^3)}\right) \\
&= C_{\mathbb{R}^3}\left(\|\Delta(\chi f)\|_{L^2(\mathbb{K}')} + \|\chi f\|_{L^2(\mathbb{K}')}\right).
\end{aligned}$$

It leads to

$$\begin{aligned}\|f\|_{L^\infty(\mathbb{K})} = \|\chi f\|_{L^\infty(\mathbb{R}^3)} &\leqslant C_{\mathbb{R}^3}\Big(\|\chi\Delta f\|_{L^2(\mathbb{K}')} + 2\|\nabla\chi\|_\infty \|\nabla f\|_{L^2(\mathbb{K}')} \\ &\qquad + \|\Delta\chi\|_\infty \|f\|_{L^2(\mathbb{K}')} + \|f\|_{L^2(\mathbb{K}')}\Big) \\ &\leqslant C_{\mathbb{R}^3}\Big(27\|\Delta f\|_{L^2(\mathbb{K})} \\ &\qquad + 54\|\nabla\chi\|_\infty \|\Delta f\|_{L^2(\mathbb{K})}^{1/2} \|f\|_{L^2(\mathbb{K})}^{1/2} \\ &\qquad + 27(\|\Delta\chi\|_\infty + 1)\|f\|_{L^2(\mathbb{K})}\Big) \\ &\leqslant 27C_{\mathbb{R}^3}\Big((1+\|\nabla\chi\|_\infty)\|\Delta f\|_{L^2(\mathbb{K})} \\ &\qquad + (\|\Delta\chi\|_\infty + \|\nabla\chi\|_\infty + 1)\|f\|_{L^2(\mathbb{K})}\Big).\end{aligned}$$

By the definition of $\mathbb{K}'$ and thus of χ, $\|\Delta\chi\|_{L^\infty(\mathbb{R}^3)}$ and $\|\nabla\chi\|_{L^\infty(\mathbb{R}^3)}$ are bounded thus we obtain that there exists $C > 0$, depending only on $\mathbb{K}$, such that

$$\|f\|_{L^\infty(\mathbb{K})} \leqslant C\left(\|-\Delta f\|_{L^2(\mathbb{K})} + \|f\|_{L^2(\mathbb{K})}\right). \tag{2.102}$$

Consequently, for any $R > 0$, it holds that

$$\|G_{\mathbb{K}} f\|_{L^2(\mathbb{K})} \leqslant \left\|G_{\mathbb{K}}\mathbb{1}_{|G_{\mathbb{K}}|\geqslant R}\right\|_{L^2(\mathbb{K})} \|f\|_{L^\infty(\mathbb{K})} + R\|f\|_{L^2(\mathbb{K})}.$$

Since $G_{\mathbb{K}} \in L^2(\mathbb{K})$, by Lemma 2.20, Lebesgue's dominated convergence theorem gives

$$\left\|G_{\mathbb{K}}\mathbb{1}_{|G_{\mathbb{K}}|\geqslant R}\right\|_{L^2(\mathbb{K})} \to 0$$

as $R \to \infty$ hence, for any $\varepsilon > 0$, it finally holds that there exists C_ε such that

$$\|G_{\mathbb{K}} f\|_{L^2(\mathbb{K})} \leqslant \varepsilon\|-\Delta f\|_{L^2(\mathbb{K})} + C_\varepsilon\|f\|_{L^2(\mathbb{K})}. \tag{2.103}$$

In particular for $0 < \varepsilon < 1$, the Rellich-Kato theorem (see e.g. [**RS75**, Theorem X.12]) implies that the operator $-\Delta_{\text{per}} - G_{\mathbb{K}}$ is self-adjoint of domain $D(-\Delta_{\text{per}}) = H^2_{\text{per}}(\mathbb{K})$ and is bounded below.

For $\beta > 0$, we then have

$$\begin{aligned}\|f\|_{H^2(\mathbb{K})} = \|(-\Delta+1)f\|_{L^2(\mathbb{K})} &\leqslant \left\|\frac{-\Delta+1}{-\Delta+\beta}\right\| \|(-\Delta+\beta)f\|_{L^2(\mathbb{K})} \\ &\leqslant \max\{1,\beta^{-1}\}\|(-\Delta+\beta)f\|_{L^2(\mathbb{K})}.\end{aligned} \tag{2.104}$$

Indeed for any $x \in \mathbb{K}$, using the Fourier series on a lattice

$$f(x) = \sum_{k\in\mathscr{L}_{\mathbb{K}}^*} \hat{f}(k)e^{-2i\pi\langle k,x\rangle},$$

with the Fourier transform on the lattice

$$\hat{f}(k) := \mathscr{F}[f](k) := |\mathbb{K}|^{-1}\int_{\mathbb{K}} f(x)e^{2i\pi\langle k,x\rangle}\,dx,$$

we have

$$\|f\|_{L^2(\mathbb{K})}^2 = |\mathbb{K}| \sum_{k \in \mathscr{L}_{\mathbb{K}}^*} |\hat{f}(k)|^2.$$

In the above, $\mathscr{L}_{\mathbb{K}}^*$ is the reciprocal lattice of $\mathscr{L}_{\mathbb{K}}$ and is generated, in the general case, by the vectors

$$(\boldsymbol{b_1}, \boldsymbol{b_2}, \boldsymbol{b_3}) = \frac{1}{\langle \boldsymbol{e_1} \wedge \boldsymbol{e_2}, \boldsymbol{e_3} \rangle} (\boldsymbol{e_2} \wedge \boldsymbol{e_3}, \boldsymbol{e_3} \wedge \boldsymbol{e_1}, \boldsymbol{e_1} \wedge \boldsymbol{e_2}).$$

In the general case we have $\langle \boldsymbol{e_i}, \boldsymbol{b_j} \rangle = \delta_i^j$ but, for or orthonormal lattice, this simplifies to $(\boldsymbol{b_1}, \boldsymbol{b_2}, \boldsymbol{b_3}) = (\boldsymbol{e_1}, \boldsymbol{e_2}, \boldsymbol{e_3})$ and thus $\mathscr{L}_{\mathbb{K}}^* = \mathscr{L}_{\mathbb{K}}$. Inequality (2.104) is then obtained by

$$\begin{aligned}
\left\| \frac{-\Delta + 1}{-\Delta + \beta} f \right\|_{L^2(\mathbb{K})}^2 &= \frac{1}{|\mathbb{K}|} \sum_{k \in \mathscr{L}_{\mathbb{K}}^*} \left| \int_{\mathbb{K}} e^{2i\pi \langle k, x \rangle} (-\Delta + 1)(-\Delta + \beta)^{-1} f(x) \, \mathrm{d}x \right|^2 \\
&= |\mathbb{K}|^{-1} \sum_{k \in \mathscr{L}_{\mathbb{K}}^*} \left(\frac{1 + 4\pi^2 |k|^2}{\beta + 4\pi^2 |k|^2} \right)^2 \left| \int_{\mathbb{K}} e^{2i\pi \langle k, x \rangle} f(x) \, \mathrm{d}x \right|^2 \\
&\leqslant \max\{1, \beta^{-2}\} |\mathbb{K}| \sum_{k \in \mathscr{L}_{\mathbb{K}}^*} |\hat{f}(k)|^2 = \max\{1, \beta^{-2}\} \|f\|_{L^2(\mathbb{K})}^2 .
\end{aligned}$$

On the other hand

$$\begin{aligned}
\|G_{\mathbb{K}} f\|_{L^2(\mathbb{K})} &\leqslant \varepsilon \|-\Delta f\|_{L^2(\mathbb{K})} + C_\varepsilon \|f\|_{L^2(\mathbb{K})} \\
&\leqslant \varepsilon \left\| \frac{-\Delta}{-\Delta + \beta} \right\| \|(-\Delta + \beta) f\|_{L^2(\mathbb{K})} + C_\varepsilon \left\| \frac{1}{-\Delta + \beta} \right\| \|(-\Delta + \beta) f\|_{L^2(\mathbb{K})} \\
&\leqslant \left(\varepsilon + C_\varepsilon \beta^{-1} \right) \|(-\Delta + \beta) f\|_{L^2(\mathbb{K})} ,
\end{aligned}$$

the last inequality being proved through Fourier series too. Consequently, since

$$(-\Delta + \beta)(-\Delta + G_{\mathbb{K}} + \beta)^{-1} = 1 + G_{\mathbb{K}} (-\Delta + G_{\mathbb{K}} + \beta)^{-1},$$

we obtain that for any $0 < \varepsilon < 1$, there exist $\beta_0 > 0$ such that for any $g \in L^2_{\mathrm{per}}(\mathbb{K})$ and any $\beta \geqslant \beta_0$, we have

$$\begin{aligned}
\left\| (-\Delta + G_{\mathbb{K}} + \beta)^{-1} g \right\|_{H^2(\mathbb{K})} &\leqslant \max\{1, \beta^{-1}\} \left\| (-\Delta + \beta)(-\Delta + G_{\mathbb{K}} + \beta)^{-1} g \right\|_{L^2(\mathbb{K})} \\
&\leqslant \max\{1, \beta^{-1}\} \left(1 - \varepsilon - \frac{C_\varepsilon}{\beta} \right)^{-1} \|g\|_{L^2(\mathbb{K})} \\
&\leqslant \max\{1, {\beta_0}^{-1}\} \left(1 - \varepsilon - \frac{C_\varepsilon}{\beta_0} \right)^{-1} \|g\|_{L^2(\mathbb{K})} .
\end{aligned}$$

Thus, for β large enough, the operator

$$(-\Delta_{\mathrm{per}} - G_{\mathbb{K}} + \beta)^{-1} : L^2_{\mathrm{per}}(\mathbb{K}) \to H^2_{\mathrm{per}}(\mathbb{K})$$

is bounded uniformly in β. ☐

LEMMA 2.80. *For any $\nu, c > 0$, the operator*

$$-\Delta_{per} - \frac{\nu}{c}\sum_{i=1}^{N} z_i G_{\mathbb{K}}(c^{-1}\cdot - R_i)$$

is self-adjoint of domain $H^2_{per}(\mathbb{K}_c)$ and, for β's large enough and $\nu \leqslant 1$,

$$\Big(-\Delta_{per} - \frac{\nu}{c}\sum_{i=1}^{N} z_i G_{\mathbb{K}}(c^{-1}\cdot - R_i) + \beta\Big)^{-1} : L^2(\mathbb{K}_c) \to H^2(\mathbb{K}_c)$$

are bounded uniformey in c, β and ν.

PROOF OF LEMMA 2.80. Let f, defined on $\mathbb{R}^3$, be in $H^2_{\rm per}(\mathbb{K}_c)$. Let $\chi \in C^\infty_c(\mathbb{R}^3)$ be such that $0 \leqslant \chi \leqslant 1$, $\chi_{|\mathbb{K}_c} \equiv 1$ and $\chi_{|\mathbb{R}^3\setminus\mathbb{K}_{c+1}} \equiv 0$. Noticing that, by the definition of χ, $\|\Delta\chi\|_{L^\infty(\mathbb{R}^3)}$ and $\|\nabla\chi\|_{L^\infty(\mathbb{R}^3)}$ are bounded independently of $\mathbb{K}_c$ (it only depends on $\mathbb{K}$) and using that by Lemma 2.20, there exist C_1 such that $|G_{\mathbb{K}}| \leqslant C_1|\cdot|^{-1}$, we can follow the same proof as for Lemma 2.79 to obtain for any $r > 0$ and with $Z = \sum_i z_i$ that

$$\begin{aligned}\left\|c^{-1}\sum_{i=1}^{N} z_i G_{\mathbb{K}}(c^{-1}\cdot - R_i) f\right\|_{L^2(\mathbb{K}_c)} &\leqslant C_1 Z\left\|\frac{1}{|\cdot|}\mathbb{1}_{|\cdot|\leqslant\frac{1}{r}}\right\|_{L^2(\mathbb{K}_c)}\|f\|_\infty + C_1 Z r\|f\|_{L^2(\mathbb{K}_c)}\\ &\leqslant C_1 C Z\sqrt{\frac{4\pi}{r}}\,\|-\Delta f\|_{L^2(\mathbb{K}_c)}\\ &\qquad + C_1 Z\left(C\sqrt{\frac{4\pi}{r}} + r\right)\|f\|_{L^2(\mathbb{K}_c)}\end{aligned}$$

where C and C_1 are independent of c. Finally, for any $\varepsilon > 0$, there exists

$$C_\varepsilon := \varepsilon + 4\pi\frac{{C_1}^3 Z^3\nu^3 C^2}{\varepsilon^2}$$

such that for any c and $0 \leqslant \nu \leqslant 1$ we have

$$\left\|\frac{\nu}{c}\sum_{i=1}^{N} z_i G_{\mathbb{K}}(c^{-1}\cdot - R_i) f\right\|_{L^2(\mathbb{K}_c)} \leqslant \varepsilon\|-\Delta f\|_{L^2(\mathbb{K}_c)} + C_\varepsilon\|f\|_{L^2(\mathbb{K}_c)}.$$

In particular for $0 < \varepsilon < 1$, the Kato-Rellich theorem (see e.g. [**RS75**, Theorem X.12]) implies that, for any c, the operator

$$-\Delta_{\rm per} - \frac{\nu}{c}\sum_{i=1}^{N} z_i G_{\mathbb{K}}(c^{-1}\cdot - R_i)$$

is self-adjoint of domain $D(-\Delta_{\rm per}) = H^2_{\rm per}(\mathbb{K}_c)$ and is bounded below.

The end of the proof is the same as for Lemma 2.79. ☐

We now show an inequality similar to (2.102) but for $\mathbb{K}_c$ and with a constant independent of c.

LEMMA 2.81. *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*

$$\|f\|_{L^\infty(\mathbb{K}_c)} \leqslant C \|f\|_{H^2(\mathbb{K}_c)}.$$

PROOF OF LEMMA 2.81. Using Fourier series, as in the proof of Lemma 2.79, we have

$$|f(x)| \leqslant \sum_{k \in \mathscr{L}^*_{\mathbb{K}_c}} \left|\hat{f}(k)\right| \leqslant \left(|\mathbb{K}_c|^{-1} \sum_{k \in \mathscr{L}^*_{\mathbb{K}_c}} (1+4\pi^2|k|^2)^{-2}\right)^{1/2} \times$$

$$\times \left(|\mathbb{K}_c| \sum_{k \in \mathscr{L}^*_{\mathbb{K}_c}} (1+4\pi^2|k|^2)^2 \left|\hat{f}(k)\right|^2\right)^{1/2},$$

for $f \in H^2(\mathbb{K}_c)$. Then, on one hand, we have

$$\begin{aligned}|\mathbb{K}_c| \sum_{k \in \mathscr{L}^*_{\mathbb{K}_c}} (1+4\pi^2|k|^2)^2 \left|\hat{f}(k)\right|^2 &= |\mathbb{K}_c| \sum_{k \in \mathscr{L}^*_{\mathbb{K}_c}} |\mathscr{F}[(1-\Delta)f](k)|^2 \\ &= \|(1-\Delta)f\|^2_{L^2(\mathbb{K}_c)} = \|f\|^2_{H^2(\mathbb{K}_c)}\end{aligned}$$

and, on the other hand, denoting by A the application sending $\mathbb{Z}^3$ onto $\mathscr{L}_{\mathbb{K}}$ hence $|\mathbb{K}| = \det A$ and ${}^tA^{-1}$ sends $\mathbb{Z}^3$ onto $\mathscr{L}^*_{\mathbb{K}}$. For $\varphi \in C^\infty_c(\mathbb{R}^3)$, we have

$$\begin{aligned}|\mathbb{K}_c|^{-1} \sum_{k \in \mathscr{L}^*_{\mathbb{K}_c}} (1+4\pi^2|k|^2)^{-2} &= \frac{c^{-3}}{|\mathbb{K}|} \sum_{k \in \mathbb{Z}^3} \left(1 + \left(2\pi c^{-1}\right)^2 |{}^tA^{-1}k|^2\right)^{-2} \\ &\leqslant \left(\frac{\|{}^tA\|}{2\pi}\right)^4 \frac{c}{|\mathbb{K}|} \sum_{k \in \mathbb{Z}^3} \left(\left(\frac{c\,\|{}^tA\|}{2\pi}\right)^2 + |k|^2\right)^{-2}.\end{aligned}$$

Moreover, the summands depending only on $|k|$, the sum can be decomposed as

$$\sum_{k \in \mathbb{Z}\times\mathbb{Z}\times\mathbb{Z}} = 8 \sum_{k \in \mathbb{N}_*\times\mathbb{N}_*\times\mathbb{N}_*} + 12 \sum_{k \in \{0\}\times\mathbb{N}_*\times\mathbb{N}_*} + 6 \sum_{k \in \{0\}\times\{0\}\times\mathbb{N}_*} + \sum_{k \in \{0\}\times\{0\}\times\{0\}}$$

where $\mathbb{N}_* = \mathbb{N}\backslash\{0\}$ and we have

$$\begin{aligned}\sum_{k \in (\mathbb{N}_*)^3} \left(\alpha^2 + |k|^2\right)^{-2} &\leqslant \int_{(\mathbb{R}_+)^3} \frac{\mathrm{d}x\,\mathrm{d}y\,\mathrm{d}z}{\left(\alpha^2+x^2+y^2+z^2\right)^2} = \frac{1}{8}\int_{\mathbb{R}^3} \frac{\mathrm{d}X}{(\alpha^2+|X|^2)^2} \\ &= \frac{\pi}{2}\int_0^\infty \frac{r^2\,\mathrm{d}r}{(\alpha^2+r^2)^2} = \frac{\pi^2}{8\alpha},\end{aligned}$$

$$\sum_{k \in (\mathbb{N}_*)^2} \left(\alpha^2 + |k|^2\right)^{-2} \leqslant \int_{(\mathbb{R}_+)^2} \frac{\mathrm{d}x\,\mathrm{d}y}{\left(\alpha^2+x^2+y^2\right)^2} = \frac{\pi}{2}\int_0^\infty \frac{r\,\mathrm{d}r}{(\alpha^2+r^2)^2} = \frac{\pi}{4\alpha^2},$$

and

$$\sum_{k\in\mathbb{N}_*}\left(\alpha^2+|k|^2\right)^{-2}\leqslant\int_{\mathbb{R}_+}\frac{\mathrm{d}r}{\left(\alpha^2+r^2\right)^2}=\frac{\pi}{4\alpha^3}.$$

It finally leads to

$$\begin{aligned}|\mathbb{K}_c|^{-1}\sum_{k\in\mathscr{L}^*_{\mathbb{K}_c}}(1+4\pi^2|k|^2)^{-2}&\leqslant\left(\frac{\|{}^tA\|}{2\pi}\right)^4\frac{c}{|\mathbb{K}|}\sum_{k\in\mathbb{Z}^3}\left(\left(\frac{c\,\|{}^tA\|}{2\pi}\right)^2+|k|^2\right)^{-2}\\&\leqslant\frac{\|{}^tA\|^3}{8\pi|\mathbb{K}|}\left[1+\frac{6}{\|{}^tA\|}c^{-1}+\frac{6\pi}{\|{}^tA\|^2}c^{-2}+\frac{8\pi}{\|{}^tA\|^3}c^{-3}\right].\end{aligned}$$

So $|\mathbb{K}_c|^{-1}\sum_{k\in\mathscr{L}^*_{\mathbb{K}_c}}(1+4\pi^2|k|^2)^{-2}$ is uniformely bounded w.r.t. $c\in[c^*;\infty)$ for any $c^*>0$ and this concludes the proof of Lemma 2.81. $\square$

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