Study of a mean-field model in quantum electrodynamics

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Étude d'un modèle de champ moyen en électrodynamique quantique

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Première partie

Introduction

Avant-Propos

Cette thèse est consacrée à l'étude théorique d'un modèle de mécanique quantique relativiste. Ces dernières années, un intérêt croissant est portée sur de tels modèles, tant par les chimistes quantiques que par les mathématiciens. D'aucuns pourraient penser que la théorie de la relativité n'est pas utile dans l'étude des propriétés chimiques ou physiques d'éléments usuels. Elle est cependant nécessaire pour expliquer des faits aussi triviaux que la couleur de l'or [1] ou l'état liquide du mercure à température ambiante [PD79, Nor91].

Dans cette thèse, on s'intéresse à la *polarisation du vide*. Ce phénomène surprenant survient lorsque l'on installe un champ électrostatique intense. Tel un réseau d'ions, le vide se déforme en sa présence, ce qui peut faire apparaître des paires de particule-antiparticule, plus précisément des paires d'électron-antiélectron (l'antiélectron est aussi connu sous le nom de *positron*).

On se place dans le cadre du modèle dit de Bogoliubov-Dirac-Fock introduit par Chaix et Iracane en 1989. Il s'agit d'une approximation de type champ moyen de l'électrodynamique quantique dans laquelle on néglige les photons ainsi que le magnétisme. Son intérêt réside en ce qu'il permet une étude variationnelle et non perturbative des systèmes électroniques.

Toute la question est de savoir s'il existe des minimiseurs de l'énergie associée, c'est-à-dire d'*états fondamentaux* dans le langage de la mécanique quantique. D'un point de vue mathématique on aboutit à un modèle d'analyse non linéaire avec défaut de compacité. La méthode privilégiée pour étudier ce genre de problème (et effectivement utilisée ici) est la méthode de concentration-compacité de P.-L. Lions.

Notons que les résultats obtenus supposent la petitesse ou la grandeur de certaines constantes physiques : par exemple on considèrera souvent que la vitesse de la lumière c est très grande. Cela correspond à se placer au voisinage de la limite non relativiste dans laquelle cette vitesse est supposée infinie [2]. Il est plus pertinent mais hélas beaucoup plus difficile de prouver les résultats pour les véritables valeurs des constantes physiques. Cette question a été laissée de côté ici.

Ce recueil de cinq articles traite de diverses situations physiques.

Dans le premier article on s'intéresse au système constitué d'un électron dans le vide. On montre l'existence d'un état fondamental sous certaines hypothèses. Ce résultat, faux en mécanique quantique (c-à-d non relativiste) s'explique par la polarisation du vide. La particule déforme le vide créant elle-même le puits de potentiel qui la lie : elle est entourée d'un nuage chargé positivement [3]

Une charge éloignée ressent ainsi la force de Coulomb due à la charge de l'électron *abaissée* de celle du nuage environnant. C'est la *renormalisation de charge* et l'objet du deuxième article. Il est possible de conserver la réaction du vide à la limite non relativiste $c \to +\infty$ et cela aboutit à un modèle Hartree-Fock altéré. Dans ce dernier la charge externe Ze est abaissée à une valeur $Ze \times Z_3 < Ze$ dans le terme d'interaction électrostatique et figure un terme attractif additionnel analogue à celui de l'énergie de Pekar-Tomasevitch [4].

Le troisième article traite du système constitué de deux électrons dans le vide. Quand la réaction du vide est trop petite elle ne peut pas contrebalancer la répulsion des deux particules : le système n'est pas stable.

Dans les deux derniers, on s'intéresse à des états excités du vide. On étudie le positronium, le système d'un électron et d'un positron, dans ses deux orientations possibles : l'ortho-positronium et le para-positronium. Le

1. Si on néglige les effets de la relativité, l'or devrait nous paraître comme l'argent !
2. Ainsi les effets relativistes ne sont plus négligeables dès lors qu'on ne peut plus supposer c infini.
3. Dans la situation analogue du cristal d'ions, ce nuage est constitué par les ions positifs qu'elle agrège et l'absence d'ions négatifs qu'elle repousse. Cette image est valide dès lors que ses dimensions sont grandes devant celles du réseau cristallin : la particule dans le milieu polarisable est alors appelé *polaron*.
4. Les modèles de Hartree-Fock et de Pekar-Tomasevitch sont rappelés dans le chapitre suivant.

premier correspond au cas où les deux particules ont des spins parallèls et le second où ceux-ci sont opposés. Le premier est le sujet du quatrième article, le cinquième article traite du second ainsi que d'autres états excités, dont le dipositronium, la molécule constituée de deux électrons et de deux positrons.

Ces articles sont regroupés en deux parties (les trois premiers puis les deux derniers). Une dernière partie est consacrée aux preuves de résultats techniques qui ont été annoncés dans les articles sans démonstration, faute de place (certains d'entre eux ne sont que des adaptations de précédents résultats).

Suit maintenant une série de rappels sur la mécanique quantique relativiste puis une présentation du modèle BDF ainsi que des principaux outils utilisés. Ceux-ci sont rappelés dans les articles. On a fait le choix de les exposer en introduction afin que le lecteur puisse passer plus rapidement les explications correspondantes dans les articles.

Chapitre 1

Rappels de mécanique quantique

1.1 Généralités

Les deux modèles présentés dans les parties 1.1.4 et 1.1.5 reviendront plusieurs fois dans l'exposé.

1.1.1 Postulats

La théorie quantique s'est développée au début du XXème siècle partant des études sur l'interaction entre le rayonnement et la matière ainsi que sur la constitution même de la matière. Certains faits demeuraient inexplicables si l'on se tenait à la théorie classique qui s'appuyait sur les lois de Newton. On a l'habitude de marquer le début de la mécanique quantique par la publication d'un article de Planck en 1900, proposant une explication du rayonnement du corps noir, corps idéal absorbant toute la lumière qu'il reçoit.

Nous n'en dirons pas plus sur les débuts de la théorie et renvoyons le lecteur intéressé à [Gri84]. Notons simplement que l'on se rendit compte alors que la lumière et les constituants de la matière se comportaient tantôt comme une onde tantôt comme une particule. Ainsi le caractère ondulatoire des électrons peut être mis en évidence lors d'une expérience de diffraction d'un faisceau de telles particules à travers un réseau cristallin (expérience [1] de Davisson-Germer 1927).

En mécanique quantique, l'état de l'électron est représenté par sa fonction d'onde. Il s'agit d'une fonction de l'espace et son évolution dans le temps est régie par la fameuse équation de Schrödinger (voir (1.1)). Mais commençons d'abord à rappeler les postulats de la mécanique quantique ainsi que son formalisme.

1. À tout système physique est associé un espace de Hilbert $(\mathcal{H}, \langle \cdot\,,\,\cdot \rangle)$. L'état du système est défini à chaque instant par un vecteur normé $\psi \in \mathcal{H}$, unique à une phase près. D'un point de vue géométrique il est équivalent de dire que l'espace des états est l'espace projectif $\mathcal{P}(\mathcal{H})$ de l'espace de Hilbert.
2. À toute grandeur physique A est associé un opérateur linéaire *autoadjoint* [2] $\widetilde{A}$ de $\mathcal{H}$. Une mesure de A ne peut donner qu'une valeur propre de l'opérateur $\widetilde{A}$, appelée observable associée à la grandeur A. Si ψ est l'état du système, la probabilité que la mesure donne μ est le carré de la norme

$$\|P_\mu \psi\|^2,$$

où P_μ est le projecteur spectral de $\widetilde{A}$ sur la valeur propre μ. Juste après la mesure ayant donnée μ, l'état du système est exactement

$$\frac{P_\mu \psi}{\|P_\mu \psi\|} \in \mathcal{H}.$$

Dans le cas d'un spectre continu, on ne peut que donner les probabilités de présence dans des plages de valeur [3] $[\mu, \mu + \delta\mu[$.

1. À noter que cette expérience ne fut pas d'abord interprétée en ces termes
2. Dans la littérature physique la notation $\widehat{A}$ est plutôt utilisée, nous avons préféré réserver cette notation à la transformée de Fourier pour éviter toute confusion ultérieure.
3. La formule de la probabilité de donner une valeur situé dans $[\mu, \mu + \delta\mu[$ utilise le théorème spectral [RS75, Vol I, Chap. VII-VIII] et la notion de mesure spectrale.

La valeur moyenne $\langle a\rangle$ de la mesure de A dans un système d'état ψ est donnée par le produit scalaire suivant :

$$\langle a\rangle = \langle \psi\,,\,\widetilde{A}\psi\rangle.$$

3. Tant qu'aucune mesure n'est faite, l'évolution de l'état dans le temps $\psi(t)$ satisfait à l'équation de Schrödinger :

$$i\hbar\partial_t\psi(t) = \widetilde{H}\psi(t), \tag{1.1}$$

où $\widetilde{H}$ est l'observable d'énergie (hamiltonien du système) et $\hbar$ la constante de Planck réduite :

$$\hbar = \frac{h}{2\pi}. \tag{1.2}$$

Le procédé de correspondance mesure-observable est appelé *quantification.*

1.1.2 Exemple d'une particule massive

Considérons le cas d'une particule (disons de masse m). L'espace de Hilbert à considérer est l'ensemble des fonctions de carré intégrable $L^2(\mathbb{R}^3)$ à valeur dans $\mathbb{C}^s$ où $s \in \mathbb{N}^*$. La valeur de s rend compte d'éventuel degré de liberté interne, tel le spin. Un vecteur normalisé de $L^2(\mathbb{R}^3)$ est appelée fonction d'onde.

Soit $\psi \in L^2(\mathbb{R}^3)$ une telle fonction. La mesure $|\psi(x)|^2dx$ s'interprète comme la probabilité de présence de la particule : sa probabilité d'être dans une zone $\mathcal{V}$ est donnée par la quantité $\int_{\mathcal{V}} |\psi(x)|^2dx$. En particulier il n'existe pas de trajectoire précise de la particule.

Aux positions x^1, x^2, x^3 de la particule suivant les trois axes d'un repère sont associées les opérateurs de multiplication par x^1, x^2, x^3 :

$$\widetilde{X^j}\psi(x) = x^j\psi(x),\ x \in \mathbb{R}^3,\ j \in \{1,2,3\}. \tag{1.3}$$

Les impulsions p^1, p^2, p^3 sont associées elles aux opérateurs de dérivations $-i\hbar\partial_{x^j}$:

$$\widetilde{P^j}\psi(x) = -i\hbar\partial_{x^j}\psi(x),\ x \in \mathbb{R}^3,\ j \in \{1,2,3\}. \tag{1.4}$$

Supposons que la particule soit placé dans un potentiel $V(x)$ fonction de la position $x = (x^1, x^2, x^3)$. L'hamiltonien classique est

$$H = \frac{p^2}{2m} + V(x)$$

où bien sûr $p = (p^1, p^2, p^3)$. Utilisant les correspondances ci-dessus, l'observable associée à l'hamiltonien est

$$\widetilde{H} = -\frac{\hbar^2}{2m}\Delta + V(x). \tag{1.5}$$

L'énergie E est associé à l'opérateur $i\hbar\partial_t$. La conservation de l'énergie au cours du temps transposée aux observables donne l'équation de Schrödinger (1.1). Ici, on obtient

$$i\hbar\partial_t\psi(x,t) = -\frac{\hbar^2}{2m_e}\Delta\psi(x,t) + V(x)\psi(x,t). \tag{1.6}$$

Cette équation implique notamment que la fonction $\rho(x,t) = |\psi(x,t)|^2$ satisfait une équation de conservation

$$\partial_t\rho + \mathrm{div}\,\vec{\jmath} = 0 \text{ avec } \vec{\jmath} = \frac{\hbar}{2mi}\big(\psi^*\nabla\psi - \psi\nabla\psi^*\big), \tag{1.7}$$

ce qui justifie l'interprétation de ρ comme densité de probabilité.

Une question fondamentale est celle de l'existence d'état stationnaire. Cela revient à rechercher les états propres de $\widetilde{H}$: si $\psi(x)$ est fonction propre de l'hamiltonien associée à la valeur propre λ, la fonction $\psi(x,t) = e^{-i\frac{\lambda}{\hbar}t}\psi(x)$ est solution de (1.6). De même on peut se demander s'il existe un état de plus basse énergie, dit fondamental. Mathématiquement la question est de savoir s'il existe un état atteignant

$$\inf\big\{\langle\psi\,,\,\widetilde{H}\psi\rangle,\ \psi \in L^2(\mathbb{R}^3),\ \|\psi\| = 1\big\}.$$

Remarque 1.1. Le potentiel $V(x)$ peut traduire plusieurs effets. Dans le cas présent, on considère surtout le potentiel électrostatique causée par des charges positives (par exemple les protons d'un noyau) dans l'espace sur les électrons de masse m_e et charge $-e$.

Dans l'approximation de Born-Oppenheimer, on étudie séparément le mouvement des noyaux et des électrons, supposant en première approximation que les protons sont immobiles lors du mouvement des électrons du fait de leur masse beaucoup plus élevée.

Ainsi on considère $V(x) = -Ze^2/(4\pi\varepsilon_0|x|)$ où ε_0 est la permittivité du vide et Z le nombre de protons du noyau dans le cas d'un atome situé à l'origine.

1.1.3 Systèmes à plusieurs particules

Considérons deux particules discernables, c'est-à-dire que l'on puisse distinguer l'une de l'autre (penser à deux atomes situés dans deux sites différents d'un réseau cristallin). La première particule est associée à l'espace $\mathcal{H}_1$ et la seconde à $\mathcal{H}_2$. L'espace de Hilbert $\mathcal{H}_{12}$ associé à l'union des deux systèmes doit pouvoir rendre compte des états de chacun d'eux, ces états étant *a priori* quelconques, l'un dans $\mathcal{H}_1$, l'autre dans $\mathcal{H}_2$ de manière décorrélée.

On peut ainsi prendre $\mathcal{H}_{12}$ comme étant le produit tensoriel $\mathcal{H}_1 \otimes \mathcal{H}_2$. Cette procédure s'apparente au produit cartésien des espaces de phases de deux particules en mécanique classique. Si on multiplie le nombre de particules, il faut considérer le produits tensoriel de tous les espaces correspondants.

La situation est tout autre pour des particules indiscernables, telles une assemblée d'électrons. Toutes ont des propriétés physiques semblables (charge $-e$, masse m_e) et aucune n'a de trajectoire précise susceptible de la distinguer. Rappelons que le principe de Pauli stipule que deux électrons (et généralement deux fermions de même type) ne peuvent avoir le même état. Dans ce cas, l'espace associé est le *produit extérieur* des espaces à une particule. Cela revient à se restreindre au sous-espace des fonctions d'onde antisymétriques dans le produit tensoriel.

Disons que l'on étudie un système à M électrons; on note $\mathcal{H} = L^2(\mathbb{R}^3)$ l'espace de Hilbert à un électron. Cet espace est isomorphe à $L^2(\mathbb{R}^3 \times [\![1, s]\!], \mathbb{C})$.

L'espace de Hilbert associé au système total est

$$\bigwedge_{1\leq j\leq M} L^2\big(\mathbb{R}^3 \times [\![1, s]\!]\big) \simeq L^2_a\big((\mathbb{R}^3 \times [\![1, s]\!])^M, \mathbb{C}\big) \subset L^2\big((\mathbb{R}^3 \times [\![1, s]\!])^M, \mathbb{C}\big),$$

où

$$L^2_a\big((\mathbb{R}^3 \times [\![1, s]\!])^M, \mathbb{C}\big) = \big\{\Psi\big((\mathbf{x}_i)_{1\leq i\leq M}\big),\ \mathbf{x}_i = (x_i, \sigma_i) \in \mathbb{R}^3 \times [\![1, s]\!],\ \forall\, \tau \in \mathcal{S}_M,\ \Psi\big((\mathbf{x}_{\tau(j)})\big) = \varepsilon(\tau)\Psi\big((\underline{x}_i)\big)\big\}.$$

En d'autres termes, pour tous $1 \leq j_1 < j_2 \leq M$ et $\mathbf{x} \in (\mathbb{R}^3 \times [\![1, s]\!])^M$ on a

$$\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_{j_2}, \ldots, \mathbf{x}_{j_1}, \ldots, \mathbf{x}_M) = -\Psi(\mathbf{x}_1, \ldots, \mathbf{x}_{j_1}, \ldots, \mathbf{x}_{j_2}, \ldots, \mathbf{x}_M).$$

Un hamiltonien est associé au système suivant une procédure systématique appelée *seconde quantification*. Nous renvoyons le lecteur à [LS10, chapitre 3] pour une présentation plus détaillée.

De manière informelle, on doit considérer la somme des énergies cinétiques, des énergies potentielles (associées au potentiel $V(x)$) et des énergies d'interaction des électrons entre eux. Dans la suite, on ne considère que les interactions électrostatiques des électrons entre eux. Cela donne

$$H_M = \sum_{1\leq j\leq M} \Big(-\frac{\hbar^2}{2m_e}\Delta_{x_j} + V(x_j)\Big) + \frac{e^2}{8\pi\varepsilon_0} \sum_{1\leq i<j\leq M} \frac{1}{|x_i - x_j|}. \tag{1.8}$$

Suivant la remarque 1.1, on prend $V(x) = -Ze^2/(4\pi\varepsilon_0|x|)$.

Comme précédemment, existe-t-il un état fondamental Ψ_0 ? Un tel état Ψ_0 doit vérifier

$$\langle \Psi_0\,,\, H_M\Psi_0\rangle = \inf\big\{\langle \Psi\,,\, H_M\Psi\rangle,\ \Psi \in L^2_a((\mathbb{R}^3)^M),\ \|\Psi\| = 1\big\} =: E_M.$$

Une conséquence du célèbre théorème HVZ (voir [Hun66, Win64, Zhi60] et [LS10, p.223-229]) permet de répondre.

Théorème 1.1. *Si $M < Z + 1$, alors il existe un état fondamental pour le système à M électrons.*

En fait le théorème [LS10, Théorème 12.2] stipule, dans ce cadre, la stabilité des atomes, des molécules neutres et des ions chargés positivement.

Nous présentons à présent une approximation du modèle revenant à se restreindre à un sous-ensemble des états admissibles : le modèle Hartree-Fock. Celui-ci a été introduit pour ses intérêts pratiques [4], mais nous l'exposons ici car il sert de référence pour le modèle BDF.

Remarque 1.2. Pour simplifier les formules, on se place dans les unités atomiques dans lesquelles $m_e = \hbar = (4\pi\varepsilon_0)^{-1} = 1$. Nous prenons aussi $e^2 = 1$. Après réduction on obtient

$$H_M = \sum_{1\le j\le M} \big(-\frac{\Delta_{x_j}}{2} - \frac{Z}{|x_j|}\big) + \frac{1}{2} \sum_{1\le i<j\le M} \frac{1}{|x_i - x_j|} \tag{1.9}$$

1.1.4 Le modèle Hartree-Fock

On reprend l'hamiltonien (1.9) et on étudie le problème variationnel restreint aux *déterminants de Slater*. Ce sont les fonctions Ψ_{sd} s'écrivant sous la forme

$$\bigwedge_{1\le j\le M} \psi_j \ \big((x_i, s_i)_{1\le i\le M}\big) := \frac{1}{\sqrt{M!}} \det\big(\psi_j(x_i, s_i)\big)_{1\le i,j\le M}$$

où $(\psi_j)_j$ est une famille orthonormale de l'espace à une particule $L^2(\mathbb{R}^3, \mathbb{C}^s)$, $x_i \in \mathbb{R}^3$ et $s_i \in [|1, s|]$.

Dans le cas $M = 2$, un déterminant de Slater s'écrit

$$\Psi_{sd}\big((x_1, s_1), (x_2, s_2)\big) \frac{1}{\sqrt{2}} \big(\psi_1(x_1, s_1)\psi_2(x_2, s_2) - \psi_1(x_2, s_2)\psi_2(x_1, s_1)\big).$$

Dans cette partie nous prenons $s = 1$ pour simplifier et notons $\underline{x} = (x_1, \dots, x_M) \in (\mathbb{R}^3)^M$.

D'un point de vue physique, cette approximation revient à supposer que les électrons n'interagissent pas entre eux mais sont soumis au champ «moyen» qu'ils créent collectivement, d'où son autre nom d'approximation de champ moyen.

L'expression de l'énergie $\langle \Psi_{sd} \,,\, H_M \Psi_{sd}\rangle$ se simplifie grandement et se réécrit en fonction de sa matrice de densité à un corps [5], $\gamma_{\Psi_{sd}}$.

Pour un état $\Psi(\underline{x})$, on définit l'opérateur positif γ_Ψ par son noyau intégral :

$$\Gamma_\Psi(x', y') := M \iint_{(\mathbb{R}^3)^{M-1}} \Psi(x', x_2, \dots, x_M)\Psi(y', x_2, \dots, x_M)^* dx_2 \cdots dx_M.$$

La densité ρ_Ψ de l'état $\Psi(\underline{x})$ est donnée par la formule

$$\rho_\Psi(x) := \Gamma_\Psi(x, x),\ x \in \mathbb{R}^3$$

La densité étant fonction de Γ_Ψ on écrira aussi ρ_{Γ_Ψ}.

Dans le cas d'un déterminant de Slater $\Gamma_{\Psi_{sd}}$ est le projecteur orthogonal sur le sous-espace engendré par les ψ_j :

$$\Gamma_{\Psi_{sd}} = \sum_{1\le j\le M} |\psi_j\rangle\langle\psi_j|,$$

et la densité vaut

$$\rho_{\Psi_{sd}}(x) = \sum_{1\le j\le M} |\psi_j(x)|^2.$$

Un simple calcul donne

$$\langle \Psi_{sd} \,,\, H_M \Psi_{sd}\rangle = \mathrm{Tr}\Big(\big(-\frac{1}{2}\Delta_{\mathbb{R}^3} - \frac{Z}{|\cdot|}\big)\Gamma_{\Psi_{sd}}\Big) + \frac{1}{2}\Big(D(\rho_{\Gamma_{\Psi_{sd}}}, \rho_{\Gamma_{\Psi_{sd}}}) - \|\Gamma_{\Psi_{sd}}\|^2_{\mathrm{Ex}}\Big), \tag{1.10}$$

4. À ce propos voir [CBM06].
5. [LS10, chapitre 1]

où $D(\rho_{\Gamma_{\Psi_{sd}}}, \rho_{\Gamma_{\Psi_{sd}}})$ et $\|\Gamma_{\Psi_{sd}}\|^2_{\mathrm{Ex}}$ sont appelés respectivement terme direct et terme d'échange et sont définies par les formules suivantes

$$D(\rho,\rho) := \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\rho(x)^*\rho(y)}{|x-y|} dxdy \text{ et } \|\Gamma\|^2_{\mathrm{Ex}} := \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\Gamma(x,y)|^2}{|x-y|} dxdy. \tag{1.11}$$

Existe-t-il des états de plus basse énergie ? On retrouve un résultat analogue au théorème 1.1 et on peut aussi statuer sur les ions chargés négativement.

Théorème 1.2 (Lieb, Simon '77)**.** *Pour $M < Z+1$, il existe un état de plus basse énergie pour le problème variationnel de Hartree-Fock à M électrons.*

Theorem 1.1 (Lieb '82)**.** *Pour $M \geq 2Z+1$, il n'y a pas d'état fondamental pour le problème à M électrons.*

Ce dernier théorème, énoncé dans [Lie84], a été amélioré (citons [Sol03] et [Nam12]).

Forme d'un minimiseur

Intéressons-nous au minimiseur du problème H_M. De la même façon qu'un état pour le système d'un électron peut être vu comme une droite complexe dans $L^2(\mathbb{R}^3)$, on peut voir l'état d'un déterminant de Slater comme un sous-espace de $L^2(\mathbb{R}^3)$ de dimension M, en d'autres termes comme un élément de la grassmannienne $\mathcal{G}_M\big(L^2(\mathbb{R}^3)\big)$. Cette correspondance est bijective.

Identifiant un espace et son projecteur orthogonal, on munit la grassmannienne de la métrique

$$\mathrm{dist}\big(\Pi_1,\Pi_2\big)^2 := \iint_{\mathbb{R}^3\times\mathbb{R}^3} \big|\mathrm{Proj}\,(\Pi_1)(x,y) - \mathrm{Proj}\,(\Pi_2)(x,y)\big|^2 dxdy,$$

où $\mathrm{Proj}\,(\Pi_j)$ est le projecteur orthogonal sur le sous-espace Π_j.

Rappelons que cette métrique est issue de la norme de Hilbert-Schmidt, $\|\cdot\|_{\mathfrak{S}_2}$ où l'espace $\mathfrak{S}_2$ désigne l'ensemble des opérateurs compacts Q dans $\mathcal{B}(L^2(\mathbb{R}^3))$ dont le noyau intégral $Q(x,y)$ est dans $L^2(\mathbb{R}^3\times\mathbb{R}^3)$.

Cela fait de cette grassmanienne une variété de Hilbert dans $\mathfrak{S}_2(\mathbb{R}^3)$.

Ainsi un minimiseur Γ de la fonctionnelle d'énergie (1.10) satisfait les équations d'Euler-lagrange :

$$\big[H_\Gamma, \Gamma\big] = 0, \tag{1.12a}$$

$$H_\Gamma = -\frac{1}{2}\Delta - \tfrac{Z}{|\cdot|} + \rho_\Gamma * \tfrac{1}{|\cdot|} - \frac{\Gamma(x,y)}{|x-y|}. \tag{1.12b}$$

Cet opérateur H_Γ est appelé *opérateur de champ moyen.* Les conditions de second ordre imposent que l'image de Γ soit engendrée par des vecteurs propres associés aux plus petites valeurs propres de l'opérateur H_Γ.

Nous verrons que le modèle BDF, qui est aussi une approximation de champ moyen, présente une structure géométrique analogue.

La section suivante est consacrée aux polarons, systèmes constitués de l'interaction d'électrons avec un cristal.

1.1.5 Le modèle de Pekar-Tomasevitch

Étudions le cas d'un électron au sein d'un milieu polarisable, supposé homogène. La situation est par exemple celle d'un électron additionnel dans un réseau d'ions. L'homogénéité du milieu suppose ici que les dimensions de l'électron sont grandes devant la maille du réseau. Comme expliqué au début de l'article [LR12], le système présente une énergie effective de la forme

$$\mathcal{E}_{PT}(\psi) = \|\nabla\psi\|^2_{L^2} - D\big(|\psi|^2, |\psi|^2\big), \tag{1.13}$$

où ψ est la fonction d'onde de l'électron.

Remarque 1.3. Cette énergie apparaît dans diverses situations physiques et l'équation variationnelle correspondante possède plusieurs noms dont Schrödinger-Newton et Choquard-Pekar. L'énergie elle-même sera dite ici de Pekar-Tomasevitch [6] suivant [FLST11].

6. Dans le cas d'un seul électron, elle sera dite parfois de Choquard-Pekar (notamment dans le premier article [Sok14b])

Le polaron est stable, il admet un état fondamental. Comme dit en introduction, cela est dû à la déformation du milieu polarisable : l'électron crée son propre trou dans le milieu agrégeant autour de lui un nuage de charge positive.

Le résultat demeure-t-il dans le cas de plusieurs électrons ? Ces derniers interagissent avec le milieu mais se repoussent l'un l'autre.

Un état du système étant toujours donné par une fonction normalisée $\Psi \in L^2_a(\mathbb{R}^3)$, l'énergie s'écrit [FLST11] :

$$\mathcal{E}^{(U,\widetilde{\alpha})}_{\mathrm{PT}}[\Psi] = \mathrm{Tr}\big(-\Delta\Gamma_\Psi\big) + U\big(D(\rho_\Psi,\rho_\Psi) - \|\Gamma_\Psi\|^2_{\mathrm{Ex}}\big) - \widetilde{\alpha}D\big(\rho_\Psi,\rho_\Psi\big), \tag{1.14}$$

où $U > 0$ est la force de la répulsion coulombienne et $\widetilde{\alpha} > 0$ la constante de couplage avec le milieu. Par un changement d'échelle [7] on peut toujours supposer $\widetilde{\alpha} = 1$ quitte à remplacer U par $\frac{U}{\widetilde{\alpha}}$. Nous considérons donc

$$\mathcal{E}^{U}_{\mathrm{PT}}[\Psi] = \mathrm{Tr}\big(-\Delta\Gamma_\Psi\big) + U\big(D(\rho_\Psi,\rho_\Psi) - \|\Gamma_\Psi\|^2_{\mathrm{Ex}}\big) - D\big(\rho_\Psi,\rho_\Psi\big). \tag{1.15}$$

Notation 1.1. On note l'infimum :

$$E^U_{\mathrm{PT}}(M) = \inf\big\{\mathcal{E}^U_{\mathrm{PT}}[\Psi],\ \Psi \in L^2_a\big((\mathbb{R}^3)^M\big)\big\}. \tag{1.16}$$

Rassemblant des résultats de [Lie77] et de [FLST11], on obtient les théorèmes suivants.

Théorème 1.3 (Lieb '77)**.** *Il existe un minimiseur du problème $E_{PT}(1)$ associé à la fonctionnelle* (1.13), *qu'on peut choisir positif et radial décroissant. C'est le seul à translation et spin (dans $\mathbb{S}^{s-1}$) près.*

Théorème 1.4 (Frank, Lieb, Seiringer, Thomas '11)**.** *Il existe une valeur critique $U_c > 0$ de U au dessus de laquelle le problème $E^U_{PT}(M)$ n'a pas de minimiseur quelle que soit la valeur de l'entier $M \geq 2$. De plus, on a l'estimation* $0 < U_c \leq 29,4$.

Remarque 1.4. Pour $E^U_{\mathrm{PT}}(1)$, l'ensemble des minimiseurs forme ainsi une sous-variété de $L^2(\mathbb{R}^3, \mathbb{C}^s)$ isomorphe à

$$\mathbb{R}^3 \times \mathbb{S}^{s-1}.$$

Considérant l'unique minimiseur $\psi_{CP}(x)$ radial positif parallèle à ${}^t(1,0,\ldots,0) \in \mathbb{C}^s$, tous les minimiseurs s'écrivent sous la forme

$$\mathcal{U}\psi_{CP}\big(x - x_0\big),\ \mathcal{U} \in \mathbf{U}(s),\ x_0 \in \mathbb{R}^3.$$

1.2 La mécanique quantique relativiste

1.2.1 Opérateur de Dirac

Dans les années 1920, Dirac essaya d'intégrer la relativité en mécanique quantique, et plus précisément de décrire un électron relativiste. Partant de la formule de l'énergie de la particule libre

$$E^2 = m_e^2c^4 + c^2p^2,$$

les mêmes règles de substitution décrites auparavant conduisent à l'équation de Klein-Gordon que doit suivre la fonction d'onde de l'électron $\psi(x,t)$:

$$-\hbar^2\partial_t^2\psi(x;t) = \big(-c^2\hbar^2\Delta + m_e^2c^4\big)\psi(x,t). \tag{1.17}$$

Cette équation pose problème lorsqu'on essaie d'en tirer une équation de conservation d'une quantité ρ *positive*, perdant alors l'interprération probabiliste.

L'idée de Dirac fut de chercher une équation aux dérivées partielles d'ordre 1 en (x,t) dont les solutions sont aussi solutions de (1.17). Il considéra

$$\frac{1}{c}\partial_t\psi + \sum_{k=1}^{3}\alpha_k\partial_{x^k}\psi + i\frac{m_ec}{\hbar}\beta\psi = 0. \tag{1.18}$$

Prenant une solution ψ de (1.18), il faut choisir β et les α_k de telle sorte qu'on ait les propriétés suivantes :

7. Écrivant $\Psi(x) = \lambda^{-3/2}\Psi'(x/\lambda)$ avec $\lambda > 0$, on réécrit l'énergie en fonction de Ψ'.

1. $|\psi|^2$ satisfait toujours une équation de conservation,
2. la fonction ψ est solution de (1.17),
3. l'équation (1.18) est invariante par les transformations du groupe de Lorentz [8].

Un tel choix est possible à condition de supposer que ces objets sont des matrices. Habituellement on prend

$$\beta := \begin{pmatrix} I_{\mathbb{C}^2} & 0 \\ 0 & -I_{\mathbb{C}^2} \end{pmatrix}, \ \alpha_k := \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix} \in \mathbb{C}^{4\times 4}, \ k \in \{1,2,3\}, \tag{1.19}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \in \mathbb{C}^{2\times 2}. \tag{1.20}$$

Les matrices σ_k sont les *matrices de Pauli*. On peut réécrire (1.18) sous la forme

$$i\hbar\partial_t\psi = D_0\psi,$$

où

$$D_0 = -i\hbar c\sum_{k=1}^{3}\alpha_k\partial_{x^k} + m_e c^2\beta = -i\hbar c\boldsymbol{\alpha}\cdot\nabla + m_e c^2\beta. \tag{1.21}$$

L'opérateur D_0 est l'opérateur de Dirac et s'interprète comme l'hamiltonien de l'électron libre. En particulier l'énergie cinétique T_ψ d'un électron dans l'état ψ est donnée par le produit scalaire

$$T_\psi = \langle D_0\psi\,,\,\psi\rangle. \tag{1.22}$$

D'un point de vue mathématique, l'opérateur D_0 est un opérateur auto-adjoint agissant sur les spineurs $L^2(\mathbb{R}^3,\mathbb{C}^4)$ de domaine $H^{1/2}(\mathbb{R}^3,\mathbb{C}^4)$. Son spectre est

$$\sigma(D_0) =]-\infty, -m_e c^2] \cup [m_e c^2, +\infty[.$$

Cela pose un grave problème dans l'égalité (1.22) car comment comprendre les états d'énergie négative, en nombre infini ? À quoi correspond un état fondamental ? L'interprétation de Dirac fut la suivante. Le vide [9] est constitué en fait d'une infinité d'électrons virtuels, chacun occupant un état d'énergie négative. Ces derniers remplissent l'espace de manière uniforme de telle sorte qu'on ne puisse les observer, constituant la *mer de Dirac*. D'après le principe d'exclusion de Pauli, les électrons réels ne peuvent avoir qu'une énergie positive.

Le point de vue moderne, celui de l'électrodynamique quantique (QED), a délaissé cette vision, mais historiquement elle a permis de prédire l'existence du positron, l'antiparticule de l'électron.

En premier lieu elle implique que le vide est un milieu polarisable. Lorsqu'on établit un champ électrostatique rendu de plus en plus intense, un électron virtuel peut passer à un état d'énergie positive. On se retrouve alors avec un électron réel et l'*absence* d'un électron virtuel dans la mer de Dirac. De manière équivalente l'absence d'électron d'énergie négative peut se voir comme la présence d'une particule de même masse mais de charge opposée (appelée positron). Elle forme avec l'électron une paire de particule-antiparticule [10].

Nous nous en tiendrons ici au point de vue de Dirac. Le vide libre est alors représenté par le projecteur spectral P_-^0

$$P_-^0 := \chi_{(-\infty,0)}(D_0). \tag{1.23}$$

Son image contient tous les états d'énergie négative et constitue la mer de Dirac libre. De même nous notons P_+^0 le projecteur spectral sur le spectre positif :

$$P_+^0 := \chi_{(0,+\infty)}(D_0). \tag{1.24}$$

Prendre en compte la réaction du vide suppose étudier un système avec nombre infini d'électrons «virtuels». C'est le point de départ du modèle BDF, exposé au chapitre suivant.

Nous terminons cette partie en présentant différentes symétries de l'opérateur D_0 et introduisons en particulier la *conjugaison de charge*.

8. comme doivent l'être les équations en relativité. Ces transformations traduisent dans les coordonnées les changements de référentiels inertiels en relativité restreinte.
9. Dirac (1934)«We make the assumption that, in the world as we know it, nearly all the states of negative energy for the electrons are occupied, with just one electron in each state, and that a uniform filling of all the negative-energy states is completely unobservable to us».
10. En QED, un positron est vu comme un électron se dirigeant vers le passé : voir [GR94, Chapitre 2]

1.2.2 Symétries de l'opérateur de Dirac

Conjugaison de charge

La symétrie entre positron et électron peut se voir de manière plus formelle. La conjugaison de charge C envoie les états de l'un sur ceux de l'autre. Il s'agit d'un opérateur anti-linéaire et isométrique de $L^2(\mathbb{R}^3, \mathbb{C}^4)$, qui au spineur $\psi = (\psi_k)_{k=1}^4$ associe

$$\mathrm{C} : \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \mapsto \begin{pmatrix} \overline{\psi_4} \\ -\overline{\psi_3} \\ -\overline{\psi_2} \\ \overline{\psi_1} \end{pmatrix}, \tag{1.25}$$

où $\overline{\psi_j}$ désigne le complexe conjugué de ψ_j ; en notation contractée on écrit $\mathrm{C}\psi = i\beta\alpha_2\overline{\psi}$. Notons que C est aussi une isométrie ponctuelle au sens où pour tout $x \in \mathbb{R}^3$, on a

$$|\mathrm{C}\psi(x)|^2 = |\psi(x)|^2. \tag{1.26}$$

En particulier, cet opérateur envoie le sous-espace $\mathrm{Im}(P_-^0)$ sur $\mathrm{Im}(P_+^0)$, c'est-à-dire envoie les états du vide libre sur les états d'énergie positive et on a $-\mathrm{C}D_0\mathrm{C}^{-1} = D_0$. Cette symétrie demeure dans un champ électromagnétique, représenté par son potentiel scalaire ϕ_{el} et son vecteur potentiel $\overrightarrow{A}$ [Tha92, partie 1.4.6]. L'opérateur de Dirac pour une particule de masse m et charge e dans le champ s'écrit

$$H(e) = c\boldsymbol{\alpha} \cdot \big(- i\nabla - \frac{e}{c}\overrightarrow{A}(t,x)\big) + \beta mc^2 + e\phi_{el}(t,x).$$

On a $-\mathrm{C}H(e)\mathrm{C} = H(-e)$ de telle sorte que la conjugaison de charge relie les états d'énergie négative pour $H(e)$ à ceux d'énergie positive pour $H(-e)$, l'opérateur de Dirac pour une particule de même masse et de charge opposée.

Si $\psi_0(t)$ est solution de $i\hbar\partial_t\psi(t) = H(e)\psi(t)$, alors $\mathrm{C}\psi_0(t)$ est solution de $i\hbar\partial_t\psi(t) = H(-e)\psi(t)$, et l'égalité (1.26) montre que l'on ne peut distinguer les mouvements de $\psi_0(t)$ de ceux de $\mathrm{C}\psi_0(t)$.

L'action de SU(2)

En mécanique quantique, l'hamiltonien libre $\frac{-\hbar^2}{2m}\Delta$ est invariant par les rotations de l'espace.

L'analogue en mécanique quantique relativiste est l'invariance de D_0 par l'action de SU(2), le groupe spécial unitaire de $\mathbb{C}^2$. Cette action est liée aux opérateurs de moments angulaires [Tha92, partie 1.3.3].

Le moment angulaire orbital est

$$\mathbf{L} = \widetilde{X} \wedge \widetilde{P} = \big(- i\hbar(x^k\partial_{x^\ell} - x^\ell\partial_{x^k})\big)_{1\le j\le 3}, \tag{1.27}$$

où (j,k,ℓ) vaut $(1,2,3)$, $(2,3,1)$ et $(3,1,2)$. Le moment de spin $\mathbf{S}$ et le moment total $\mathbf{J}$ sont définis par

$$\mathbf{S} = -\frac{i}{4}\boldsymbol{\alpha} \wedge \boldsymbol{\alpha} = \left(\begin{pmatrix} \sigma_k & 0 \\ 0 & \sigma_k \end{pmatrix}\right)_{1\le k\le 3} \text{ et } \mathbf{J} := \mathbf{L} + \mathbf{S}. \tag{1.28}$$

Les opérateurs $-iJ_1, -iJ_2$ et $-iJ_3$ constituent une représentation de l'algèbre de Lie $\mathfrak{su}(2)$ induisant la représentation unitaire $\Phi_{\mathrm{SU}} : \mathrm{SU}(2) \to \mathbf{U}(L^2)$ [Tha92, partie 4.6.1]

$$e^{-i\phi\mathbf{J}\cdot n}\psi(x) = e^{-i\phi\mathbf{S}\cdot n}\psi\big(R_{\phi,n}^{-1}x\big),\ \phi \in [0, 4\pi) \tag{1.29}$$

où $R_{\phi,n}$ est la rotation de $\mathbb{R}^3$ d'axe $n \in \mathbb{S}^2$ et d'angle ϕ.

L'opérateur D_0 est invariant par l'action du groupe : pour tout élément U dans l'image $\mathrm{Im}(\Phi_{\mathrm{SU}})$ on a

$$UD_0U^{-1} = D_0.$$

Aidé de [Tha92, partie 4.4.6], on peut étudier les sous-représentations irréductibles de Φ_{SU}. Cela est fait dans le chapitre 7 et une telle sous-représentation est associée à deux nombres : une valeur propre de $\mathbf{J}^2$ et une valeur propre de l'opérateur de spin-orbite $\mathbf{K}$ définit comme suit :

$$\mathbf{K} := \beta\big(2\mathbf{S}\cdot\mathbf{L} + 1\big). \tag{1.30}$$

Renversement temporel et structure symplectique

Il existe une autre symétrie envoyant $\mathrm{Im}(P_-^0)$ sur $\mathrm{Im}(P_+^0)$. Elle est donnée par l'action sur les spineurs de la matrice

$$\mathrm{I_s} = \begin{pmatrix} 0 & -\mathrm{I}_{\mathbb{C}^2} \\ \mathrm{I}_{\mathbb{C}^2} & 0 \end{pmatrix}.$$

L'opérateur $\mathrm{L}_T := i\mathrm{I_s}$ est l'opérateur de renversement temporel [Tha92, partie 2.5.7] dans l'espace des spineurs [11].

Ici reprenons l'exemple de la partie (1.2.2) d'une particule chargée dans un champ électromagnétique : sa fonction d'onde ψ_0 vérifie l'équation de Dirac $i\hbar\partial_t\psi = H(e)\psi$.

La fonction d'onde $\mathrm{L}_T\psi_0$ satisfait alors l'équation $-i\hbar\partial_t\psi = H(-e)\psi$, représentant l'évolution d'une particule de charge oppposée qui remonte le temps.

Le fait que $\mathrm{A} : \mathrm{Im}(P_\pm^0) \to \mathrm{Im}(P_\mp^0)$ avec $\mathrm{A} \in \{\mathrm{I_s}, \mathrm{C}\}$ est une isométrie n'est pas difficile à montrer. Des équations $P_\pm^0 f = f$, on obtient

$$\begin{cases} f = \begin{pmatrix} f_\uparrow \\ f_\downarrow \end{pmatrix} \in \mathrm{Im}(P_-^0) \cap L^2(\mathbb{R}^3, \mathbb{C}^2) \oplus L^2(\mathbb{R}^3, \mathbb{C}^2) & \iff \quad f_\uparrow = \frac{i\boldsymbol{\sigma}\cdot\nabla}{1+|D_0|} f_\downarrow, \\ f = \begin{pmatrix} f_\uparrow \\ f_\downarrow \end{pmatrix} \in \mathrm{Im}(P_+^0) \cap L^2(\mathbb{R}^3, \mathbb{C}^2) \oplus L^2(\mathbb{R}^3, \mathbb{C}^2) & \iff \quad f_\downarrow = -\frac{i\boldsymbol{\sigma}\cdot\nabla}{1+|D_0|} f_\uparrow, \end{cases} \tag{1.31}$$

où on a décomposé f en spineur haut et spineur bas (tous deux dans $L^2(\mathbb{R}^3, \mathbb{C}^2)$).

Il est alors clair que

$$f \in \mathrm{Im}(P_\pm^0) \iff \mathrm{I_s} f \in \mathrm{Im}(P_\mp^0), \text{ idem pour C.}$$

Soulignons aussi les faits suivants : $-\mathrm{I_s} D_0 \mathrm{I_s}^{-1} = D_0$ et $|\mathrm{I_s}\psi(x)|^2 = |\psi(x)|^2$.

La matrice $\mathrm{I_s}$ vérifie également

$$\mathrm{I_s}^2 = -1,$$

conférant à $L^2(\mathbb{R}^3, \mathbb{C}^4)$ une structure presque complexe. En toute rigueur, il faudrait se placer sur un espace de Hilbert *réel*, mais tel est le cas pour $L^2(\mathbb{R}^3, \mathbb{C}^4)$ si on le munit du produit scalaire $\mathfrak{Re}\langle \cdot\,,\,\cdot\rangle$. Elle lui confère aussi une structure symplectique par la 2-forme (c-à-d bilinéaire antisymétrique)

$$\forall\, f, g \in L^2(\mathbb{R}^3, \mathbb{C}^4),\ \omega_{\mathrm{I_s}}(f, g) := \mathfrak{Re}\langle f\,,\, \mathrm{I_s} g\rangle.$$

De ce point de vue, le sous-espace $\mathrm{Im}(P_-^0)$ est une lagrangienne pour $\omega_{\mathrm{I_s}}$, c'est-à-dire qu'il est son propre orthogonal selon la 2-forme $\omega_{\mathrm{I_s}}$.

Ces remarques sur $\mathrm{I_s}$ ne sont données qu'à titre indicatif, nous n'utiliserons pas ces structures géométriques. La matrice $\mathrm{I_s}$ est utilisée dans la dernière partie pour trouver un état de *para-positronium*, système méta-stable constitué d'un électron et d'un positron de spins opposés. Il est possible de traduire le raisonnement de l'article en termes géométriques, utilisant la notion d'indice de Maslov [Fur04].

11. vu comme représentation du groupe de Poincaré.

Chapitre 2

Le modèle BDF

Notation 2.1. Pour simplifier les notations, on écrit $\mathfrak{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$. Suivant [Tha92, chapitre 10], on considère une décomposition orthogonale $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$ où les sous-espaces $\mathfrak{H}_\pm$ sont de dimension infinie. Dans l'idée, $\mathcal{F}_+^{(1)} = \mathfrak{H}_+$ est l'espace de Hilbert d'une particule et $\mathcal{F}_-^{(1)} = \mathrm{C}\mathfrak{H}_-$ celui d'une antiparticule. On prendra ici

$$\mathfrak{H}_\pm = \mathrm{Im}(P_\pm^0).$$

Notation 2.2. On se place dans le système d'unités où les constantes $\hbar, 4\pi\varepsilon_0$ et c sont fixées à 1. Nous gardons la charge élémentaire e, dans le modèle celle-ci n'apparaît qu'à travers la constante de structure fine α qui physiquement vaut

$$\alpha = \frac{e^2}{\hbar c 4\pi\varepsilon_0} \approx \frac{1}{137}.$$

Ici $\alpha > 0$ est considéré comme un paramètre du modèle, toujours de petite valeur.

2.1 Description du modèle

2.1.1 Définition de l'énergie

Le but est de décrire des électrons relativistes en interaction avec le vide polarisé, en présence d'un champ électrostatique et on néglige l'action des photons. Il s'agit d'une approximation de l'électrodynamique quantique (QED).

En QED, le nombre de particules n'est plus invariant et peut fluctuer au gré de créations spontanées de paires particule-antiparticule. Formellement, l'espace de Hilbert d'un système électronique est l'*espace de Fock*, noté $\mathcal{F}_{el}$. On peut le définir comme

$$\begin{cases} \mathcal{F}_{el} & := \bigoplus_{n,m\in\mathbb{N}} \mathcal{F}^{(n,m)}, \\ \mathcal{F}^{(n,m)} & := \left(\mathcal{F}_+^{(1)}\right)^{\wedge n} \otimes \left(\mathcal{F}_-^{(1)}\right)^{\wedge m}, \end{cases} \tag{2.1}$$

où les deux espaces $\mathcal{F}_+^{(1)}$ et $\mathcal{F}_-^{(1)}$ sont définis ci-dessus (Notations (2.1)). L'espace $\mathcal{F}^{(n,m)}$ est l'espace à n électrons et m positrons. On associe à $\mathcal{F}_{el}$ un hamiltonien $\mathbb{H}$: son expression est compliquée et nous renvoyons le lecteur intéressé à [CI89], [HLS05a, Appendice] et [Gra11, chapitre II]. On ne prend en compte dans cet exposé que les interactions électrostatiques, en particulier $\mathbb{H}$ fait intervenir un potentiel électrostatique externe $\alpha\nu * \frac{1}{|\cdot|}$ où α est la constante de structure fine et ν la densité de charge externe (telle celle d'un noyau atomique).

Le modèle BDF consiste en la restriction de $\mathbb{H}$ à des états particuliers de $\mathcal{F}_{el}$, les états dits BDF. La définition précise de ces états fait appel aux opérateurs de création et d'annihilation : là encore nous renvoyons le lecteur aux articles pré-cités pour de plus amples détails. Retenons toutefois les faits suivants.

— Un état BDF est entièrement déterminé par sa matrice de densité à un corps $P \in \mathcal{B}(\mathfrak{H})$. Dans ce cas, l'opérateur P est un projecteur orthogonal de rang infini.

— Soit $(f_i)_{i\in\mathbb{N}}$ une base orthonormée (BON) d'un tel projecteur P. Il faut penser l'état comme un déterminant de Slater infini $f_1 \wedge f_2 \wedge \cdots$, représentant les électrons virtuels du vide et d'éventuels électrons réels.

— Pour qu'une projection orthogonale P représente un état BDF, il faut et il suffit que l'opérateur $Q = P - P_-^0$ soit de Hilbert-Schmidt, c-à-d que Q soit compact et que son noyau intégral satisfait

$$\iint |Q(x,y)|^2 dxdy < +\infty,$$

L'état BDF associé à P_-^0 est donné par un vecteur unitaire $\Omega_0 \in \mathcal{F}^{(0,0)}$.

À noter aussi une subtilité de taille : pour un état $\Omega \in \mathcal{F}_{el}$ l'énergie $\langle \Omega \,,\, \mathbb{H}\Omega\rangle_{\mathcal{F}_{el}}$ n'est pas bien définie. En un certain sens sa valeur est toujours $-\infty$! Les premières manipulations sont formelles, le but étant de parvenir à un modèle variationnel rigoureux.

De manière formelle donc on soustrait à l'énergie d'un état BDF Ω_P celle de l'état Ω_0 pris comme état de référence. Le projecteur P étant la matrice de densité à un corps de Ω_P, la différence donne une expression $\mathcal{E}(Q)$ de $Q = P - P_-^0$:

$$\mathcal{E}(Q) = \mathrm{Tr}\big(D_0 Q\big) - \alpha D\big(\nu, \rho_Q\big) + \frac{\alpha}{2}\Big(D(\rho_Q, \rho_Q) - \|Q\|_{\mathrm{Ex}}^2\Big), \tag{2.2}$$

où

$$\rho_Q(x) = \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big), \tag{2.3}$$

et les fonctions $D(\cdot,\cdot)$ et $\|\cdot\|_{\mathrm{Ex}}$ sont définies comme pour le modèle Hartree-Fock. Nous supposons naturellement que la densité ν est d'énergie électrostatique finie : $D(\nu,\nu) < +\infty$. On reconnaît la même décomposition que pour le modèle Hartree-Fock.

La fonction ρ_Q est la densité de Q. Sa formule n'est valide *a priori* que si Q est à trace ou localement à trace et pose problème quand Q est simplement de Hilbert-Schmidt.

Passons outre et supposons que les termes sont bien définis, en particulier que $D_0 Q$ est à trace. Des manipulations algébriques montrent qu'un minimiseur $\overline{P} = \overline{Q} + P_-^0$ doit satisfaire l'équation

$$\overline{P} = Q_0 + P_-^0 = \chi_{(-\infty,0)}\big(H_{Q_0}\big). \tag{2.4}$$

où H_Q est l'*opérateur de champ moyen* associé à Q

$$H_Q = D_0 + \alpha\Big(\big(\rho_Q - \nu\big) * \frac{1}{|\cdot|} - \frac{Q(x,y)}{|x-y|}\Big). \tag{2.5}$$

On peut trouver la forme (2.4) en faisant un calcul perturbatif sans se soucier du sens. On a

$$\begin{aligned}\mathcal{E}\big(Q_0 + \delta Q\big) &= \mathcal{E}(Q_0) + \mathrm{Tr}\big(H_{Q_0}\,\delta Q\big) + \frac{\alpha}{2}\big(D(\rho_{\delta Q}, \rho_{\delta Q}) - \|\delta Q\|_{\mathrm{Ex}}^2\big)\\ &= \mathcal{E}(Q_0) + \mathrm{Tr}\big(H_{Q_0}\,\delta Q\big) + o(\delta Q).\end{aligned}$$

Pour $\delta Q = P - \overline{P}$ où P est un projecteur, on fait le calcul de la trace $\mathrm{Tr}\big(H_{Q_0}\delta Q\big)$ relativement à la décomposition $\mathrm{Ker}\,\overline{P} \oplus \mathrm{Im}\,\overline{P}$:

$$\begin{aligned}\mathrm{Tr}\big(H_{Q_0}\delta Q\big) &= \mathrm{Tr}\Big((1-\overline{P})H_{Q_0}\delta Q(1-\overline{P}) + \overline{P}H_{Q_0}\delta Q\overline{P}\Big),\\ &= \mathrm{Tr}\Big(|H_{Q_0}|\big((1-\overline{P})\delta Q(1-\overline{P}) - \overline{P}\delta Q\overline{P}\big)\Big),\\ &= \mathrm{Tr}\Big(|H_{Q_0}|(\delta Q)^2\Big) \geq 0.\end{aligned} \tag{2.6}$$

Le retour à l'Analyse est brutal. Dès que la charge externe ν n'est pas nulle, l'opérateur Q_0 de (2.4) n'est pas à trace. Pour rendre ces calculs valides une coupure en fréquence est nécessaire : au lieu de considérer l'espace $\mathfrak{H}$ en entier, on se restreint à

$$\mathfrak{H}_\Lambda := \big\{\psi \in \mathfrak{H},\ \mathrm{supp}\,\widehat{\psi} \subset B_{\mathbb{R}^3}(0,\Lambda)\big\}, \tag{2.7}$$

où $\Lambda > 0$ est le niveau de *cut-off* et $\widehat{\psi}$ désigne la transformée de Fourier de ψ.

Notation 2.3. Dans cet exposé, la transformée de Fourier $\mathscr{F}$ est définie selon la formule

$$\forall\, f \in L^1(\mathbb{R}^3),\ \widehat{f}(p) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(x) e^{-ix\cdot p} dx. \tag{2.8}$$

Gardant (2.6) à l'esprit, on étend alors la notion de trace de la manière suivante.

Definition 2.1. Soit P_0 un projecteur. Un opérateur de Hilbert-Schmidt Q est dit à P_0-trace si les deux applications P_0QP_0 et $(1-P_0)Q(1-P_0)$ sont à trace. Dans ce cas la P_0-trace de Q est

$$\mathrm{Tr}_{P_0}(Q) := \mathrm{Tr}\big(P_0QP_0 + (1-P_0)Q(1-P_0)\big).$$

Ici on prend bien sûr $P_0 := P^0_-$. Le cut-off impose qu'un opérateur Q à P^0_--trace satisfasse la condition

$$\mathrm{supp}\, \widehat{Q}(\cdot,\cdot) \subset B_{\mathbb{R}^3}(0,\Lambda) \times B_{\mathbb{R}^3}(0,\Lambda), \tag{2.9}$$

où $\widehat{Q}$ est la transformée de Fourier de Q. Dans ce cas on peut donner un sens à ρ_Q et au terme direct $D(\rho_Q,\rho_Q)$. Une première définition de l'énergie BDF est ainsi :

Definition 2.2 (Énergie BDF, première version)**.**
Soit P un projecteur tel que $Q := P - P^0_-$ est Hilbert-Schmidt et satisfait (2.9). L'énergie BDF de l'état Ω_P est

$$\mathcal{E}^{\nu}_{\mathrm{BDF}}(Q) := \mathrm{Tr}_0\big(D_0Q\big) - \alpha D(\nu,\rho_Q) + \frac{\alpha}{2}\Big(D(\rho_Q,\rho_Q) - \|Q\|^2_{\mathrm{Ex}}\Big). \tag{2.10}$$

C'est la définition choisie dans les articles [HLS05a, HLS05b]. Elle suppose que l'état fondamental du vide libre est P^0_- conformément à la vision de Dirac. Toutefois Hainzl, Lewin et Solovej ont montré dans [HLS07] que la situation était légèrement différente.

Prenant acte de la nécessité du cut-off, ils ont étudié le système dans une boîte de taille finie $[-L/2, L/2[^3$ (avec des conditions aux bords périodiques) et pris ensuite la limite $L \to +\infty$. En d'autres termes ils ont pris *la limite thermodynamique* du modèle. Cette procédure réduit le problème à un problème de dimension finie où l'énergie associé à l'hamiltonien correspondant $\mathbb{H}^{\nu}_L$ est une fonction bien définie. Le vide libre correspond à $\nu = 0$: pour L assez grand, ils ont montré l'existence d'un unique minimiseur $\mathcal{P}^0_L$. De plus, lorsque L tend vers l'infini, ce minimiseur tend (dans un certain sens) vers un projecteur $\mathcal{P}^0_- \in \mathcal{B}(\mathfrak{H}_\Lambda)$.

Le projecteur $\mathcal{P}^0_-$ est interprété comme l'état fondamental du vide libre. Il est différent de P^0_- et satisfait l'équation

$$\begin{cases} \mathcal{P}^0_- &= \chi_{(-\infty,0)}\big(\mathcal{D}^0\big), \\ \mathcal{D}^0 &= D_0 - \alpha \frac{(\mathcal{P}^0_- - \frac{1}{2})(x,y)}{|x-y|}. \end{cases} \tag{2.11}$$

La vision de Dirac demeure à ceci près que l'état du vide libre correspond au projecteur spectral négatif de l'opérateur $\mathcal{D}^0$. Celui-ci est comme D_0 un multiplicateur de Fourier à valeur matricielle, il s'écrit

$$\widehat{\mathcal{D}^0}(p) = \beta g_0(p) + g_1(p)\boldsymbol{\alpha}\cdot\frac{p}{|p|},\ p \in B(0,\Lambda), \tag{2.12}$$

où g_0 et g_1 sont des fonctions lisses et radiales. Pour α et $\alpha\log(\Lambda)$ suffisamment petits, elles satisfont les équations suivantes :

$$\forall\, p \in B_{\mathbb{R}^3}(0,\Lambda)^*,\ \omega_p := \tfrac{p}{|p|} \text{ et } \begin{cases} g_0(p) &= 1 + \frac{\alpha}{4\pi^2}\int_{B(0,\Lambda)} \frac{dq}{|p-q|}\frac{g_0(q)}{\sqrt{g_0(q)^2+g_1(q)^2}}, \\ g_1(p) &= |p| + \frac{\alpha}{4\pi^2}\int_{B(0,\Lambda)} \frac{\langle \omega_p\,,\omega_q\rangle_{\mathbb{R}^3}\, dq}{|p-q|}\frac{g_1(q)}{\sqrt{g_0(q)^2+g_1(q)^2}}, \end{cases} \tag{2.13}$$

En présence d'un potentiel externe $\alpha\nu * \frac{1}{|\cdot|}$, la limite thermodynamique conduit à la définition de l'énergie BDF. Plus précisément, soit $E_L(\nu)$ l'infimum de l'énergie de $\mathbb{H}^{\nu}_L$ et $E_L(0)$ celle de H^0_L (celle de $\mathcal{P}^0_L$).

Il est montré dans [HLS07] que la différence $E_L(\nu) - E_L(0)$ a une limite quand L tend vers l'infini, et que celle-ci n'est autre que l'infimum d'une énergie $\mathcal{E}^{\nu}_{\mathrm{BDF}}$, définie sur

$$\mathscr{N} = \{\text{projecteurs orthogonaux}\} \cap \big(\mathcal{P}^0_- + \mathfrak{S}_2(\mathfrak{H}_\Lambda)\big), \tag{2.14}$$

où $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ désigne l'espace des opérateurs de Hilbert-Schmidt dans $\mathfrak{H}_\Lambda$.

Definition 2.3 (Énergie BDF)**.** Soit $P \in \mathscr{N}$ et $Q = P - \mathcal{P}^0_- \in \mathfrak{S}_2$. L'énergie BDF de l'état P est

$$\mathcal{E}^{\nu}_{\mathrm{BDF}}(Q) := \mathrm{Tr}_{\mathcal{P}^0_-}\big(\mathcal{D}^0 Q\big) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2}\big(D(\rho_Q, \rho_Q) - \|Q\|^2_{\mathrm{Ex}}\big). \tag{2.15}$$

Dans la suite nous allons travailler avec cette définition [1].

Remarque 2.1. L'étude mathématique des deux énergies définies en 2.2 et 2.3 diffèrent peu. Seulement, elles ne sont pas définies dans le même espace : avec la première on compose avec un sous-espace de l'espace affine

$$\Pi_\Lambda P^0_- + \mathfrak{S}_2(\mathfrak{H}_\Lambda),$$

où Π_Λ est la projection orthogonale sur $\mathfrak{H}_\Lambda$ (voir Notation 2.4). Avec la seconde on se retrouve dans

$$\mathscr{N} \subset \mathcal{P}^0_- + \mathfrak{S}_2(\mathfrak{H}_\Lambda).$$

Remarque 2.2. L'opérateur $\mathcal{D}^0$ apparaît la première fois dans l'article [LS00], mais dans un autre contexte que le modèle BDF.

Terminons cette partie par quelques notations utilisées dans la suite.

Notation 2.4. On écrit Π_Λ la projection orthogonale sur $\mathfrak{H}_\Lambda$. C'est le multiplicateur de Fourier

$$\Pi_\Lambda := \mathscr{F}^{-1}\, \chi_{B(0,\Lambda)}\, \mathscr{F}. \tag{2.16}$$

En particulier elle commute avec D_0 donc avec P^0_-.

Notation 2.5. On définit

$$\mathcal{P}^0_+ = \chi_{(0,+\infty)}(\mathcal{D}^0), \tag{2.17}$$

et on a $\Pi_\Lambda = \mathcal{P}^0_- + \mathcal{P}^0_+$. Comme on se place dans $\mathfrak{H}_\Lambda$, on confond parfois 1 et Π_Λ.

Notation 2.6. Pour un opérateur $Q \in \mathcal{B}(\mathfrak{H}_\Lambda)$, on écrit

$$\forall\, \varepsilon_1, \varepsilon_2 \in \{+,-\},\ Q^{\varepsilon_1\,\varepsilon_2} := \mathcal{P}^0_{\varepsilon_1} Q \mathcal{P}^0_{\varepsilon_2}. \tag{2.18}$$

Décomposant Q suivant $\mathfrak{H}_\Lambda = \mathrm{Im}(\mathcal{P}^0_+) \oplus \mathrm{Im}(\mathcal{P}^0_-)$ on a, en notation matricielle

$$Q = \begin{pmatrix} Q^{++} & Q^{+-} \\ Q^{-+} & Q^{--} \end{pmatrix} \tag{2.19}$$

Un opérateur $Q \in \mathcal{B}(\mathfrak{H}_\Lambda)$ est à $\mathcal{P}^0_-$-trace si $Q^{+-}, Q^{-+} \in \mathfrak{S}_2$ et $Q^{++}, Q^{--} \in \mathfrak{S}_1$. Ces opérateurs forment un espace de Banach $\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$ avec la norme

$$|Q\|_{\mathfrak{S}_1^{\mathcal{P}^0_-}} := \|Q^{+-}\|_{\mathfrak{S}_2} + \|Q^{-+}\|_{\mathfrak{S}_2} + \|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1}. \tag{2.20}$$

Notation 2.7. Pour un opérateur $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, l'opérateur $\frac{Q(x,y)}{|x-y|}$ est noté R_Q.

Pour une densité ρ, la fonction $\rho * \frac{1}{|\cdot|}$ est notée v_ρ.

Pour un opérateur $Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$, on écrit $B_Q = v_{\rho_Q} - v_\nu - R_Q$ et

$$D_Q := \mathcal{D}^0 + \alpha B_Q. \tag{2.21}$$

C'est l'opérateur de champ moyen dans le cas où Q définit un état BDF.

Notation 2.8. L'énergie de Coulomb $D(\nu,\nu)$ correspond à 4π fois le carré de la norme $\|\cdot\|_{\mathcal{C}}$:

$$D(\nu,\nu) = 4\pi \int_{\mathbb{R}^3} \frac{|\widehat{\nu}(k)|^2}{|k|^2} dk =: 4\pi \|\nu\|^2_{\mathcal{C}}.$$

L'espace des densités d'énergie de Coulomb finie est l'espace de Sobolev homogène $\dot{H}^{-1}(\mathbb{R}^3)$, noté aussi $\mathcal{C}$.

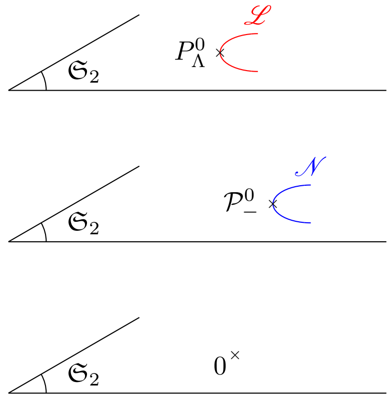

FIGURE 2.1 – Différentes feuilles pour différentes énergies

Dans la figure 2.1, $\mathscr{L}$ représente la variété des projecteurs qui sont perturbation Hilbert-Schmidt de $P^0_\Lambda := P^0_-\Pi_\Lambda$ et $\mathscr{N}$ celle des projecteurs projecteurs qui sont perturbation Hilbert-Schmidt de $\mathcal{P}^0_-$.

Remarque 2.3 (Chronologie non exhaustive). Ce modèle a été introduit par Chaix et Iracane en 1989 dans [CI89], puis étudié par ces derniers et Lions dans [CIL89].

Bach, Barbaroux, Helffer et Siedentop reprennent l'étude dans [BBHS98b, BBHS98a]. En particulier ils donnent dans [BBHS98a] un cadre rigoureux au modèle BDF dans lequel la polarisation du vide est négligée. Dans [BFHS05], Barbaroux, Farkas, Helffer et Siedentop étudient le problème de minimisation.

La prise en compte de la polarisation conduit à des difficultés mathématiques. Un grand pas est effectué par Hainzl et Siedentop dans [HS03].

Dans [HLS05a, HLS05b], Hainzl, Lewin et Séré démontrent l'existence d'un état stable pour le vide polarisé, en présence d'un champ électrostatique externe.

C'est le point de départ de l'étude d'autres problèmes variationnels : citons notamment [HLS07, HLS09, GLS09].

2.1.2 Minimiseurs

Notation 2.9. Soit

$$\mathscr{V} := \mathscr{N} - \mathcal{P}^0_- \subset \mathfrak{S}_2(\mathfrak{H}_\Lambda). \tag{2.22}$$

Nous ferons souvent la confusion entre un état BDF, sa matrice de densité à un corps dans $\mathscr{N}$, et sa matrice de densité réduite dans $\mathscr{V}$.

Notation 2.10. Dès à présent la lettre m désigne

$$m = \inf \sigma\big(|\mathcal{D}^0|\big). \tag{2.23}$$

Pour α et $\alpha \log(\Lambda)$ suffisamment petits, m coïncide avec $g_0(0)$ (voir [HLS07]).

Problèmes variationnels et résultats antérieurs

L'énergie BDF $\mathcal{E}^\nu_{\mathrm{BDF}}$ étant définie, étudions les problèmes variationnels. Par commodité on peut étendre $\mathcal{E}^\nu_{\mathrm{BDF}}$ à l'envelopppe convexe fermée de $\mathscr{V}$ sous la topologie $\mathfrak{S}_1^{\mathcal{P}^0_-}$ (voir (2.20) ci-dessus). On la note $\mathcal{K}$:

$$\mathcal{K} = \overline{\mathrm{Conv}(\mathscr{V})}^{\mathfrak{S}_1^{\mathcal{P}^0_-}}.$$

1. Une troisième définition est utilisée dans le troisième article. Elle correspond à un autre choix de cut-off et est plus adaptée pour étudier la répartition spatiale des minimiseurs.

Sous la condition technique

$$\alpha\frac{\pi}{4} < 1, \tag{2.24}$$

l'énergie BDF est bornée inférieurement. Cela découle de l'inégalité de Kato utilisée pour contrôler le terme d'échange [BBHS98a] :

$$\iint \frac{|Q(x,y)|^2}{|x-y|}dxdy \leq \frac{\pi}{2}\mathrm{Tr}\big(|\nabla||Q|^2\big). \tag{2.25}$$

Un premier résultat est l'existence de minimiseurs globaux.

Théorème 2.1 (Hainzl, Lewin, Séré '05)**.** *Si $\alpha\pi/4 < 1$ et $D(\nu,\nu) < +\infty$, alors il existe un minimiseur $\overline{P} = \overline{Q} + \mathcal{P}_-^0$ de $\mathcal{E}_{BDF}^{\nu}$ sur $\mathcal{K}$. C'est un projecteur satisfaisant l'équation*

$$\overline{P} = \chi_{(-\infty,0)}\big(\Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda\big).$$

Pour $\alpha\sqrt{D(\nu,\nu)}$ assez petit, le minimiseur est unique, et neutre au sens où

$$\mathrm{Tr}_{\mathcal{P}_-^0}\big(\overline{P} - \mathcal{P}_-^0\big) = 0.$$

Ce théorème compose avec la première définition 2.2, mais le résultat s'applique *mutatis mutandis* avec la deuxième 2.3. La remarque sur la neutralité vient de ce que pour un état BDF, représenté par sa matrice de densité à un corps P, sa charge est donnée par :

$$\text{Charge de } P = \mathrm{Tr}_{\mathcal{P}_-^0}\big(P - \mathcal{P}_-^0\big). \tag{2.26}$$

On en vient tout naturellement à s'intéresser aux états fondamentaux pour des systèmes à charge fixées. Soit

$$\mathcal{Q}(q) := \big\{Q \in \mathcal{K},\ \mathrm{Tr}_{\mathcal{P}_-^0}(Q) = q\big\},\ q \in \mathbb{R}, \tag{2.27}$$

on recherche des minimiseurs du problème variationnel

$$E_{\mathrm{BDF}}^{\nu}(q) := \inf\big\{\mathcal{E}_{\mathrm{BDF}}^{\nu}(Q),\ Q \in \mathcal{Q}(q)\big\}. \tag{2.28}$$

Le principe variationnel de Lieb [HLS09, Proposition 3] assure que l'on peut rechercher les minimiseurs dans $\mathscr{V}$ quand q est entier, et plus généralement dans

$$\big\{Q \in \mathcal{K},\ Q = P - \mathcal{P}_-^0 + (q - \mathrm{E}(q))|\psi\rangle\langle\psi|,\ P^* = P^2 = P,\ \|\psi\|_{L^2} = 1 \text{ et } P\psi = 0\big\}.$$

Cela justifie au passage l'extension de $\mathscr{V}$ à son enveloppe convexe. Un minimiseur $Q_0 = \overline{P} - \mathcal{P}_-^0$ de l'énergie correspondante satisfait l'équation suivante [HLS09, Proposition 1]

$$\overline{P} = \chi_{]-\infty,\mu]}\big(\Pi_\Lambda D_{Q_0}\Pi_\Lambda\big),\ \mu \in [-m,m] \tag{2.29}$$

Pour simplifier l'écriture, on écrira

$$D_{Q_0}^{(\Lambda)} := \Pi_\Lambda D_{Q_0}\Pi_\Lambda. \tag{2.30}$$

Les cas où $q = M$ est un entier naturel correspondent à des systèmes à M électrons, avec $\nu \in L^1(\mathbb{R}^3,\mathbb{R}^+)$ et $Z = \int\nu$ entier ils modélisent des atomes ou des molécules.

Le projecteur $\chi_{]\infty,0[}(D_{Q_0}^{(\Lambda)})$ s'interprète comme le *vide habillé*, une déformation du *vide nu* $\mathcal{P}_-^0$ due à la présence des charges. Les M «électrons réels» sont représentés par $\chi_{]0,\mu]}(D_{Q_0}^{(\Lambda)})$, qui sous certaines hypothèses est effectivement un projecteur de rang M. Nous renvoyons le lecteur à [HLS09] et particulièrement aux théorèmes d'existence (2 et 3 de l'article) pour plus de détails.

Ces résultats sont obtenus grâce à la méthode de concentration-compacité [HLS09, théorème 1], déplaçant le problème à la vérification des *inégalités de liaison*

$$\forall\, k \in \mathbb{R}^*,\ E_{\mathrm{BDF}}^{\nu}(q) < E_{\mathrm{BDF}}^{\nu}(q-k) + E_{\mathrm{BDF}}^{0}(k). \tag{2.31}$$

Théorème 2.2. *Il y a équivalence entre les deux assertions :*

— *Les inégalités* (2.31) *sont satisfaites.*

— *Toute suite minimisante pour le problème $E^\nu(q)$ admet une sous-suite convergente et la limite est un minimiseur. Pour $\nu = 0$, le résultat demeure moyennant (éventuellement) translation des fonctions tests.*

Cette équivalence s'explique simplement. Les inégalités de liaison impliquent qu'il n'est pas favorable d'un point de vue énergétique de décomposer le système en deux sous-parties, l'un restant autour de la densité ν, l'autre s'échappant à l'infini.

Dès lors toute suite minimisante reste d'un seul tenant, rendant possible l'extraction d'une sous-suite convergente. Réciproquement, si une inégalité est mise en défaut on construit aisément une suite minimisante non convergente. C'est par cette méthode que dans la partie II on montre l'existence de minimiseurs.

2.1.3 Résultats de la partie II

On y démontre les résultats suivants sous les hypothèses techniques de petitesse [2] de α et de $\alpha\log(\Lambda)$.

1. Le problème $E^0_{\rm BDF}(1)$ admet un minimiseur. La limite non relativiste est le modèle de Pekar-Tomasevitch à un électron. Un électron dans le vide est un système stable.
2. Le problème $E^\nu_{\rm BDF}(M)$ admet un minimiseur pour $0 < M < \int \nu + 1$, sous des conditions techniques moins restrictives que [HLS09, Théorème 3]. La limite non relativiste est un modèle Hartree-Fock altéré.
3. Avec un nouveau choix de cut-off, on montre que le problème $E^0_{\rm BDF}(2)$ n'admet pas de minimiseur. Deux électrons dans le vide n'est pas un système stable si la réaction du vide est trop faible.
4. Les densités des minimiseurs des deux premiers points sont des fonctions intégrables. Les intégrales valent $Z_3(M - \int \nu)$ où Z_3 est une fonction de α et Λ, appelée *constante de renormalisation.* On a

$$1 - Z_3 \approx \frac{\frac{2}{3\pi}\alpha\log(\Lambda)}{1 + \frac{2}{3\pi}\alpha\log(\Lambda)}. \tag{2.32}$$

La concision de ces énoncés fait pendant avec la difficulté de leurs preuves. L'idée directrice est de se placer près de la limite non relativiste afin d'utiliser les résultats connus des modèles limites.

Malgré les apparences le dernier point — certes technique — n'est absolument pas évident : les minimiseurs ne sont pas des opérateurs à trace.

Sur la limite non relativiste Le passage aux modèles non relativistes s'effectue en prenant la limite $c \to +\infty$ c'est-à-dire $\alpha \to 0$ dans notre choix d'unités [3] : un simple changement d'échelle

$$\psi(x) \longrightarrow \alpha^{-3/2}\psi(x/\alpha)$$

permet de passer du choix de paramètres $(c = 1, \alpha, \Lambda)$ aux choix de paramètres $(c = \frac{1}{\alpha}, 1, \frac{\Lambda}{\alpha})$. Pour un état $Q \in \mathcal{K}$, cela correspond à la transformation

$$Q(x,y) \longrightarrow \frac{1}{\alpha^3} Q\Big(\frac{x}{\alpha}, \frac{y}{\alpha}\Big). \tag{2.33}$$

Dans [HLS09], la limite non relativiste est prise en fixant le niveau de cut-off à une certaine valeur $\Lambda_0 > 0$.

Nous montrons dans le chapitre 4 que l'amplitude de la réaction du vide dépend du nombre $\alpha\log(\Lambda)$, dans le sens où une charge électronique $-1 \times e$ agrège autour d'elle un nuage de charge positive $Z_3 \times e$.

Cela a été prouvé rigoureusement dans le modèle BDF réduit [GLS09], dans lequel le terme d'échange est négligé. La présence de ce dernier complique (beaucoup) les calculs mais le résultat demeure.

Ainsi dans l'article [HLS09] où $1 \gg \alpha$ et $\Lambda_0 > 0$ fixe, on a $\alpha\log(\Lambda_0) \ll 1$ et à la limite $0 \times \log(\Lambda_0) = 0$. On perd la polarisation du vide. Nous montrons que l'on peut également prendre la limite $\alpha \to 0$ mais en fixant $L := \alpha\log(\Lambda)$ à une valeur $L_0 > 0$, petite mais pas nulle. Notant $Z := \int \nu$ et

$$1 - Z_3^0 := \frac{\frac{2}{3\pi}L_0}{1 + \frac{2}{3\pi}L_0},$$

2. Il existe $\alpha(\nu, M)$ et L_0 tels que pour $\alpha \le \alpha(\nu, M)$ et $\alpha\log(\Lambda) \le L_0$, etc.
3. voir la première partie de la preuve du [HLS09, Théorème 3] pour la correspondance

pour $0 < M < Z+1$ on a le résultat suivant.

La famille (indicée par α) des minimiseurs rééchelonnés [4] tend à extraction près vers un minimiseur de la fonctionnelle d'énergie

$$\mathcal{E}_{nr}^{Z}(\Gamma) := \tfrac{1}{2}\mathrm{Tr}\big(-\Delta\Gamma\big) - Z \times Z_3^0 \mathrm{Tr}\Big(\tfrac{1}{|\cdot|}\Gamma\Big) + \frac{1}{2}\Big(D(\rho_\Gamma,\rho_\Gamma) - \|\Gamma\|_{\mathrm{Ex}}^2\Big) - \frac{1-Z_3^0}{2}D(\rho_\Gamma,\rho_\Gamma), \tag{2.34}$$

sous les contraintes

$$0 \le \Gamma \le 1, \quad \mathrm{Tr}(\Gamma) = M \quad \text{ et } \quad \tfrac{1-\beta}{2}\Gamma = 0. \tag{2.35}$$

On reconnaît dans (2.34) les termes de l'énergie Hartree-Fock où la charge externe Z est abaissée à $Z(1-Z_3^0)$ avec un terme additionnel $-\frac{1}{2}(1-Z_3^0)D(\rho_\Gamma,\rho_\Gamma)$, de type Pekar-Tomasevitch. La dernière contrainte de (2.35) signifie que les spineurs bas sont nuls, le problème se posant donc dans $L^2\big(\mathbb{R}^3,\mathbb{C}^2\big)$.

2.1.4 Structure géométrique

Nous reformulons les résultats dans un langage géométrique. Les preuves figurent dans la partie III, au moins en puissance.

Commençons peut-être par un théorème de structure [HLS09, Appendice].

Théorème 2.3. *Soit P_0, P_1 deux projecteurs orthogonaux d'un espace de Hilbert tels que la différence $Q = P_1 - P_0$ soit compacte. Alors*

1. *L'espace $\mathrm{Im}(P_1)\cap\mathrm{Ker}(P_0)$ (resp. $\mathrm{Im}(P_0)\cap\mathrm{Ker}(P_1)$) de dimension M_+ (resp. M_-) est engendré par $\underline{a_+} = (a_j)_{1\le j\le M_+}$ resp. $\underline{a_-} = (a_{-j})_{1\le j\le M_-}$.*
2. *Il existe deux familles orthonormales $\underline{e_+} = (e_j)_{j\in\mathbb{N}^*}$ dans $\mathrm{Ker}(P_0)$ et $\underline{e_-} = (e_{-j})_{j\in\mathbb{N}^*}$ dans $\mathrm{Im}(P_0)$ telles que $\underline{a_+}\cup\underline{a_-}\cup\underline{e_+}\cup\underline{a_+}$ est une BON de l'image de Q.*
3. *Chaque plan $\Pi_j = \mathrm{Vect}(e_j, e_{-j})$ est engendré par deux vecteurs $e'_j \in \mathrm{Ker}(P_1)$ et $e'_{-j} \in \mathrm{Im}(P_1)$, mais aussi par deux vecteurs propres f_j et f_{-j} associés aux valeurs propres respectives λ_j et $-\lambda_j$.*
4. *Le nombre λ_j vaut $\sin(\theta_j)$ où $\theta_j \in [0,\frac{\pi}{2}]$ est l'angle que font les deux droites $\mathbb{C}e_j$ et $\mathbb{C}e'_j$.*
5. *Si Q est Hilbert-Schmidt, alors la suite $(\lambda_j)_{j\in\mathbb{N}}$ (que l'on peut supposer décroissante) est dans ℓ^2 et le nombre $\mathrm{Tr}_{P_0}(Q)$ est un entier valant*

$$\mathrm{Tr}_{P_0}(Q) = M_+ - M_- \in \mathbb{Z}.$$

Fort de ce résultat on énonce :

Théorème 2.4. *L'ensemble $\mathscr{N}$ (et donc également $\mathscr{V}$) est une variété de Hilbert de $\mathcal{P}_-^0 + \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ (resp. $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$). Pour tout $P \in \mathscr{N}$, on a*

$$\mathrm{T}_P\mathscr{N} = \big\{v \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ v^* = v \text{ et } PvP = (1-P)v(1-P) = 0\big\}.$$

La famille des composantes connexes de $\mathscr{N}$ est $\big(\mathscr{N}\cap(\mathcal{P}_-^0 + \mathcal{Q}(M))\big)_{M\in\mathbb{Z}}$, elle est indicée par les différentes valeurs de $\mathrm{Tr}_{\mathcal{P}_-^0}(P - \mathcal{P}_-^0)$. Soit $P_0 \in \mathscr{N}$ et soit

$$\mathfrak{m}_{P_0} := \big\{[v, P_0],\ v \in \mathrm{T}_P\mathscr{N}\big\}.$$

Tout projecteur P_1 dans la même composante connexe que P_0 s'écrit sous la forme $e^A P_0 e^{-A}$ où $A \in \mathfrak{m}_{P_0}$.

Revoyons maintenant l'énergie BDF d'un point de vue géométrique.

Théorème 2.5. *Soit une densité $\nu \in \mathcal{C}$. L'énergie BDF $\mathcal{E}_{\mathrm{BDF}}^\nu$ est une fonction lisse dans $\mathscr{N}$. Le gradient [5] $\nabla\mathcal{E}_{\mathrm{BDF}}^\nu$ au point $P = Q + \mathcal{P}_-^0$ est*

$$\nabla\mathcal{E}_{\mathrm{BDF}}^\nu(P) = \big[\big[D_Q^{(\Lambda)}, P\big], P\big] \in \mathrm{T}_P\mathscr{N}.$$

4. comme dans (2.33) mais avec α remplacé par $\alpha\frac{m}{g_1'(0)^2}$.
5. suivant le produit scalaire $\mathrm{Tr}(A^*B)$ de $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$.

Un point critique pour $\mathcal{E}^{\nu}_{\rm BDF}$ vérifie donc

$$\big[\big[D_Q^{(\Lambda)},P\big],P\big]=0.$$

On rappelle que pour tout opérateur borné $T\in\mathcal{B}$

$$\begin{cases}\big[T,P\big] &=& (1-P)TP-PT(1-P),\\ \big[\big[T,P\big],P\big] &=& (1-P)TP+PT(1-P).\end{cases}$$

D'où l'équation d'Euler-Lagrange

$$\big[D_Q^{(\Lambda)},P\big]=0.$$

De même, en notant $a=[v,P]$ pour $v\in \mathrm{T}_P\mathscr{N}$, la hessienne est :

$$\mathrm{Hess}(\mathcal{E}^{\nu}_{\rm BDF},P)\cdot(v,v)=\mathrm{Tr}\Big(\nabla\mathcal{E}^{\nu}_{\rm BDF}(P)\big(\frac{1}{2}\{a^2,P\}-aPa\big)\Big)+\frac{\alpha}{2}\big(D(\rho_v,\rho_v)-\|v\|^2_{\rm Ex}\big).$$

Soit v_0 de la forme

$$v_0=|\psi_+\rangle\langle\psi_-|+|\psi_-\rangle\langle\psi_+|,\ \|\psi_\pm\|_{L^2}=1 \text{ et } (1-P)\psi_-=P\psi_+=0,$$

on obtient

$$\mathrm{Hess}(\mathcal{E}^{\nu}_{\rm BDF},P)\cdot(v_0,v_0)=\langle D_Q^{(\Lambda)}\psi_+\,,\,\psi_+\rangle-\langle D_Q^{(\Lambda)}\psi_-\,,\,\psi_-\rangle-\frac{\alpha}{2}\iint_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\psi_+\wedge\psi_-(x,y)|^2}{|x-y|}dxdy. \tag{2.36}$$

Les conditions de premier ordre (équation d'Euler-Lagrange) et de second ordre (hessienne positive) imposent donc bien qu'un minimum local satisfait (2.29).

2.1.5 Résultats de la partie III

Dans cette partie, on s'intéresse à la composante connexe

$$\mathscr{M}:=\mathscr{N}\cap(\mathcal{P}^0_-+\mathcal{Q}(0))$$

représentant les états possibles du vide. Le but est de rechercher des états excités s'interprétant comme le positronium (resp. le dispositronium), système métastable d'un électron et un positron (resp. deux électrons et deux positrons).

D'un point de vue géométrique on recherche des points critiques de la fonctionnelle d'énergie différents du minimiseur global $\mathcal{P}^0_-$. Pour ce faire, on se restreint à des sous-variétés de $\mathscr{M}$ obtenues en imposant les symétries décrites dans la partie 1.2.2.

On se restreint successivement aux sous-variétés

$$\mathscr{M}_{\mathscr{C}}:=\big\{P\in\mathscr{M},\ P+\mathrm{C}P\,\mathrm{C}^{-1}=\Pi_\Lambda\big\}, \tag{2.37a}$$

$$\mathscr{M}_{\mathscr{I}}:=\big\{P\in\mathscr{M},\ P+\mathrm{I_s}P\,\mathrm{I_s}^{-1}=\Pi_\Lambda\big\}, \tag{2.37b}$$

$$\mathscr{W}:=\big\{P\in\mathscr{M}_{\mathscr{C}},\ \forall U\in\mathrm{Im}\,\Phi_{\rm SU},\ UPU^{-1}=P\big\}. \tag{2.37c}$$

Nous remarquons que $\mathcal{P}^0_-$ est dans toutes ces sous-variétés et que toutes sont invariantes par le flot du gradient.

La sous-variété $\mathscr{M}_{\mathscr{C}}$ a deux composantes connexes et $\mathscr{W}$ en a une infinité dénombrable. La recherche de minimiseurs dans les composantes connexes non-triviales fournit des points critiques de l'énergie BDF. C'est de cette façon qu' on obtient l'ortho-positronium et le dipositronium. On rappelle que dans l'ortho-positronium, l'électron et le positron ont des spins parallèles.

La sous-variété $\mathscr{M}_{\mathscr{I}}$ n'a qu'une composante connexe mais un argument de point col va fournir un point critique différent de $\mathcal{P}^0_-$, interprété comme le para-positronium où les deux particules ont des spins opposés.

En fin de compte on énonce :

Théorème 2.6. *Il existe $\alpha_0, L_0 > 0$ tels que pour $\alpha \le \alpha_0$ et $\alpha \log(\Lambda) \le L_0$ il existe deux point critiques de l'énergie BDF $P_C \in \mathscr{M}_{\mathscr{C}}$ et $P_I \in \mathscr{M}_{\mathscr{I}}$. Ils s'écrivent sous la forme suivante où A dénote C ou $\mathrm{I_s}$ et $P_{\mathrm{A}} = Q_{\mathrm{A}} + \mathcal{P}^0_-$.*

$$\begin{cases} P_{\mathrm{A}} &= \chi_{]-\infty,0[}(D^{(\Lambda)}_{Q_{\mathrm{A}}}) + |\psi\rangle\langle\psi| - |\mathrm{A}\psi\rangle\langle\mathrm{A}\psi|, \\ D^{(\Lambda)}_{Q_{\mathrm{A}}}\psi &= \mu_{\mathrm{A}}\psi, \\ \inf\sigma\big(|D^{(\Lambda)}_{Q_{\mathrm{A}}}|\big) &= \mu_{\mathrm{A}} \in]0,m[\end{cases} \tag{2.38}$$

De même pour tous $j \in \mathbb{N} + \frac{1}{2}$ et $k \in \{j + \frac{1}{2}, -(j+\frac{1}{2})\}$, il existe $\alpha_{j,k} > 0$ tel que pour $\alpha \le \alpha_{j,k}$ il existe un point critique

$$P_{j,k} = \Gamma_{j,k} + \mathcal{P}^0_- \in \mathscr{W}$$

de l'énergie BDF qui s'écrit sous la forme suivante.

$$\begin{cases} P_{j,k} &= \chi_{]-\infty,0[}(D^{(\Lambda)}_{\Gamma_{j,k}}) + \mathrm{Proj}\big(\Phi_{\mathrm{SU}}\psi_{j,k}\big) - \mathrm{Proj}\big(\mathrm{C}\,\Phi_{\mathrm{SU}}\psi_{j,k}\big), \\ D^{(\Lambda)}_{\Gamma_{j,k}}\psi_{j,k} &= \mu_{j,k}\psi_{j,k}, \\ \inf\sigma\big(|D^{(\Lambda)}_{\Gamma_{j,k}}|\big) &= \mu_{j,k} \in]0,m[, \end{cases} \tag{2.39}$$

où $\Phi_{\mathrm{SU}}\psi_{j,k}$ définit une représentation irréductible de Φ_{SU} associée aux valeurs propres $j(j+1)$ de $\mathbf{J}^2$ et k de $\mathbf{K}$.

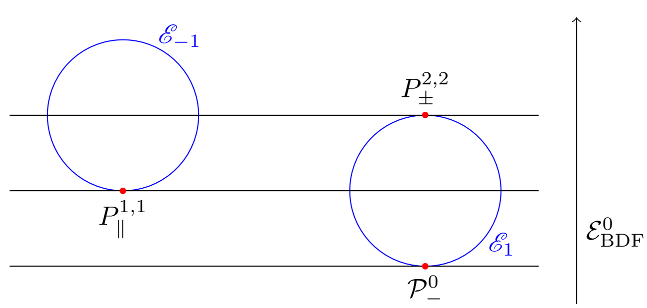

FIGURE 2.2 – Représentation de la variété $\mathscr{M}_{\mathscr{C}}$

Dans la figure 2.2, on représente les deux composantes connexes de $\mathscr{M}_{\mathscr{C}}$ par deux cercles. On peut s'imaginer la variété $\mathscr{M}$ comme un tore légèrement tourné et l'ensemble des états C-symétriques comme son intersection avec un plan vertical.

La fonction altitude représente l'énergie BDF et on y a figuré trois points critiques : le minimiseur global $\mathcal{P}^0_-$, puis l'ortho-positronium $P^{1,1}_{\parallel}$ et enfin le dipositronium $P^{2,2}_{\pm}$. Pour ce dernier le signe $\pm$ correspond au signe de la valeur propre de $\mathbf{K}$.

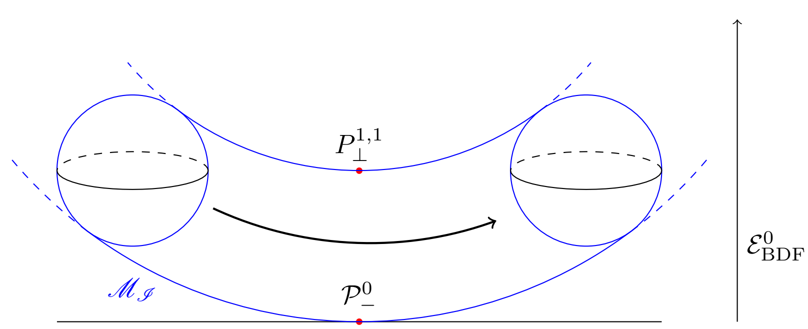

FIGURE 2.3 – Représentation de la variété $\mathscr{M}_{\mathscr{I}}$

Dans la figure 2.3, on représente $\mathscr{M}_{\mathscr{I}}$ comme une portion de $\mathbb{R}^4$ représentant la trajectoire d'un pendule sphérique. On a figuré les points critiques de la fonction altitude $(t, x, y, z) \mapsto z$. On a représenté le projecteur $\mathcal{P}^0_-$ comme le minimiseur global et le para-positronium $P^{1,1}_{\perp}$ comme un point critique. On peut trouver ce dernier par un argument de point col, à l'aide de la fonction d'angle θ de la sphère en coordonnées sphériques.

2.2 Outils

2.2.1 Cadre fonctionnel

Espace de banach

Un grand nombre d'espaces de Banach est utilisé ici. Nous renvoyons le lecteur aux ouvrages [LL97], [RS75, Vol. 1 Chap VI] et [Sim79] pour plus de détails.

Espaces de fonctions et distributions Rappelons que pour $1 \leq p \leq +\infty$ l'espace $L^p(\mathbb{R}^3)$ désigne l'ensemble des fonctions f pour qui

$$\int_{\mathbb{R}^3} |f(x)|^p dx < +\infty. \tag{2.40}$$

Le cas $p = 2$ correspond à l'espace de Hilbert $\mathfrak{H}$ déjà vu précédemment.

Pour $s \in \mathbb{R}$, $H^s(\mathbb{R}^3)$ est l'espace de Sobolev, que l'on définit grâce à la transformée de Fourier [6]

$$H^s(\mathbb{R}^3) = \Big\{ f \in \mathcal{S}'(\mathbb{R}^3),\ \|f\|^2_{H^p} := \int E(p)^{2s} |\widehat{f}(p)|^2 < +\infty \Big\} \tag{2.41}$$

où l'on rappelle que $E(p) := \sqrt{1 + |p|^2}$. Les espaces de Sobolev homogènes $\dot{H}^s(\mathbb{R}^3)$ sont définis de manière analogue en remplaçant $E(p)^{2s}$ par $|p|^{2s}$ dans (2.41). Tous ces espaces sont des espaces de Hilbert.

Pour toute fonction $w : \mathbb{R}^3 \to [1, \infty[$, nous définissons aussi les espaces de Hilbert $\mathfrak{C}_w$ comme suit

$$\mathfrak{C}_w = \Big\{ f \in \mathcal{S}'(\mathbb{R}^3),\ \int \frac{w(k)}{|k|^2} |\widehat{f}(k)|^2 dk < +\infty \Big\}. \tag{2.42}$$

On a utilisé par commodité l'espace des distributions de Schwartz $\mathcal{S}'(\mathbb{R}^3)$, pris comme «l'espace vectoriel des objets dont on peut prendre la transformée de Fourier, et ce de manière cohérente avec la définition usuelle dans les espaces $L^1(\mathbb{R}^3)$ et $L^2(\mathbb{R}^3)$ ».

Espaces d'opérateurs On rappelle que $\mathcal{B}(\mathfrak{H})$ désigne l'ensemble des opérateurs linéaires bornés de $\mathfrak{H}$. On notera Comp$(\mathfrak{H})$ ou $\mathfrak{S}_\infty(\mathfrak{H})$ le sous-ensemble des opérateurs compacts. L'espace $\mathfrak{S}_1(\mathfrak{H})$ désigne l'espace des opérateurs à trace, c'est-à-dire des opérateurs Q pour qui

$$\mathrm{Tr}\big(|Q|\big) = \sum_i \langle |Q| e_i\,,\, e_i \rangle < +\infty$$

où $(e_i)_{i \in \mathbb{N}}$ est une quelconque base hilbertienne de $\mathfrak{H}$ et $|Q| = \sqrt{Q^* Q}$ (à prendre au sens du calcul fonctionnel).
– Il existe toute une échelle de sous-espaces intermédiaires, les espaces de Schatten $\mathfrak{S}_p(\mathfrak{H})$ $(1 \leq p < +\infty)$, définis par

$$\mathfrak{S}_p(\mathfrak{H}) = \big\{ Q \in \mathfrak{S}_\infty(\mathfrak{H}),\ \|Q\|^p_{\mathfrak{S}_p} := \mathrm{Tr}\, |Q|^p < +\infty \big\}. \tag{2.43}$$

Comme pour les espaces ℓ^p on a des résultats d'inclusions : pour $1 \leq p \leq q \leq +\infty$ on a l'injection continue $\mathfrak{S}_p \subset \mathfrak{S}_q$ (de norme 1). De même si

$$\tfrac{1}{p} + \tfrac{1}{q} \geq \tfrac{1}{r},$$

alors le produit TS est dans $\mathfrak{S}_r$ dès que $T \in \mathfrak{S}_p$ et $S \in \mathfrak{S}_q$.

Le cas $p = 2$ correspond aux opérateurs de Hilbert-Schmidt.
– Nous avons aussi introduit l'espace $\mathfrak{S}_1^{\mathcal{P}^0_-}$ des opérateurs à $\mathcal{P}^0_-$-trace, dans lequel on définit la fonctionnelle d'énergie.

6. Pour $s \in \mathbb{N}$, on peut en donner une autre définition, strictement équivalente.

– La formule du terme d'échange définit aussi un espace de Hilbert, fait déjà souligné à travers la notation $\|\cdot\|_{\rm Ex}^2$.
– On est aussi amené à introduire des espaces de Sobolev à poids. Pour toute fonction $f : \mathbb{R}^3 \to [1, \infty[$, on définit

$$\mathbf{Q}_w := \Big\{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ \iint \big(\widetilde{E}\,(p) + \widetilde{E}\,(q)\,\big) f(p-q)|\widehat{Q}(p,q)|^2 dpdq < +\infty\Big\}$$

où $\widetilde{E}\,(p) := \sqrt{g_0(p)^2 + g_1(p)^2}$. Dans ces espaces, on traite différemment les directions $\frac{p+q}{2}$ et $p-q$ dont les variables duales sont respectivement $x-y$ et $\frac{x+y}{2}$. Typiquement la fonction poids $w(p-q)$ est $E(p-q)^{2s}$: pour s grand, il faut penser l'espace comme constitué de noyaux intégraux $Q(x,y)$ lisses dans la direction $\frac{x+y}{2}$, mais peut-être singulier dans la direction $x-y$.

Quelques inégalités

Les inégalités suivantes sont souvent utilisées dans les articles.

La lettre K désigne une constante dont on ne précise pas la valeur mais qui est indépendante des différents paramètres considérés. Sa valeur peut changer d'une ligne à l'autre. Quand on écrit par exemple $K(a,b)$, on indique qu'elle dépend uniquement des paramètres mis entre parenthèse.

Inégalités de Sobolev On se place dans l'espace $\mathbb{R}^3$: l'inégalité de Sobolev usuelle [LL97, Théorème 8.3] affirme que

$$\forall f \in H^1(\mathbb{R}^3),\ \|f\|_{L^6} \le K\|\nabla f\|_{L^2} \tag{2.44}$$

pour une certaine constante K. On rappelle aussi les inégalités de Sobolev fractionnaires suivantes [BCD11, Théorème 1.38] :

$$\forall\, s \in]0,1[,\ \forall\, f \in H^s(\mathbb{R}^3),\ \|f\|_{L^p} \le K(s)\||\nabla|^s f\|_{L^2},\ \frac{1}{p} + \frac{s}{3} = \frac{1}{2}. \tag{2.45}$$

Les cas utilisés $p=3$ et $p=4$ correspondent à $s=\frac{1}{2}$ et $s=\frac{3}{4}$.

Critère d'appartenance à $\mathfrak{S}_p$ L'inégalité de Kato-Seiler-Simon (KSS) [Sim79, Chapitre 3] stipule que pour tout $p \in [2, +\infty[$ et $m \in \mathbb{N}^*$, on a

$$\forall\, f, g \in L^p(\mathbb{R}^m),\ \|f(x)g(-i\nabla)\|_{\mathfrak{S}_p} \le (2\pi)^{-m/p}\|f\|_{L^p}\|g\|_{L^p}.$$

Contrôle de l'énergie Un mot d'abord sur le terme direct : l'application linéaire

$$Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda) \mapsto \rho_Q \in \mathcal{C}$$

est continue où on rappelle que ρ_Q est définie [7] par (2.3). Une preuve de ce fait figure dans [GLS09, Proposition 2], nous prouvons dans le chapitre 5 que la constante de continuité est d'ordre $\sqrt{\log(\Lambda)}$.

Pour contrôler le terme d'échange, on utilise l'inégalité de Kato et l'inégalité de Hardy stipulant, dans l'ordre :

$$\forall\, \phi \in H^{1/2}(\mathbb{R}^3),\ \int \frac{|f(x)|^2}{|x|}dx \le \frac{\pi}{2}\langle|\nabla|\phi\,,\,\phi\rangle, \tag{2.46a}$$

$$\forall\, \phi \in H^1(\mathbb{R}^3),\ \int \frac{|f(x)|^2}{|x|^2}dx \le 4\langle(-\Delta)\phi\,,\,\phi\rangle. \tag{2.46b}$$

Contrôle de l'opérateur de champ moyen Pour $\rho \in \mathcal{C}$ et $Q \in \mathfrak{S}_2$, on considère

$$D^{(\Lambda)}_{\rho,Q} = \Pi_\Lambda\Big(\mathcal{D}^0 + \alpha\big(v_\rho - R_Q\big)\Big)\Pi_\Lambda. \tag{2.47}$$

Par les inégalités de Sobolev on a

$$\begin{aligned}\|v_\rho \tfrac{1}{|\nabla|^{1/2}}\psi\|_{L^2} &\le \|v_\rho\|_{L^6}\|\tfrac{1}{|\nabla|^{1/2}}\psi\|_{L^3}\\ &\le K\|\nabla v_\rho\|_{L^2}\|\psi\|_{L^2} \le K\|\rho\|_{\mathcal{C}}\|\psi\|_{L^2}.\end{aligned} \tag{2.48}$$

7. Grâce au cut-off Q est un opérateur localement à trace : il suffit d'utiliser l'inégalité de KSS ci-dessus.

De même l'inégalité de Cauchy-Schwartz dans l'espace direct [8] montre que

$$\|\tfrac{1}{|\nabla|^{1/2}}R_Q\|_{\mathfrak{S}_2} \leq K\|Q\|_{\mathrm{Ex}}. \tag{2.49}$$

Ces deux inégalités permettent alors d'avoir les inégalités (d'opérateurs auto-adjoints)

$$|\mathcal{D}^0|^2\big(1-2\alpha K(\|\rho\|_{\mathcal{C}}+\|Q\|_{\mathrm{Ex}})\big) \leq |D^{(\Lambda)}_{\rho,Q}|^2 \leq |\mathcal{D}^0|^2\big(1+\alpha K(\|\rho\|_{\mathcal{C}}+\|Q\|_{\mathrm{Ex}})\big)^2 \tag{2.50}$$

2.2.2 Le développement de Cauchy et la méthode de point fixe

Comme indiqué précédemment, le vide *habillé* d'un état fondamental ou excité est représenté par un projecteur

$$\boldsymbol{\pi}^-_{\rho,Q} := \chi_{]-\infty,0[}\big(D^{(\Lambda)}_{\rho,Q}\big), \tag{2.51}$$

avec $Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}$, $\rho \in \mathcal{C}$ et $D^{(\Lambda)}_{\rho,Q}$ défini à (2.47). Le but est d'obtenir des estimées d'un tel état.

Comme dans les articles [HLS05a, GLS09], on obtient une expression de $\boldsymbol{\pi}^-_{\rho,Q} - \mathcal{P}^0_-$ en puissance de α en développant une formule de Cauchy.

Ainsi, supposant que$|D^{(\Lambda)}_{\rho,Q}| \geq K > 0$, on a [9]

$$\begin{aligned}
\boldsymbol{\pi}^-_{\rho,Q} - \mathcal{P}^0_- &= \frac{1}{2i\pi}\int_{i\mathbb{R}} dz\Big(\frac{1}{z-D^{(\Lambda)}_{\rho,Q}} - \frac{1}{z-\mathcal{D}^0}\Big)\\
&= -\frac{1}{2\pi}\int_{\mathbb{R}} d\eta\Big(\frac{1}{D^{(\Lambda)}_{\rho,Q}+i\eta} - \frac{1}{\mathcal{D}^0+i\eta}\Big)\\
&= \sum_{j=1}^{+\infty}\alpha^j Q_j(\rho,Q),
\end{aligned} \tag{2.52}$$

où

$$Q_j(\rho,Q) = -\frac{1}{2\pi}\int_{\mathbb{R}}\frac{d\eta}{\mathcal{D}^0+i\eta}\Big(\Pi_\Lambda(R_Q - v_\rho)\Pi_\Lambda\frac{1}{\mathcal{D}^0+i\eta}\Big)^j. \tag{2.53}$$

Développant l'opérateur Q_j en somme de polynômes homogènes en v_ρ et R_Q, on écrit

$$Q_j(\rho,Q) = \sum_{k=0}^{j} Q_{k,j-k}(\rho,Q), \tag{2.54}$$

où

$$\deg_{v_\rho}\big(Q_{k,j-k}(\rho,Q)\big) = k \quad\text{et}\quad \deg_{R_Q}\big(Q_{k,j-k}(\rho,Q)\big) = j-k. \tag{2.55}$$

Grâce aux inégalités (2.48)-(2.49), on peut donner un sens à la série (2.52), au moins quand la quantité $\alpha(\|\rho\|_{\mathcal{C}}+\|Q\|_{\mathrm{Ex}})$ est suffisament petite : la série converge alors en norme d'opérateurs.

Tout le jeu va être de lui donner un sens dans d'autres espaces de Banach afin d'adapter l'équation (2.29) en schéma de point fixe à la Banach-Picard.

Soyons plus précis : soit $Q_0 \in \mathcal{Q}(M)$ un minimiseur pour $E^\nu_{\mathrm{BDF}}(M)$, où $\nu \in \mathcal{C}$. On scinde Q_0 en la partie du vide

$$\gamma := \boldsymbol{\pi}^-_{\rho_{Q_0}-\nu,\,Q_0} - \mathcal{P}^0_- \tag{2.56}$$

et la partie électronique

$$N := \chi_{[0,\mu]}\big(D^{(\Lambda)}_{\rho_{Q_0}-\nu,\,Q_0}\big). \tag{2.57}$$

On écrit $Q_0 = \gamma + N$ et $\rho_{Q_0} = \rho_\gamma + n$.

Dans [HLS05a], Hainzl, Lewin et Séré réécrivent les équations sous la forme

$$(Q_0,\rho_{Q_0}) = \big(F_Q(Q_0,\rho_{Q_0}), F_\rho(Q_0,\rho_{Q_0})\big), \tag{2.58}$$

où la fonction $F_1 := F_Q \times F_\rho$ a pour paramètres [10] ν et N.

8. Le calcul est effectué au chapitre 3.

9. «On enserre l'intervalle $\mathbb{R}^*_-$ par le cercle infini $i\mathbb{R}$». Cette formule n'est valide que parce qu'on considère la différence de deux projecteurs spectraux de la forme $\chi_{]-\infty,0[}(\mathrm{Op})$.

10. En fait cet article traite du minimiseur global, donc dans ce cas $N = 0$.

Première méthode Dans le chapitre 3, on montre que l'on peut appliquer le schéma de point fixe F_1 dans une boule $B(0, K(\Lambda))$ d'un espace de Banach de type

$$\mathcal{X}_w := \mathbf{Q}_w \times \mathfrak{C}_w,$$

avec $w : \mathbb{R}^3 \mapsto [1, +\infty[$ une fonction poids satisfaisant une hypothèse de sous-additivité.

Le cas $w \equiv 1$ correspond aux normes naturelles du problème. On peut ensuite construire une procédure *bootsrap* à partir des équations (2.56)-(2.57) comme expliqué dans cette partie.

Seconde méthode Dans le chapitre 4, on définit un nouveau schéma de point fixe, dans l'optique de prouver que ρ_{Q_0} est intégrable. On écrit

$$\rho_{Q_0} = F_2(\rho_{Q_0}) \tag{2.59}$$

où F_2 est une fonction de paramètres Q_0 et ν, définie dans une boule $B(0, K(\Lambda))$ de $\mathcal{C} \cap L^1(\mathbb{R}^3)$ ou de $\mathcal{C}$. L'unicité de la solution dans les deux cas impose le résultat.

Deuxième partie

Existence et absence d'états fondamentaux

Chapitre 3

Sur un électron dans le vide

Existence of ground state of an electron in the BDF approximation

Abstract

The Bogoliubov-Dirac-Fock (BDF) model allows to describe relativistic electrons interacting with the Dirac sea. It can be seen as a mean-field approximation of Quantum Electro-dynamics (QED) where photons are neglected.

This paper treats the case of an electron together with the Dirac sea in the absence of any external field. Such a system is described by its one-body density matrix, an infinite rank, self-adjoint operator which is a compact pertubation of the negative spectral projector of the free Dirac operator.

The parameters of the model are the coupling constant $\alpha > 0$ and the ultraviolet cut-off $\Lambda > 0$: we consider the subspace of squared integrable functions made of the functions whose Fourier transform vanishes outside the ball $B(0,\Lambda)$. We prove the existence of minimizers of the BDF-energy under the charge constraint of one electron and no external field provided that α, Λ^{-1} and $\alpha\log(\Lambda)$ are sufficiently small. The interpretation is the following : in this regime the electron creates a polarization in the Dirac vacuum which allows it to bind.

We then study the non-relativistic limit of such a system in which the speed of light tends to infinity (or equivalently α tends to zero) with $\alpha\log(\Lambda)$ fixed : after rescaling the electronic solution tends to the Choquard-Pekar ground state.

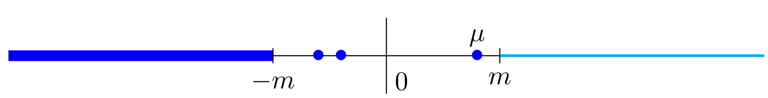

FIGURE 3.1 – Spectre du système {électron+ vide}

Contents

3.1 Introduction

The relativistic quantum theory of electrons is based on the free Dirac operator $D^0 = -i\hbar c\boldsymbol{\alpha} \cdot \nabla + mc^2\beta$. Here β and α_k are the $\mathbb{C}^4 \times \mathbb{C}^4$ matrices :

$$\beta := \begin{pmatrix} \mathrm{Id}_2 & 0 \\ 0 & -\mathrm{Id}_2 \end{pmatrix}, \ \alpha_k = \begin{pmatrix} 0 & \sigma_j \\ \sigma_k & 0 \end{pmatrix},$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The free Dirac operator D^0 acts on 4-spinors, that is on $\mathfrak{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ which is the Hilbert space of one relativistic electron. It is self-adjoint with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and form domain $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Moreover $(D^0)^2 = m^2c^4 - \hbar^2c^2\Delta$. We write :

$$P^0_- = 1 - P^0_+ := \chi_{(-\infty,0)}(D^0). \tag{3.1}$$

It is well known that its spectrum is $\sigma(D^0) = (-\infty, -mc^2] \cup [mc^2, +\infty)$ leading to difficulties in relativistic quantum mechanics. This operator was introduced by Dirac to describe the energy of a free particle with spin $\frac{1}{2}$ (*e.g.* an electron). To explain why electrons with negative energies are not observed, Dirac postulated that all the negative energy states are already occupied by virtual electrons, the so-called Dirac sea. By the Pauli principle, a real electron cannot have a negative energy.

We study an approximation of no-photon Quantum Electrodynamics (QED) allowing to describe the behavior of relativistic electrons in an external field interacting with the virtual electrons of the Dirac sea via the electrostatic potential in a mean-field type theory. This so-called Bogoliubov-Dirac-Fock (BDF) model was introduced by Chaix and Iracane [CI89] and then studied by Bach *et al.* in [BBHS98a], by Hainzl *et al.* in [HS03, HLS05a, HLS05b, HLS07, HLS09] and by Lewin *et al.* in [GLS09]. In particular in those last papers, the authors are interested in the existence of ground states for this variational model.

Let us sketch how the BDF model is derived from full QED. We use relativistic units $\hbar = c = 1$ and set the bare particle mass equal to 1 and $\alpha = e^2/(4\pi)$. When photons are neglected, the (formal) Hamiltonian $\mathbb{H}^\phi$ of QED acts on the Fock space $\mathcal{F}$ of $\mathfrak{H}$ [Tha92] :

$$\mathbb{H}^\phi = \int \Psi^*(x) D^0 \Psi(x) dx - \int \phi(x)\rho(x)dx + \frac{\alpha}{2} \iint \frac{\rho(x)\rho(y)}{|x-y|} dxdy. \tag{3.2}$$

Here $\Psi(x)$ is the second-quantized field operator, ϕ is the external field and $\rho(x)$ is the density operator :

$$\rho(x) = \sum_{\sigma=1}^{4} \big\{ \Psi^*(x)_\sigma \Psi(x)_\sigma - \Psi(x)_\sigma \Psi^*(x)_\sigma \big\}. \tag{3.3}$$

In the presence of an external density ν, the corresponding external field is $\phi = \alpha\nu * \frac{1}{|\cdot|}$. This Hamiltonian is not bounded from below and it is not possible to solve the corresponding minimization problems.

The BDF variational model is obtained from this Hamiltonian by making several approximations.

The first one consists in restricting the energy to special states in $\mathcal{F}$, the so-called Bogoliubov-Dirac-Fock (BDF) states. They are states Ω_P which are fully described by their one-body density matrix P :

$$P(x,y)_{\sigma,\tau} = \langle \Omega_P | \Psi^*(x)_\sigma \Psi(y)_\tau | \Omega_P \rangle_{\mathcal{F}}. \tag{3.4}$$

For instance the vacuum state Ω_0 (no electron and no positron) in $\mathcal{F}$ is a BDF state with one-body density matrix P^0_-.

One must consider them as an infinite Slater determinant $f_1 \wedge f_2 \wedge \cdots$ where $(f_i)_{i\geq 1}$ is an orthonormal basis of the range $\mathrm{Ran}(P)$ of P. We will write P instead of Ω_P for a BDF state : the QED energy can be written in terms of P.

In [HLS07], Hainzl *et al.* study the corresponding minimization problem of $\mathbb{H}^0$ in the space $\mathfrak{H}^L_\Lambda$ of functions in $L^2([-L/2, L/2)^3, \mathbb{C}^4)$ (with periodic boundary conditions) whose Fourier transform vanishes outside the ball $B(0,\Lambda)$; the constant $\Lambda > 0$ is the so-called ultraviolet cut-off. This space has finite dimension and the corresponding Hamiltonian $\mathbb{H}^0_L$ is continuous.

It is then shown that, for each $L > 0$ and $0 < \alpha < 4/\pi$, there exists a minimizer $P_L = \gamma_L + \frac{1}{2}$ among BDF states (with energy $E_L(0)$) and that in the thermodynamic limit $L \to +\infty$, Γ_L tends in some sense to a self-adjoint, translation-invariant operator Γ_0 of $\mathfrak{H}_\Lambda$:

$$\mathfrak{H}_\Lambda := \{f \in \mathfrak{H},\ \mathrm{supp}\,\widehat{f} \subset B(0,\Lambda)\}. \tag{3.5}$$

Moreover Γ_0 satisfies the following self-consistent equations :

$$\begin{cases} \Gamma_0 &= -\dfrac{\mathrm{sign}(\mathcal{D}^0)}{2}, \\ \mathcal{D}^0 &= D^0 - \alpha \dfrac{\Gamma_0(x,y)}{|x-y|}. \end{cases} \tag{3.6}$$

The operator $\mathcal{P}^0_- = \Gamma_0 + \frac{1}{2}$ is the orthogonal projection $\chi_{(-\infty,0)}(\mathcal{D}^0)$ and we write $\mathcal{P}^0_+ = 1 - \mathcal{P}^0_-$. The operator $\mathcal{D}^0$ has been previously introduced in [LS00] but in another context.

We will now take $\mathcal{P}^0_-$ as reference state. For a one-body density matrix P, the formal difference between the QED energies $\mathcal{E}^\nu_{\mathrm{QED}}(P - \frac{1}{2})$ and $\mathcal{E}^0_{\mathrm{QED}}(\mathcal{P}^0_- - \frac{1}{2})$ gives the following function of $Q := P - \mathcal{P}^0_-$:

$$\begin{cases} \mathcal{E}^\nu_{\mathrm{BDF}}(Q) = \mathrm{Tr}\Big\{\mathcal{D}^0(\mathcal{P}^0_- Q \mathcal{P}^0_- + \mathcal{P}^0_+ Q \mathcal{P}^0_+)\Big\} - \alpha \displaystyle\int \phi(x)\rho_Q(x)dx + \frac{\alpha}{2}\Big[D(\rho_Q,\rho_Q) - \mathrm{Ex}[Q]\Big], \\ D(\rho_Q,\rho_Q) := \displaystyle\iint \frac{\rho_Q(x)^*\rho_Q(y)}{|x-y|}dxdy,\ \mathrm{Ex}[Q] := \iint \frac{|Q(x,y)|^2}{|x-y|}dxdy. \end{cases}$$

The function $\mathcal{E}^\nu_{\mathrm{BDF}}$ is the BDF energy we will deal with in this paper. Throughout this paper we write $\mathcal{P}^0_\varepsilon Q \mathcal{P}^0_{\varepsilon'} = Q^{\varepsilon\,\varepsilon'}$ where $\varepsilon, \varepsilon' \in \{+/-\}$. For an operator Q with integral kernel $Q(x,y)$, we define R_Q by its integral kernel : $R_Q(x,y) := \frac{Q(x,y)}{|x-y|}$. There holds : $\|Q\|^2_{\mathrm{Ex}} := \mathrm{Ex}[Q] = \mathrm{Tr}(R_Q^* Q)$. We write $\mathcal{C}$ the Hilbert space of densities with finite Coulomb energy :

$$\mathcal{C} := \big\{\zeta \in \mathcal{S}'(\mathbb{R}^3),\ \|\zeta\|^2_{\mathcal{C}} := 4\pi \int \frac{|\widehat{\zeta}(k)|^2}{|k|^2}dk < +\infty\big\}. \tag{3.7}$$

The squared norm $\|\zeta\|^2_{\mathcal{C}}$ coincides with $\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \zeta^*(x)\zeta(y)\frac{dxdy}{|x-y|}$ whenever this last integral converges.

A justification to study the BDF energy – stated in [HLS07] – is the following. In the presence of an external charge density ν such that $D(\nu,\nu) < +\infty$ and that $\widehat{\nu}$ continuous is in $B(0,\Lambda)$, one can consider the corresponding minimization problem of $\mathbb{H}^\phi$ in $\mathfrak{H}^L_\Lambda$. There also exists a minimizer with energy $E_L(\phi)$ and in the thermodynamic limit :

$$\begin{cases} \lim\limits_{L\to+\infty}(E_L(\phi) - E_L(0)) = \inf\limits_{Q\in\mathcal{Q}_\Lambda} \mathcal{E}^\nu_{BDF}(Q), \\ \text{where } \mathcal{Q}_\Lambda := \{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ -\mathcal{P}^0_- \le Q \le \mathcal{P}^0_+, Q^{++}, Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\}. \end{cases}$$

We recall that for each $1 \le p \le +\infty$, $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ is the subspace of compact operators $A \in \mathcal{B}(\mathfrak{H}_\Lambda)$ with $\mathrm{Tr}|A|^p < +\infty$. The case $p = 1$ gives trace-class operators and $p = 2$ gives Hilbert-Schmidt operators. We recall Q is Hilbert-Schmidt if and only if its integral kernel is in $L^2(\mathfrak{H}_\Lambda \times \mathfrak{H}_\Lambda)$.

Instead of minimizing over all states in $\mathcal{Q}_\Lambda$, we may minimize over sector charge $\mathcal{Q}_\Lambda(q)$, $q \in \mathbb{R}$:

$$\mathcal{Q}_\Lambda(q) := \{Q \in \mathcal{Q}_\Lambda, \mathrm{Tr}(Q^{++} + Q^{--}) = q\}. \tag{3.8}$$

The number q is interpreted as the number of electrons (if $q \in \mathbf{N}^*$) or the number of positrons (if $q \in \mathbb{Z}\backslash\mathbf{N}$). In the presence of an external field ν, the energy function is then defined as

$$E^\nu_{\mathrm{BDF}}(q) := \inf\big\{\mathcal{E}^\nu_{\mathrm{BDF}}(Q),\ Q \in \mathcal{Q}_\Lambda(q)\big\}. \tag{3.9}$$

In [HLS09], Hainzl *et al.* have shown that for any $q_0 \in \mathbb{R}$, the problem $E^\nu_{\mathrm{BDF}}(q_0)$ admits a minimizer as soon as there hold binding inequalities :

$$\forall\ q \in \mathbb{R}\backslash\{0\},\ E^\nu_{\mathrm{BDF}}(q_0) < E^\nu_{\mathrm{BDF}}(q_0 - q) + E^0_{\mathrm{BDF}}(q). \tag{3.10}$$

A more difficult task is to check these inequalities hold for some q_0. In [HLS09], by this method it is proved that for any $\nu \in L^1(\mathbb{R}^3,\mathbb{R}_+) \cap \mathcal{C}$ and any integer M such that $0 \le M < \int \nu + 1$, the problem $E^\nu_{\mathrm{BDF}}(M)$ admits a minimizer (a so-called ground state) close to the limit $\alpha \to 0$ with $\Lambda = \Lambda_0 > 0$ kept *fixed*.

In this paper we show there exists a minimizer for $E^0_{\mathrm{BDF}}(1)$, provided α, Λ^{-1} and $\alpha\log(\Lambda)$ are sufficiently small. It is remarkable that the system of one electron in the Dirac sea can bind in the absence of any external field : this answers an open question stated in [HLS07] (page 19). The presence of the electron induces the polarization of the Dirac sea : it is locally repelled in the neighbourhood of the particle. This fact is illustrated by the inequality $E^0_{\mathrm{BDF}}(1) < m(\alpha)$ where $m(\alpha)$ is the infimum of the BDF energy among configurations where the Dirac sea, represented by $\mathcal{P}^0_-$, is not polarized :

$$m(\alpha) = \inf_{\phi\in \mathrm{Ker}\,\mathcal{P}^0_-} \mathcal{E}^0_{\mathrm{BDF}}(|\phi\rangle\langle\phi|) = \inf\sigma(|\mathcal{D}^0|).$$

We are then interested in the non-relativistic limit $\alpha\to 0$ with $\alpha\log(\Lambda)$ kept fixed to a small value (it may not be 0). The wave function ψ of the real electron has a specific behaviour. There exists $c(\alpha,\Lambda) > 0$ with $c = O(\alpha^{-2}\log(\Lambda)^{-1})$ such that up to translation and up to scaling by $c > 0$, the upper spinor of the wave function ψ tends to a minimizer of the Choquard-Pekar energy E_{CP} [Lie77] :

$$E_{\mathrm{CP}} := \inf_{\phi\in H^1(\mathbb{R}^3):\|\phi\|_{L^2}=1} \left\{ \mathcal{E}_{\mathrm{CP}}(\phi) := \int |\nabla\phi|^2 dx - D(|\phi|^2, |\phi|^2) \right\} < 0. \tag{3.11}$$

More precisely the Choquard-Pekar energy $\mathcal{E}_{\mathrm{CP}}$ of $\underline{\psi}(x) := c^{3/2}\psi(cx)$ tends to E_{CP}. The link with a model of polaron is natural : the Dirac sea is a polarizable system and like a lattice of ions reacts to the presence of an electron. The smallness of $\alpha\log(\Lambda)$ corresponds to a small charge renormalisation. As explained in [HLS05b, part 4], the *physical* coupling constant α_{phys} is different from its "bare" value α. More precisely in the reduced BDF model, where the exchange term is neglected, a minimizer of $\mathcal{E}^\nu_{\mathrm{BDF}}$ with $\nu\geq 0$ radial (interpreted for instance as $\int\nu = Z$ protons) and $D(\nu,\nu)$ small enough has radial density ρ_γ [GLS09], the potential induced by ν at infinity is not $\alpha Z\frac{1}{|x|}$ as it should be but rather $(\nu-\rho_\gamma) * \frac{1}{|\cdot|}(x) \underset{|x|\to+\infty}{\sim} \alpha_{\mathrm{phys}} Z\frac{1}{|x|}$ where

$$\alpha_{\mathrm{phys}} = \alpha Z_3,\ Z_3 = \frac{1}{1+\alpha B^0_\Lambda(0)} \text{ and } B^0_\Lambda(0) = \frac{2}{3\pi}\log(\Lambda) + O(1). \tag{3.12}$$

The quantity $B_\Lambda(0)^0$ is the value at $k=0$ of the function defined in Notation 3.3 below and Z_3 is the charge renormalization constant. If we assume the charge renormalization in the full model to be a perturbation of (3.12), fixing $0 < \alpha\log(\Lambda) = L_0 \ll 1$ corresponds to considering $0 < 1 - Z_3 \ll 1$.

In this paper we have chosen the model of [HLS07] with $\mathcal{P}^0_-$ as reference state instead of that of [HLS05a, HLS05b] with P^0_- as reference state, but all the results proved here are also true in this last model with the same proofs.

The paper is organized as follows : in the next section we properly state the variational problem $E^0_{\mathrm{BDF}}(1)$ and state the main theorems. Subsections 3.3.1 and 3.3.2 are devoted to introduce the Banach spaces and the inequalities used throughout the paper. Theorem 3.1 gives an upper bound of $E^0_{\mathrm{BDF}}(1)$ which is the BDF energy of a test function Γ. This test function is defined by adapting the fixed point scheme in [HLS05a] : the method is explained in Subsection 3.3.3 and the needed estimates in Appendices 3.B.2 and 3.B.3. Then Proposition 3.1 states that the binding inequalities at level 1 are true for $\mathcal{E}^0_{\mathrm{BDF}}$, as a consequence there exists a minimizer for $E^0_{\mathrm{BDF}}(1)$. Theorem 3.2 gives a lower bound of $E^0_{\mathrm{BDF}}(1)$ by computing the BDF energy of a minimizer. The two theorems and the proposition are proved in Section 3.4. At last we look at the nonrelativistic limit in Theorem 3.3. Appendix 3.A is devoted to prove estimates linked to the use of the operator $\mathcal{D}^0$.

3.2 Description of the model and main results

We start with some definitions and notations. Our convention for the Fourier transform $\mathscr{F}$ is :

$$\forall f\in\mathfrak{H}_\Lambda\cap L^1(\mathbb{R}^3,\mathbb{C}^4),\ \widehat{f}(p) := \frac{1}{(2\pi)^{3/2}}\int f(x)e^{-ix\cdot p}dx.$$

In Fourier space $\mathcal{D}^0$ takes the following form

$$\widehat{\mathcal{D}^0}(p) = \boldsymbol{\alpha}\cdot\omega_p g_1(|p|) + g_0(|p|)\beta,\ \omega_p = \frac{p}{|p|}, \tag{3.13}$$

where $g_0, g_1 : [0, \Lambda) \to \mathbb{R}_+$ are real and smooth functions satisfying

$$x \le g_1(x) \le x g_0(x). \tag{3.14}$$

It is possible to improve estimations of [LS00] in the regime $L := \alpha \log(\Lambda) = O(1)$: we get estimates of the derivatives of g_0, g_1 by using their self-consistent equation (*cf* Appendix A). We write $m(\alpha)$ for the bottom of $\sigma(|\mathcal{D}^0|)$:

$$m(\alpha) := g_0(0) = \min(\sigma(|\mathcal{D}^0|)). \tag{3.15}$$

We introduce the following notations concerning the Dirac operator :

Notation 3.1. We write $\widetilde{E}\,(p) := \sqrt{g_0(p)^2 + g_1(p)^2} = |\mathcal{D}^0(p)|$ and
$E\,(p) := \sqrt{1 + |p|^2} = |D^0(p)|$.

We write g_0 (respectively g_1) for both functions
$g_\star : x \in [0, \Lambda] \to g_\star(x) \in \mathbb{R}^+$ and $g_\star : p \in B(0, \Lambda) \to g_\star(|p|) \in \mathbb{R}^+$. The (g_0)'s are in $\mathcal{C}^\infty$ while $g_1 \in \mathcal{C}^1(B(0, \Lambda))$ (*cf* Appendix 3.A).

At last we write

$$\begin{cases} \mathbf{g_1} : p \in B(0, \Lambda) \to g_1(|p|)\omega_p \in \mathbb{R}^3 \\ \mathbf{g} : p \in B(0, \Lambda) \to \begin{pmatrix} g_0(p) \\ \mathbf{g_1}(p) \end{pmatrix} \in \mathbb{R}^4. \end{cases}$$

Notation 3.2. $C_1 \ge 1$ denotes a constant satisfying $g_1(r) \le C_1 |r|$ and $|g_0|_\infty \le C_1$.

Notation 3.3. A recurrent function of this problem is

$$B_\Lambda(k) := \frac{1}{\pi^2 |k|^2} \int\limits_{|p = l + \frac{k}{2}|, |q = l - \frac{k}{2}| \le \Lambda} \frac{\widetilde{E}\,(p)\,\widetilde{E}\,(q) - \mathbf{g}(p)\cdot\mathbf{g}(q)}{\widetilde{E}\,(p)\,\widetilde{E}\,(q)\,(\widetilde{E}\,(p) + \widetilde{E}\,(q))} dl. \tag{3.16}$$

If we replace $\widetilde{E}\,(\cdot)$ by $E(\cdot)$ we get the function B^0_Λ of [HLS05a, GLS09]. We define the function $b_\Lambda(k)$ by the formula

$$b_\Lambda(k) := \tfrac{\alpha B_\Lambda(k)}{1 + \alpha B_\Lambda(k)}. \tag{3.17}$$

In Appendix 3.A it is shown that $B_\Lambda(k) = O(\log(\Lambda))$ and that for $L \ll 1$ there holds $B_\Lambda(0) = \frac{2}{3\pi}\log(\Lambda) + O(L\log(\Lambda) + 1)$.

We consider then the $\mathcal{P}^0_-$-trace ($\mathcal{P}^0_-$ is defined in the introduction) :

$$\mathrm{Tr}_0(Q) := \mathrm{Tr}(\mathcal{P}^0_- Q \mathcal{P}^0_-) + \mathrm{Tr}(\mathcal{P}^0_+ Q \mathcal{P}^0_+),\ \mathcal{P}^0_+ := 1 - \mathcal{P}^0_-. \tag{3.18}$$

As shown in[HLS05a] we know the operators $Q^{--} = \mathcal{P}^0_- Q \mathcal{P}^0_-$ and $Q^{++} = \mathcal{P}^0_+ Q \mathcal{P}^0_+$ are trace-class when $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ is a difference of two orthogonal projectors of the form $Q = P - \mathcal{P}^0_-$. In this case :

$$|Q|^2 = Q^2 = Q^{++} - Q^{--}.$$

We introduce the set of $\mathcal{P}^0_-$-trace class operators :

$$\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda) = \big\{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) : Q^{++}, Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\big\}.$$

The variational set $\mathcal{Q}_\Lambda$ (*cf* introduction) is a convex set of $\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$ and its extremal points are that of the form $Q = P - \mathcal{P}^0_-$ where P is an orthogonal projector.

The density of an operator $Q \in \mathcal{Q}_\Lambda$ is $\rho_Q(x) = \mathrm{Tr}_{\mathbb{C}^4}(Q(x,x))$. It is mathematically well defined since Q is locally trace-class (thanks to the cut-off). The Fourier transform of ρ_Q is :

$$\widehat{\rho_Q}(k) := \frac{1}{(2\pi)^{3/2}} \int\limits_{|u + \frac{k}{2}|, |u - \frac{k}{2}| \le \Lambda} \mathrm{Tr}_{\mathbb{C}^4}(\hat{Q}(u + \tfrac{k}{2}, u - \tfrac{k}{2}))du, \tag{3.19}$$

In the absence of external field, the energy functional defined on $\mathcal{Q}_\Lambda$ is

$$\mathcal{E}^0_{\rm BDF}(Q) = \mathrm{Tr}_0(\mathcal{D}^0 Q) + \frac{\alpha}{2}\left(D(\rho_Q,\rho_Q) - \|Q\|^2_{\rm Ex}\right).$$

The trace part is the kinetic energy while the two others are respectively the *direct term* and the *exchange term*. Moreover the following inequalities hold [BBHS98a, HLS05a, HLS07]

$$\mathrm{Tr}_0(\mathcal{D}^0 Q) = \mathrm{Tr}(|\mathcal{D}^0|(Q^{++} - Q^{--})) \geq \mathrm{Tr}(|\mathcal{D}^0|Q^2), \tag{3.20a}$$

$$\iint \frac{|Q(x,y)|^2}{|x-y|}dxdy \leq \frac{\pi}{2}\mathrm{Tr}(|\mathcal{D}^0|Q^2). \tag{3.20b}$$

Inequality (3.20b) is due to Kato's inequality(3.37b). We assume that $\alpha < \frac{4}{\pi}$: in this case $\mathcal{E}^0_{\rm BDF}$ is bounded from below [HLS05a].

We study the variational problem $E^0_{\rm BDF}(1)$. To ensure the existence of a minimizer for $E^0_{\rm BDF}(1)$, it suffices to prove the following binding inequalities [HLS09].

Proposition 3.1. *There exist three constants $\alpha_0, L_0, \Lambda_0 > 0$ such that if $0 < \alpha \leq \alpha_0, 0 < L \leq L_0$ and $\Lambda \geq \Lambda_0$, then :*

$$\forall\, q \in \mathbb{R}\backslash\{0,1\} : \;\; E^0_{BDF}(1) < E^0_{BDF}(1-q) + E^0_{BDF}(q). \tag{3.21}$$

This Proposition comes as a corollary of the following Theorem.

Theorem 3.1. *There exist three constants $\alpha_0, L_0, \Lambda_0 > 0$ such that if $\alpha \leq \alpha_0, L \leq L_0, \Lambda \geq \Lambda_0$ then :*

$$E^0_{BDF}(1) \leq m(\alpha) + \frac{(\alpha b_\Lambda(0))^2 m(\alpha)}{2g_1'(0)^2}E_{CP} + o((\alpha b_\Lambda(0))^2) < m(\alpha), \tag{3.22}$$

where E_{CP} is the Choquard-Pekar energy (see (3.11)*).*

Remark 3.1. For sufficiently small $\alpha\log(\Lambda)$ we have $g_1'(0) > \varepsilon > 0$. More generally all the results we need about g_0 and g_1 are proved in Appendix 3.A.

Notation 3.4. Throughout this paper we work in the regime

$$\alpha \ll 1,\;\; \Lambda \gg 1,\;\; \alpha\log(\Lambda) = L \leq \varepsilon_0, \tag{3.23}$$

so whenever we write $o(\cdot)$ and $O(\cdot)$ without specifying the limit it is understood that it holds in the regime (3.23). Moreover, K denotes a constant which is independent of α and Λ. The inequality $a \lesssim b$ means that $a \leq Kb$ where a and b are positive real numbers.

To understand what happens in Theorem 3.1 let us see what should be a minimizer of $E^0_{\rm BDF}(1)$. We have the following lemma (proved in Section 3.4.3, see Lemma 3.11)

Lemma 3.1. *A minimizer Q for $E^0_{BDF}(1)$ can be decomposed as $Q = \gamma + |\psi\rangle\langle\psi|$ where γ, ψ satisfy the self-consistent equations :*

$$\left\{\begin{array}{ll} \gamma + \mathcal{P}^0_- & = \chi_{(-\infty,0)}(\mathcal{D}_Q),\;\; \mathcal{D}_Q := \mathcal{D}^0 + \alpha\Big(\rho_Q * |\cdot|^{-1} - \frac{Q(x,y)}{|x-y|}\Big), \\ |\psi\rangle\langle\psi| & = \chi_{[0,\mu]}(\mathcal{D}_{\mathcal{Q}}). \end{array}\right. \tag{3.24}$$

The number $0 < \mu < m(\alpha)$ can be chosen such that $\mathcal{D}_Q\psi = \mu\psi$.

Thanks to Proposition 1 of [HLS09], there only remains to prove $\chi_{[0,\mu]}(\mathcal{D}_{\mathcal{Q}})$ has rank 1 : as $\gamma + \mathcal{P}^0_-$ is a compact perturbation of $\mathcal{P}^0_-$, its essential spectrum is the same and necessarily $0 \leq \mu < m(\alpha)$ and $\chi_{[0,\mu]}(\mathcal{D}_{\mathcal{Q}})$ is the projection onto an eigenspace of $\mathcal{D}_Q$. It suffices to prove $\|\gamma\|_{\mathfrak{S}_2} = o(1)$ to get :

$$\mathrm{Tr}\big(\chi_{[0,\mu]}(\mathcal{D}_{\mathcal{Q}})\big) = \mathrm{Tr}_0\big(\chi_{[0,\mu]}(\mathcal{D}_{\mathcal{Q}})\big) = \mathrm{Tr}_0(\gamma') - \mathrm{Tr}_0(\gamma) = 1.$$

The strategy for Theorem 3.1 is to take a test function Γ which satisfies an equation similar to (3.24). To this end let us first take ϕ_1' the *unique* positive radial minimizer of the Choquard-Pekar energy (*cf* Introduction) and consider $\phi_1 := \frac{P_{\mathfrak{H}_\Lambda}\phi_1'}{\|P_{\mathfrak{H}_\Lambda}\phi_1'\|_{L^2}}$ where $P_{\mathfrak{H}_\Lambda}$ is the projector onto $\mathfrak{H}_\Lambda$. We consider the spinor : $\psi_1 := \begin{pmatrix}\phi_1\\ 0\end{pmatrix}$. For $\lambda^{-1} := \frac{\alpha b_\Lambda(0)m(\alpha)}{g_1'(0)^2}$ we write

$$\psi_\lambda := \lambda^{-3/2}\psi_1(\lambda^{-1}(\cdot)),\ N = N_\lambda := |\psi_\lambda\rangle\langle\psi_\lambda| \text{ and } n_\lambda := |\psi_\lambda|^2 = \rho_N. \tag{3.25}$$

It is possible to adapt the fixed point method of [HLS05a] to define γ as the solution to

$$\gamma = \chi_{(-\infty,0)}\Big(\mathcal{D}^0 + \alpha((\rho_\gamma + n) * |\cdot|^{-1} - R[\gamma + N])\Big) - \mathcal{P}_-^0, \tag{3.26}$$

provided α and $\alpha\log(\Lambda)$ are small enough. In fact this paper [HLS05a] treats the case of D^0 but in Appendix 3.B it is shown that replacing it by $\mathcal{D}^0$ is harmless (*cf* Lemmas 3.7 and 3.8).

We chose the test function Γ defined by the formulae

$$\Gamma := \gamma + N',\ \pi = \gamma + \mathcal{P}_-^0, \text{ and } N' = \frac{|(1-\pi)\psi_\lambda\rangle\langle(1-\pi)\psi_\lambda|}{1 - \|\pi\psi_\lambda\|_{L^2}^2}. \tag{3.27}$$

We then compute compute $\mathcal{E}_{\mathrm{BDF}}^0(\Gamma)$ using that an electron does not see its own field (that is here $D(|\psi|^2, |\psi|^2) - \mathrm{Ex}\big[|\psi\rangle\langle\psi|\big] = 0$).

Lemma 3.2. *Let Γ be as above (3.26), (3.27). Then the following estimate holds :*

$$\mathcal{E}_{BDF}^0(\Gamma) = m(\alpha) + \frac{\alpha b_\Lambda(0)}{2\lambda}E_{CP} + o\left(\frac{\alpha b_\Lambda(0)}{\lambda}\right). \tag{3.28}$$

More precisely, writing $I = \|\rho_\Gamma\|_{\mathcal{C}}^2 - \|\rho_{N'}\|_{\mathcal{C}}^2$ and $J = Ex[\Gamma] - \|\rho_{N'}\|_{\mathcal{C}}^2$ we have

$$\left|\begin{array}{rl} \mathrm{Tr}_0(\mathcal{D}^0 N') & = m(\alpha) + \frac{g_1'(0)^2}{2\lambda^2 m}\displaystyle\int |\nabla\psi_1|^2 dx + o(\lambda^{-2}),\\ \mathrm{Tr}_0(D\gamma) & = \frac{\alpha(b_\Lambda(0) - b_\Lambda(0)^2)}{2\lambda}D(n_1, n_1) + o\left(\frac{\alpha b_\Lambda(0)}{\lambda}\right),\\ \dfrac{\alpha}{2}I & = -\frac{\alpha(2b_\Lambda(0) - b_\Lambda(0)^2)}{2\lambda}D(n_1, n_1) + o\left(\frac{\alpha b_\Lambda(0)}{\lambda}\right),\\ \alpha J & = o\left(\frac{\alpha b_\Lambda(0)}{\lambda}\right). \end{array}\right.$$

Lemma 3.2 is proved in Section 3.4.1. Theorem 3.1 is an obvious corollary.

At this point we know there exists a minimizer $\gamma' = \gamma + |\psi\rangle\langle\psi|$ for $E_{\mathrm{BDF}}^0(1)$ and it satisfies Eq. (3.24). The computation of its energy in terms of ψ gives a lower bound of $E_{\mathrm{BDF}}^0(1)$ of the same form as the right hand side of (3.28).

Theorem 3.2. *There exist three constants $\alpha_1, L_1, \Lambda_1 > 0$ such that for $\alpha \le \alpha_1$, $L \le L_1$, $\Lambda \ge \Lambda_1$, there holds*

$$E_{BDF}^0(1) = m(\alpha) + \frac{(\alpha b_\Lambda(0))^2 m(\alpha)}{2(g_1'(0))^2}E_{CP} + o\left((\alpha b_\Lambda(0))^2\right). \tag{3.29}$$

Theorem 3.3. *Writing $C_0^2 := \frac{2g_1'(0)^2}{(\alpha b_\Lambda(0))^2 m(\alpha)}$ in the regime (3.23) we have :*

$$\liminf_{\alpha,\Lambda^{-1}\to 0} C_0^2(E_{BDF}^0(1) - m(\alpha)) = \limsup_{\alpha,\Lambda^{-1}\to 0} C_0^2(E_{BDF}^0(1) - m(\alpha)) = E_{CP}. \tag{3.30}$$

Assume Q is a minimizer for $E_{BDF}^0(1)$: as in (3.24) we can write : $Q = \gamma + |\psi\rangle\langle\psi|$. In the limit $\alpha \to 0$ where $\alpha\log(\Lambda) = L'$ is kept fixed *and for L' small enough the following holds :*

Up to translation, the upper spinor $\underline{\varphi} \in H^1(\mathbb{R}^3, \mathbb{C}^2)$ of $\underline{\psi}(x) := c^{3/2}\psi(cx)$ tends to a minimizer of the Choquar-Pekar energy E_{CP}.

Remark 3.2. This paper uses heavily estimates and proofs of [HLS05a]. For convenience Lemma 3.17 is not fully proved : it is an adaptation of [HLS05a], the whole proof is in the thesis [Sok14c] of the author.

3.3 Preliminary results

3.3.1 Banach spaces

In this paper several Banach spaces are used.

As usual $\|\cdot\|_{L^p}$ and $\|\cdot\|_{H^s}$ for $p \in [1,+\infty)$ and $s \in \mathbb{R}_+$ are the usual norms of L^p and Sobolev functions. Moreover $\|\cdot\|_{\mathfrak{S}_p}$ is the norm of the space of Schatten-class operators $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ and $\|\cdot\|_{\mathcal{B}}$ is the usual norm of bounded linear operators in $\mathcal{B}(\mathfrak{H}_\Lambda)$. The norms $\|\cdot\|_{\mathcal{C}}$ and $\|\cdot\|_{\mathrm{Ex}}$ are defined in the introduction.
A large part of the paper is devoted to estimate Sobolev norms of test functions Q and among them the norm

$$\|Q\|_{\mathrm{Kin}}^2 := \mathrm{Tr}(|\mathcal{D}^0||Q|^2) \tag{3.31}$$

is linked to the kinetic energy of Q.

In [HLS05a] Hainzl *et al.* introduce the following norms for $(Q,\rho) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \times \mathcal{C} \cap L^2$:

$$\begin{cases} \|Q\|_{\mathcal{Q}}^2 & := \iint \widetilde{E}(p-q)^2\, \widetilde{E}(p+q)\, |\widehat{Q}(p,q)|^2 dpdq, \\ \|\rho\|_{\mathfrak{C}}^2 & := \displaystyle\int \frac{\widetilde{E}(k)^2\, |\widehat{\rho}(k)|^2}{|k|^2} dk \lesssim \|\rho\|_{\mathcal{C}}^2 + \|\rho\|_{L^2}^2. \end{cases} \tag{3.32}$$

Strictly speaking, the authors use $E(\cdot)$ instead of $\widetilde{E}(\cdot)$. However thanks to (3.14) and (3.15) these norms are equivalent :

$$\exists K>0,\ \forall\, p \in B(0,\Lambda),\ \frac{1}{K}E(p) \le \widetilde{E}(p) \le KE(p).$$

Moreover we write for an operator $R(x,y)$:

$$\|R\|_{\mathcal{R}}^2 := \iint \tfrac{\widetilde{E}(p-q)^2}{\widetilde{E}(p+q)} |\widehat{R}(p,q)|^2 dpdq. \tag{3.33}$$

As in [HLS05a], we will estimate the above norm of $R_Q(x,y) = \frac{Q(x,y)}{|x-y|}$.

Unfortunately this is not sufficient and intermediate norms between $\|\cdot\|_{\mathrm{Kin}}$ and $\|\cdot\|_{\mathcal{Q}}$ (respectively $\|\cdot\|_{\mathcal{C}}$ and $\|\cdot\|_{\mathfrak{C}}$) are necessary :

$$\begin{cases} \|Q\|_{q_1}^2 & := \iint \widetilde{E}(p-q)\, \widetilde{E}(p+q)\, |\widehat{Q}(p,q)|^2 dpdq, \\ \|Q\|_{q_0}^2 & := \iint \widetilde{E}(p+q)\, |\widehat{Q}(p,q)|^2 dpdq, \\ \|\rho\|_{\mathfrak{C}_1}^2 & := \displaystyle\int \frac{\widetilde{E}(k)\, |\widehat{\rho}(k)|^2}{|k|^2} dk. \end{cases} \tag{3.34}$$

The numbers 0 and 1 refer to the exponent of $\widetilde{E}(p-q)$ and $\widetilde{E}(k)$.

We also introduce :

$$\|Q\|_E^2 := \iint \max\left\{\widetilde{E}(p),\, \widetilde{E}(p-q)^2,\, \widetilde{E}(p-q)\, \widetilde{E}(p+q)\right\} |\widehat{Q}(p,q)|^2 dpdq. \tag{3.35}$$

For any operator $Q \in \mathfrak{S}_2$ we have :

$$\sqrt{\frac{2}{\pi}}\|Q\|_{\mathrm{Ex}} \le \|Q\|_{\mathrm{Kin}} \le \|Q\|_E \le \|Q\|_{\mathcal{Q}}. \tag{3.36}$$

For some function $f : \mathbb{R}^3 \to [1,+\infty)$, we write :

$$\|Q\|_{\mathcal{Q}_f}^2 := \int f(p-q)\widetilde{E}(p+q)\, |\widehat{Q}(p,q)|^2 dpdq, \quad \|\rho\|_{\mathfrak{C}_f}^2 := \int \frac{f(k)}{|k|^2} |\widehat{\rho}(k)|^2 dk.$$

3.3.2 Some inequalities

Let us recall Hardy's and Kato's inequalities we will use throughout this paper. For $\phi \in L^2(\mathbb{R}^3)$, the following inequalities hold :

$$\int \frac{|\phi(x)|^2}{|x|^2} dx \leq 4\langle |\nabla|^2 \phi\,,\,\phi\rangle, \tag{3.37a}$$

$$\int \frac{|\phi(x)|^2}{|x|} dx \leq \frac{\pi}{2}\langle |\nabla| \phi\,,\,\phi\rangle, \tag{3.37b}$$

Another recurrent inequality is Kato-Seiler-Simon's inequality (K.-S.-S.) [Sim79] :
for any $f, g \in \mathcal{B}(\mathbb{R}^3, \mathbb{C}^{\mathbf{4}})$ (Borelian functions), we have :

$$\|f(x)g(i\nabla)\|_{\mathfrak{S}_p} \leq (2\pi)^{-\frac{3}{p}} \|f\|_{L^p}\|g\|_{L^p},\, 2 \leq p < \infty. \tag{3.38}$$

We use the following Sobolev inequalities in this paper (*cf* [BCD11] Theorem 1.38 p.29) : for suitable f ($f \in H^1(\mathbb{R}^3)$ for instance)

$$\|f\|_{L^6} \lesssim \|\nabla f\|_{L^2},\ \|f\|_{L^4} \lesssim \big\|\,|\nabla|^{3/4} f\big\|_{L^2},\ \|f\|_{L^3} \lesssim \big\|\,|\nabla|^{1/2} f\big\|_{L^2}. \tag{3.39}$$

An immediate result of (3.38) ($p = 6$) and (3.39) ($p = 3$) is the following Lemma.

Lemma 3.3. *Let $\rho \in \mathcal{C}$ and $\varphi_\rho := \rho * |\cdot|^{-1}$. For any $t > 1/2$ there exists $K_t > 0$ such that*

$$\|\varphi_\rho |\mathcal{D}^0|^{-t}\|_{\mathfrak{S}_6} \leq K_t \|\rho\|_{\mathcal{C}}.$$

Moreover we have :

$$\|\varphi_\rho |\mathcal{D}^0|^{-\frac{1}{2}}\|_{\mathfrak{S}_6} \lesssim (\log(\Lambda))^{\frac{1}{6}} \|\rho\|_{\mathcal{C}}, \quad \|\varphi_\rho |\nabla|^{-\frac{1}{2}}\|_{\mathcal{B}} \lesssim \|\rho\|_{\mathcal{C}}$$

Remark 3.3. The notation φ_ρ is used throughout the paper.
Let us consider $R = R_Q$ with $Q \in \mathcal{Q}_\Lambda$. The Lemma 8 of [HLS05a] states that :

$$\|R_Q\|_{\mathcal{R}} \lesssim \|Q\|_{\mathcal{Q}}. \tag{3.40}$$

The following Lemma generalizes this result :

Lemma 3.4. *Let $t \geq 0$. Then we have :*

$$\||\nabla|^{-1/2} R_Q\|_{\mathfrak{S}_2} \lesssim \|Q\|_{Ex}, \tag{3.41a}$$

$$\iint \frac{\widetilde{E}\,(p-q)^t}{\widetilde{E}\,(q)^2} |\widehat{R}(p,q)|^2 dpdq \lesssim \iint \widetilde{E}\,(p-q)^t\, \widetilde{E}\,(p+q)\, |\widehat{Q}(p,q)|^2 dpdq, \tag{3.41b}$$

$$\iint \frac{|\widehat{R}(p,q)|^2}{\widetilde{E}\,(q)} dpdq \lesssim \iint \widetilde{E}\,(p-q)\, \widetilde{E}\,(p+q)\, |\widehat{Q}(p,q)|^2 dpdq. \tag{3.41c}$$

Proof : Ineq. (3.41c) is a consequence of (3.40) for $\widetilde{E}\,(q)^{-1} \lesssim \frac{\widetilde{E}(p-q)}{\widetilde{E}(p+q)}$. Ineq. (3.41b) can be proved by adapting the proof of Lemma 8.[HLS05a] (see Lemma 3.15). This gives :

$$\iint \frac{\widetilde{E}\,(p-q)^t}{\widetilde{E}\,(q)^2} |\widehat{R}(p,q)|^2 dpdq \leq 8 \iint \widetilde{E}\,(2v)^t\, \widetilde{E}\,(2\ell)\, w(\ell, v) |\widehat{Q}(\ell+v, \ell-v)|^2 d\ell dv,$$

where $w(\ell, v)$ is a weight lesser than

$$\widetilde{E}\,(2\ell)\,(2\pi^2)^{-2} \iint dud\ell' \big\{\widetilde{E}\,(u-v)^2\, \widetilde{E}\,(2\ell')^{1+1} |\ell-u|^2 |\ell'-u|^2\big\}^{-1} \lesssim 1.$$

Ineq. (3.41a) is proved as follows : up to a constant the operator $|\nabla|^{-1}$ acts in Direct space as a convolution by $\frac{1}{|\cdot|^2}$ (*cf* [LL97], p.130).

The operator $R_Q^* \frac{1}{|\nabla|} R_Q$ is nonnegative and by Cauchy-Schwartz inequality :

$$\begin{aligned}
\mathrm{Tr}\big\{R_Q^* \tfrac{1}{|\nabla|} R_Q\big\} &\leq \iiint_{(\mathbb{R}^3)^3} \frac{|Q(x,y)|}{|x-y|} \frac{dxdydz}{|y-z|^2} \frac{|Q(z,x)|}{|z-x|} \\
&\leq \left\{ \iiint_{(\mathbb{R}^3)^3} |Q(x,y)|^2 \frac{dxdydz}{|y-z|^2|z-x|^2} \right\}^2 \\
&\lesssim \iint \frac{|Q(x,y)|^2}{|x-y|} dxdy.
\end{aligned}$$

□

Lemma 3.5. *There exist $0 < \varepsilon < 1$ and $K_0 > 0$ such that, for all $(Q,\rho) \in Ex \times \mathcal{C}$, if $\alpha(\|Q\|_{Ex} + \|\rho\|_{\mathcal{C}}) < \varepsilon$, then*

$$|\mathcal{D}^0|\big(1 - \alpha K_0(\|Q\|_{Ex} + \|\rho\|_{\mathcal{C}})\big) \leq |\mathcal{D}^0 + \alpha(\varphi_\rho - R_Q)| \leq |\mathcal{D}^0|\big(1 + \alpha K_0(\|Q\|_{Ex} + \|\rho\|_{\mathcal{C}})\big). \tag{3.42}$$

Proof : We have

$$\|R_Q|\mathcal{D}^0|^{-1}\|_{\mathcal{B}} \leq \|R_Q|\mathcal{D}^0|^{-1}\|_{\mathfrak{S}_2} \lesssim \|Q\|_{\mathrm{Ex}} \text{ and } \|\varphi_\rho|\mathcal{D}^0|^{-1}\|_{\mathcal{B}} \lesssim \|\rho\|_{\mathcal{C}}.$$

As shown in [HLS05a], it suffices to take the square root of

$$|\mathcal{D}^0|\big(1 - 2\alpha K(\|Q\|_{\mathrm{Ex}} + \|\rho\|_{\mathcal{C}})\big) \leq |\mathcal{D}^0 + \alpha(\varphi_\rho - R_Q)|^2 \leq |\mathcal{D}^0|^2\big(1 + \alpha K(\|Q\|_{\mathrm{Ex}} + \|\rho\|_{\mathcal{C}})\big)^2.$$

□

3.3.3 The fixed point method

In [HLS05a] the authors prove the existence of a global minimizer of $\mathcal{E}^\nu_{\mathrm{BDF}}$ under some assumptions on $\alpha, \Lambda, \|\nu\|_{\mathcal{C}}$. The authors show there exists a solution to the self-consistent equation that should satisfy a minimizer Q_0 of E^ν_{BDF} (when P^0_- is taken as reference state). This equation is :

$$Q_0 + P^0_- = \chi_{(-\infty,0)}\big(D^0 + \alpha((\rho_{Q_0} - \nu) * \tfrac{1}{|\cdot|}) - R_{Q_0}\big).$$

To this end a fixed-point scheme based on this equation is used : let us adapt this proof to our problem.

As shown in [HLS05a] we can use the Cauchy's expansion to write (at least formally)

$$\widetilde{Q} = \chi_{(-\infty,0)}(\mathcal{D}^0 + \alpha(\varphi_Q - R_Q)) - \chi_{(-\infty,0)}(\mathcal{D}^0) = \sum_{k=1}^{\infty} \alpha^k Q_k, \tag{3.43a}$$

$$Q_k = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}\eta \frac{1}{\mathcal{D}^0 + i\eta} \Big((R_Q - \varphi_Q) \frac{1}{\mathcal{D}^0 + i\eta} \Big)^k. \tag{3.43b}$$

We also expand $(R-\varphi)^k$, $Q_k := \sum_{j=0}^k Q_{j,j-k}$: the function $Q_{j,j-k}(\cdot,\cdot)$ is polynomial of degree j in R_Q and polynomial of degree $(j-k)$ in φ_Q. Thanks to Lemmas 3.3 and 3.4 we know that each integral converges at least in $\mathfrak{S}_6(\mathfrak{H}_\Lambda)$. If we take the density of each Q_k, we also obtain a (formal) expansion of $\rho[\widetilde{Q}]$:

$$\rho[\widetilde{Q}] = \sum_{k=1}^{+\infty} \alpha^k \rho_k = \sum_{k=1}^{+\infty} \sum_{j=0}^{k} \alpha^k \rho_{j,j-k}. \tag{3.44}$$

In [HLS05a] it is proved that provided $\alpha(\|Q\|_{\mathcal{Q}} + \|\rho_Q\|_{\mathfrak{C}})$ is small enough, those sums converge in $\mathcal{Q}$ for $\widetilde{Q}$ and in $\mathfrak{C}$ for $\rho[\widetilde{Q}]$. In fact the authors show :

Proposition 3.2. *For any $k \in \mathbb{N}^*$ and any $0 \leq j \leq k$, the function*

$$F_{k,j} : \begin{array}{ccc} \mathcal{Q} \times \mathfrak{C} & \to & \mathcal{Q} \times \mathfrak{C} \\ (Q,\rho) & \to & \big(Q_{j,k-j}[Q,\rho], \rho_{j,k-j}[Q,\rho]\big) \end{array}$$

is a continuous *polynomial operator (with estimates of the norm precised in Lemmas 3.16 and 3.17 in Appendix 3.B.2).*

We prove a similar result in the cited Lemmas.

It is necessary to precise the particular form of $\rho_{0,1}[\rho]$. A direct computation in Fourier space gives the following formula [HLS05a].

Lemma 3.6. *For $\rho \in \mathcal{C}$ we have :*

$$\widehat{\rho}_{0,1}(\rho;k) = -B_\Lambda(k)\widehat{\rho}(k) \in \mathcal{C}.$$

If ρ is in $\mathfrak{C}$ (respectively $\mathfrak{C}_1$) then so is $\rho_{0,1}[\rho]$.

The last statement follows from the fact that $|B_\Lambda(k)| \lesssim \log(\Lambda)$, proved in Appendix 3.A.

Let us describe a fixed-point scheme adapted to our problem in the spirit of [HLS05a]. Given the projector N that corresponds to the "real" electrons and $n = \rho_N$ its density, we try to define the dressed vacuum Q surrounding it. We seek a solution to

$$Q + \mathcal{P}^0_- = \chi_{(-\infty,0)}\big(\mathcal{D}^0 + \alpha(\varphi_{Q+N} - R(Q+N))\big). \tag{3.45}$$

For convenience we write $\rho' = \rho'_\gamma := \rho + n$, $Q' = Q + N$, $\varphi'_Q = \varphi_{Q'}$; Eq. (3.45) can be rewritten :

$$F_Q(Q',\rho') := \chi_{(-\infty,0)}(\mathcal{D}^0 + \alpha(\varphi'_Q - R'_Q)) - \chi_{(-\infty,0)}(\mathcal{D}^0) + N = N + \sum_{k=1}^{\infty} \alpha^k Q_k(Q',\rho'). \tag{3.46}$$

Taking the density ρ of both sides and using Lemma 3.6 we get $\rho_{Q'} = F_\rho(Q',\rho')$ with :

$$\widehat{F_\rho}(k) := \frac{1}{1+\alpha B_\Lambda(k)}\Big(\widehat{n}(k) + \alpha\widehat{\rho}_{1,0}(Q';k) + \sum_{\ell\geq 2}\alpha^\ell \widehat{\rho}_\ell(Q',\rho';k)\Big). \tag{3.47}$$

We must precise the domain of the function

$$F := F_Q \times F_\rho. \tag{3.48}$$

Following [HLS05a] we first consider the Banach space $\mathcal{X} = \mathcal{Q}\times\mathfrak{C}$ with the norm

$$\|(Q,\rho)\|_{\mathcal{X}} = 2C_1^{3/2}(2\sqrt{2}\|\rho\|_{\mathfrak{C}} + C_R\sqrt{2}\|Q\|_{\mathcal{Q}}),$$

where $C_R > 0$ is defined in [HLS05a] and $C_1 \geq 1$ is defined in Notation 3.2.

Lemma 3.7. *There exist $R_\Lambda, \varepsilon_1, \varepsilon_2 > 0$ such that if $\sqrt{L\alpha} \leq \varepsilon_1, \alpha\|(N,n)\|_{\mathcal{X}} \leq \varepsilon_2$ then $B_{\mathcal{X}}(0,R_\Lambda)$ is F-invariant. The number R_Λ is $O(\sqrt{\log(\Lambda)})$. Moreover in this ball F is Lipschitz with constant $\nu_0 = O(\sqrt{L\alpha})$. In other words the fixed point theorem can be applied to F on $B_{\mathcal{X}}(0,R_\Lambda)$.*

This lemma and the next one are proved in Appendix 3.B.2.

Remark 3.4. As explained and proved in Appendix 3.B.2, by adapting the estimates of [HLS05a] we realize that another choice of norms for F is possible and so another choice of Banach space on which applying the Banach fixed point theorem. Indeed let us take a radial function $f : \mathbb{R}^3 \to [1,+\infty)$: as long as there exists a constant $C(f) \geq 1$ such that

$$\sqrt{f(p-q)} \leq C(f)(\sqrt{f(p-p_1)} + \sqrt{f(p_1-q)}), \tag{3.49}$$

we can apply the fixed point theorem with the norms

$$\|Q\|^2_{\mathcal{Q}_f} := \iint f(p-q)\widetilde{E}(p+q)\,|\widehat{Q}(p,q)|^2 dpdq,\ \ \|\rho\|^2_{\mathfrak{C}_f} := \int \frac{f(k)|\widehat{\rho}(k)|^2}{|k|^2}dk.$$

Here we are interested in the case $f(p-q) = \widetilde{E}(p-q)$ and $f(p-q) = 1$.

Let $\mathcal{X}_f \subset \mathfrak{S}_2(\mathfrak{H}_\Lambda)\times\mathcal{C}$ be the Banach space with norm
$\|(Q,\rho)\|_{\mathcal{X}_f} := K(f)(\|Q\|_{q_1} + \|\rho\|_{\mathcal{X}_1})$, for some $K(f) > 0$ depending on f (Appendix 3.B.2).

Lemma 3.8. *There exist $R'_\Lambda, \varepsilon'_1, \varepsilon'_2 > 0$ such that if $L \leq \varepsilon'_1, \alpha\|(N,n)\|_{\mathcal{X}_1} \leq \varepsilon'_2$ then $B_{\mathcal{X}_f}(0,R'_\Lambda)$ is F-invariant. The number R'_Λ is $O(\sqrt{\log(\Lambda)})$. Moreover in this ball F is Lipschitz with constant $\nu'_0 = O(\sqrt{L\alpha})$.*

3.4 Proofs

We will use the following Lemma, proved in Appendix 3.B (Subsection 3.B.3).

Lemma 3.9. *Let $\psi_\lambda, \gamma, \rho_\gamma$ defined in* (3.25) *and* (3.26). *Then the following estimates hold :*

$$\begin{aligned} \|\gamma\|_{\mathcal{Q}} &\lesssim \alpha & \|\gamma\|_{E} &\lesssim L\alpha, & \|\gamma\|_{\mathfrak{S}_2} &\lesssim \alpha\sqrt{L\alpha},\\ \|\rho_\gamma\|_{\mathfrak{C}} &\lesssim L\sqrt{L\alpha}, & \|\rho_\gamma\|_{\mathcal{C}} &\lesssim L\sqrt{L\alpha}. \end{aligned} \tag{3.50}$$

Moreover :

$$\|\gamma|\mathcal{D}^0|\psi_\lambda\|_{L^2} + \|\gamma\psi_\lambda\|_{L^2} \lesssim \alpha\sqrt{L\alpha} \text{ and } \big\|\big[|\mathcal{D}^0|, \gamma\big]\big\|_{\mathfrak{S}_2} \lesssim L\alpha. \tag{3.51}$$

3.4.1 Proof of Lemma 3.2

We recall N and n are defined in (3.25).

Notation 3.5. For convenience we write

$$\phi_\lambda := \frac{(1-\pi)\psi_\lambda}{\|(1-\pi)\psi_\lambda\|_{L^2}} = \frac{(1-\pi)\psi_\lambda}{\sqrt{1-\|\pi\psi_\lambda\|_{L^2}^2}}.$$

So we have $N' = |\phi_\lambda\rangle\langle\phi_\lambda|$. Moreover we write

$$\tau := \alpha b_\Lambda(0). \tag{3.52}$$

Remark 3.5. Here λ^{-1} and τ are of the same order $L\alpha$. A direct calculation shows that $\|\mathcal{P}^0_-|\mathcal{D}^0|\psi_\lambda\|_{L^2} = O(\lambda^{-1})$ and $\||\mathcal{D}^0|\psi_\lambda\|_{L^2} = O(1)$. We will often use

$$\|\pi\psi_\lambda\|_{L^2} \le \|\gamma\psi_\lambda\|_{L^2} + \|\mathcal{P}^0_-\psi_\lambda\|_{L^2} \lesssim (o(\tau) + \lambda^{-1}). \tag{3.53}$$

1. Estimation of J

Lemma 3.9 gives $\|\gamma\|_{\text{Ex}}^2 \lesssim \|\gamma\|_E^2 = O(\tau^2)$. By Cauchy-Schwarz inequality and Ineq. (3.37a) : for any $G = |f\rangle\langle g|$ with $f, g \in H^1$

$$|\mathrm{Tr}\big(G^* R_\gamma\big)| \le \min(\|\gamma\|_{\text{Ex}}\|G\|_{\text{Ex}}, 2\|\gamma\|_{\mathfrak{S}_2}\big\|\nabla f\big\|_{L^2}\|g\|_{L^2}).$$

Now thanks to Ineq. (3.37b) and Lemma 3.9 :

$$\begin{aligned} \big\|\,|\pi\psi_\lambda|^2\big\|_{\mathcal{C}}^2 &\lesssim \|\pi\psi_\lambda\|_{L^2}^2\langle|\mathcal{D}^0|\pi\psi_\lambda\,,\,\pi\psi_\lambda\rangle\\ \langle|\mathcal{D}^0|\pi\psi_\lambda\,,\,\pi\psi_\lambda\rangle &\le 2\|\psi_\lambda\|_{L^2}\Big(\big\|\,\big[|\mathcal{D}^0|,\gamma\big]\,\big\|_{\mathfrak{S}_2} + \big\|\gamma|\mathcal{D}^0|\psi_\lambda\big\|_{L^2}\Big) = O((L\alpha)^2). \end{aligned}$$

Similarly we have :

$$\begin{aligned} &\big|D\big(|\psi_\lambda|^2, |\pi\psi_\lambda|^2\big)\big| \lesssim \|\pi\psi_\lambda\|_{L^2}^2\langle|\nabla|\psi_\lambda\,,\,\psi_\lambda\rangle \lesssim \tfrac{(\tau+\lambda^{-1})}{\lambda},\\ &\text{and : } |\mathrm{Tr}(R_\gamma^* N')| \le 2\|\gamma\|_{\mathfrak{S}_2}\|\nabla\psi_\lambda\|_{L^2}\|\psi_\lambda\|_{L^2} \lesssim \tau\lambda^{-1}. \end{aligned}$$

Thus $J = O(\tau^2 + \lambda^{-2}) = O((L\alpha)^2)$.

2. Estimation of I

According to the self-consistent equation satisfied by ρ_γ, we write

$$\widehat{\rho}(\gamma;k) = -b_\Lambda(k)\widehat{n}(k) + (1-b_\Lambda(k))\widehat{\rho}_{1,0}(\gamma;k) + (1-b_\Lambda(k))\sum_{\ell=2}^{\infty}\alpha^\ell\widehat{\rho}_\ell(\gamma;k) \tag{3.54}$$

where we recall that $b_\Lambda(p) = \frac{\alpha B_\Lambda(p)}{1+\alpha B_\Lambda(p)}$. We write $\rho_\ell := \rho_\ell(\gamma)$ and $\sum := \sum_{\ell=2}^{+\infty}\alpha^\ell\rho_\ell$ for short. There holds :

$$\begin{aligned} D(\rho_\gamma,\rho_\gamma) = 4\pi\int_k\frac{dk}{|k|^2}\Big(&b_\Lambda(k)^2|\widehat{n}(k)|^2 + (1-b_\Lambda(k))^2|\alpha\widehat{\rho}_{1,0}(k)|^2 + (1-b_\Lambda(k))^2\big|\widehat{\textstyle\sum}\big|^2\\ &+2\Re\Big(b_\Lambda(k)(1-b_\Lambda(k))\overline{\widehat{n}(k)}\Big(\alpha\widehat{\rho}_{1,0}(k) + \widehat{\textstyle\sum}\Big) + (1-b_\Lambda(k))^2\overline{\alpha\widehat{\rho}_{1,0}(k)}\widehat{\textstyle\sum}\Big)\Big). \end{aligned}$$

By Cauchy-Schwarz inequality it suffices to study $\int\frac{|\widehat{\rho}(k)|^2}{|k|^2}dk$ for $\rho \in \{n, \rho_{1,0}, \sum\}$. We recall $\|b_\Lambda\|_{L^\infty} \lesssim L < 2^{-1}$ for sufficiently small L.

Lemma 3.10. *Let $i \in \{1,2\}$, then there holds :*

$$4\pi \int_p b_\Lambda(p)^i \frac{|\widehat{n_\lambda}(p)|^2}{|p|^2} dp = b_\Lambda(0)^i \frac{D(n_1,n_1)}{\lambda} + \underset{\lambda\to\infty}{o}(L^i \lambda^{-1}). \tag{3.55}$$

Moreover :

$$\begin{aligned} \alpha\|\rho_{1,0}(\gamma)\|_{\mathcal{C}} &\lesssim \sqrt{L\alpha}\|\gamma\|_E \lesssim (L\alpha)^{-3/2}, \\ \|\textstyle\sum\|_{\mathcal{C}} &\lesssim \alpha^2. \end{aligned} \tag{3.56}$$

Before proving this Lemma, we show the estimation of I. First there holds :

$$\|\rho_\gamma\|_{\mathcal{C}}^2 = \frac{b_\Lambda(0)^2}{\lambda} D(n_1,n_1) + \underset{\lambda\to\infty}{o}\left(\frac{L}{\lambda}\right).$$

Then $|\phi_\lambda|^2(x) = \frac{1}{1-\|\pi\psi_\lambda\|_{L^2}^2}(|\psi_\lambda(x)|^2 + |\pi\psi_\lambda(x)|^2 - 2\Re\,\psi_\lambda^*(x)(\pi\psi_\lambda)(x))$. By Cauchy-Schwarz and Kato inequalities the two last terms are $O(L(L\alpha)^2)$. In fact :

$$\begin{aligned} \big\|\, |\pi\psi_\lambda|^2 \,\big\|_{\mathcal{C}}^2 &\lesssim \|\pi\psi_\lambda\|_{L^2}^2 \langle |\nabla| \pi\psi_\lambda\,,\, \pi\psi_\lambda\rangle \lesssim (L\alpha)^4 \\ \big\|\, |\pi\psi_\lambda||\psi_\lambda| \,\big\|_{\mathcal{C}}^2 &\leq 2\|\pi\psi_\lambda\|_{L^2}^2 \|\nabla\psi_\lambda\|_{L^2}\|\psi_\lambda\|_{L^2} \lesssim (L\alpha)^3, \end{aligned}$$

so $\big|D\big(\rho_\gamma, |\pi\psi_\lambda|^2 - 2\Re\{\psi_\lambda^*(\pi\psi_\lambda)\}\big)\big| \lesssim L\sqrt{L\alpha}(L\alpha)^{3/2}$.

Then $D(\rho_\gamma, n_\lambda) = -4\pi \int b_\Lambda(k)|\widehat{n_\lambda}(k)|^2 \frac{dk}{|k|^2} + O\big\{(\alpha\|\rho_{1,0}\|_{\mathcal{C}} + \|\sum\|_{\mathcal{C}})\|n_\lambda\|_{\mathcal{C}}\big\}$.

In the same way :

$$D(\rho_\gamma, |\phi_\lambda|^2) = -b_\Lambda(0) D(n_\lambda, n_\lambda) + \underset{\lambda\to\infty}{o}(\tfrac{L}{\lambda}).$$

Since $\frac{1}{1-\|\pi\psi_\lambda\|_{L^2}^2} = 1 + O((\tau+\lambda^{-1})^2)$, we finally obtain :

$$I = -\frac{2b_\Lambda(0) + b_\Lambda(0)^2}{\lambda} D(n_1,n_1) + \underset{\lambda\to\infty}{o}\left(\frac{L}{\lambda}\right) \tag{3.57}$$

Proof of Lemma 3.10. We use Proposition 3.6 (Appendix 3.A). In the regime (3.23) and for $\varepsilon = \frac{1}{6}$, in a neighbourhood $B(0, r_\varepsilon)$ of 0 *independent* of α, Λ we have :

$$\forall\, k \in\; B(0,r_\varepsilon)\backslash\{0\},\; \frac{|B_\Lambda(|k|) - B_\Lambda(0)|}{|k|} \lesssim (\Lambda^{-1} + |k|^{1/2}) =: z(|k|). \tag{3.58}$$

Then

$$\int_k \frac{b_\Lambda(k)^2 |\widehat{n_\lambda}(k)|^2}{|k|^2} dk = \frac{1}{\lambda}\int_k \frac{b_\Lambda(\frac{k}{\lambda})^2|\widehat{n_1}(k)|^2}{|k|^2} dk,$$

For $\lambda \geq r_\varepsilon^{-4}$ and $k \in B(0,\lambda^{3/4})$: $|B_\Lambda(k/\lambda) - B_\Lambda(0)| \leq \frac{|k|}{\lambda}(z(\lambda^{-1/4}) + K\Lambda^{-1})$. As $f_1 : t \in \mathbb{R}^+ \to \frac{t}{1+t}$ and $f_2 = f_1^2$ have bounded derivatives (by 1 and 2 respectively), for k with $B_\Lambda(p) \neq B_\Lambda(0)$,

$$|b_\Lambda(k) - b_\Lambda(0)| \leq \alpha|B_\Lambda(k) - B_\Lambda(0)|, \quad |b_\Lambda(k)^2 - b_\Lambda(0)^2| \leq 2\alpha|B_\Lambda(k) - B_\Lambda(0)|,$$

so

$$\begin{aligned} \int_{|k|\leq\lambda^{3/4}} |f_i(\alpha B_\Lambda(k)) - f_i(\alpha B_\Lambda(0))| \frac{|\widehat{n_\lambda}(k)|^2 dk}{|k|^2} &\leq 2\alpha \frac{z(\lambda^{-1/4}) + K\Lambda^{-1}}{\lambda} \int \frac{|\widehat{n_1}(k)|^2 dk}{|k|} \\ &\lesssim \alpha \frac{z(\lambda^{-1/4}) + \Lambda^{-1}}{\lambda} \|n_1\|_{\mathcal{C}} \|\psi_1\|_{L^4}^2. \end{aligned}$$

As $f_1(t), f_2(t) \leq t^2$ then

$$\int_{|k|>\lambda^{3/4}} b_\Lambda(k)^i \frac{|\widehat{n_1}(k)|^2}{|k|^2} dk \lesssim \lambda^{-3/2} L^i \int |\widehat{n_1(k)}|^2 dk \lesssim \lambda^{-3/2} L^i \|\psi_1\|_{H^1}^2 = O(L^i \lambda^{-3/2})$$

and

$$\int_k b_\Lambda(k)^i \frac{|\widehat{n_\lambda}(k)|^2}{|k|^2} dk = b_\Lambda(0)^i \frac{D(n_1, n_1)}{\lambda} + \underset{\lambda\to\infty}{o}(L^i \lambda^{-1}).$$

There holds $\int_k \alpha^2(1-b_\Lambda(k))^2 \frac{|\widehat{\rho}_{1,0}(k)|^2}{|k|^2} dk \lesssim \alpha^2\|\rho_{1,0}\|_{\mathcal{C}}^2$. Then estimates of $\|\rho_{1,0}\|_{\mathcal{C}}$ and $\|\sum\|_{\mathcal{C}}$ are proved in Appendix 3.B.3. □

3. Estimation of $\mathrm{Tr}_0(\mathcal{D}^0 N')$

We emphasize that ψ_λ *has no lower part* as a spinor.

There holds

$$\begin{aligned}\langle \mathcal{D}^0 \pi\psi_\lambda\,,\,\pi\psi_\lambda\rangle &= -\langle |\mathcal{D}^0|\mathcal{P}^0_-\psi_\lambda\,,\,\mathcal{P}^0_-\psi_\lambda\rangle + \langle \mathcal{D}^0\gamma\psi_\lambda\,,\,\gamma\psi_\lambda\rangle + 2\Re\langle \mathcal{D}^0\mathcal{P}^0_-\psi_\lambda\,,\,\gamma\psi_\lambda\rangle\\ &= -\langle |\mathcal{D}^0|\psi_\lambda\,,\,\psi_\lambda\rangle + O\Big\{\|\gamma\psi_\lambda\|_{L^2}\big(\big\|\,|\mathcal{D}^0|\gamma\psi_\lambda\big\|_{L^2} + \big\|\,|\mathcal{D}^0|\mathcal{P}^0_-\psi_\lambda\big\|_{L^2}\big)\Big\}\\ &= -\langle |\mathcal{D}^0|\psi_\lambda\,,\,\psi_\lambda\rangle + o((L\alpha)^2).\end{aligned}$$

Then we have :

$$\begin{aligned}\langle \mathcal{D}^0\psi_\lambda\,,\,\pi\psi_\lambda\rangle &= \langle \mathcal{D}^0\psi_\lambda\,,\,\gamma\psi_\lambda\rangle - \langle |\mathcal{D}^0|\mathcal{P}^0_+\psi_\lambda\,,\,\psi_\lambda\rangle\\ &= \langle |\mathcal{D}^0|\psi_\lambda\,,\,\mathcal{P}^0_+\gamma\mathcal{P}^0_+\psi_\lambda\rangle + \langle |\mathcal{D}^0|\psi_\lambda\,,\,\mathcal{P}^0_+\gamma\mathcal{P}^0_-\psi_\lambda\rangle - \langle |\mathcal{D}^0|\mathcal{P}^0_+\psi_\lambda\,,\,\psi_\lambda\rangle\\ &= -\langle |\mathcal{D}^0|\mathcal{P}^0_+\psi_\lambda\,,\,\psi_\lambda\rangle + O(\|\mathcal{D}^0\psi_\lambda\|_{L^2}\|\gamma\|^2_{\mathfrak{S}_2} + \|\mathcal{D}^0\psi_\lambda\|_{L^2}\|\gamma\|_{\mathcal{B}}\|\mathcal{P}^0_-\psi_\lambda\|_{L^2})\\ &= -\langle |\mathcal{D}^0|\mathcal{P}^0_+\psi_\lambda\,,\,\psi_\lambda\rangle + o((L\alpha)^2).\end{aligned}$$

Hence $\langle \mathcal{D}^0\phi_\lambda\,,\,\phi_\lambda\rangle = \frac{\langle \mathcal{D}^0\psi_\lambda\,,\,\psi_\lambda\rangle}{1-\|\pi\psi_\lambda\|^2_{L^2}} + \langle |\mathcal{D}^0|\mathcal{P}^0_-\psi_\lambda\,,\,\psi_\lambda\rangle + o((L\alpha)^2)$.

Notation 3.6. We write $\langle g_\star\psi\,,\,\psi\rangle$ for $\langle g_\star(-i\nabla)\psi\,,\,\psi\rangle$ for $\star\in\{0,1\}$.

As $g_0'(0)=0$ and $\|g_0''\|_\infty \lesssim \alpha$ and the $(g_1')_{\alpha,\Lambda}$'s are uniformly continuous in a neighbourhood of 0 (*cf* Proposition 3.3 in Appendix A)

$$\begin{aligned}\frac{\langle \mathcal{D}^0\psi_\lambda\,,\,\psi_\lambda\rangle}{1-\|\pi\psi_\lambda\|^2_{L^2}} &= \langle g_0\psi_\lambda\,,\,\psi_\lambda\rangle(1+\langle \mathcal{P}^0_-\psi_\lambda\,,\,\psi_\lambda\rangle) + o((L\alpha)^2)\\ &= g_0(0) + \frac{g_0(0)}{4}\langle \frac{g_1^2}{g_0^2}\psi_\lambda\,,\,\psi_\lambda\rangle + o((L\alpha)^2)\\ &= g_0(0) + \frac{g_1'(0)}{4g_0(0)\lambda^2}\langle |\nabla|^2\psi_1\,,\,\psi_1\rangle + o((L\alpha)^2).\end{aligned}$$

Furthermore

$$\langle |\mathcal{D}^0|\mathcal{P}^0_-\psi_\lambda\,,\,\psi_\lambda\rangle = \tfrac{1}{2}\langle (|\mathcal{D}^0|-g_0)\psi_\lambda\,,\,\psi_\lambda\rangle = \tfrac{1}{4g_0(0)}\langle g_1^2\psi_\lambda\,,\,\psi_\lambda\rangle + o(\lambda^{-2}).$$

Finally

$$\begin{aligned}\mathrm{Tr}_0(\mathcal{D}^0 N') &= \langle \mathcal{D}^0\phi_\lambda\,,\,\phi_\lambda\rangle\\ &= g_0(0) + \tfrac{g_1'(0)^2}{2\lambda^2 g_0(0)}\langle |\nabla|^2\psi_1\,,\,\psi_1\rangle + o((L\alpha)^2).\end{aligned} \tag{3.59}$$

4. Estimation of $\mathrm{Tr}_0(D\gamma)$

Notation 3.7. Let us write $B = R'_\gamma - \varphi'_\gamma = R(\gamma+N) - (\rho_\gamma+n)*|\cdot|^{-1}$.

Remark 3.6. Let us recall Lemma 1.[HLS05a] : if P,Π are two projectors such that :
$P-\Pi\in\mathfrak{S}_2$ then
$Q\in\mathfrak{S}_1^P \iff Q\in\mathfrak{S}_1^\Pi$ and then $\mathrm{Tr}_P(Q)=\mathrm{Tr}_\Pi(Q)$.

We apply this Lemma for $P=\mathcal{P}^0_-$ and $\Pi := \chi_{(-\infty,0)}(\mathcal{D}^0+\alpha B)$: formally

$$\mathrm{Tr}_0((\mathcal{D}^0+\alpha B)\gamma) = \mathrm{Tr}(|\mathcal{D}^0|\gamma^2) + \alpha\mathrm{Tr}_0(B\gamma) \tag{3.60a}$$

$$\mathrm{Tr}_0((\mathcal{D}^0+\alpha B)\gamma) = -\mathrm{Tr}(|\mathcal{D}^0+\alpha B|\gamma^2) = -\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) + o(\mathrm{Tr}(|\mathcal{D}^0|\gamma^2)). \tag{3.60b}$$

So we would like to show that

$$\begin{aligned}\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) &= -\tfrac{\alpha}{2}\mathrm{Tr}_0(B\gamma) + o((L\alpha)^2),\\ &= -\tfrac{\alpha}{2}\big(D(\rho_\gamma+n,\rho_\gamma) - \mathrm{Tr}(R'_\gamma\gamma)\big) + o((L\alpha)^2),\\ &= -\tfrac{\alpha}{2}D(\rho_\gamma+n,\rho_\gamma) + o((L\alpha)^2).\end{aligned} \tag{3.61}$$

We have to prove that $B\gamma$ in $\mathfrak{S}_1^{\mathcal{P}^0_-}$ and $\mathrm{Tr}\big\{(|\mathcal{D}^0+\alpha B|-|\mathcal{D}^0|)\gamma^2\big\} = O(\alpha(L\alpha)^2)$.

Supposing those facts are true we get $\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) = -\frac{\alpha}{2}\mathrm{Tr}_0(B\gamma) + O(\alpha\tau^2)$. We use (3.41c) :

$$\|R'_\gamma\gamma\|_{\mathfrak{S}_1} \leq \|R(\gamma)|\mathcal{D}^0|^{-1/2}\|_{\mathfrak{S}_2}\||\mathcal{D}^0|^{1/2}\gamma\|_{\mathfrak{S}_2} + \|R(N)\|_{\mathfrak{S}_2}\|\gamma\|_{\mathfrak{S}_2} \lesssim (\tau+\lambda^{-1})\tau.$$

First let us prove that $\mathrm{Tr}(|\mathcal{D}^0+\alpha B|\gamma^2) = \mathrm{Tr}(|\mathcal{D}^0|\gamma^2) + O(\alpha(L\alpha)^2)$.

Thanks to Lemma 3.5, there holds :

$$\begin{cases} |\mathcal{D}^0+\alpha B| \geq |\mathcal{D}^0|\big(1-\alpha K(\|\gamma\|_{\mathrm{Kin}} + \|\rho_\gamma\|_{\mathcal{C}} + \||\nabla|^{1/2}\psi_\lambda\|_{L^2})\big),\\ |\mathcal{D}^0+\alpha B| \leq |\mathcal{D}^0|\big(1+\alpha K(\|\gamma\|_{\mathrm{Kin}} + \|\rho_\gamma\|_{\mathcal{C}} + \||\nabla|^{1/2}\psi_\lambda\|_{L^2})\big).\end{cases}$$

Then we multiply by $\gamma^*=\gamma$ on the left and by γ on the right : this does not change the inequalities. To conclude it suffices to take the trace.

Let us prove $\mathrm{Tr}_0(\varphi'_\gamma\gamma) = D(\rho_\gamma+n_\lambda,\rho_\gamma)$. In fact if $Q\in\mathfrak{S}_1^{\mathcal{P}^0_-}$ and if $\int \mathrm{Tr}(\widehat{Q}(p,p))dp$ exists then this last integral is equal to $\mathrm{Tr}_0(Q)$, because $\mathcal{P}^0_- = f(i\nabla)$, in Fourier space we have $\mathrm{Tr}_{\mathbb{C}^4}(\widehat{\mathcal{P}^0_-}(p)\widehat{Q}(p,p)\widehat{\mathcal{P}^0_+}(p)) = \mathrm{Tr}_{\mathbb{C}^4}(\widehat{\mathcal{P}^0_+}(p)\widehat{Q}(p,p)\widehat{\mathcal{P}^0_-}(p)) = 0$. Here, the trace $\mathrm{Tr}_0(\varphi'_\gamma\gamma)$ is formally equal to

$$\begin{aligned}(2\pi)^{-3/2}&\iint_{|p|,|q|<\Lambda}\widehat{\varphi'_\gamma}(p-q)(\mathrm{Tr}(\widehat{\gamma}(p,q)))^*dpdq\\ &= (2\pi)^{-3/2}\iint_{|u+\frac{k}{2}|,|u-\frac{k}{2}|<\Lambda}\widehat{\varphi'_\gamma}(k)(\mathrm{Tr}(\widehat{\gamma}(u+k/2,u-k/2)))^*dudk\\ &= \int_k \widehat{\varphi'_\gamma}(k)\widehat{\rho_\gamma}(k)^*dk = 4\pi\int_k\frac{\widehat{\rho'_\gamma}(k)\widehat{\rho_\gamma}(k)^*}{|k|^2}dk = D(\rho_\gamma,\rho'_\gamma).\end{aligned}$$

As shown in the estimation of I, there holds

$$D(\rho_\gamma,\rho_\gamma+n_\lambda) = \tfrac{b_\Lambda(0)^2-b_\Lambda(0)}{\lambda}D(n_1,n_1) + o\big(\tfrac{L}{\lambda}\big),$$

so we get

$$\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) = \alpha\tfrac{b_\Lambda(0)^2-b_\Lambda(0)}{2\lambda}D(n_1,n_1) + o\left(\frac{L}{\lambda}\right). \tag{3.62}$$

Remark 3.7. The calculation above is correct if $\widehat{\gamma}(p,q)\in\mathcal{C}^0(B(0,\Lambda)^2)$:

$$\iint_{|u\pm\frac{k}{2}|<\Lambda}\frac{|\widehat{\rho}(k)|}{|k|^2}|\widehat{\gamma}(u+\tfrac{k}{2},u-\tfrac{k}{2})|dudk \lesssim \Lambda^{3/2}\|\rho\|_{\mathcal{C}}(\Lambda^{3/2}\|\widehat{\gamma}\|_{L^\infty}+\|\gamma\|_{\mathfrak{S}_2}).$$

We conclude by continuity of $Q\in\mathfrak{S}_1^{\mathcal{P}^0_-}\mapsto\rho_Q\in\mathcal{C}$ shown in [HLS09], that of $Q\in\mathfrak{S}_1^{\mathcal{P}^0_-}\mapsto\mathrm{Tr}_0(\varphi'_\gamma Q)$ and the density of $\mathcal{C}^0(B(0,\Lambda)^2)$ in $\mathscr{F}(\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda))$.

Let us prove $\varphi'_\gamma Q\in\mathfrak{S}_1^{\mathcal{P}^0_-}$. We have :

$$(\varphi'_\gamma Q)^{--} = \underbrace{(\mathcal{P}^0_-[\varphi'_\gamma,\mathcal{P}^0_+]|\mathcal{D}^0|^{-1/2})}_{\in\mathfrak{S}_2(\mathfrak{H}_\Lambda)}\underbrace{|\mathcal{D}^0|^{1/2}Q^{+-}}_{\in\mathfrak{S}_2(\mathfrak{H}_\Lambda)} + \underbrace{(\varphi'_\gamma|\mathcal{D}^0|^{-1/2})^{--}}_{\in\mathcal{B}(\mathfrak{H}_\Lambda)}\underbrace{|\mathcal{D}^0|^{1/2}Q^{--}}_{\in\mathfrak{S}_1(\mathfrak{H}_\Lambda)} \in\mathfrak{S}_1(\mathfrak{H}_\Lambda) \tag{3.63}$$

and so $|\mathrm{Tr}_0(\varphi'_\gamma Q)| \leq (\Lambda^{1/2}+\sqrt{\log(\Lambda)})\|\rho'_\gamma\|_{\mathcal{C}}\big\|Q\big\|_{\mathfrak{S}_{1,\mathcal{P}^0_-}}$ with

$$\big\|Q\big\|_{\mathfrak{S}_{1,\mathcal{P}^0_-}} := \|Q^{--}\|_{\mathfrak{S}_1} + \|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{-+}\|_{\mathfrak{S}_2} + \|Q^{+-}\|_{\mathfrak{S}_2}. \tag{3.64}$$

To see $\mathcal{P}^0_-[\varphi'_\gamma,\mathcal{P}^0_+]|\mathcal{D}^0|^{-1/2}$ is Hilbert-Schmidt, it suffices to prove the kernel of its Fourier transform is in $L^2(B(0,\Lambda)^2)$: this is easy with the help of Lemma 3.14.

To conclude this section there remains to deal with $R'_\gamma\gamma$, we recall this operator is trace-class (*cf* Lemma 3.4) :

$$R'_\gamma\gamma = \underbrace{(R'_\gamma)|\mathcal{D}^0|^{-1/2}}_{\in\mathfrak{S}_2(\mathfrak{H}_\Lambda)}\underbrace{|\mathcal{D}^0|^{1/2}\gamma}_{\in\mathfrak{S}_2(\mathfrak{H}_\Lambda)}$$

and

$$\mathrm{Tr}\big\{R'_\gamma\gamma\big\} = O(\|R_N\|_{\mathfrak{S}_2}\|\gamma\|_{\mathfrak{S}_2} + \|R_\gamma|\mathcal{D}^0|^{-1/2}\|_{\mathfrak{S}_2}\||\mathcal{D}^0|^{1/2}\gamma\|_{\mathfrak{S}_2}) = O\Big(\frac{\alpha\sqrt{L\alpha}}{\lambda} + (L\alpha)^2\Big). \tag{3.65}$$

Remark 3.8. As $\Lambda\to+\infty$ there holds $\langle|\mathcal{D}^0|^2\psi_1\,,\,\psi_1\rangle - D(n_1,n_1) = E_{\mathrm{CP}} + o(1)$. In fact $\psi_1 = (\phi_1,0)^T$ where $\phi_1 = P_{\mathfrak{H}_\Lambda}\phi'_1/\|P_{\mathfrak{H}_\Lambda}\phi'_1\|_{L^2}$ and ϕ'_1 is the minimizer of Choquard-Pekar energy. $P_{\mathfrak{H}_\Lambda}$ is the projector onto $\mathfrak{H}_\Lambda$. So we have $\phi_1 \underset{\Lambda\to+\infty}{\overset{H^1}{\to}} \phi'_1$. Writing $n' = |\phi'_1|^2$ there holds by Kato's inequality (3.37b)

$$\begin{aligned}\big|\|n_1\|_{\mathcal{C}} - \|n'\|_{\mathcal{C}}\big| &\le \|n_1 - n'\|_{\mathcal{C}} \lesssim \Big(\langle|\nabla|\psi_1\,,\,\psi_1\rangle + \langle|\nabla|\phi'_1\,,\,\phi'_1\rangle\Big)\big|\|\psi_1\|^2_{L^2} - \|\phi'_1\|^2_{L^2}\big|\\ &\lesssim \langle|\nabla|\phi'_1\,,\,\phi'_1\rangle\Big|\|\psi_1\|^2_{L^2} - \|\phi'_1\|^2_{L^2}\Big| \underset{\Lambda\to\infty}{\to} 0.\end{aligned}$$

3.4.2 Proof of Proposition 3.1

In this part we write $E(\cdot)$ for $E^0_{\mathrm{BDF}}(\cdot)$.

Let us prove now the binding inequalities for $0<q<1$. According to Lieb's principle (Proposition 3.[HLS09]) for each q we can take minimizing sequences for $E(q)$ of the form

$$\begin{cases} Q_{(k)} = P_{(k)} - \mathcal{P}^0_- + q|\psi_k\rangle\langle\psi_k|, k\in\mathbb{N}\\ \text{with } (P_{(k)} - \mathcal{P}^0_-)\in\mathcal{Q}_\Lambda(0) \text{ and } P_k^2 = P_k, P_k\psi_k = 0.\end{cases} \tag{3.66}$$

We write as before $\gamma_k = P_k - \mathcal{P}^0_-, n_k = |\psi_k|^2, N_k = |\psi_k\rangle\langle\psi_k|$. We will forget to emphasize the dependence in k. Writing $I_\gamma(N) = \alpha\Re\Big(D(\rho_\gamma, n) - \mathrm{Tr}(R_N^*\gamma)\Big)$, $\mathcal{E}^0_{\mathrm{BDF}}(Q)$ can be written :

$$\mathcal{E}^0_{\mathrm{BDF}}(Q) = \mathcal{E}^0_{\mathrm{BDF}}(\gamma) + q\langle\mathcal{D}^0\psi\,,\,\psi\rangle + qI_\gamma(N) = (1-q)\mathcal{E}^0_{\mathrm{BDF}}(\gamma) + q\mathcal{E}^0_{\mathrm{BDF}}(\gamma+N).$$

Taking the lim inf, we obtain

$$E(q) = \liminf_{k\to\infty}((1-q)\mathcal{E}^0_{\mathrm{BDF}}(\gamma) + q\mathcal{E}^0_{\mathrm{BDF}}(\gamma+N)) \ge (1-q)\liminf_{k\to\infty}\mathcal{E}^0_{\mathrm{BDF}}(\gamma) + qE(1).$$

Either $x = \liminf_{k\to\infty}\mathcal{E}^0_{\mathrm{BDF}}(\gamma) > 0$ and $E(q) > qE(1)$ or $x=0$. What happens in the second case? Up to the extraction of a subsequence we can assume that $\liminf\mathcal{E}^0_{\mathrm{BDF}}(\gamma)$ is a limit. Thanks to (3.20) it implies $\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) + D(\rho_\gamma,\rho_\gamma) \underset{k\to\infty}{\to} 0$. As $P_k\psi_k = 0$, there holds $\mathcal{P}^0_-\psi_k = \gamma\psi_k$, in particular

$$\|\mathcal{P}^0_+\psi\|^2 = \|\psi\|^2 - \|\mathcal{P}^0_-\psi\|^2 = 1 - \|\gamma\psi\|^2 \to 1$$

and $\langle\mathcal{D}^0\psi\,,\,\psi\rangle = \langle|\mathcal{D}^0|\psi^+\,,\,\psi^+\rangle - \langle|\mathcal{D}^0|\gamma\psi\,,\,\gamma\psi\rangle$ where $\psi^\varepsilon = \mathcal{P}^0_\varepsilon\psi$.
As $\||\mathcal{D}^0|^{1/2}\gamma\psi\|^2_{L^2} \le \mathrm{Tr}(|\mathcal{D}^0|\gamma^2)\|\psi\|^2_{L^2}$ and $\|\psi\|_2 = 1$: up to extraction we have

$$\lim_{k\to\infty}\langle\mathcal{D}^0\psi\,,\,\psi\rangle = \lim_{k\to\infty}\langle|\mathcal{D}^0|\psi^+\,,\,\psi^+\rangle \ge m(\alpha).$$

The sequence $(\langle\mathcal{D}^0\psi_k\,,\,\psi_k\rangle)_k$ is bounded, else by Cauchy-Schwarz and Kato's inequality

$$\begin{aligned}\mathcal{E}^0_{\mathrm{BDF}}(\gamma+N) &\ge \mathcal{E}^0_{\mathrm{BDF}}(\gamma) + \langle\mathcal{D}^0\psi\,,\,\psi\rangle - \frac{1}{2}\big(\|\rho_\gamma\|^2_{\mathcal{C}} + \|\gamma\|^2_{\mathrm{Ex}} + \pi\alpha^2\langle|\nabla|\psi\,,\,\psi\rangle\big)\\ &\underset{k\to+\infty}{\longrightarrow} +\infty.\end{aligned}$$

By Cauchy-Schwartz inequality $I_\gamma(N)\to 0$ and

$$\liminf_{k\to\infty}\mathcal{E}^0_{\mathrm{BDF}}(Q_k) = E(q) \ge \liminf_{k\to\infty}\mathcal{E}^0_{\mathrm{BDF}}(\gamma) + q\liminf_{k\to\infty}I_\gamma(N) + q\liminf_{k\to\infty}\langle\mathcal{D}^0\psi\,,\,\psi\rangle \ge qm(\alpha).$$

It implies $E(q) = qm(\alpha)$, but we can use the method of Section 3.4.1. to prove that $E(q) < qm(\alpha)$ for sufficiently small α and L in regard with q : we define $\overline{Q}$ by the formulae

$$\begin{cases} \overline{\Pi} := \overline{\gamma} + \mathcal{P}^0_- = \chi_{(-\infty,0)}\Big(\mathcal{D}^0 + \alpha\big(\varphi_{\overline{\gamma}} + qn * |\cdot|^{-1} - R(\overline{\gamma} + qN)\big)\Big), \\ \overline{Q} := \overline{\gamma} + \frac{q}{1 - \|\overline{\Pi}\psi_\lambda\|^2_{L^2}} |(1-\overline{\Pi})\psi_\lambda\rangle\langle(1-\overline{\Pi})\psi_\lambda|. \end{cases}$$

If we assume that $E(q) = qm(\alpha)$ once $E(1) < m(\alpha)$ has been proven, we also obtain $E(q) > qE(1)$. We thus get $E(q) + E(1-q) > qE(1) + (1-q)E(1) = E(1)$.

There remains the case $q > 1$. However it has been proved in [HLS09] that for each integer M, $E_{\text{BDF}}(\cdot)$ is concave on $[M, M+1]$. Besides thanks to (3.20) there holds

$$E(q) \geq q(1 - \alpha\tfrac{\pi}{4})m(\alpha).$$

So it suffices that $2(1-\alpha\frac{\pi}{4})m(\alpha) > E(1)$ to get $E(q) > E(1)$ for $q > 1$. For $\alpha < \frac{2}{\pi}$ it is true and as $E(q) > 0$ for $q \neq 0$ the binding inequalities for $q > 1$ are proved.

3.4.3 Proof of Theorems 3.2 and 3.3

Notations

Let $Q = \gamma' = \gamma + N$ be a minimizer written with the notation of (3.24). As before we write $n := \rho_N$.

We have $N = \chi_{(0,\mu]}(D_Q)$ with $D_Q := \mathcal{D}^0 + \alpha(R'_\gamma - \varphi'_\gamma)$. We have to show that $N = |\psi\rangle\langle\psi|$, then we can choose μ such that $D_Q\psi = |D_Q|\psi = \mu\psi$ with $\mu \leq m(\alpha)$.

We split ψ in two : $\psi = \begin{pmatrix}\varphi \\ \chi\end{pmatrix}$. The wave function $\varphi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ is the upper spinor and $\chi \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ the lower spinor.

We write $C_0^2 := \frac{2g_1'(0)^2}{(\alpha b_\Lambda(0))^2 m(\alpha)}$ and $c := \frac{(g_1'(0))^2}{\alpha b_\Lambda(0) m(\alpha)}$.

As $(R(N) - \psi_{|\psi|^2})\psi = 0$, there holds

$$(\mathcal{D}^0 + \alpha(\varphi_\gamma - R_\gamma))\psi = \mu\psi = |\mathcal{D}^0 + \alpha(\varphi_\gamma - R_\gamma)|\psi. \tag{3.67}$$

We write $v^\star_\gamma := \varphi^\star_\gamma, b^\star_\gamma := v^\star_\gamma - R^\star_\gamma$, where $\star$ is a prime symbol or no prime. Moreover we write $d := \mathcal{D}^0$. We recall :

$$\langle v_\gamma\psi\,,\,\psi\rangle = D(\rho_\gamma, n) \text{ and } |\langle R_\gamma\psi\,,\,\psi\rangle| \leq \|\gamma\|_{\text{Ex}}\|n\|_{\mathcal{C}}, \tag{3.68}$$

We recall the notation $\langle g_\star\psi\,,\,\psi\rangle := \langle g_\star(-i\nabla)\psi\,,\,\psi\rangle$ with $\star \in \{0, 1\}$.

Strategy of the proof

The proof of Theorem 3.2 relies on bootsrap arguments enabling us to get appropriate estimates of $\|\,|\nabla|^s\psi\|_{L^2}$ for $s = \frac{1}{2}, 1, \frac{3}{2}$. The starting point is *a priori* estimates of $\|\,|\nabla|^{1/2}\psi\|_{L^2}, \|\nabla\psi\|_{L^2}, \text{Tr}(|\mathcal{D}^0|\gamma^2)$. It is possible to use an adaptation of the fixed point method of [HLS05a] to get estimates of

$$\iint \widetilde{E}\,(p-q)^{2s}\,\widetilde{E}\,(p+q)\,|\widehat{g}(p,q)|^2 dpdq \text{ and } \int \frac{\widetilde{E}\,(k)^{2s}\,|\widehat{\rho}_\gamma(k)|^2}{|k|^2}dk$$

in terms of the Sobolev norms $\|\psi\|_{H^{s+1/2}}$ at least for $s = 0, \frac{1}{2}, 1$. Then the second part of Eq. (3.24) enables to get estimates of $\|\,|\nabla|^{s+1}\psi\|_{L^2}$ in terms of $\|\,|\nabla|^{s+1/2}\psi\|_{L^2}$ and the (squared) norms above. It is possible to keep going as explained in the thesis of the author [Sok14c], provided α, L are small enough.

More precisely the steps are the following.

1. We first prove *a priori* estimates and get $\|\rho_Q\|_{\mathcal{C}}, \|Q\|_{\text{Kin}}$ are $O(1)$ and then show that $\|\gamma\|_{\text{Kin}} = o(1)$. As a consequence Lemma 3.1 holds and we get $\|\rho_\gamma\|_{\mathcal{C}}, \|\gamma\|_{q_0}, \langle|\mathcal{D}^0|\psi\,,\,\psi\rangle$ are O(1). This enables us to show that we can apply the fixed point method (Lemma 3.8, $f = 1$) and that the minimizer $\gamma + N$ and its density $\rho_\gamma + n$ form a fixed point (at least in the space associated to $\|\cdot\|_{q_0}$ and $\|\cdot\|_{\mathcal{C}}$).
2. We then prove

$$\|\psi\|_{H^{3/2}}, \|n\|_{\mathfrak{C}} = O(1). \tag{3.69}$$

Thus we can apply the fixed-point method (Lemma 3.7) with $n = |\psi|^2$ and $N = |\psi\rangle\langle\psi|$ and so to construct $(\gamma + N; \rho_\gamma + \rho_N)$ as a fixed point in (a ball of) $\mathcal{X}$.
3. Using the estimates that we deduce from the fixed-point method and Eq. (3.24) we then prove that

$$\langle |\nabla|^2 \psi\,,\, \psi\rangle = O((\alpha b_\Lambda(0))^2).$$

4. Following [HLS09], we apply a scaling transform to the minimizer with the scaling factor $c = O(\alpha b_\Lambda(0))$ defined in Subsection 3.4.3 :
we get $\underline{\psi}(x) := c^{3/2}\psi(cx) \in H^1(\mathbb{C}^4)$. The previous results will give

$$\|\underline{\psi}\|_{H^{3/2}} = O(1),\ \|\underline{\chi}\|_{H^1} = O(L\alpha),$$

where $\underline{\chi} \in H^1(\mathbb{R}^3, \mathbb{C}^2)$ is the lower spinor of $\underline{\psi}$.
5. At last we compute the energy and show the asymptotic expansion.

A priori estimates

The first step is the following result.

Lemma 3.11. *For $Q = \gamma + N$ a minimizer of $E^0_{BDF}(1)$, then N has rank 1 and there holds the following* a priori *estimates :*

$$\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) + \alpha D(\rho_\gamma, \rho_\gamma) + \langle |\mathcal{D}^0|\psi\,,\,\psi\rangle \lesssim 1.$$

The decomposition $\gamma + N$ is the same as in (3.24)*, Section 3.2 with $N = |\psi\rangle\langle\psi|$.*

Assuming this result is true we can go further : we know that
$F(Q, \rho_Q) = (Q, \rho_Q)$ where F is the function defined in (3.46) and (3.47). Using the estimates of Appendix 3.B.3 we get that :

$$\|\rho_\gamma\|_{\mathcal{C}} \lesssim L\|n\|_{\mathcal{C}} + \sqrt{L\alpha}\|Q\|_{q_0} + \sum_{j=2}^{+\infty} (\alpha K(\|\rho_Q\|_{\mathcal{C}} + \|Q\|_{q_0}))^j \lesssim L = O(1).$$

We then apply Lemma 3.8 (with $f = 1$) : we get that (Q, ρ_Q) is in fact the *unique* fixed point of F in a ball of $\mathcal{X}_0$.
Proof of Lemma 3.11 : As Q is a minimizer and that $E^0_{\mathrm{BDF}}(1) \leq m(\alpha)$ then there holds :

$$m(\alpha) \geq \mathcal{E}^0_{\mathrm{BDF}}(Q) \geq \big(1 - \alpha\frac{\pi}{4}\big)\mathrm{Tr}(|\mathcal{D}^0|Q^2) + \frac{\alpha}{2} D(\rho_Q, \rho_Q), \tag{3.70}$$

and $\|Q\|_{\mathrm{Kin}}, \sqrt{\alpha}\|\rho_Q\|_{\mathcal{C}} = O(1)$. As $\gamma = \chi_{(-\infty,0)}(\mathcal{D}^0_Q) - \mathcal{P}^0_-$, using estimates of Lemmas 3.16 and 3.17 we get :

$$\|\gamma\|_{\mathfrak{S}_2} \lesssim \alpha(\|\rho_Q\|_{\mathcal{C}} + \|Q\|_{\mathrm{Ex}}) \lesssim \sqrt{\alpha}.$$

Thus $|\mathrm{Tr}_0(\gamma)| \leq \|\gamma\|^2_{\mathfrak{S}_2} \lesssim \alpha < 1$, as a consequence $\mathrm{Tr}_0(\gamma) = 0$ and N has rank 1.
Thanks to (3.68) and Kato's inequality there holds

$$\langle \mathcal{D}^0\psi\,,\,\psi\rangle = \langle D_Q\psi\,,\,\psi\rangle - \alpha\langle b_\gamma\psi\,,\,\psi\rangle = \langle |D_Q|\psi\,,\,\psi\rangle + O(\alpha\|\psi\|_{H^{1/2}}(\|\gamma\|_{\mathrm{Ex}} + \|\rho_\gamma\|_{\mathcal{C}})). \tag{3.71}$$

We apply Lemma 3.5 on $|D_Q|$:

$$\langle |D_Q|\psi\,,\,\psi\rangle \geq \big(1 - K(\alpha\|Q\|_{\mathrm{Ex}} + \alpha^{1/2} \times \alpha^{1/2}\|\rho_Q\|_{\mathcal{C}})\big)\langle |\mathcal{D}^0|\psi\,,\,\psi\rangle, \tag{3.72}$$

and :

$$\langle \mathcal{D}^0\psi\,,\,\psi\rangle \geq (1 - K\sqrt{\alpha})\langle |\mathcal{D}^0|\psi\,,\,\psi\rangle + O\big(\alpha(\|\rho_Q\|_{\mathcal{C}} + \|Q\|_{\mathrm{Kin}})\|\psi\|_{H^{1/2}}\big). \tag{3.73}$$

By Cauchy-Schwartz inequality and Kato's inequality :

$$\begin{aligned}\mathcal{E}^0_{\mathrm{BDF}}(Q) &= \mathcal{E}^0_{\mathrm{BDF}}(\gamma) + \langle \mathcal{D}^0\psi\,,\,\psi\rangle + \alpha\Re\big(D(\rho_\gamma, n) - \mathrm{Tr}(R_\gamma N)\big)\\ &\geq (1 - \alpha\tfrac{\pi}{4})\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) + \tfrac{\alpha}{2}D(\rho_\gamma, \rho_\gamma) + (1 - C_2\sqrt{\alpha})\langle |\mathcal{D}^0|\psi\,,\,\psi\rangle\\ &\qquad -\alpha\|\psi\|_{H^{1/2}}(\|\gamma\|_{\mathrm{Kin}} + \|\rho_\gamma\|_{\mathcal{C}}).\end{aligned}$$

As $\mathcal{E}^0_{\mathrm{BDF}}(Q) \leq m(\alpha)$ we have

$$\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) + \alpha D(\rho_\gamma, \rho_\gamma) + \langle |\mathcal{D}^0|\psi\,,\,\psi\rangle = O(1). \tag{3.74}$$

□

Estimates around the fixed point method

Let us prove that we can construct (Q, ρ_Q) as a fixed point in $\mathcal{X}$. We have to show $\|n\|_{\mathfrak{C}}, \|N\|_{\mathcal{Q}} = O(1)$ and as $\|N\|_{\mathcal{Q}} \lesssim \|\psi\|^2_{H^{3/2}}$ it suffices to prove (3.69).

By Sobolev inequality (3.39) :

$$\|n\|_{L^2} = \|\psi\|^2_{L^4} \lesssim \big\| \, |\nabla|^{3/4}\psi\big\|^2_{L^2} \lesssim \|\nabla\psi\|^{3/2}_{L^2}\|\psi\|^{1/2}_{L^2} = O(\sqrt{\alpha}).$$

Moreover there holds $D(n,n) \le \frac{\pi}{2}\langle|\nabla|\psi\,,\,\psi\rangle \lesssim 1$ and $\|n\|_{\mathfrak{C}} = O(1)$.

At this point we have : $\|n\|_{\mathfrak{C}_1}, \|N\|_{q_1} \lesssim 1$: we can apply Lemma 3.8 with $f(p-q) = \widetilde{E}\,(p-q)$ and construct (Q, ρ_Q) as a fixed point in $\mathcal{X}_1$. As shown in Appendix 3.B.3, there holds $\|\gamma\|_{\mathfrak{C}_1} + \|\rho_\gamma\|_{\mathfrak{C}_1} \lesssim 1$.

Let us now prove that $\|\psi\|_{H^{3/2}} \lesssim 1$. By (3.67) we have $|d|^2\psi = \mu d\psi - \alpha d b_\gamma \psi$, therefore :

$$\langle |d|^3\psi\,,\,\psi\rangle = \mu\langle |d|d\psi\,,\,\psi\rangle + \alpha\langle |d|^{1/2}(R_\gamma - v_\gamma)|d|^{-3/2}|d|^{3/2}\psi\,,\,d|d|^{1/2}\psi\rangle.$$

Then thanks to (3.41b) and Lemma 3.12 below, writing

$$|d|^{1/2}b_\gamma|d|^{-3/2} = [\,|d|^{1/2}, b_\gamma]|d|^{-3/2} + b_\gamma|d|^{-1}$$

we get $\big\||d|^{1/2}b_\gamma|d|^{-3/2}\big\|_{\mathcal{B}} \lesssim (\|\gamma\|_{\text{Ex}} + \|\rho_\gamma\|_{\mathcal{C}}) + \|\gamma\|_{q_1}$.

We obtain at last $\|\psi\|_{H^{3/2}} \lesssim 1$. In particular we can apply Lemma 3.7 and construct (Q, ρ_Q) as a fixed point in $\mathcal{X}$ and get $\|\gamma\|_{\mathcal{Q}}, \|\rho_\gamma\|_{\mathfrak{C}} \lesssim 1$.

Lemma 3.12. *Let (γ_0', ρ_0') be in $\mathcal{Q}\times\mathcal{C}$ and $b_0 := \rho_0' * \frac{1}{|\cdot|} - \gamma_0'$, $v_0' := \rho_0' * \frac{1}{|\cdot|}$. Then there holds :* $\left\| |\mathcal{D}^0|^{-\frac{3}{2}}\left[b_0, |\mathcal{D}^0|^{\frac{1}{2}}\right]\right\|_{\mathcal{B}} + \left\| |\mathcal{D}^0|^{-1}\left[b_0, |\mathcal{D}^0|^{\frac{1}{4}}\right]\right\|_{\mathcal{B}} \lesssim (\|\gamma_0'\|_{\mathcal{Q}} + \|\rho_0'\|_{\mathcal{C}})$.

Proof : The estimation for the term $R(\gamma_0')$ comes from (3.41b) in Lemma 3.4 : indeed we have

$$|\widetilde{E}\,(p)^s - \widetilde{E}\,(q)^s\,| \le K\frac{|p-q|}{\widetilde{E}\,(p)^{1-s} + \widetilde{E}\,(q)^{1-s}} \text{for } s = \frac{1}{2^k},\, k \in \mathbb{N}^*.$$

We write $f \in \mathfrak{H}_\Lambda$ and $\Phi = |\mathcal{D}^0|^{-\frac{3}{2}}\left[v_0', |\mathcal{D}^0|^{\frac{1}{2}}\right]$, the following holds :

$$\int_p |\widehat{\Phi f}(p)|^2 dp \le K\iint \frac{dpdq}{\widetilde{E}\,(p)^3}\frac{|\widetilde{E}\,(p) - \widetilde{E}\,(q)\,|^2}{|p-q|^4}\frac{|\widehat{\rho_0'}(p-q)|^2}{\widetilde{E}\,(p) + \widetilde{E}\,(q)}\int|\widehat{f}(q)|^2 dq.$$

To deal with last term we use the same method. □

Let us prove $\langle|\nabla|^2\psi\,,\,\psi\rangle = O((\alpha b_\Lambda(0))^2)$.

We write $x = x(N) = \|g_1(-i\nabla)\psi\|_{L^2}$. By Lemma 3.19 we have :

$$\|\rho_\gamma\|_{\mathcal{C}} \lesssim Lx^{1/2} + \alpha x + L\alpha, \tag{3.75a}$$

$$\|\gamma\|_{\text{Ex}} \lesssim \sqrt{L\alpha}x^{1/2} + \alpha x + L\alpha. \tag{3.75b}$$

Taking $\|\cdot\|_{L^2}$-norm of $d\psi = \mu\psi - \alpha b_\gamma\psi$, we have (*cf* Proposition 3.3 for $\|g_0''\|_\infty$) :

$$\begin{aligned}
&\langle d^2\psi\,,\,\psi\rangle = x^2 + m(\alpha)^2 + O(\|g_0''\|_\infty x^2) = x^2 + m(\alpha)^2 + O(\alpha x^2)\\
&\alpha|\langle b_\gamma\psi\,,\,\psi\rangle| + \alpha^2\|b_\gamma\psi\|^2_{L^2} \le K_1L\alpha^2x^{1/2} + K_2L\alpha x + K_3\alpha^2x^{3/2} + K_4(L\alpha^3)x^2 + K_6\alpha^4x^3\\
&\mu^2\|\psi\|^2_{L^2} \le m(\alpha)^2.
\end{aligned}$$

For the first equality we have used Taylor's Formula (order 2) and the fact that $g_0'(0) = 0$. As $x = O(1)$ we have $\alpha^4x^3 = O(\alpha^4x^2)$ and

$$x^2 \le k_1L\alpha^2x^{1/2} + k_2(L\alpha)x + k_3\alpha^2x^{3/2}. \tag{3.76}$$

Finally we obtain

$$x^{1/2} \leq k_1^{1/3}(L\alpha^2)^{1/3} + k_2^{1/2}(L\alpha)^{1/2} + k_3\alpha^2 \lesssim (L\alpha)^{1/2}, \tag{3.77}$$

and there holds $x^2 \leq K(L\alpha)^2 = O(c^{-2})$.

By Lemma 3.19 the following estimates hold for the minimizer :

$$\begin{array}{l|l} \|\gamma\|_{\mathcal{Q}} \lesssim \alpha, & \|\rho_\gamma\|_{\mathfrak{C}} \lesssim (L + w(N))\sqrt{L\alpha}, \\ \|\gamma\|_E \lesssim L\alpha, & \|\rho_\gamma\|_{\mathcal{C}} \lesssim L\sqrt{L\alpha} \end{array}$$

where we recall :

$$w(N) := \left\{ \iint |p-q|^2|p+q||\widehat{N}(p,q)|^2 dpdq \right\}^{1/2} \lesssim \left\| |\nabla|^{3/2}\psi \right\|_{L^2}.$$

Scaling

We have considered so far the problem associated with $E_{c=1,\alpha,\Lambda}$(BDF energy where the parameters are : speed of light 1, fine structure constant α and cut-off Λ). We link it to the BDF energy in another choice of parameters : speed of light c, fine structure constant αc and cut-off $c\Lambda$, with $c > 0$ defined in Subsection 3.4.3.

As in [HLS09] we write

$$U_c^* : \begin{array}{ccc} \mathfrak{H}_\Lambda & \to & \mathfrak{H}_{c\Lambda} \\ \phi & \mapsto & c^{3/2}\phi(c(\cdot)), \end{array}$$

and so $U_c\phi(x) = c^{-3/2}\phi(x/c)$. There holds a scaling correspondence between $(1, \alpha, \Lambda)$ and $(c, c\alpha, c\Lambda)$:

$$E_{c,c\alpha,c\Lambda}(U_c^* Q U_c) = c^2 E_{1,\alpha,\Lambda}(Q).$$

To distinguish the corresponding objects of $(c, c\alpha, c\Lambda)$ we underline them :

$$\begin{array}{l|l} \underline{\psi}(x) = U_c^*\psi(x) = c^{3/2}\psi(cx), & \underline{\mathcal{D}^0} = c^2\, U_c^*\mathcal{D}^0 U_c = \underline{m}c^2\beta + cT, \\ \underline{\gamma}(x,y) = U_c^*\gamma U_c(x,y) = c^3\gamma(cx,cy), & \underline{m} = g_0(-i\nabla/c), \\ \rho_{\underline{\gamma}}(x) = c^3\rho_\gamma(cx), \underline{v} = \rho_\gamma * |\cdot|^{-1}, & T_{\boldsymbol{\alpha}} = cg_1(-i\nabla/c)\boldsymbol{\alpha}\cdot\frac{-i\nabla}{|\nabla|}, \\ \underline{R}(x,y) = \underline{\gamma}(x,y)|x-y|^{-1}, & T_\sigma = cg_1(-i\nabla/c)\sigma\cdot\frac{-i\nabla}{|\nabla|}. \end{array}$$

There holds $|\nabla| \leq |T_\sigma| \leq C_1|\nabla|$ and

$$\left\{ \begin{array}{l} \|\underline{\gamma}\|_{\mathrm{Ex}} = \sqrt{c}\|\gamma\|_{\mathrm{Ex}} \\ \|\rho_{\underline{\gamma}}\|_{\mathcal{C}} = \sqrt{c}\|\rho_\gamma\|_{\mathcal{C}} \end{array}\right., \text{so} \left\{ \begin{array}{l} \|\underline{R}|D^0|^{-1/2}\|_{\mathcal{B}} \lesssim \|\gamma\|_{\mathrm{Ex}} = \sqrt{c}\|\gamma\|_{\mathrm{Ex}} \\ \|\underline{v}|D^0|^{-1/2}\|_{\mathcal{B}} \lesssim \|\rho_{\underline{\gamma}}\|_{\mathcal{C}} = \sqrt{c}\|\rho_\gamma\|_{\mathcal{C}} \end{array}\right.$$

We have shown $\langle g_1^2\psi\,,\,\psi\rangle = O((L\alpha)^2)$, so for $c := \frac{g_1'(0)^2}{\alpha b_\Lambda(0)}$, $\underline{\psi}$ has uniformly bounded H^1 norm with respect to the parameters in the regime (3.23).

Remark 3.9. Here the constant of scaling c corresponds to λ of the test function.

First we we prove the following middle results.

Lemma 3.13. *Let $Y = Y(\psi) := \|g_1^{3/2}\psi\|_{L^2}$ where ψ is defined as above. Then we have*

$$\|\chi\|_{L^2} \lesssim c^{-1} \text{ and } \|\nabla\chi\|_{L^2} \lesssim \alpha Y + c^{-1}.$$

Moreover $\mu = m(\alpha) + O(c^{-2})$ and $E^0_{BDF}(1) = \mathcal{E}^0_{BDF}(\gamma') = m(\alpha) + O(c^{-2})$.

Proof : Thanks to (3.67) we have

$$\underline{m}c^2\beta\underline{\psi} + cT_{\boldsymbol{\alpha}}\underline{\psi} + \alpha c(\underline{v} - \underline{R})\underline{\psi} = \mu c^2\underline{\psi}. \tag{3.78}$$

Considering the upper part φ and the lower part χ of ψ :

$$\underline{m}c^2\underline{\varphi} + cT_\sigma\underline{\chi} + \alpha c\underline{v}\underline{\varphi} - \alpha c(\underline{R}\underline{\psi})_1 = \mu c^2\underline{\varphi} \tag{3.79a}$$

$$-\underline{m}c^2\chi + cT_\sigma\varphi + \alpha c\underline{v}\chi - \alpha c(\underline{R}\underline{\psi})_2 = \mu c^2\underline{\chi} \tag{3.79b}$$

From (3.79b) we obtain

$$\underline{\chi} = \frac{T_\sigma}{\underline{m}c+\mu c}\underline{\varphi} + \frac{\alpha}{\underline{m}c+\mu c}((\underline{R}\underline{\psi})_2 - \underline{v}\underline{\chi}).$$

We take the L^2-norm :

$$\|\underline{\chi}\|_{L^2} \lesssim \frac{\|\underline{\psi}\|_{H^1}}{c} + \frac{\alpha}{\sqrt{c}}(\|\rho_\gamma\|_{\mathcal{C}} + \|\gamma\|_{\mathrm{Ex}}) \lesssim \frac{1}{c} + \frac{\alpha L\sqrt{L\alpha}}{\sqrt{c}} + \frac{\alpha L\alpha}{\sqrt{c}} \lesssim \frac{1}{c}.$$

In particular we have $\|\chi\|_{L^2} = \|\underline{\chi}\|_{L^2} = O(c^{-1})$.

We write $S_{\mathbf{x}} = \boldsymbol{g}_1(-i\nabla)\cdot\mathbf{x}$ with $\mathbf{x}$ either σ or $\boldsymbol{\alpha}$. As $T_{\boldsymbol{\alpha}}$ exchanges upper and lower spinors, by Cauchy-Schwarz inequality the following holds :

$$\begin{aligned}\langle \mathcal{D}^0\psi\,,\,\psi\rangle &= \langle g_0\varphi\,,\,\varphi\rangle - \langle g_0\chi\,,\,\chi\rangle + 2\Re\langle S_\sigma\varphi\,,\,\chi\rangle \\ &= m(\alpha)\|\varphi\|_{L^2}^2 + O(c^{-2}) \\ &= m(\alpha) + O(c^{-2}).\end{aligned}$$

It enables us to estimate

$$\mu = m(\alpha) + O(c^{-2}) \text{ and } E^0_{\mathrm{BDF}}(1) = \mathcal{E}^0_{\mathrm{BDF}}(\gamma') = m(\alpha) + O(c^{-2}). \tag{3.80}$$

From Eq. (3.79a) we get

$$T_\sigma\underline{\chi} = \frac{(\mu c^2 - \underline{m}c^2)\underline{\varphi}}{c} + \alpha[(\underline{R}\psi)_1 - \underline{V}\underline{\varphi}].$$

As $\mu = m(\alpha) + O(c^{-2})$, the L^2-norm of $T_\sigma\underline{\chi}$ has the following upper bound :

$$\|T_\sigma\underline{\chi}\|_{L^2} \lesssim \alpha + c^{-1} + \alpha\sqrt{c}(L\alpha + L\sqrt{L\alpha}) \lesssim \alpha,$$

writing $Y^2 = Y(\psi)^2 := \langle g_1^3\psi\,,\,\psi\rangle$, we get the middle estimates

$$\|\underline{\chi}\|_{H^1} \lesssim \alpha \tag{3.81a}$$

$$\|\underline{\chi}\|_{H^1} \lesssim (\alpha Y + c^{-1}). \tag{3.81b}$$

Indeed writing $\mu = m(\alpha) + \delta m$, $c^2 \times \frac{\delta m}{c}\underline{\varphi}$ has L^2-norm lesser than Kc^{-1}. Then :

$$\Big|g_0(p/c) - g_0(0)\Big| = \begin{cases} \Big|\displaystyle\int_0^1 g_0'(tp/c)dt\frac{|p|}{c}\Big| & \le K\alpha\frac{|p|}{c}, \\ \Big|\displaystyle\int_0^1 g_0''(tp/c)(1-t)dt\frac{|p|^2}{c^2}\Big| & \le K\alpha\frac{|p|^2}{c^2}, \end{cases}$$

and $|g_0(p/c) - g_0(0)| \lesssim \alpha|p|^3/c^3$. In particular

$$\langle g_1\chi\,,\,\chi\rangle \le \sqrt{\langle\chi\,,\,\chi\rangle\langle g_1^2\chi\,,\,\chi\rangle} = O(c^{-1}\times(\alpha Y + c^{-1})c^{-1}) = O(\alpha Yc^{-2} + c^{-3}) \tag{3.82}$$

and there also holds the middle estimate : $\|\nabla\chi\|_{L^2} \lesssim \alpha c^{-1}$. □

Let us prove that $\|U_c^*\psi\|_{H^{3/2}} = O(1)$. The method is the following : we take the scalar product of $|\nabla|\psi$ with each part of the equation $|\mathcal{D}^0|^2\psi = \mathcal{D}^0(\mu - \alpha b_\gamma)\psi$. Then we cancel the leading terms in order to get an inequality involving $Y^2 = \langle g_1^3\psi\,,\,\psi\rangle$ of the form :

$$Y^2 \le O(c^{-3} + Yc^{-3/2} + Y^{3/2}c^{-3/4}).$$

As a consequence we get $Y^2 = O(c^{-3})$.

Let us first deal with $\langle|\mathcal{D}^0|^2\psi\,,\,|\nabla|\psi\rangle$.

Thanks to estimate (3.82) there holds

$$\Big|\mu\langle g_1\boldsymbol{\alpha}\cdot\tfrac{-i\nabla}{|i\nabla|}\psi\,,\,|\nabla|\psi\rangle\Big|\lesssim\|\,|\nabla|^{3/2}\varphi\|_{L^2}\|\,|\nabla|^{1/2}\chi\|_{L^2}=O(Yc^{-3/2}+Y^{3/2}\sqrt{\alpha}c^{-1}).$$

We recall that $|g_0(p)-m(\alpha)|\le\min(\|g_0'\|_{L^\infty}|p|,2\|g_0\|_{L^\infty})$: it is $O(\min(1,\alpha|p|))$. Then we have :

$$\begin{aligned}\langle g_0^2\psi\,,\,|\nabla|\psi\rangle&=m(\alpha)^2\langle|\nabla|\psi\,,\,\psi\rangle+2m(\alpha)\langle(g_0-m(\alpha))\psi\,,\,|\nabla|\psi\rangle+\langle(g_0-m(\alpha))^2\psi\,,\,|\nabla|\psi\rangle\\&=m(\alpha)^2+O(\alpha Y^2),\end{aligned}$$

Thus we have :

$$\langle|\mathcal{D}^0|^2\psi\,,\,|\nabla|\psi\rangle=m(\alpha)^2\langle|\nabla|\psi\,,\,\psi\rangle+\langle g_1^2|\nabla|\psi\,,\,\psi\rangle+O(\alpha Y^2).$$

Let us now treat the term $\langle\mathcal{D}^0(\mu-\alpha b_\gamma)\psi\,,\,|\nabla|\psi\rangle$ and first the term $\mu\langle\mathcal{D}^0\psi\,,\,|\nabla|\psi\rangle$.

$$\begin{aligned}\langle g_0\beta\psi\,,\,|\nabla|\psi\rangle&=\langle g_0\psi\,,\,|\nabla|\psi\rangle-2\langle g_0\chi\,,\,|\nabla|\chi\rangle=\langle g_0\psi\,,\,|\nabla|\psi\rangle+O(\alpha Yc^{-2}+c^{-3})\\&=m(\alpha)\langle|\nabla|\psi\,,\,\psi\rangle+O(\alpha Y^2+\alpha Yc^{-2}+c^{-3}),\\\langle\mathcal{D}^0\psi\,,\,|\nabla|\psi\rangle&=\langle g_0\beta\psi\,,\,|\nabla|\psi\rangle+2\Re(\langle S_\sigma\varphi\,,\,|\nabla|\chi\rangle)\\&=m(\alpha)\langle|\nabla|\psi\,,\,\psi\rangle+O(\alpha Y^2+\alpha Yc^{-2}+c^{-3}+Yc^{-3/2}+Y^{3/2}\sqrt{\alpha}c^{-1}),\\\mu\langle\mathcal{D}^0\psi\,,\,|\nabla|\psi\rangle&=m(\alpha)^2\langle|\nabla|\psi\,,\,\psi\rangle+O(\alpha Y^2+Y^{3/2}\sqrt{\alpha}c^{-1}+Yc^{-3/2}+c^{-3}).\end{aligned}$$

We write :

$$|d|^{1/2}R_\gamma\psi=\big[|d|^{1/2},R_\gamma\big]|d|^{-1}|d|\psi+R_\gamma|d|^{1/2}\psi,$$

and thanks to Lemma 3.4 we have :

$$\big\|\,\big[|d|^{1/2},R_\gamma\big]|d|^{-1}\big\|_{\mathfrak{S}_2}^2\lesssim\|\gamma\|_{q_1}^2\lesssim\|\gamma\|_E^2\lesssim c^{-2}.$$

By adapting the proof of Lemma 3.12 we can prove the follwing estimates :

$$\Big\|[|\nabla|,v_\gamma]\tfrac{1}{|\nabla||\mathcal{D}^0|^{1/2}}\Big\|_{\mathcal{B}},\Big\|[|\nabla|^{1/2},v_\gamma]\tfrac{1}{|\nabla|^{1/2}|\mathcal{D}^0|^{1/2}}\Big\|_{\mathcal{B}}\lesssim\|\rho_\gamma\|_{\mathcal{C}}\sqrt{\log(\Lambda)}.$$

We use Lemmas 3.3 and 3.4 to get estimates of $\|b_\gamma\psi\|_{L^2}$. First we deal with the terms with $S_{\boldsymbol{\alpha}}$:

$$\begin{aligned}|\langle R_\gamma\psi\,,\,S_{\boldsymbol{\alpha}}|\nabla|\psi\rangle|&\le\big|\big\langle\big[|\nabla|^{1/2},R_\gamma\big]|d|^{-1}|d|\psi,\,S_{\boldsymbol{\alpha}}|\nabla|^{1/2}\psi\big\rangle\big|+|\langle R_\gamma|\nabla|^{1/2}\psi\,,\,S_{\boldsymbol{\alpha}}|\nabla|^{1/2}\psi\rangle|\\&\lesssim Y\|\gamma\|_{\mathrm{Ex}}(1+\|\nabla\psi\|_{L^2})\lesssim Y(L\alpha).\end{aligned}$$

The operator $S_{\boldsymbol{\alpha}}$ exchanges upper and lower spinors, so we get :

$$\begin{aligned}|\langle S_\sigma v_\gamma\varphi\,,\,|\nabla|\chi\rangle|&=\big|\langle|\nabla|v_\gamma\varphi\,,\,S_\sigma\chi\rangle\big|\le\big\|\,|\nabla|v_\gamma\varphi\big\|_{L^2}\|S\chi\|_{L^2}\\&\le\alpha c^{-1}\Big\{\big\|\big[\,|\nabla|,v_\gamma\big]\varphi\big\|_{L^2}+\|v_\rho|\nabla|\varphi\|_{L^2}\Big\}\\&\lesssim\alpha c^{-1}\Big\{\sqrt{\log(\Lambda)}\|\rho_\gamma\|_{\mathcal{C}}\times\big\|\,|\nabla||d|^{1/2}\varphi\big\|_{L^2}+\|\rho_\gamma\|_{\mathcal{C}}Y\Big\}\\&\le Lc^{-5/2}(\|\nabla\varphi\|_{L^2}+\|\,|\nabla|^{3/2}\varphi\|_{L^2})\lesssim Lc^{-7/2}+Lc^{-5/2}Y.\end{aligned}$$

Similarly the following holds :

$$\begin{aligned}|\langle S_\sigma v_\gamma\chi\,,\,|\nabla|\varphi\rangle|&=\big|\langle|\nabla|^{1/2}v_\gamma\chi\,,\,|\nabla|^{1/2}S_\sigma\varphi\rangle\big|\\&\le\Big\{\big\|\big[|\nabla|^{1/2},v_\gamma\big]\chi\big\|_{L^2}+\|v_\gamma|\nabla|^{1/2}\chi\|_{L^2}\Big\}\big\|\,|\nabla|^{3/2}\varphi\big\|_{L^2}\\&\lesssim\big(\sqrt{\log(\Lambda)}\|\rho_\gamma\|_{\mathcal{C}}\||\nabla|^{1/2}|d|^{1/2}\chi\|_{L^2}+\|\rho_\gamma\|_{\mathcal{C}}\big\|\,|\nabla|^{3/2}\chi\big\|_{L^2}\big)Y\\&\lesssim(L\sqrt{\log(\Lambda)}c^{-1/2}(c^{-3/2}+c^{-1}\sqrt{\alpha Y}+\alpha c^{-2}Y))Y.\end{aligned}$$

We treat now the terms with $g_0(-i\nabla)$:

$$\begin{array}{rcccl}|\langle v_\gamma\varphi\,,\,|\nabla|g_0\varphi\rangle|&\lesssim&\|\rho_\gamma\|_{\mathcal{C}}\big\|\,|\nabla|^{1/2}\varphi\big\|_{L^2}\big\|\,|\nabla|g_0\varphi\big\|_{L^2}&\lesssim&Lc^{-2}\\|\langle v_\gamma\chi\,,\,|\nabla|g_0\chi\rangle|&\lesssim&\|\rho_\gamma\|_{\mathcal{C}}\big\|\,|\nabla|^{1/2}\chi\big\|_{L^2}\big\|\,|\nabla|g_0\chi\big\|_{L^2}&\lesssim&Lc^{-2},\\|\langle R_\gamma\psi\,,\,|\nabla|g_0\psi\rangle|&\lesssim&\|\gamma\|_{\mathrm{Ex}}\big\|\,|\nabla|^{1/2}\psi\big\|_{L^2}\big\|\,|\nabla|g_0\psi\big\|_{L^2}&\lesssim&c^{-5/2}.\end{array}$$

It is clear that $\alpha(Lc^{-2}+c^{-5/2}) = O(c^{-3})$. At last :

$$\langle \mathcal{D}^0(\mu-\alpha b_\gamma)\psi\,,\,|\nabla|\psi\rangle = m(\alpha)^2\langle|\nabla|\psi\,,\,\psi\rangle + O(\alpha Y^2 + Y^{3/2}\sqrt{\alpha}c^{-1} + Yc^{-3/2}+c^{-3}),$$

and :

$$Y^2(1-K\alpha) \le K_0c^{-3} + K_1(L\alpha^2)Y + K_3\sqrt{\alpha}c^{-1}Y^{3/2}.$$

As $\sqrt{\alpha}c^{-1} = O(c^{-3/4})$ (because $\alpha(\log(\Lambda))^{1/4} = o(1)$ in the regime (3.23)), we deduce $\langle|\nabla|^3\psi\,,\,\psi\rangle = O(c^{-3})$, equivalently

$$\|\underline{\psi}\|_{H^{3/2}} = O(1).$$

We now improve estimate (3.81a) as written before :

$$\begin{aligned} g_0(p/c)-g_0(0) &= \int_0^1 g_0'(tp/c)\frac{|p|}{c}dt = \int_0^1 (1-t)g_0''(tp/c)\frac{|p|^2}{c^2}dt\\ |g_0(p/c)-g_0(0)|^2 &= \Big|\int_0^1 g_0'(tp/c)dt\int_0^1(1-u)g_0''(up/c)du\Big|\frac{|p|^3}{c^3}, \end{aligned}$$

and therefore

$$\|(m(\alpha)-\underline{m})c\underline{\psi}\|_{L^2} \le K\sqrt{\frac{\|g_0'\|_\infty\,\|g_0''\|_\infty}{c}} = K\alpha\sqrt{L\alpha} = o(c^{-1}). \tag{3.83}$$

So

$$\|\underline{\chi}\|_{H^1} = O(c^{-1}) \text{ and } \|\,|\nabla|\chi\|_{L^2} = O(c^{-2}). \tag{3.84}$$

Estimation of $E^0_{\mathbf{BDF}}(1)$.

Thanks to Eq. (3.79b)

$$\chi = \frac{S_\sigma}{g_0+\mu}\varphi + \frac{\alpha}{g_0+\mu}\big((R_\gamma\psi)_2 - v_\gamma\chi\big) = \frac{S_\sigma}{g_0+\mu}\varphi + \delta\chi,$$

where the remainder $\delta\chi$ is such that $\|\delta\chi\|_{L^2}$ is lesser than $K\alpha(\|\gamma\|_{\mathrm{Ex}}\||\nabla|^{1/2}\psi\|_{L^2} + \|\rho\|_{\mathcal{C}}\||\nabla|^{1/2}\chi\|_{L^2}) = O(\alpha c^{-3/2}) = o(c^{-1})$. Thanks to Proposition 3.3, as $\|g_1\psi\|_{L^2} = O(c^{-1})$, we have the following asymptotic expansion :

$$\begin{aligned} E^0_{\mathrm{BDF}}(1) + \tfrac{\alpha b_\Lambda(0)}{2c}D(\underline{n},\underline{n}) &= \langle g_0\varphi\,,\,\varphi\rangle - \langle \tfrac{g_0}{g_0+\mu}S_\sigma\varphi\,,\,\tfrac{1}{g_0+\mu}S_\sigma\varphi\rangle + 2\Re\langle\tfrac{1}{g_0+\mu}S_\sigma\varphi\,,\,S_\sigma\varphi\rangle + o(c^{-2})\\ &= m(\alpha)(1-2\langle\tfrac{g_1^2}{(g_0+\mu)^2}\varphi\,,\,\varphi\rangle) + 2\langle\tfrac{g_1^2}{g_0+\mu}\varphi\,,\,\varphi\rangle + o(c^{-2})\\ &= m(\alpha) - \langle\tfrac{g_1^2}{2m(\alpha)}\varphi\,,\,\varphi\rangle + \langle\tfrac{g_1^2}{m(\alpha)}\varphi\,,\,\varphi\rangle + o(c^{-2})\\ &= m(\alpha) + \tfrac{1}{2m(\alpha)}\langle g_1^2\varphi\,,\,\varphi\rangle + o(c^{-2})\\ &= m(\alpha) + \tfrac{1}{2m(\alpha)}\langle g_1^2\psi\,,\,\psi\rangle + o(c^{-2}). \end{aligned}$$

To deal with g_0 we use both results $\langle|\nabla|^3\varphi\,,\,\varphi\rangle = O(c^{-3})$ and $|g_0'| = O(\alpha)$ and treat the $((g_0+\mu)^{-1})$'s one after the other. For the last line we use the fact that $\langle|\nabla|^2\chi\,,\,\chi\rangle = O(c^{-3})$. Writing in terms of $\underline{\psi}$:

$$C_0^2(E^0_{\mathrm{BDF}}(1)-m(\alpha)) = \frac{1}{(g_1'(0))^2(2\pi)^3}\int c^2 g_1\left(\frac{p}{c}\right)^2|\widehat{\underline{\psi}}(p)|^2dp - \iint\frac{|\underline{\psi}(x)|^2|\underline{\psi}(y)|^2}{|x-y|}dxdy + o(1). \tag{3.85}$$

We recall (*cf* Proposition 3.4, Appendix 3.A) the $(g_1')_{\alpha,\Lambda}$'s are *uniformly* continuous in a neighbourhood of 0 ;

splitting in Fourier space at level $|p| = \sqrt{c}$ we get

$$\begin{aligned}
\int\limits_{|p|\le\sqrt{c}} c^2 g_1(p/c)^2 |\widehat{\underline{\psi}}(p)|^2 dp = & \int\limits_{|p|\le\sqrt{c}} g_1'(0)^2 |p|^2 |\widehat{\underline{\psi}}(p)|^2 dp \\
& + \int\limits_{|p|\le\sqrt{c}} \left(\int_{t=0}^1 (g_1'(tp/c) - g_1'(0))dt\right)^2 |p|^2 |\widehat{\underline{\psi}}(p)|^2 dp \\
& + 2g_1'(0) \int_{|p|\le\sqrt{c}} \left(\int_{t=0}^1 (g_1'(tp/c) - g_1'(0))dt\right) |p|^2 |\widehat{\underline{\psi}}(p)|^2 dp \\
= & \int\limits_{|p|\le\sqrt{c}} g_1'(0)^2 |p|^2 |\widehat{\underline{\psi}}(p)|^2 dp + O\big(\| \, |\nabla|\underline{\psi}\|^2 \sup_{|q|\le c^{-\frac{1}{2}}} \{|g_1'(q) - g_1'(0)|\}\big) \\
= & \int\limits_{|p|\le\sqrt{c}} g_1'(0)^2 |p|^2 |\widehat{\underline{\psi}}(p)|^2 dp + \underset{c\to+\infty}{o}(1).
\end{aligned}$$

Moreover :

$$\begin{aligned}
\int_{|p|\ge\sqrt{c}} c^2 g_1(p/c)^2 |\widehat{\underline{\psi}}(p)|^2 dp & \lesssim \int_{|p|\ge\sqrt{c}} \frac{|p|^3}{|p|} |\widehat{\underline{\psi}}(p)|^2 dp \\
& \lesssim \tfrac{1}{\sqrt{c}} \langle |\nabla|^3 \underline{\psi} \,,\, \underline{\psi}\rangle \lesssim c^{-1/2} \underset{c\to+\infty}{\to} 0.
\end{aligned}$$

Thus

$$\frac{1}{(g_1'(0)^2)} \langle c^2 g_1^2(\cdot/c)\underline{\psi} \,,\, \underline{\psi}\rangle - D(\underline{n},\underline{n}) \quad = \langle |\nabla|^2 \underline{\psi} \,,\, \underline{\psi}\rangle - D(\underline{n},\underline{n}) + o(1),$$

By unicity of the asymptotic expansion and by definition of E_{CP} we thus have

$$E^0_{\mathrm{BDF}}(1) = m(\alpha) + C_0^{-2} E_{\mathrm{CP}} + o((\alpha b_\Lambda(0))^2). \tag{3.86}$$

As a consequence, the Choquard-Pekar energy wave function $\underline{\psi}$ (more specifically $\underline{\varphi}$) tends to the minimizer. It is known [Lie77] there is but one minimizer in $H^1(\mathbb{R}^3, \mathbb{C})$ up to translation. The fact that we work with spinors is harmless. By using convexity inequality for gradients [LL97] (Theorem 7.8 p.177) and Riesz's rearrangements inequality (sharp version in [Lie77]), we have that there is but one minimizer of the Choquard-Pekar energy in $H^1(\mathbb{R}^3, \mathbb{C}^4)$ up to translation and *overall* rotation in $\mathbb{C}^4$. Keeping track of the mass of $\underline{\psi}$ with the help of some translation we get that necessarily it tends to a Choquard-Pekar minimizer.
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3.A The operator $\mathcal{D}^0$

Remark 3.10. In this part the scalar product in $\mathbb{R}^d$ is written $\langle \cdot \,,\, \cdot\rangle$ for $d = 3, 4$.

3.A.1 The functions g_0 and g_1

As established in [HLS07], $\mathcal{D}^0$ is a solution to the following equation in the Fourier space

$$\widehat{\mathcal{D}^0} = \widehat{D^0} + \frac{\alpha}{4\pi^2} \frac{\widehat{\mathcal{D}^0}}{|\mathcal{D}^0|} * \frac{1}{|\cdot|^2} \quad \text{in } \mathcal{B}(B(0,\Lambda), \mathrm{End}(\mathbb{C}^4)) \tag{3.87}$$

and by a bootstrap argument $\widehat{\mathcal{D}^0} \in \cap_{m\ge1} H^m\big(B(0,\Lambda)\big)$. With the notation of 3.1 (Subsection 3.2) it shows that $g_0, \mathbf{g_1}$ are smooth while $g_1(p) = \mathbf{g_1}(p) \cdot \omega_p$ is *a priori* in $\mathcal{C}^\infty(B(0,\Lambda)\backslash\{0\})$ and we have

$$g_0(|p|) = 1 + \frac{\alpha}{4\pi^2} \int_{|r|<\Lambda} dr \frac{1}{|p-r|^2} \frac{g_0(|r|)}{\sqrt{g_1(|r|)^2 + g_0(|r|)^2}}, \tag{3.88a}$$

$$g_1(|p|) = |p| + \frac{\alpha}{4\pi^2}\int_{|r|<\Lambda} dr \frac{\langle \omega_p, \omega_r\rangle}{|p-r|^2}\frac{g_1(|r|)}{\sqrt{g_1(|r|)^2 + g_0(|r|)^2}}. \tag{3.88b}$$

Remark 3.11. We recall here that $C_1 > 0$ is a constant such that $g_1(r) \le C_1 r$ and $|g_0|_\infty \le C_1$.

Proposition 3.3. *We have* $g_1 \in \mathcal{C}^1([0,\Lambda],\mathbb{R})$ *and* $g_0'(0) = 0$.
Writing $\|\mathrm{d}^2 g_1\|_\star = \sup_{0<|p|\le\Lambda} \big| |p| \mathrm{d}^2 g_1(p)\big|$ *the following holds :*

$$\left\{\begin{array}{l} \|g_0'\|_\infty = O(\alpha) \\ \|g_1'\|_\infty = O(1) \end{array}\right. \quad \text{and} \quad \left\{\begin{array}{l} \|g_0''\|_\infty = O(\alpha) \\ \|\mathrm{d}^2 g_1\|_\star = O(1) \end{array}\right. .$$

Moreover there exists $K > 0$ *such that*

$$\forall\, q \in B(0,\Lambda)\backslash B(0,1), \quad \left\{\begin{array}{ll} |g_0(0) - 1| & \le K\alpha\Big\{\log\dfrac{\Lambda}{|q|} + 1\Big\} \\ |g_1'(q) - 1| & \le K\alpha\Big\{\log\dfrac{\Lambda}{|q|} + 1\Big\}, \end{array}\right.$$

and we have

$$g_0(0) = 1 + \frac{L}{\pi} + O(L^2 + \alpha), \quad g_1'(0) = 1 + \frac{2L}{3\pi} + O(\alpha).$$

In fact it suffices to differentiate (3.87) to get $g_0'(p)$ and $g_1'(p)$, we take the norm to obtain the first part; then we differentiate once more to get the second part. The third part is a consequence of those parts. Proposition 3.3 enables us to prove the following result.

Lemma 3.14. *Let* $p, q \in B(0,\Lambda)$ *and* $k = p - q$. *There holds*

$$\frac{\widetilde{E}(p)\,\widetilde{E}(q) - \langle \mathbf{g}(p), \mathbf{g}(q)\rangle}{\widetilde{E}(p)\,\widetilde{E}(q)\,(\widetilde{E}(p) + \widetilde{E}(q))} \le \min\Big(2, \frac{2K|k|^2}{\widetilde{E}(p)^2}, \frac{2K|k|^2}{\widetilde{E}(q)^2}\Big).$$

where we can choose $K \le 2$ *for* $\alpha\log(\Lambda)$ *sufficiently small.*

Proof : In fact we can write for $a, b, t = b - a \in \mathbb{R}^3$: $|a||b| - \langle a, b\rangle = \frac{a^2t^2 - \langle t, a\rangle^2}{|a||b| + \langle a,b\rangle}$. If $\langle a, b\rangle > -\frac{|a||b|}{2}$ then $A = \frac{|a||b| - \langle a,b\rangle}{|a||b|} \le \frac{2a^2t^2}{a^2b^2}$, by symmetry we also have $A \le \frac{2b^2t^2}{a^2b^2}$.
Else $-|a||b| \le \langle a, b\rangle \le -\frac{|a||b|}{2}$, then $\big\{|a||b|(|a||b| + \langle a, b\rangle)\big\}^{-1} \ge 2(a^2b^2)^{-1}$, so :

$$\begin{array}{l} 2\frac{t^2}{b^2} \ge 2\frac{a^2+b^2+|a||b|}{b^2} \ge 2 \\ 2\frac{t^2}{a^2} \ge 2\frac{a^2+b^2+|a||b|}{a^2} \ge 2. \end{array}$$

□

Proposition 3.4. *The function*

$$\mathrm{d}\mathbf{g_1}(p) = id + \frac{\alpha}{4\pi^2}\int_{|r|<\Lambda} \frac{dr}{|p-r|\widetilde{E}(r)}\Big(\mathrm{d}\mathbf{g_1}(r) - \mathbf{g_1}(r)\frac{g_0(r)\mathrm{d}g_0(r) + g_1(r)\mathrm{d}g_1(r)}{\widetilde{E}(r)^2}\Big)$$

is in $\mathcal{C}^0(B(0,\Lambda), L(\mathbb{R}^3,\mathbb{C}^4))$ *and*

$$|\mathrm{d}\mathbf{g_1}(p) - \mathrm{d}\mathbf{g_1}(q)| \le KL|p-q|.$$

In particular the same holds for $g_1'(t) = \langle \mathrm{d}\mathbf{g_1}(t\omega), \omega\rangle$.

Proof of Proposition 3.3

1. We can define $\mathrm{d}g_1(p)$ for $p \ne 0$. First we have

$$\mathrm{d}g_0(p)h = \frac{\alpha}{4\pi^2}\int \frac{dq}{|p-q|^2}\left(\frac{\mathrm{d}g_0(q)h}{\widetilde{E}(q)} - \frac{g_0(q)\mathrm{d}g_0(q)h + g_1(q)\mathrm{d}g_1(q)h}{\widetilde{E}(q)^2}\frac{g_0(q)}{\widetilde{E}(q)}\right).$$

We remark that for $p \neq 0$ we have :

$$\begin{cases} \mathrm{d}g_\star(p)h = g'_\star(|p|)\langle \omega_p\,,\, h\rangle, \ \star \in \{0,1\}, \\ \langle \mathrm{d}\mathbf{g_1}(p)\cdot\omega_p\,,\,\omega_p\rangle = g'_1(|p|). \end{cases}$$

Then

$$\mathrm{d}\mathbf{g_1}(p)\cdot h = h + \frac{\alpha}{4\pi^2}\int \frac{dq}{|p-q|^2}\left(\frac{\mathrm{d}\mathbf{g_1}(q)\cdot h}{\widetilde{E}\,(q)} - \frac{g_0(q)\mathrm{d}g_0(q)h + g_1(q)\mathrm{d}g_1(q)h}{\widetilde{E}\,(q)^2}\frac{\mathbf{g_1}(q)}{\widetilde{E}\,(q)}\right).$$

So for any $\omega \in \mathbb{S}^2$ we have

$$\begin{aligned} g'_1(x) \quad &= 1 + \frac{\alpha}{4\pi^2}\int_{|q|\le\Lambda}\frac{dq}{|x\omega - q|^2}\Big\{\Big(\frac{g_1(q)}{|q|}(1-\langle\omega,\omega_q\rangle^2)\Big)\frac{1}{\widetilde{E}\,(q)} \\ &+\Big(g'_1(q)\langle\omega_q,\omega\rangle^2\big(1-\tfrac{g_1^2(q)}{\widetilde{E}(q)^2}\big)\Big)\frac{1}{\widetilde{E}\,(q)} - \frac{g_1(q)}{\widetilde{E}\,(q)}\frac{\langle\omega,\omega_q\rangle^2}{\widetilde{E}\,(q)}\frac{g_0(q)g'_0(q)}{\widetilde{E}\,(q)}\Big\}. \end{aligned} \tag{3.89}$$

The regularity of g_1 (as a function of $\mathbb{R}^+$) will come from the continuous extension to $x = 0$ of the formula above.

We have

$$|g'_0(|p|)| \le \frac{\alpha}{4\pi^2}\int\frac{dq}{|p-q|^2}\left(\frac{|g'_0|_\infty}{\widetilde{E}\,(q)} + |g_0|_\infty\frac{|g'_0|_\infty + |g'_1|_\infty}{\widetilde{E}\,(q)^2}\right) \tag{3.90a}$$

$$|g'_1(|p|)| \le 1 + \frac{\alpha}{4\pi^2}\int\frac{dq}{|p-q|^2}\left(\frac{|g'_1|_\infty}{\widetilde{E}\,(q)} + \frac{|g'_0|_\infty + |g'_1|_\infty}{\widetilde{E}\,(q)}\right). \tag{3.90b}$$

Thus

$$\begin{cases} |g'_0|_\infty \le K_1\alpha\log(\Lambda)|g'_0|_\infty + K_2\alpha|g'_1|_\infty \\ |g'_1|_\infty \le 1 + K_3\alpha\log(\Lambda)(|g'_0|_\infty + |g'_1|_\infty). \end{cases}$$

So $|g'_0|_\infty \lesssim \alpha$ and $|g'_1|_\infty \le 1 + K\alpha\log(\Lambda)$.
Since $g_0 \in \mathcal{C}^\infty(B(0,\Lambda),\mathbb{R})$ *and* radial, necessarily

$$\mathrm{d}g_0(0) = 0 \text{ and } g'_0(0) = \mathrm{d}g_0(0)\,\omega = 0,\ \forall\omega\in\mathbb{S}^2.$$

2. We treat now the second derivative $\mathrm{d}^2\mathcal{D}^0$. We write $h_\star = \frac{g_\star}{\widetilde{E}(\cdot)}$ and $\mathcal{J} = \widetilde{E}\,(\cdot)^{-1}$. The coefficient of β in $\mathrm{d}^2\mathcal{D}^0(p)\,h^2$ is

$$\mathrm{d}^2 g_0(p)\,h^2 = \frac{\alpha}{4\pi^2}\int_q\frac{dq}{|p-q|^2}\mathrm{d}^2h_0(q)\,h^2,$$

where

$$\begin{aligned} \mathrm{d}^2h_0(q)\,h^2 \quad &= \frac{\mathrm{d}^2g_0(p)\cdot h^2}{\widetilde{E}\,(q)} - \frac{2}{\widetilde{E}\,(q)^3}\mathrm{d}g_0(q)h\,[g_0(q)\mathrm{d}g_0(q)h + g_1(q)\mathrm{d}g_1(q)h] \\ &-\frac{g_0(q)}{\widetilde{E}\,(q)^3}\left[(\mathrm{d}g_0(q)h)^2 + g_0(q)\mathrm{d}^2g_0(q)h^2 + (\mathrm{d}g_1(q)h)^2 + g_1(q)\mathrm{d}^2g_1(q)h^2\right] \\ &+3\frac{g_0(q)}{\widetilde{E}\,(q)^5}[g_0(q)\mathrm{d}g_0(q)h + g_1(q)\mathrm{d}g_1(q)h]^2. \end{aligned}$$

Furthermore, we have

$$\mathrm{d}^2\mathbf{g}_1(p)h^2 = \frac{\alpha}{4\pi^2}\int\frac{dq}{|p-q|^2}\Big(\frac{\mathrm{d}^2\mathbf{g}_1(q)h^2}{\widetilde{E}\,(q)} + 2\mathrm{d}\mathbf{g}_1(q)h\,\mathrm{d}\mathcal{J}(q)h + \mathbf{g}_1(q)\mathrm{d}^2\mathcal{J}(q)h^2\Big).$$

Since we have $\langle |p|\mathrm{d}^2\mathbf{g_1}(p)h^2, \omega_p\rangle = |p|\mathrm{d}^2 g_1^p\cdot h^2 + \frac{g_1(p)}{|p|}\left(\langle\omega_p, h\rangle^2 - |h|^2\right)$, by taking the scalar product with ω_p we get

$$\begin{aligned}
|p||\mathrm{d}^2 g_1(p)| &\le C_1 + \frac{\alpha}{4\pi^2}\int \frac{|p|dq}{|p-q|^2|q|E(q)}\|\mathrm{d}^2 g_1\|_\star + \frac{\alpha}{4\pi^2}\int \frac{|p|dq}{|p-q|^2E(q)^2}\|\mathrm{d}^2 g_1\|_\star \\
&+\frac{\alpha}{4\pi^2}\int_q \frac{|p|dq}{|p-q|^2}\Big\{\frac{1}{E(q)^2}(|\mathrm{d}g_0|^2+|\mathrm{d}g_1|^2) + \frac{g_0(q)}{E(q)^2}|\mathrm{d}^2 g_0| \\
&+\frac{3}{E(q)^2}(|\mathrm{d}g_0|+|\mathrm{d}g_1|)^2 + 2(|\mathrm{d}g_1|+C_1)\frac{|\mathrm{d}g_0|+|\mathrm{d}g_1|}{E(q)^2} + \frac{1}{E(q)}\frac{2|\mathrm{d}g_1|+4C_1}{|q|}\Big\}.
\end{aligned}$$

We also have :

$$\begin{aligned}
|\mathrm{d}^2 g_0(p)| &\le \frac{\alpha}{4\pi^2}\Big\{\int \frac{C_1 dq}{E(q)^2|p-q|^2}\|\mathrm{d}^2 g_1\|_\star \\
&\int_q \frac{dq}{|p-q|^2}\Big(\frac{|\mathrm{d}^2 g_0|}{E(q)} + 2\frac{|\mathrm{d}g_0|(|\mathrm{d}g_0|+|\mathrm{d}g_1|)}{E(q)^2} + \frac{g_0(q)}{E(q)}\frac{|\mathrm{d}g_0|^2+|\mathrm{d}g_1|^2}{E(q)^2} \\
&+\frac{g_0(q)^2}{E(q)^2}\frac{|\mathrm{d}^2 g_0|}{E(q)} + 3\frac{g_0(q)}{E(q)}\frac{(|\mathrm{d}g_0|+|\mathrm{d}g_1|)^2}{E(q)^2}\Big)\Big\}.
\end{aligned}$$

As $\frac{|p|}{|p-q|^2|q|} \le 2\max(\frac{1}{|p-q||q|}, \frac{1}{|p-q|^2})$, we have

$$\int_{|q|\le\Lambda} \frac{dq|p|}{|p-q|^2|q|E(q)} \le 2\left(\int_{|q|\le\Lambda}\frac{dq}{|p-q||q|E(q)} + \int_{|q|\le\Lambda}\frac{dq}{|p-q|E(q)}\right).$$

We recall then that the convolution of radial nonnegative functions is radial nonnegative. So the following holds :

$$\begin{cases} \|g_0''\|_\infty \le K\alpha \\ \|\mathrm{d}^2 g_1\|_\star \le C_1 + K\alpha\log(\Lambda) \end{cases}$$

3. By Ineq (3.88a) and for $p\in\mathbb{R}^3$, $1\le|p|<\Lambda$ we get that :

$$\begin{aligned}
\frac{4\pi^2|g_0(p)-1|}{\alpha} &= \int\limits_{|q|<\Lambda}\frac{dq}{|p-q|^2}\frac{g_0(q)}{\sqrt{g_0(x)^2+g_1(q)^2}} \le \int\limits_{|q|<\Lambda}\frac{dq}{|p-q|^2}\frac{1}{\sqrt{1+\frac{|q|^2}{|g_0|_\infty^2}}} \\
&\le \int\limits_{|q|<2\Lambda}\frac{dq}{|q|^2}\frac{1}{\sqrt{1+\frac{|p+q|^2}{|g_0|_\infty^2}}} \le \int\limits_{|q|<2\Lambda}\frac{dq}{|q|^2}\frac{|g_0|_\infty}{|p+q|} \\
&= 2\pi|g_0|_\infty\int_0^\Lambda \frac{dr}{r|p|}\log\left|\frac{r+|p|}{r-|p|}\right| = 2\pi|g_0|_\infty\int_0^\Lambda \frac{r+|p|-\big|r-|p|\big|}{r|p|} \\
&\lesssim 1+\log\frac{\Lambda}{|p|}.
\end{aligned}$$

To deal with g_1' we use Eq. (3.89). The integral of the integrand in the second line is $O(1)$: as we multiply by α its contribution is $O(\alpha)$. For $1\le|p|<\Lambda$ there holds :

$$\int\limits_{|q|<\Lambda}\frac{dq}{|p-q|^2|\widetilde{E}(q)}\frac{g_1(q)}{|q|} \le \int\limits_{|q|<2\Lambda}\frac{dq}{|q|^2|p+q|} \lesssim 1+\log\frac{\Lambda}{|p|}.$$

For $g_0(0)$ we have :

$$\begin{aligned}
\frac{\pi|g_0(0)-1|}{\alpha} &= \int_0^\Lambda \frac{g_0(r)dr}{\sqrt{g_0(r)^2+g_1(r)^2}} = \int_1^\Lambda dr\Big\{\frac{1+O(\alpha\log\frac{\Lambda}{r})}{\sqrt{1+r^2}}\Big\} + O(1) \\
&= \log(\Lambda) + O(1+\alpha\log(\Lambda)^2).
\end{aligned}$$

Let us prove the estimation of $g_1'(0)$. There holds for any $0<x<\Lambda$ and $\omega\in\mathbb{S}^2$:

$$\begin{aligned}
\int\limits_{|q|<\Lambda}\frac{\langle\omega,\omega_q\rangle^2 dq}{|x\omega-q|^2\widetilde{E}(q)}\frac{g_1(q)}{|q|} &= 2\pi\int_0^\Lambda dr\frac{x^2+r^2}{2x^2}\left[\frac{x^2+r^2}{2rx}\log\left|\frac{x+r}{x-r}\right|-1\right]\frac{g_1(r)}{r\widetilde{E}(r)}, \\
&= 2\pi\int_0^{\Lambda/x} dr\frac{1+r^2}{2r}\left[\frac{1+r^2}{2r}\log\left|\frac{1+r}{1-r}\right|-1\right]\frac{g_1(xr)}{\widetilde{E}(xr)}.
\end{aligned}$$

We split at two levels : e^{-1} and e. The integral over (e^{-1}, e) is $O(1)$ for log is integrable on $(0, e)$. For $x \in (0, e^{-1})$ there holds the following expansion :

$$\frac{1+r^2}{r}(\log(1+r) - \log(1-r)) - 1 = \frac{4}{3}r^2 + \underset{r\to 0}{O}(r^3),$$

thus the integration over $(0, e^{-1})$ is $O(1)$. For $x \in (e, \Lambda/x)$ there holds :

$$\frac{1+r^2}{r}(\log(1+r^{-1}) - \log(1-r^{-1})) - 1 = \frac{4}{3r^2} + \underset{r\to +\infty}{O}(r^{-3}).$$

If we multiply by $\dfrac{1+r^2}{2r}$ we get $\dfrac{2}{3r} + \underset{r\to +\infty}{O}(r^{-2})$. Thus the integration over (e, Λ) gives :

$$\frac{4\pi}{3}\int_e^{\Lambda/x} \frac{g_1(rx)dr}{\widetilde{E}\,(rx)\,r} + O(1) = \frac{4\pi}{3}\int_{ex}^{\Lambda} \frac{g_1(r)dr}{\widetilde{E}\,(r)\,r} + O(1).$$

At last we get :

$$g_1'(0) - 1 = \frac{\alpha}{\pi}\int_0^{\Lambda} \frac{g_1(r)dr}{r\widetilde{E}\,(r)}\Big[1 - \frac{1}{3}\Big] + O(\alpha) = \frac{2\alpha\log(\Lambda)}{3\pi} + O(\alpha).$$

□

Proof of Proposition 3.4 In fact it suffices to use another formulae for $\mathrm{d}^2\mathbf{g}_1$ and $\mathrm{d}^2 g_0$ consisting in replacing $g_1(q)\mathrm{d}g_1(q)$ by

$$\langle \mathbf{g}_1(q)\,,\, \mathrm{d}\mathbf{g}_1(q)\rangle.$$

By the same method as for $\mathrm{d}g_0, \mathrm{d}g_1$, we get that

$$\left\|\mathrm{d}^2\mathbf{g}_1\right\|_\infty \lesssim L. \tag{3.91}$$

□

3.A.2 The function B_Λ

We recall that

$$B_\Lambda(k) = \frac{1}{\pi^2|k|^2}\int_{|p=l-\frac{k}{2}|,|q=l+\frac{k}{2}|<\Lambda} \frac{\widetilde{E}\,(p)\,\widetilde{E}\,(q) - \langle \mathbf{g}(p), \mathbf{g}(q)\rangle}{\widetilde{E}\,(p)\,\widetilde{E}\,(q)\,(\widetilde{E}\,(p) + \widetilde{E}\,(q))}dl \geq 0. \tag{3.92}$$

This formula holds only for $k \neq 0$: our first purpose is to extend it continuously to 0. Thanks to Lemma 3.14 we can say that $B_\Lambda(k) \leq K\log(\Lambda)$.

Notation 3.8. Throughout this part, $p = \ell + \frac{k}{2}, q = \ell - \frac{k}{2}$.

Proposition 3.5. *Let ω be any in $\mathbb{S}^2$. For $\ell \in B(0,\Lambda)$ we write :*

$$\mathbf{g}_\ell^\omega := \begin{pmatrix} g_0'(|\ell|)\omega_\ell\cdot\omega \\ \mathrm{d}\mathbf{g_1}(\ell)\cdot\omega \end{pmatrix} \text{ and } \widetilde{E}_\ell^\omega := |\mathbf{g}_\ell^\omega|.$$

Then we have

$$B_\Lambda(k) \underset{k\to 0}{\to} \frac{1}{\pi^2}\int_{|\ell|\leq\Lambda} \frac{|\mathbf{g}_\ell^\omega \wedge \mathbf{g}_\ell|^2}{4\widetilde{E}\,(\ell)^5}d\ell =: B_\Lambda(0), \tag{3.93}$$

Moreover

$$B_\Lambda(0) = \frac{2}{3\pi}\log(\Lambda) + O(L\log(\Lambda) + 1).$$

Proof : Let us write $I = \pi^2|k|^2 B_\Lambda(k)$, its integrand $f(\ell)$ and $x = |k|$. Let us consider $0 < \varepsilon < \frac{2}{3}$ and $s = \frac{1}{3} + \varepsilon$. We assume $x < 1$ and split the domain in three :

$$\begin{aligned} &B = \{\ell : |\ell| \le x^s\}, A = \{\ell : x^s < |\ell| < \Lambda - \tfrac{x}{2}\}, \\ &C = \{\ell : |\ell - \tfrac{k}{2}|, |\ell + \tfrac{k}{2}| < \Lambda\} \backslash \{\ell : |\ell| < \Lambda - \tfrac{x}{2}\} \subset \{\ell : \Lambda - \tfrac{x}{2} < |\ell| < \Lambda\} = C'. \end{aligned}$$

Using Lemma 3.14 we get the following behaviour *independent* of α, Λ in the regime (3.23) :

$$|I_B| \le K x^{2+3s} = K x^{3+3\varepsilon} = \underset{x\to 0}{o}(x^3), \quad |I_C| \le K x^2 \log\left(\frac{\Lambda}{\Lambda - \frac{x}{2}}\right) \underset{x\to 0}{\sim} \frac{Kx^3}{\Lambda}. \tag{3.94}$$

There remains to deal with I_A : we rewrite $f(\ell)$ as follows :

$$f(\ell) = \frac{|\mathbf{g}(p) \wedge \mathbf{g}(q)|^2}{\widetilde{E}(p)\,\widetilde{E}(q)\,(\widetilde{E}(p) + \widetilde{E}(q))(\widetilde{E}(p)\,\widetilde{E}(q) + \mathbf{g}(p)\cdot\mathbf{g}(q))} \tag{3.95}$$

where $|\mathbf{g}(p) \wedge \mathbf{g}(q)|^2 = \sum_i |\Delta_{0i}|^2 + \sum_{i,j} |\Delta_{ij}|^2$,

$$\Delta_{0i} = \begin{vmatrix} g_0(p) & g_0(q) \\ (\mathbf{g_1}(p))_i & (\mathbf{g_1}(q))_i \end{vmatrix} = \begin{vmatrix} \delta g_0 & g_0(q) \\ (\delta \mathbf{g_1})_i & (\mathbf{g_1}(q))_i \end{vmatrix} \tag{3.96a}$$

$$\Delta_{ij} = \begin{vmatrix} (\mathbf{g_1}(p))_i & (\mathbf{g_1}(q))_i \\ (\mathbf{g_1}(p))_j & (\mathbf{g_1}(q))_j \end{vmatrix} = \begin{vmatrix} (\delta \mathbf{g_1})_i & (\mathbf{g_1}(q))_i \\ (\delta \mathbf{g_1})_j & (\mathbf{g_1}(q))_j \end{vmatrix} \tag{3.96b}$$

$\delta g_\star = g_\star(p) - g_\star(q)$.

If we take k along a *fixed* half-line : $k = x\omega$ we have

$$\begin{aligned} \tfrac{1}{x}\delta g_0(k,\ell) &= \int_{t=0}^{1} \mathrm{d}g_0(\ell + (t-1/2)k)\cdot\omega dt \underset{x\to 0}{\to} g_0'(|\ell|)\omega_\ell\cdot\omega \\ \tfrac{1}{x}\delta \mathbf{g_1}(k,\ell) &= \int_{t=0}^{1} \mathrm{d}\mathbf{g_1}(\ell + (t-1/2)k)\cdot\omega dt \underset{x\to 0}{\to} \mathrm{d}\mathbf{g_1}(\ell)\cdot\omega. \end{aligned}$$

In fact, as A, g_0, g_1 are radial symmetrics so is $I_A(k)$ and for $\omega \in \mathbb{S}^2$ *fixed* and $p' = \ell + \frac{x\omega}{2}$, $q' = \ell - \frac{x\omega}{2}$ there holds

$$I_A(k = x\omega_k) = \frac{1}{\pi^2 x^2} \int_{x^s < |\ell| < \Lambda - \frac{x}{2}} \frac{\widetilde{E}(p')\,\widetilde{E}(q') - \langle \mathbf{g}(p'), \mathbf{g}(q')\rangle}{\widetilde{E}(p')\,\widetilde{E}(q')\,(\widetilde{E}(p') + \widetilde{E}(q'))} dl,$$

$f_0(\ell) = \frac{f(\ell)}{x^2}\chi_{\ell\in A}$ is also symmetric. By Proposition 3.3 we have
$|f_0(\ell)| \le K\frac{1}{(1+|\ell|^2)^{3/2}}\chi_{|\ell|\le\Lambda - x/2}$. By dominated convergence we get the integral formula (3.93).
As there holds by symmetry

$$\int_{\mathbf{n}\in\mathbb{S}^2} \langle \mathbf{n}, \omega\rangle^2 d\mathbf{n} = \frac{4}{3}\pi, \quad \int_{\mathbf{n}\in\mathbb{S}^2} |\mathrm{d}\mathbf{g_1}(|\ell|\mathbf{n})\cdot\omega|^2 d\mathbf{n} = \frac{4}{3}\pi\left((g_1')^2(\ell) + 2\frac{g_1(\ell)^2}{|\ell|^2}\right) \tag{3.97}$$

we have

$$\begin{aligned} B_\Lambda(0) = \tfrac{1}{3\pi}\Bigg(\int_{u=0}^{\Lambda} u^2 \frac{((g_0')^2(u) + (g_1')^2(u) + 2\frac{g_1(u)^2}{|u|^2})(g_0^2(u) + g_1^2(u))}{(g_0(u)^2 + g_1(u)^2)^{5/2}} du \\ - \int_{u=0}^{\Lambda} u^2 \frac{(g_0 g_0'(u) + g_1 g_1'(u))^2}{(g_0(u)^2 + g_1(u)^2)^{5/2}} du\Bigg), \end{aligned}$$

and

$$B_\Lambda(0) = \frac{1}{3\pi}\left(\int_{u=0}^{\Lambda} u^2 \frac{(g_0')^2(u) + (g_1')^2(u) + 2\frac{g_1(|u|)^2}{|u|^2}}{(g_0(u)^2 + g_1(u)^2)^{3/2}} du - \int_{u=0}^{\Lambda} u^2 \frac{(g_0 g_0'(u) + g_1 g_1'(u))^2}{(g_0(u)^2 + g_1(u)^2)^{5/2}} du\right).$$

Thanks to Proposition 3.3, we get the estimate of $B_\Lambda(0)$. □

Let us look at the variations $|k|^{-1}|B_\Lambda(k) - B_\Lambda(0)|$.

Proposition 3.6. *There exists* $0 < r_\varepsilon \in \mathbb{R}^+$, independent *of* α, Λ *in the regime* (3.23) *such that for* $|k| < r_\varepsilon$ *:*

$$|k|^{-1}|B_\Lambda(k) - B_\Lambda(0)| \le K(\Lambda^{-1} + L^2|k| + |k|^{3\varepsilon} + |k|^{2/3-\varepsilon}).$$

Choosing $\varepsilon := 6^{-1}$ *there holds :*

$$|k|^{-1}|B_\Lambda(k) - B_\Lambda(0)| \le K(\Lambda^{-1} + |k|^{1/2}).$$

Proof : For $k \in B(0,1)$ we write $|k| = x$. We reconsider the domains A, B and C of the proof of Proposition 3.5 and write f_1 the integrand in (3.92).

We have $|\int_B f_1| \le K x^{3s} = \underset{x\to 0}{O}(x^{1+3\varepsilon})$ and $|\int_C f_1| \le K \log(\frac{\Lambda}{\Lambda - x/2}) = \underset{x\to 0}{O}(\frac{x}{\Lambda})$. There remains the integration over A. For $|\ell| \ge x^s$ we have $\frac{x}{|\ell|} = O(x^{2/3-\varepsilon})$ so we can expand the integrand of $I_A(x)$ at order 1. Indeed :

$$\widetilde{E}(p)^{-1} = \widetilde{E}(\ell)^{-1}\Big\{1 + \frac{\widetilde{E}(p) - \widetilde{E}(\ell)}{\widetilde{E}(\ell)}\Big\}^{-1} = \widetilde{E}(\ell)^{-1}\Big\{1 + \frac{\widetilde{E}(\ell) - \widetilde{E}(p)}{\widetilde{E}(\ell)} + \underset{x\to 0}{O}\big(\frac{x^2}{\widetilde{E}(\ell)^2}\big)\Big\},$$

where the $\underset{x\to 0}{O}(\cdot)$ is independent of ℓ (because $\widetilde{E}(\ell) \ge 1$) . The same holds for $\widetilde{E}(q)^{-1}$ and $(\widetilde{E}(p) + \widetilde{E}(q))^{-1}$. Writing $h(\ell,k) = \widetilde{E}(p)\widetilde{E}(q) - \mathbf{g}(p)\cdot\mathbf{g}(q)$ we have :

$$\begin{aligned} I_A(x) = \quad & \frac{1}{x^2}\int_A \frac{h(\ell,k)}{2\widetilde{E}(\ell)^3}d\ell + \frac{1}{x^2}\int_A \frac{h(\ell,k)}{2\widetilde{E}(\ell)^3}\Big(\frac{2\widetilde{E}(\ell) - \widetilde{E}(p) - \widetilde{E}(q)}{\widetilde{E}(\ell)} \\ & + \frac{2\widetilde{E}(\ell) - \widetilde{E}(p) - \widetilde{E}(q)}{2\widetilde{E}(\ell)} + O\big(\frac{x^2}{\widetilde{E}(\ell)^2}\big)\Big). \end{aligned}$$

By Taylor formula (at order 2) :

$$|2\widetilde{E}(\ell) - (\widetilde{E}(p) + \widetilde{E}(q))| \le \int_t\int_u dtduKx^{1+2/3-\varepsilon} = Kx^{1+2/3-\varepsilon}.$$

By Proposition 3.4 and by Taylor formula at order 1 we have :

$$\left|\frac{\mathbf{g}(p) - \mathbf{g}(q)}{x} - \mathbf{g}_l^\omega\right| \lesssim Lx.$$

Thus $|k|^{-1}|B_\Lambda(k) - B_\Lambda(0)| = \underset{k\to 0}{O}(\Lambda^{-1} + L + |k|^{3\varepsilon})$. □

3.B The fixed point method : estimations

3.B.1 Estimation about the $R.$ operator

Let us generalize Lemma 8.[HLS05a] that states the inequality : $\|R_Q\|_{\mathcal{R}} \lesssim \|Q\|_{\mathcal{Q}}$. Further generalisations are detailed in [Sok14c].

Lemma 3.15. *Let* f *be some function* $f : B(0,\Lambda) \to \mathbb{R}_+$ *and* $Q \in \mathcal{Q}_f$. *Then we have :*

$$\iint f(p-q)\frac{|\widehat{R}_Q(p,q)|^2}{|p+q|}dpdq \lesssim \iint f(p-q)|p+q||\widehat{Q}(p,q)|^2dpdq. \tag{3.98}$$

Proof : The kernel $\widehat{R}(p,q) := \widehat{R}_Q(p,q)$ is equal to :

$$\widehat{R}(p,q) = \frac{1}{2\pi^2}\int \frac{\widehat{Q}(p-\ell, q-\ell)}{|\ell|^2}d\ell.$$

We remark the Fourier multiplier :

$$A(x,y) \mapsto \mathscr{F}^{-1}\Big\{f(p-q)\widehat{A}(p,q)\Big\}$$

commutes with $R_\cdot : A \mapsto R_A$. So it suffices to show that :

$$\iint \frac{|\widehat{R}(p,q)|^2}{|p+q|} dpdq \lesssim \iint |p+q||\widehat{Q}(p,q)|^2 dpdq.$$

To this end we follow the proof in [HLS05a], for any $\theta \in (0,2)$:

$$\begin{aligned}
\iint \frac{|\widehat{R}(p,q)|^2}{|p+q|} dpdq &= 8 \iint \frac{dudv}{|2u|} |\widehat{R}(u+v,u-v)|^2 \\
&\leq \tfrac{8}{(2\pi^2)^2} \iiiint \frac{|\widehat{Q}(\ell+v,\ell-v)||\widehat{Q}(\ell'+v,\ell'-v)|}{|2u||\ell-u|^2|\ell'-u|^2} dudvd\ell d\ell' \\
&\leq \tfrac{8}{(2\pi^2)^2} \iiiint \frac{1}{|2u|} \frac{|\widehat{Q}(\ell+v,\ell-v)|^2}{|\ell-u|^2|\ell'-u|^2} \frac{|2\ell|^{1+\theta}}{|2\ell'|^{1+\theta}} dudvd\ell d\ell' \\
&\leq \tfrac{8}{(2\pi^2)^2} \iint |2\ell||\widehat{Q}(\ell+v,\ell-v)|^2 w_\theta(\ell) dvd\ell,
\end{aligned}$$

where the weight $w_\theta(\ell)$ is :

$$w_\theta(\ell) := |2\ell|^\theta \iint \frac{dud\ell'}{|2u||2\ell'|^{1+\theta}|\ell-u|^2|\ell'-u|^2}.$$

Then we have :

$$\begin{aligned}
w_\theta(\ell) &\leq \int_u \frac{du}{|2u|^{1+\theta}|u-\ell|^2} \Big(|2u|^\theta \int_{\ell'} \frac{d\ell'}{|2\ell'|^{1+\theta}|\ell'-u|^2} \Big) \\
&\leq \Big(\frac{1}{2} \int \frac{dx}{|x|^{1+\theta}|x-\mathbf{e}|^2} \Big)^2,
\end{aligned}$$

where $\mathbf{e} \in \mathbb{R}^3$ is any vector satisfying $|\mathbf{e}| = 1$. □

3.B.2 Estimates for the fixed point method

Let $N_0 \geq 0$ be in $\mathfrak{S}_1(\mathfrak{H}_\Lambda)$ and let γ_0 be in $\mathfrak{S}_1^{\mathcal{P}_-^0}(\mathfrak{H}_\Lambda)$.
We write $n_0 := \rho_{N_0}$ and $x(N_0) := \|\nabla N_0\|_{\mathfrak{S}_2}$. We assume that

$$\mathrm{Tr}(N_0) \lesssim 1 \tag{3.99}$$

to simplify. In our problem $N_0 = |\psi\rangle\langle\psi|$ with $\|\psi\|_{L^2} = 1$.

In this part f is some function $f : \mathbb{R}^3 \mapsto [1,+\infty)$ satisfying condition (3.49) and we consider the Fourier multiplier m_f :

$$Q(x,y) \in L^2(\mathfrak{H}_\Lambda \times \mathfrak{H}_\Lambda) \mapsto \mathscr{F}^{-1}(f(p-q)\widehat{Q}(p,q)).$$

For $Q_0 \in \mathcal{Q}_f, \rho_0 \in \mathfrak{C}_f$ we write :

$$\|(Q_0,\rho_0)\|_{\mathcal{X}_f} := K_{(0)}(f)(\|Q_0\|_{\mathcal{Q}_f} + \|\rho_0\|_{\mathfrak{C}_f}),$$

where $K_{(0)}(f) > 0$ to be precised later.
By Kato's inequality and Sobolev inequality (3.39) $\|n_0\|_{\mathcal{C}} \lesssim x^{1/2}$ and $\|n_0\|_{L^2} \lesssim x^{3/2}$. For the last inequality it suffices to write $N_0 := \sum a_i |f_i\rangle\langle f_i|$, $a_i \geq 0$ and $\|f_i\|_{L^2} = 1$. Then :

$$\|n_0\|_{L^2} \leq \sum_i a_i \|\nabla f_i\|_{L^2}^{3/2} \lesssim (\sum_i a_i \|\nabla f_i\|_{L^2}^2)^{3/4}.$$

The same method enables us to prove that $\|R_{N_0}\|_{\mathfrak{S}_2} \lesssim x$.

Lemma 3.16. *Let N_0 and γ_0 be as above. Then we have :*

$$\begin{aligned}
\|Q_{0,1}[\rho_{\gamma_0}]\|_{\mathcal{Q}_f} &\lesssim \sqrt{\log(\Lambda)} \|\rho_{\gamma_0}\|_{\mathfrak{C}_f}, \\
\|Q_{1,0}[\gamma_0]\|_{\mathcal{Q}_f} &\lesssim \|\gamma_0\|_{\mathcal{Q}_f}, \\
\|\rho_{1,0}[\rho_{\gamma_0}]\|_{\mathfrak{C}_f} &\lesssim \sqrt{\log(\Lambda)} \|\gamma_0\|_{\mathcal{Q}_f}.
\end{aligned}$$

Moreover :

$$\begin{aligned}\|Q_{1,0}[N_0]\|_E &\lesssim x,\\ \|\rho_{1,0}[N_0]\|_{\mathcal{C}} &\lesssim x.\end{aligned}$$

Lemma 3.17. *Let (Q_0,ρ_0) be in $\mathcal{X}_f$. There exist constants $K_{(1)},K_{(2)}>0$ such that, writing*

$$G_f(Q,\rho) := K_{(1)}C(f)(\|Q\|_{\mathfrak{Q}_f}+\|\rho\|_{\mathfrak{C}_f})$$

we have :

$$\forall \ell\geq 2:\ \|(Q_\ell,\rho_\ell)[Q_0,\rho_0]\|_{\mathcal{X}_f}\leq \frac{K_{(2)}}{\sqrt{\ell}}G_f(Q_0,\rho_0)^\ell. \tag{3.100}$$

Assuming these lemmas hold, we follow [HLS05a] to find a ball $B(0,R_f)$ invariant under the function $F=F_Q\times F_\rho$ of the fixed point method ((3.46) and (3.47)) and on which F is a contraction. Indeed for some $K_{(4)}>0$, we have :

$$\begin{cases} \|F_Q[Q_0,\rho_0]\|_{\mathfrak{Q}_f}\leq \|N\|_{\mathfrak{Q}_f}+K_{(4)}\sqrt{L\alpha}(\|Q_0\|_{\mathfrak{Q}_f}+\|\rho_0\|_{\mathfrak{C}_f})+K_{(2)}\displaystyle\sum_{\ell=2}^{+\infty}\ell^{1/2}(\alpha G_f(Q_0,\rho_0))^\ell,\\ \|F_\rho[Q_0,\rho_0]\|_{\mathfrak{C}_f}\leq \|n\|_{\mathfrak{C}_f}+K_{(4)}\sqrt{L\alpha}(\|Q_0\|_{\mathfrak{Q}_f}+\|\rho_0\|_{\mathfrak{C}_f})+K_{(2)}\displaystyle\sum_{\ell=2}^{+\infty}\ell^{1/2}(\alpha G_f(Q_0,\rho_0))^\ell,\end{cases}$$

these upper bounds are finite provided $\alpha G_f(Q_0,\rho_0)<1$ where G_f is defined in Lemma 3.17. Moreover :

$$\|\mathrm{d}F[Q_0,\rho_0]\|_{\mathrm{L}(\mathcal{X}_f)}\leq 2\big\{K_{(4)}\sqrt{L\alpha}+\alpha K_{(3)}(f)\sum_{\ell=2}^{+\infty}\ell^{3/2}(\alpha G_f(Q_0,\rho_0))^{\ell-1}\big\}$$

where $K_{(3)}(f)=K_{(1)}K_{(2)}C(f)A(f)$. The supremum of the above upper bound on $B_{\mathcal{X}_f}(0,R)$ is written $\nu=\nu(f,R)$.

We take $K_{(0)}(f):=K_{(1)}C(f)$, $R_f=\varepsilon_f\sqrt{\log(\Lambda)}$ for some $\varepsilon_f>0$ and assume $(\|N\|_{\mathfrak{Q}_f}+\|n\|_{\mathfrak{C}_f})\leq\varepsilon_n\sqrt{\log(\Lambda)}$ (with $0<\varepsilon_n<\varepsilon_f$).

For any $(Q_0,\rho_0)\in B_{\mathcal{X}_f}(0,R_f)$ the following holds :

$$\begin{aligned}\|F(Q_0,\rho_0)\|_{\mathcal{X}_f} &\leq \nu(f,R_f)\|(Q_0,\rho_0)\|_{\mathcal{X}_f}+\|F(0,0)\|_{\mathcal{X}_f}\\ &\leq \nu(f,R_f)\varepsilon_f\sqrt{\log(\Lambda)}+K_{(0)}(f)\varepsilon_n\sqrt{\log(\Lambda)}.\end{aligned}$$

We have :

$$\nu(f,\varepsilon_f\sqrt{\log(\Lambda)})\leq 2K_{(4)}\sqrt{L\alpha}+2\alpha K_{(3)}(f)\sum_{\ell=2}^{+\infty}\ell^{1/2}\Big(\frac{\alpha\varepsilon_f\sqrt{\log(\Lambda)}}{C(f)}\Big)^{\ell-1}$$

To apply the Banach fixed point Theorem it suffices to have :

$$\nu(f,\varepsilon_f\sqrt{\log(\Lambda)})<1 \text{ and } \frac{\nu(f,\varepsilon_f\sqrt{\log(\Lambda)})+K_{(1)}C(f)\varepsilon_n}{\varepsilon_f}<1.$$

For $f_j(p-q)=\widetilde{E}(p-q)^j$ with $j\in\{0,1,2\}$ and provided $\alpha\sqrt{\log(\Lambda)}\varepsilon_f$ is small enough we have :

$$\nu(f_1,\varepsilon_f\sqrt{\log(\Lambda)})\lesssim\sqrt{L\alpha}(1+\alpha\sqrt{\log(\Lambda)}\varepsilon_f)=O(\sqrt{L\alpha}).$$

In the case $\alpha\log(\Lambda)\ll 1$, it suffices to take $\frac{\varepsilon_n}{\varepsilon_f}$ small enough to apply the fixed point Theorem.

Proof of Lemma 3.16 Let $M(\cdot,\cdot)$ be the function

$$(p,q)\in B(0,\Lambda)^2\mapsto M(p,q):=\frac{1}{\widetilde{E}(p)+\widetilde{E}(q)}\Big(\frac{\widehat{\mathcal{D}^0}(p)}{\widetilde{E}(p)}\frac{\widehat{\mathcal{D}^0}(q)}{\widetilde{E}(q)}-1\Big).$$

We write $S(p) := \frac{\widehat{\mathcal{D}^0}(p)}{\widetilde{E}(p)}$ for short. A direct computation in Fourier space (and Cauchy's formula) gives like in [HLS05a] :

$$\begin{cases} \widehat{Q}_{0,1}(\rho;p,q) &= \frac{1}{2^{5/2}\pi^{3/2}}\widehat{\varphi}_\rho(p-q)M(p,q), \\ \widehat{Q}_{1,0}(\gamma;p,q) &= -\frac{1}{2}\big(S(p)\widehat{R}_\gamma(p,q)S(q)-\widehat{R}_\gamma(p,q)\big). \end{cases} \tag{3.101}$$

We will use Lemma 3.14 : it gives an estimation of $M(p,q)$:

$$|M(p,q)| \lesssim \frac{|p-q|}{(\widetilde{E}\,(p)+\widetilde{E}\,(q))^2}.$$

The estimation of $\|Q_{0,1}(\rho_{\gamma_0})\|_{\mathcal{Q}_f}$ is then easy. In (3.101), it suffices to use Lemma 3.15 to get estimation of $\|Q_{1,0}(\gamma_0)\|_{\mathcal{Q}_f}$.

Then, as $\|R_N\|_{\mathfrak{S}_2} \lesssim x$, the estimation of $\|Q_{1,0}(N_0)\|_{\mathrm{Kin}}$ follows from a simple computation of $\iint |\widehat{Q}_{1,0}(N_0)|^2$.

Then the norm $\|\rho_{1,0}[\gamma_0]\|_{\mathfrak{C}_f}$ is dealt with in the same way as in [HLS05a] :

$$\rho_{1,0}[\gamma_0;k] = -\frac{1}{2^{5/2}\pi^{3/2}}\int\limits_{|u\pm\frac{k}{2}|<\Lambda} \mathrm{Tr}_{\mathbb{C}^4}\Big\{\widehat{R}_{\gamma_0}\big(u+\frac{k}{2},u-\frac{k}{2}\big)M\big(u-\frac{k}{2},u+\frac{k}{2}\big)\Big\}.$$

By Cauchy-Schwartz inequality we have :

$$\begin{aligned}|\rho_{1,0}[\gamma_0;k]|^2 \le \frac{1}{2^5\pi^3}&\int \widetilde{E}\,(2u)^{-1}\,|\widehat{R}_{\gamma_0}(u+\tfrac{k}{2},u-\tfrac{k}{2})|^2du\ \times \\ &\int \widetilde{E}\,(2u)\,|M(u-\tfrac{k}{2},u+\tfrac{k}{2})|^2du.\end{aligned}$$

By Lemma 3.15 $\|\rho_{1,0}[\gamma_0]\|_{\mathfrak{C}_f} \lesssim \sqrt{\log(\Lambda)}\|\gamma_0\|_{\mathcal{Q}_f}$.

□

Proof of Lemma 3.17 We only sketch the proof of Lemma 3.17 in this paper : we refer the reader to [HLS05a, Sok14c] for full details.

The main idea is to use the K.-S.-S. inequality (3.38) together with the Hölder inequality for $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$. For instance, let us take the Hilbert-Schmidt norm of $Q_{0,3}[\rho_0]$: writing $h_{\rho_0} := \mathscr{F}^{-1}(|\widehat{\varphi}_{\rho_0}|)$ we have

$$\Big\|\frac{1}{(|\mathcal{D}^0|^2+\eta^2)^{1/4}}h_{\rho_0}\frac{1}{(|\mathcal{D}^0|^2+\eta^2)^{1/4}}\Big\|_{\mathfrak{S}_6} \lesssim \frac{1}{\widetilde{E}\,(\eta)^{1/2}}\|h_{\rho_0}\|_{L^6}.$$

By Sobolev inequality we get $\|h_{\rho_0}\|_{L^6} \lesssim \|\rho_0\|_{\mathcal{C}}$ and thus there holds :

$$\begin{aligned}\|Q_{0,3}[\rho_0]\|_{\mathfrak{S}_2} &\le \frac{1}{2\pi}\int_{-\infty}^{+\infty}\Big\|\frac{1}{(|\mathcal{D}^0|^2+\eta^2)^{1/4}}h_{\rho_0}\frac{1}{(|\mathcal{D}^0|^2+\eta^2)^{1/4}}\Big\|_{\mathfrak{S}_6}^3\frac{d\eta}{\widetilde{E}\,(\eta)} \\ &\lesssim \|\rho_0\|_{\mathcal{C}}^3.\end{aligned}$$

Let us first estimate $\|Q_\ell\|_{\mathcal{Q}_f},\ \ell\ge 2$.

The term Q_2 is dealt with the same way as in [HLS05a] : we refer to this paper for details.

The difference between the example above $\|Q_{0,3}[\rho_0]\|_{\mathfrak{S}_2}$ and $\|Q_\ell[Q_0,\rho_0]\|_{\mathcal{Q}_f}$ is that we have to multiply $\widehat{Q}_\ell(p,q)$ by the weight

$$\sqrt{f(p-q)\widetilde{E}\,(p+q)}$$

before taking the Hilbert-Schmidt norm. Besides this fact the main idea is the same :

— We consider $\sqrt{f(p-q)\widetilde{E}\,(p+q)}\widehat{Q}_\ell$,

— We take its Hilbert-Schmidt norm and get an upper bound of it using K.-S.-S. and Hölder inequalities.

To deal with $\sqrt{f(p-q)}$ we use condition (3.49) :

$$\sqrt{f(p-q)} \le C(f)^{\ell-1}\{\sqrt{f(p-p_1)}+\sqrt{f(p_1-p_2)}+\cdots+\sqrt{f(p_{\ell-1}-q)}\} \tag{3.102}$$

and to deal with $\sqrt{\widetilde{E}\,(p+q)}$ we use the following trick :

$$\frac{1}{\{(\widetilde{E}\,(p)^2+\eta^2)(\widetilde{E}\,(q)^2+\eta^2)\}^{1/4}} \lesssim \frac{1}{\sqrt{\widetilde{E}\,(p+q)\,\widetilde{E}\,(\eta)}}. \tag{3.103}$$

We consider the integral representation of each term of $\widehat{Q}_{j,\ell-j}[Q_0,\rho_0]$; for convenience we write $R_0 := R[Q_0]$ and $\varphi_0 := \varphi[\rho_0]$.

For instance let us treat the term where the j operators R_0 are on the left, we take the modulus and get the upper bound :

$$\begin{aligned}\int_{-\infty}^{+\infty}\frac{d\eta}{(2\pi)^{1+3(\ell-j)/2}}\int_{B(0,\Lambda)^{\ell-1}} dp_1\cdots dp_{\ell-1}\frac{|\widehat{R}_0(p,p_1)|}{\sqrt{\widetilde{E}\,(p)^2+\eta^2}}\prod_{i=1}^{j}\frac{|\widehat{R}_0(p_i,p_{i+1})|}{\sqrt{\widetilde{E}\,(p_i)^2+\eta^2}}\times\\ \prod_{k=j+1}^{\ell-1}\frac{|\widehat{\varphi}_0(p_k-p_{k+1})|}{\sqrt{\widetilde{E}\,(p_{k+1})^2+\eta^2}}.\end{aligned} \tag{3.104}$$

We write $p_0 := p$ and $p_\ell := q$.

We multiply (3.104) by $\sqrt{f(p-q)\widetilde{E}\,(p+q)}$ and use tricks (3.102) and (3.103). We then use (3.103) for the terms involving p_i and p_{i+1} $(0 \le i \le j-1)$ and get :

$$\big\|f(p'-q')^{1/2}|\widehat{R}_0(p',q')|/\sqrt{\widetilde{E}\,(p'+q')}\big\|_{\mathfrak{S}_2} \quad \lesssim \|Q_0\|_{\mathcal{Q}_f}. \tag{3.105}$$

Moreover we have by the K.-S.-S. inequality :

$$\begin{aligned}&\big\|(\widetilde{E}\,(p')^2+\eta^2)^{-1/4}|\sqrt{f(p'-q')}\widehat{\varphi}_0(p'-q')|(\widetilde{E}\,(q')^2+\eta^2)^{-1/4}\big\|_{\mathfrak{S}_6} \lesssim \frac{\|\rho_0\|_{\mathfrak{C}_f}}{\widetilde{E}\,(\eta)^{1/2}},\\ &\big\|(\widetilde{E}\,(p')^2+\eta^2)^{-1/4}|\sqrt{f(p'-q')}\widehat{\varphi}_0(p'-q')|(\widetilde{E}\,(q')^2+\eta^2)^{-1/4}\big\|_{\mathfrak{S}_\infty}\\ &\qquad \le \big\|(\widetilde{E}\,(p')^2+\eta^2)^{-1/4}|\sqrt{f(p'-q')}\widehat{\varphi}_0(p'-q')|(\widetilde{E}\,(q')^2+\eta^2)^{-1/4}\big\|_{\mathfrak{S}_6}.\end{aligned} \tag{3.106}$$

By using those K.-S.-S. inequalities under the integral sign $\int_\eta$ in (3.104) (multiplied by the weight $\sqrt{f(p-q)\widetilde{E}\,(p+q)}$), we get an upper bound of the form :

$$\int_{-\infty}^{+\infty}\frac{d\eta}{\widetilde{E}\,(\eta)^{(1+j+\ell-j)/2}}\ell K^\ell C(f)^\ell \|Q_0\|_{\mathcal{Q}_f}^j\|\rho_0\|_{\mathfrak{C}_f}^{\ell-j}.$$

This upper bound is valid provided $(\ell+1)/2 > 1$ and $\ell \ge 3$ *ie* if $\ell \ge 3$.

In fact the same method gives :

$$\begin{aligned}\|Q_{2,0}[Q_0]\|_{\mathcal{Q}_f} &\lesssim C(f)^2\|Q_0\|_{\mathcal{Q}_f}^2,\\ \|Q_{1,1}[Q_0,\rho_0]\|_{\mathcal{Q}_f} &\lesssim C(f)^2\|Q_0\|_{\mathcal{Q}_f}\|\rho_0\|_{\mathfrak{C}_f}.\end{aligned}$$

Let us now deal with the densities $\rho_\ell[Q_0,\rho_0]$. First remark : as recalled in [HLS05a], Furry's Theorem states that for all $\ell = 2\ell_1 \in 2\mathbb{N}^*$ *even*, we have

$$\rho_{0,2\ell_1} = 0.$$

As in [HLS05a], we deal with the other terms *by duality* : the dual $\mathfrak{C}_f'$ of $\mathfrak{C}_f$ is :

$$\mathfrak{C}_f' = \Big\{\zeta \in \mathcal{S}'(\mathbb{R}^3)\ :\ \int\frac{|\widehat{\zeta(k)}|^2}{|k|f(k)}dk < +\infty\Big\}.$$

For any $\zeta \in \mathfrak{C}'_f \cap L^2$ and $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ we have

$$Q\zeta = (Q|\mathcal{D}^0|^2)(\tfrac{1}{|\mathcal{D}^0|^2}\zeta) \in \mathfrak{S}_1(L^2(\mathbb{R}^3)).$$

Above, it is understood that $\frac{1}{|\mathcal{D}^0|^2}$ is the Fourier multiplier

$$\frac{1}{|\mathcal{D}^0|^2} : \phi \in L^2(\mathbb{R}^3) \mapsto \mathscr{F}^{-1}\big\{\frac{\chi_{|p|<\Lambda}}{\widetilde{E}(p)^2}\widehat{\phi}(p)\big\} \in L^2(\mathbb{R}^3).$$

Then the following holds :

$$|\langle \rho_Q\,,\,\zeta\rangle| = |\mathrm{Tr}(Q\zeta)| = |\mathrm{Tr}(\widehat{Q\zeta})| \le \int |\widehat{Q\zeta}(p,p)|dp.$$

The idea is to get an upper bound depending only on the $\mathfrak{C}'_f$-norm of ζ and to conclude by density of $\mathfrak{C}'_f \cap L^2$ in $\mathfrak{C}'_f$.

The ingredients are the same but we treat $\rho_{1,1}$ and $\rho_{0,3}$ differently (as in [HLS05a]). We use the same K.-S.-S. inequalities and (3.102).

For instance, for $\ell \ge 5$:

$$|\widehat{Q_{0,5}\zeta}(p,p)| \le \frac{1}{(2\pi)^{1+3(\ell+1)/2}}\int_{-\infty}^{+\infty}\int_{B(0,\Lambda)^{\ell-1}} d\mathbf{p}\,\frac{|\widehat{\varphi}_0(p-p_1)|}{(\widetilde{E}(p)^2+\eta^2)^{1/4}}\prod_{k=1}^{\ell-1}\frac{|\widehat{\varphi}_0(p_k-p_{k+1})|}{\sqrt{\widetilde{E}(p_k)^2+\eta^2}}\times$$
$$\frac{|\widehat{\zeta}(p_{\ell-1}-p)|}{(\widetilde{E}(p)^2+\eta^2)^{1/4}}.$$

We write

$$|\widehat{\zeta}(p_{\ell-1}-p)| = \frac{\sqrt{f(p_{\ell-1}-p)}}{\sqrt{f(p_{\ell-1}-p)}}|\widehat{\zeta}(p_{\ell-1}-p)| = \sqrt{f(p_{\ell-1}-p)}\widehat{\zeta}'(p_{\ell-1}-p)$$

and use (3.102) :

$$\sqrt{f(p_{\ell-1}-p)} \le C(f)^{\ell-1}(\sqrt{f(p_1-p)}+\cdots+\sqrt{f(p_{\ell-1}-p_{\ell-2})}).$$

Then it suffices to use 6 times the first inequality of (3.106) and $(\ell+1-6)$ times the second.

We refer the reader to [HLS05a, Sok14c] for the other terms. □

3.B.3 Estimates of a fixed point

Let $(N,n) \in \mathcal{X}_\star$ be given where $\star$ means $0, 1$ or no subscript. Let us assume that the norms of N and n are $O(1)$ such that we can apply the fixed point Theorem (*cf* Lemmas 3.7 and 3.8). From now on ν is Lipschitz constant in Lemma 3.7 that is the one corresponding to F applied on some ball $B_{\mathcal{X}}(0,R)$. We write : $x = \sqrt{\mathrm{Tr}(-\Delta|N|)}$.

We apply the Banach theorem with initial data $(0,0) \in \mathcal{X}_\star$: iterations are written $(\gamma'_{(\ell)}, \rho'_{(\ell)})$ and $\gamma_{(\ell)}, \rho_{(\ell)}$ are defined as follows :

$$\gamma'_{(\ell)} = \gamma_{(\ell)} + N,\ \ \rho'_{(\ell)} = \rho_{(\ell)} + n \tag{3.107}$$

with $\gamma_{(\ell+1)} = \chi_{(-\infty,0)}(\mathcal{D}^0 + \alpha(\varphi_{\rho'_{(\ell)}} - R(\gamma'_{(\ell)}))) - \mathcal{P}^0_-$. The fixed point is written :

$$(\gamma', \rho'_\gamma) = (\gamma, \rho_\gamma) + (N, n).$$

Lemma 3.18. *Let $N, n, \gamma, \rho_\gamma$ be as above. If $\|(N,n)\|_{\mathcal{X}_\star} = O(1)$ then so is $\|(\gamma,\rho_\gamma)\|_{\mathcal{X}_\star}$.*

Proof : In the regime (3.23), the Lipschitz constant ν_0 in Lemmas 3.7, 3.8 is $o(1)$. So :

$$\begin{aligned}\|(\gamma',\rho'_\gamma)-(0,0)\|_{\mathcal{X}_\star} &\le \sum_{\ell=0}^{+\infty}\|(\gamma'_{(\ell+1)},\rho'_{\gamma_{(\ell+1)}})-(\gamma'_{(\ell)},\rho'_{\gamma_{(\ell)}})\|_{\mathcal{X}_\star}\\ &\le \sum_{\ell=0}^{+\infty}\nu_0^\ell\|(\gamma'_{(1)},\rho'_{\gamma_{(1)}})-(\gamma'_{(0)},\rho'_{\gamma_{(0)}})\|_{\mathcal{X}_\star}\\ &\le \tfrac{\|F(0,0)\|_{\mathcal{X}_\star}}{1-\nu_0} \le \tfrac{\|(N,n)\|_{\mathcal{X}_\star}}{1-\nu_0}.\end{aligned}$$

□

We want to be more precise and prove Lemma 3.9. We first have :

Lemma 3.19. *Let $N, n, \gamma, \rho_\gamma, x(N) =: x$ be as above. Let us write :*

$$w(N) := \sqrt{\iint |p-q|^2 |p+q| |\widehat{N}(p,q)|^2 dp dq}.$$

Then the following estimates hold :

$$\begin{array}{ll|ll} \|\gamma\|_E & \lesssim \sqrt{L\alpha} x^{1/2} + \alpha x + L\alpha, & \|\rho_\gamma\|_{\mathcal{C}} & \lesssim L x^{-1/2} + \alpha x + L\alpha, \\ \|\gamma\|_{\mathcal{Q}} & \lesssim \sqrt{L\alpha} x^{1/2} + \alpha, & \|\rho_\gamma\|_{\mathfrak{C}} & \lesssim L x^{-1/2} + \alpha x + w(N)\sqrt{L\alpha} + L\alpha. \end{array}$$

Proof : The first point is devoted to Lemma 3.19 and the second to the end of Lemma 3.9.
1. We write $\overline{n} := \mathscr{F}^{-1}(\widehat{n}(k)/(1+\alpha B_\Lambda(k)))$. There holds : $F(0,0) = (N, \overline{n})$; in particular $\gamma_{(1)} = 0$ and $\rho_{(1)} = \overline{n} - n = -\mathscr{F}^{-1}(b_\Lambda) * n$.
Writing $\gamma = \sum_{\ell=1}^{+\infty} (\gamma_{(\ell+1)} - \gamma_{(\ell)}) + \gamma_{(1)}$ we have :

$$\begin{aligned} \|\gamma\|_E & \le \textstyle\sum_{\ell=2}^{+\infty} \|\gamma_{(\ell+1)} - \gamma_{(\ell)}\|_{\mathcal{Q}} + \|\gamma_{(2)} - \gamma_{(1)}\|_E + \|\gamma_{(1)}\|_E \\ & \le \textstyle\sum_{\ell=2}^{+\infty} \nu^\ell \|F(0,0)\|_{\mathcal{X}_f} + \|F_Q(N,\overline{n}) - N\|_E. \end{aligned}$$

The first term on the right hand side is equal to $\frac{\nu^2}{1-\nu}\|N,\overline{n}\|_{\mathcal{X}_f} = O(L\alpha)$. The second term is the $\|\cdot\|_E$ norm of :

$$\sum_{j=1}^{+\infty} \alpha^j Q_j[N, \overline{n}].$$

By Lemmas 3.16 and 3.17 the following inequalities hold : $\alpha\|Q_1[N,\overline{n}]\|_E \lesssim \sqrt{L\alpha} x^{-1/2} + \alpha x$ and

$$\sum_{j=2}^{+\infty} \alpha^j \|Q_j[N,\overline{n}]\|_E \le \sum_{j=2}^{+\infty} \alpha^j \|Q_j[N,\overline{n}]\|_{\mathcal{Q}} \lesssim \alpha^2 \|(N,\overline{n})\|_{\mathcal{X}} = O(\alpha^2) = O(L\alpha).$$

Using the same method for $\|\cdot\|_{\mathcal{Q}}$, we have $\alpha\|Q_1[N,\overline{n}]\|_{\mathcal{Q}} \lesssim \sqrt{L\alpha} x^{-1/2} + \alpha\|N\|_{\mathcal{Q}}$ and :

$$\begin{aligned} \|\gamma\|_E & \lesssim \sqrt{L\alpha} x^{-1/2} + \alpha x + L\alpha \lesssim \sqrt{L\alpha} x^{-1/2} + \alpha x + L\alpha, \\ \|\gamma\|_{\mathcal{Q}} & \lesssim \sqrt{L\alpha} x^{-1/2} + \alpha\|N\|_{\mathcal{Q}} + L\alpha \lesssim \sqrt{L\alpha} x^{-1/2} + \alpha. \end{aligned} \tag{3.108}$$

There remains to check that $x = O(L\alpha)$ to get $\|\gamma\|_E \lesssim L\alpha$ and $\|\gamma\|_{\mathcal{Q}} \lesssim \alpha$.
For the density we have :

$$\begin{aligned} \|\rho_\gamma\|_{\mathcal{C}} & \le \sum_{\ell=2}^{+\infty} \|\rho_{(\ell+1)} - \rho_{(\ell)}\|_{\mathfrak{C}} + \|\rho_{(2)} - \rho_{(1)}\|_{\mathcal{C}} + \|\rho_{(1)}\|_{\mathcal{C}} \\ & \le \sum_{\ell=2}^{+\infty} \nu^\ell \|F(0,0)\|_{\mathcal{X}_f} + \|F_\rho(N,\overline{n}) - \overline{n}\|_{\mathcal{C}} + \|n - \overline{n}\|_{\mathcal{C}}. \end{aligned}$$

It is clear that $\|n - \overline{n}\|_{\mathcal{C}} \le \|b_\Lambda\|_{L^\infty} \|n\|_{\mathcal{C}} \lesssim L x^{-1/2}$. The first term is $O(\alpha^2)$. The last term is the norm of :

$$\mathscr{F}^{-1}\Big\{ \frac{1}{1+\alpha B_\Lambda(k)} \Big(\alpha \widehat{\rho}_{1,0}(N,k) + \sum_{j=2}^{+\infty} \alpha^j \widehat{\rho}_j(N,\overline{n};k) \Big) \Big\}.$$

We use Lemmas 3.16 and 3.17 to get :

$$\begin{aligned} \alpha\|(\delta_0 - b_\Lambda) * \rho_{1,0}(N)\|_{\mathcal{C}} & \lesssim \alpha x, \\ \sum_{j=2}^{+\infty} \alpha^j \|(\delta_0 - b_\Lambda) * \rho_j(N,\overline{n})\|_{\mathfrak{C}} & \lesssim \alpha^2 \|(N,\overline{n})\|_{\mathcal{X}}^2 \lesssim \alpha^2 \lesssim L\sqrt{L\alpha}. \end{aligned}$$

Here δ_0 is the usual Dirac's generalized function.

If we consider the norm $\|\cdot\|_{\mathfrak{C}}$, there holds :

$$\alpha\|(\delta_0 - b_\Lambda) * \rho_{1,0}(N)\|_{L^2} \lesssim \sqrt{L\alpha}\sqrt{\iint |p+q||p-q|^2|\widehat{N}(p,q)|^2 dpdq} =: \sqrt{L\alpha}w(N)$$

where we have used Lemma 3.15 with $f(p-q) = |p-q|^2$. Provided $x = O(L\alpha)$ and $w(N) = O(L)$ the following estimate hold :

$$\|\rho_\gamma\|_{\mathfrak{C}}, \|\rho_\gamma\|_{\mathcal{C}} \lesssim L\sqrt{L\alpha}.$$

For the test function defined by (3.25) and (3.26), it is clear that $x = O(L\alpha)$ and $w(N) = O((L\alpha)^{3/2})$.

2. The estimate of $\|\gamma\|_{\mathfrak{S}_2}$ follows from these estimates. First by computing in Fourier space it is clear that :

$$\forall \rho_0 \in \mathcal{C}: \ \|Q_{0,1}[\rho_0]\|_{\mathfrak{S}_2} \lesssim \|\rho_0\|_{\mathcal{C}}.$$

Then :

$$\begin{aligned}
\|\gamma\|_{\mathfrak{S}_2} &\leq \sum_{j=1}^{+\infty} \alpha^j \|Q_j[\gamma', \rho'_\gamma]\|_{\mathfrak{S}_2} \\
&\leq \alpha(\|Q_{0,1}[\rho'_\gamma]\|_{\mathfrak{S}_2} + \|Q_{1,0}[\gamma']\|_{\mathfrak{S}_2}) + \sum_{j=2}^{+\infty} \alpha^j \|Q_j[\gamma', \rho'_\gamma]\|_E \\
&\lesssim \alpha\|\rho'_\gamma\|_{\mathcal{C}} + \alpha(\|R_N\|_{\mathfrak{S}_2} + \|\gamma\|_{\mathrm{Ex}}) + O(\alpha^2\|(\gamma', \rho'_\gamma)\|^2_{\mathcal{X}}) \lesssim \alpha\sqrt{L\alpha}.
\end{aligned}$$

Moreover :

$$\iint |\widetilde{E}(p) - \widetilde{E}(q)|^2 |\widehat{\gamma}(p,q)|^2 dpdq \lesssim \iint |p-q|^2 |\widehat{\gamma}(p,q)|^2 dpdq \lesssim \|\gamma\|_E^2 \lesssim (L\alpha)^2.$$

To conclude this part, there remains to estimate $\|\gamma|\mathcal{D}^0|\psi_\lambda\|_{L^2}$ and $\|\gamma\psi_\lambda\|_{L^2}$. We have :

$$\begin{aligned}
\|\gamma|\mathcal{D}^0|\psi_\lambda\|_{L^2} &\leq \|\gamma\|_{\mathfrak{S}_2}\| \, |\mathcal{D}^0|\psi_\lambda\|_{L^2} \lesssim \alpha\sqrt{L\alpha}, \\
\|\gamma\psi_\lambda\|_{L^2} &\leq \|\gamma\|_{\mathfrak{S}_2}\|\psi_\lambda\|_{L^2} \lesssim \alpha\sqrt{L\alpha}.
\end{aligned}$$

We can get better upper bounds [Sok14c] but we do not need them here. □

Chapitre 4

Sur la renormalisation de charge

Charge renormalisation in a mean-field approximation of QED

Abstract

We study the Bogoliubov-Dirac-Fock (BDF) model, a no-photon, mean-field approximation of quantum electrodynamics that allows to study relativistic electrons interacting with the vacuum. It is a variational model in which states are represented by Hilbert-Schmidt operators. We prove a charge renormalisation formula that holds close to the non-relativistic limit : the density of a ground state is shown to be integrable although such a state is known not to be trace-class. We prove that we can take the non-relativistic limit by keeping track of the vacuum polarisation. We get an altered Hartree-Fock model due to the screening effect.

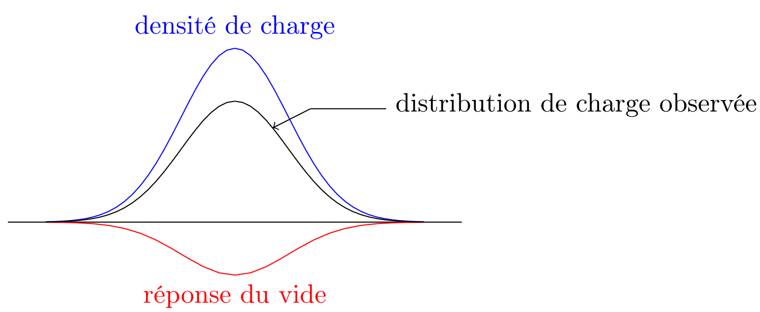

Figure 4.1 – Représentation de la renormalisation de charge

Contents

4.1 Introduction

The relativistic quantum theory of electrons is based on the Dirac operator [Tha92] : $mc^2\beta - \sum_{j=1}^3 i\hbar c\alpha_j \cdot \partial_j$. Here c is the speed of light, m the mass of electron, $\hbar$ the Planck's constant,

$$\beta := \begin{pmatrix} \mathrm{id}_{\mathbf{C}^2} & 0 \\ 0 & -\mathrm{id}_{\mathbf{C}^2} \end{pmatrix},\ \alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \in \mathrm{End}(\mathbf{C}^4),$$

where the σ_j's are the Pauli matrices :

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{4.1}$$

The Dirac operator is a self-adjoint operator acting on $\mathfrak{H} := L^2(\mathbb{R}^3, \mathbf{C}^4)$ and whose domain is $H^1(\mathbb{R}^3, \mathbf{C}^4)$. In the one-particle theory, the energy of a free particle $\psi \in L^2(\mathbb{R}^3, \mathbf{C}^4)$ is given by $\langle D_0\psi\,,\,\psi\rangle$, while the spectrum of D_0 is $(-\infty, -mc^2] \cup [mc^2, +\infty)$. According to Dirac's interpretation, all the negative energy states are already occupied by "virtual" electrons, the so-called Dirac sea. By the Pauli principle a real electron can only have positive energy.

In this paper we study the Bogoliubov-Dirac-Fock (BDF) model which is a mean-field approximation of Quantum Electrodynamics (QED). This model, introduced by Chaix and Iracane in [CI89], enables us to consider a system of relativistic electrons interacting with the vacuum in the presence of an electrostatic field.This paper is a continuation of previous works by Hainzl, Gravejat, Lewin, Séré, Siedentop, Solovej [HS03, HLS05a, HLS05b, HLS07, HLS09, GLS09] and Sok (unpublished work [Sok14b]). In this paper we will extend some results of [GLS09] and of [HLS09].

We use relativistic units $\hbar = c = 4\pi\varepsilon_0 = 1$ and set the bare particle mass equal to 1. The fine structure constant is written α. The free Dirac operator is written $D^0 = -i\boldsymbol{\alpha}\cdot\nabla + \beta$, furthermore we write $\mathfrak{H} := L^2(\mathbb{R}^3, \mathbf{C}^4)$ and define P_-^0 (resp. P_+^0) as the negative (resp. positive) spectral projector of D_0.

We will not recall here how the BDF energy is derived from QED but refer the reader to [CI89] or [HLS05a, Appendix]. Let us just say that the starting point is the Hamiltonian of QED $\mathbb{H}_{\mathrm{QED}}$, defined on the electronic Fock space $\mathcal{F}_{el}$. The mean-field approximation consists in restricting the Hamiltonian of QED $\mathbb{H}_{\mathrm{QED}}$ to "Hartree-Fock" states, the so-called BDF states.

These BDF states are fully characterized by their one-body density matrix (1pdm) P, an orthogonal projector of $L^2(\mathbb{R}^3, \mathbf{C}^4)$. For instance, the projector P_-^0 is the 1pdm of the free vacuum Ω_0 of the Fock space $\mathcal{F}_{el}$. Taking P_-^0 as a reference state, we consider the reduced 1pdm $Q := P - P_-^0$. Not all projectors are admissible : a projector P defines a BDF states if and only if the difference $P - P_-^0$ is Hilbert-Schmidt.

Remark 4.1. We recall that a Hilbert-Schmidt operator is a compact operator Q whose integral kernel $Q(x, y)$ is square-integrable, or equivalently whose singular values form a sequence in ℓ^2. If this sequence is in ℓ^1, then the corresponding operator is trace-class.

Let Ω_P be a BDF state with 1pdm P. The *formal* difference of the energy $\langle\Omega_P|\mathbb{H}|\Omega_P\rangle$ of the state Ω_P and that of Ω_0 gives a function of Q, the so-called BDF energy.

We assume the presence of an external density of charge ν (real-valued) of finite Coulomb norm :

$$D(\nu,\nu) = \|\nu\|_{\mathcal{C}}^2 := 4\pi \int \frac{|\widehat{\nu}(k)|^2}{|k|^2} dk = \iint \frac{\nu(x)\nu(y)^*}{|x-y|} dxdy. \tag{4.2}$$

The last equality holds for suitable ν (for instance $\nu \in \mathcal{C} \cap L^{6/5}(\mathbb{R}^3)$).

Formally the BDF energy of a state with reduced 1pdm Q is :

$$\begin{cases} \mathrm{Tr}_{P_-^0}(D_0 Q) - \alpha D(\rho_Q, \nu) + \frac{\alpha}{2}\Big(D(\rho_Q, \rho_Q) - \mathrm{Ex}[Q]\Big), \\ \mathrm{Tr}_{P_-^0}(D_0 Q) := \mathrm{Tr}\big\{P_-^0(D_0 Q)P_-^0 + P_+^0(D_0 Q)P_+^0\big\}, \\ \mathrm{Ex}[Q] := \iint \frac{|Q(x,y)|^2}{|x-y|} dxdy. \end{cases} \tag{4.3}$$

Here, $\alpha > 0$ is the coupling constant, $Q(x, y)$ the integral kernel of the operator Q and ρ_Q is its density : $\rho_Q(x) = \mathrm{Tr}_{\mathbf{C}^4}(Q(x, x))$. We recognize the kinetic energy, the interaction energy with ν, the direct term and the exchange term as in Hartree-Fock theory.

This expression is not always well defined, in particular the formula for the density ρ_Q makes sense *a priori* only if Q is (locally) trace-clas.

An ultraviolet cut-off $\Lambda > 0$ is needed : many choices are possible. In [HLS05a, HLS05b, HLS07, HLS09], Hainzl *et al.* have considered a "sharp" cut-off in which $L^2(\mathbb{R}^3, \mathbb{C}^4)$ is replaced by its subspace $\mathfrak{H}_\Lambda$ made of functions whose Fourier transforms vanish outside a ball $B(0,\Lambda)$.

In [HLS07], Hainzl *et al.* proposed another BDF energy based on an altered Dirac operator $\mathcal{D}^0$ and on its spectral projectors

$$\mathcal{P}^0_\pm := \chi_{\mathbb{R}^*_\pm}(\mathcal{D}^0) \tag{4.4}$$

In fact Hainzl *et al.* studied the periodized Hamiltonian $\mathbb{H}_{\mathrm{L}}$ in a finite box $[-\frac{\mathrm{L}}{2}, \frac{\mathrm{L}}{2})$ (with periodic boundary conditions). Setting an ultraviolet cut-off, the problem becomes finite dimensional : for L large enough they prove there exists a unique ground state which tends to $\mathcal{P}^0_-$ as L tends to $+\infty$. Thus the BDF energy with respect to this minimizer ("substracting $\langle \Omega_{\mathcal{P}^0_-} | \mathbb{H} | \Omega_{\mathcal{P}^0_-} \rangle$") gives a more relevant model.

The operator $\mathcal{D}^0$ has the same structure as the Dirac operator : $\mathcal{D}^0 := \boldsymbol{\alpha} \cdot \mathbf{g}_1(-i\nabla) + \beta g_0(-i\nabla)$ and it satisfies the following equation :

$$\mathcal{D}^0 = D_0 + \frac{\alpha}{2} \frac{\mathrm{sgn}(\mathcal{D}^0)(x,y)}{|x-y|}. \tag{4.5}$$

Here g_0 and $\mathbf{g}_1$ are smooth functions of $B(0,\Lambda)$.

In this paper the energy functional $\mathcal{E}^\nu_{\mathrm{BDF}}$ is defined on a subspace $\mathcal{K}$ of $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$, made of convex combinations of reduced 1pdm's of form $P - \mathcal{P}^0_-$. The set $\mathcal{K}$ is properly defined in the next section and $\mathcal{E}^\nu_{\mathrm{BDF}}$ is defined as in (4.3) except that we replace the P^0_--trace by a $\mathcal{P}^0_-$-trace :

$$\mathrm{Tr}_0(\mathcal{D}^0 Q) := \mathrm{Tr}\big\{\mathcal{P}^0_-(\mathcal{D}^0 Q)\mathcal{P}^0_- + \mathcal{P}^0_+(\mathcal{D}^0 Q)\mathcal{P}^0_+\big\}, \tag{4.6}$$

A global minimizer of $\mathcal{E}^\nu_{\mathrm{BDF}}$ is interpreted as the polarized vacuum in the presence of ν.

The charge of a state $Q \in \mathcal{K}$ is given by $\mathrm{Tr}_0(Q)$. Thus the ground state of a system with M electrons is given by a minimizer of $\mathcal{E}^\nu_{\mathrm{BDF}}$ over the corresponding charge sector.

Furthermore, we define then the energy functional for $q \in \mathbb{R}$:

$$\begin{cases} E^\nu_{\mathrm{BDF}}(q) & := \inf\{\mathcal{E}^\nu_{\mathrm{BDF}}(Q),\, Q \in \mathcal{Q}(q)\}, \\ \quad\mathcal{Q}(q) & := \{Q \in \mathcal{K},\, \mathrm{Tr}_0(Q) = q\}. \end{cases}$$

The question becomes : does there exist a minimizer for $E^\nu_{\mathrm{BDF}}(q)$?

In [HLS09], Hainzl *et al.* proved that a sufficient condition for the existence is the validity of binding inequalities at level q :

$$\forall\, q' \in \mathbb{R}\backslash\{0, q\},\ E^\nu_{\mathrm{BDF}}(q) < E^\nu_{\mathrm{BDF}}(q - q') + E^0_{\mathrm{BDF}}(q'). \tag{4.7}$$

A much more difficult task is to check that these inequalities hold.

In [HLS09], the authors showed the following.

Let a density $\nu \in L^1(\mathbb{R}^3, \mathbb{R}_+) \cap \mathcal{C}$, an integer $0 \le M < \int \nu + 1$ and a cut-off level $\Lambda_0 > 0$ be given, then there exists minimizer for $E^\nu_{\mathrm{BDF}}(M)$ provided $\alpha \le \varepsilon_0(\nu, \Lambda_0)$ for some number $\varepsilon_0(\nu, \Lambda_0) > 0$.

In [Sok14b] we proved that $E^0_{\mathrm{BDF}}(1)$ admits a minimizer provided that α, Λ^{-1} and $L := \alpha \log(\Lambda)$ are small enough. In other words, surprisingly an electron can bind alone in the Dirac sea without any external density, due to the vacuum polarisation.

In both cases the results hold in the non-relativistic regime $\alpha \ll 1$.

Let $M \in \mathbb{Z}$: a minimizer for $E^\nu_{\mathrm{BDF}}(M)$ satisfies a self-consistent equation of the form [HLS09]

$$Q + \mathcal{P}^0_- = \chi_{(-\infty,\mu]}\Big(\mathcal{D}^0 + \alpha\big((\rho_Q - \nu) * \tfrac{1}{|\cdot|} - \tfrac{Q(x,y)}{|x-y|}\big)\Big) =: \chi_{(-\infty,\mu)}(D_Q). \tag{4.8}$$

Here, μ is a Lagrange multiplier due to the charge constraint M, interpreted as a chemical potential. For $M > 0$, it is positive, the projector $\chi_{(-\infty,0)}(D_Q)$ is interpreted as the 1pdm of the polarized vacuum while $\chi_{[0,\mu]}(D_Q)$ is the 1pdm of the "real" electrons. For α sufficiently small, the last projector is indeed of rank M. Furthermore in the limit $\alpha \to 0$, $\Lambda_0 > 0$ fixed, its scaling by α^{-1} tends (up to extraction) to a minimizer of the Hartree-Fock energy $\mathcal{E}^Z_{\mathrm{HF}}$ for M electrons and $Z := \int \nu$, restricted to $L^2(\mathbb{R}^3, \mathbb{C}^2 \oplus 0)$.

In [Sok14b], a similar result is obtained with a minimizer for $\mathcal{E}^0_{\mathrm{BDF}}(1)$ in the non-relativistic limit $\alpha \to 0,\ \alpha\log(\Lambda) := L_0$ fixed, the limit is then the Choquard-Pekar model [Lie77].

In this paper we show that, assuming $L = \alpha\log(\Lambda) \leq L_0$, there exists a minimizer for $E^\nu_{\mathrm{BDF}}(M)$ as soon as $M < \int\nu + 1$ and $\alpha \leq \alpha_1(\nu, L)$. The nonrelativistic limit is an altered Hartree-Fock model : writing $Z = \int\nu$ and $a = (\frac{2}{3\pi}L)/(1+\frac{2}{3\pi}L) < 1$ the energy is

$$\forall\,\Gamma \in \mathfrak{S}_1(L^2(\mathbb{R}^3, \mathbf{C}^4)),\ 0 \leq \Gamma \leq 1,\ \mathrm{Tr}(\Gamma) = M :$$
$$\mathcal{E}^Z_{nr}(\Gamma) := \tfrac{1}{2}\mathrm{Tr}(-\Delta\Gamma) - Z(1-a)\mathrm{Tr}\Big(\tfrac{1}{|\cdot|}\Gamma\Big) + \tfrac{1}{2}\Big\{\|\rho_\Gamma\|^2_{\mathcal{C}} - \mathrm{Ex}[\Gamma]\Big\} - \tfrac{a}{2}\|\rho_\Gamma\|^2_{\mathcal{C}}.$$

The vacuum polarizes due to the presence of ν and the electrons : the positive charge ν attracts a cloud of negative charge which makes it appear smaller (hence the term $Z(1-a)$) while the electrons repelled them resulting to an attractive well created by the distortion (hence the term $-\frac{a}{2}\|\rho_\Gamma\|^2_{\mathcal{C}}$ like in a polaron model). This result gives a wider range of existence of ground state in the space of parameters (α, Λ) compared to that of [HLS09], where the quantity $\alpha\log(\Lambda_0)$ is neglected and considered as $\underset{\alpha\to 0}{o}(1)$.

To prove it, it is necessary to have a good understanding of a minimizer Q_0 and of its density ρ_{Q_0}. In [GLS09] the authors proved that, in the simplified model without the exchange term, the density of a minimizer is integrable. This is a natural result : the distortion of the vacuum due to a finite number of charged particles with finite Coulomb energy should also be finite.

Mathematically speaking however this is a non-trivial fact because a minimizer for $E^\nu_{\mathrm{BDF}}(M)$ is *not* trace-class. As in [GLS09] we prove that, assuming that L is small enough and $M, \|\nu\|^2_{\mathcal{C}} \lesssim \log(\Lambda)$, then the density ρ_Q of a minimizer Q is in $L^1 \cap \mathcal{C}$. Moreover, the following *charge renormalisation* formula holds :

$$\int(\rho_Q - \nu) =: Z_3(M - Z) \simeq \frac{M-Z}{1+\frac{2}{3\pi}L}, \tag{4.9}$$

where Z_3 is interpreted as the *renormalization constant* [GLS11]. This means that the total observed charge $\int(\rho_Q - \nu)$ is different from the real charge $M - Z$ of the system.

The quantity $L = \alpha\log(\Lambda)$ is related to Z_3. In the reduced BDF model where the exchange term is neglected, Gravejat *et al.* showed in [GLS09] that the density ρ_Q of a minimizer of the reduced energy $E^\nu_{\mathrm{rBDF}}(M)$ is radial as soon as ν is radial and that, in this case, away from the origin, the electrostatic potential of the system is

$$\alpha(\rho_Q - \nu) * \frac{1}{|\cdot|}(x) \underset{x\to+\infty}{\sim} \frac{\alpha Z_3(M-Z)}{|x|}.$$

In the full model we were unable to prove such behaviour at infinity but we think this is true. Taking L small corresponds then to considering Z_3 close to 1.

The main contribution of this paper is the integrability result stating that the density of a minimizer is in L^1 together with the charge renormalisation formula (4.9). It cannot be easily obtained from [GLS09], the presence of the exchange term complicates the study. In our results, we were unable to remove the technical conditions $M, \|\nu\|^2_{\mathcal{C}} \lesssim \log(\Lambda)$. We emphasize here that we can prove the same results with another choice of cut-off considered in [GLS09], the one consisting in replacing $\mathcal{D}^0$ by $D_0(1 - \frac{\Delta}{\Lambda^2})$ in $L^2(\mathbb{R}^3, \mathbf{C}^4)$.

The paper is organized as follows : in the next section we properly define the variational problem $\mathcal{E}^\nu_{\mathrm{BDF}}$ and states the main results.

In Section 4.3, we derive two fixed point schemes from the equation satisfied by a minimizer, using the Cauchy expansion. Moreover *a priori* estimates are proved in Subsection 4.3.2.

In Section 4.4 we prove important estimates on a term of the Cauchy expansion ("$Q_{1,0}$") and prove Theorem 4.1.

Section 4.5 is devoted to prove estimates for the fixed point method and apply it to prove that the density of a minimizer is in L^1 (under some assumptions).

We prove the formula of charge renormalization (Theorem 4.2) and the existence of minimizers close to the nonrelativistic limit (Theorem 4.3) in Section 4.6.

The nonrelativistic energy is studied in Appendix 4.B. The very technical Appendix 4.C is devoted to prove Proposition 4.1. We prove Lemma 4.8 which is used for Sections 4.4 and 4.5 in Appendix 4.A.

Remark 4.2 (Fourier transform). Throughout this paper, the Fourier transform $\mathscr{F}$ is defined as the extension of

$$\forall\ f \in\ L^2(\mathbb{R}^3) \cap L^1(\mathbb{R}^3):\ \widehat{f}(p) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} f(x) e^{-ip\cdot x} dx.$$

Remark 4.3 (Form of $\mathcal{D}^0$). The operator $\mathcal{D}^0$ was first studied by Lieb and Siedentop in [LS00] in another context. We know $\mathbf{g}_1(-i\nabla) = \frac{-i\nabla}{|-i\nabla|} g_1(-i\nabla)$ and g_0, g_1 are radial functions satisfying

$$\forall p \in B(0,\Lambda),\ |p| \leq g_1(p) \leq g_0(p)|p| \text{ and } 1 \leq g_0(p) \leq 1 + \text{Cst} \times \alpha \log(\Lambda). \tag{4.10}$$

We define

$$m := \inf\ \sigma\big(|\mathcal{D}^0|\big). \tag{4.11}$$

For $\alpha \log(\Lambda)$ and α sufficiently small, m is equal to $g_0(0)$.

Useful estimates on $g_0, \mathbf{g}_1$ are proved in [Sok14b].

4.2 Description of the model and main results

BDF Energy We assume there is an external density of charge ν (real-valued) of finite Coulomb norm ($\|\nu\|_{\mathcal{C}} < +\infty$).

Let us recall our choice of cut-off : following [HLS09], we replace D_0 by $\mathcal{D}^0$ and work in $\mathfrak{H}_\Lambda$, defined by

$$\mathfrak{H}_\Lambda := \big\{\psi \in L^2(\mathbb{R}^3, \mathbb{C}^4),\ \operatorname{supp} \widehat{\psi} \subset B_{\mathbb{R}^3}(0,\Lambda)\big\},\ \Lambda > 0.$$

We write $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ the Schatten class of compact operators A in $\mathfrak{H}_\Lambda$ such that $\text{Tr}(|A|^p) < +\infty$ [Sim79]. The set of $\mathcal{P}^0_-$-trace operators is [HLS09] :

$$\mathfrak{S}_1^{\mathcal{P}^0_-} := \{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), Q^{++}, Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\} \tag{4.12}$$

where $Q^{\varepsilon_1\varepsilon_2} := \mathcal{P}^0_{\varepsilon_1} Q \mathcal{P}^0_{\varepsilon_2}$. This set is a Banach space with

$$\|Q\|_{\mathfrak{S}_1^{\mathcal{P}^0_-}} := \|Q^{+-}\|_{\mathfrak{S}_2} + \|Q^{-+}\|_{\mathfrak{S}_2} + \|Q^{--}\|_{\mathfrak{S}_1} + \|Q^{++}\|_{\mathfrak{S}_1}. \tag{4.13}$$

We recall that $\text{Tr}_0\big(|\mathcal{D}^0|(Q^{++} - Q^{--})\big)$ is the kinetic energy functional.

We work in a subset of this space, namely

$$\mathcal{K} := \{Q,\ -\mathcal{P}^0_- \leq Q \leq \mathcal{P}^0_+\} \cap \mathfrak{S}_1^{P^0_-} \subset \{Q,\ Q^* = Q\} \cap \mathfrak{S}_1^{P^0_-}. \tag{4.14}$$

It is the closed convex hull of the $P - \mathcal{P}^0_- \in \mathfrak{S}_1^{\mathcal{P}^0_-}$, where P is an orthogonal projection.

The density ρ_Q must be defined consistently with the usual formula when Q is (locally) trace-class and it must also be of finite Coulomb energy.

Let Q be in $\mathfrak{S}_1^{\mathcal{P}^0_-}$, then ρ_Q is defined by duality :

$$\forall\ V \in \mathcal{C}',\ QV \in \mathfrak{S}_1^{\mathcal{P}^0_-} \text{ and } \text{Tr}_0(QV) = {}_{\mathcal{C}'}\langle V\ ,\ \rho_Q\rangle_{\mathcal{C}}. \tag{4.15}$$

The map $Q \in \mathfrak{S}_1^{\mathcal{P}^0_-} \mapsto \rho_Q \in \mathcal{C}$ is continuous [GLS09, Proposition 2].
The exchange term is well defined : thanks to Kato's inequality [BBHS98a, HLS07, HLS05a]

$$\begin{aligned} \frac{2}{\pi} \iint \frac{|Q(x,y)|^2}{|x-y|} dxdy \quad &\leq \text{Tr}(|\nabla|Q^2) \leq \text{Tr}(|D_0|Q^2) = \text{Tr}\{|D_0|^{1/2} Q^2 |D_0|^{1/2}\} \\ \text{and for } Q \in \mathcal{K}: \quad &\leq \text{Tr}\{|D_0|^{1/2}(Q^{++} - Q^{--})|D_0|^{1/2}\} \leq \text{Tr}_{P^0_-}(\mathcal{D}^0 Q), \end{aligned} \tag{4.16}$$

The BDF energy is defined as follows :

$$\mathcal{E}^\nu_{\text{BDF}}(Q) := \text{Tr}_{P^0_-}(\mathcal{D}^0 Q) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2}\Big(D(\rho_Q, \rho_Q) - \iint \frac{|Q(x,y)|^2}{|x-y|} dxdy\Big),\ Q \in \mathcal{K}. \tag{4.17}$$

As said in the introduction we define the energy functional $E^{\nu}_{\rm BD}(q)$ by the infimum over $\mathcal{Q}(q) = \{Q \in \mathcal{K},\ \mathrm{Tr}_{P^0_-}(Q) = q\}$.

For $M \in \mathbb{N}^*$, let us say that the problem $E^{\nu}_{\rm BDF}(M)$ has a minimizer : as pointed out in [HLS09, GLS09] such a minimizer $\gamma' = \gamma + N$ must be of the following form :

$$\begin{cases} \gamma + P^0_- = \chi_{(-\infty,0)}\big\{\mathcal{D}^0 + \alpha((\rho[\gamma'] - \nu) * \frac{1}{|\cdot|} - R[\gamma'])\big\} =: \chi_{(-\infty,0)}(D_{\gamma'}), \\ N = \chi_{(0,\mu]}\big\{\mathcal{D}^0 + \alpha\big((\rho_{\gamma'} - \nu) * \frac{1}{|\cdot|} - (R_{\gamma'})\big)\big\} = \sum_{j=1}^{M_0} |\psi_j\rangle\langle\psi_j|, \\ \text{so } D_{\gamma'}\psi_j = \mu_j\psi_j \text{ and we write} : n := \rho_N = \sum_j |\psi_j|^2. \end{cases} \tag{4.18}$$

We choose $0 \le \mu_1 \le \mu_2 \le \cdots \le \mu_{M_0} = \mu < m$. *A priori* $M_0 \neq M$ but in our regime they are equal (Lemma 4.3). Indeed in the spirit of [HLS05a] the equation of the dressed vacuum γ enables us to say that $(\gamma', \rho_{\gamma'} - \nu)$ is the only fixed point of some function $F^{(1)}$ defined in (a ball of) the Banach space $\mathcal{X}_1 = \mathbf{Q}_1 \times \mathcal{C}$ where

$$||Q||^2_{\mathbf{Q}_1} = \|Q\|^2_{\mathrm{T}} := \iint (\widetilde{E}\,(p) + \widetilde{E}\,(q))|\widehat{Q}(p,q)|^2 dp dq.$$

Notation 4.1. For a density $\rho \in \mathcal{C}$ we write : $v_\rho = v[\rho] := \rho * \frac{1}{|\cdot|}$.

For an operator $Q \in \mathfrak{S}_1^{P^0_-}$ with integral kernel $Q(x,y)$ we define the operator $R_Q = R[Q]$ by the formula :

$$R_Q(x,y) := \frac{Q(x,y)}{|x-y|}.$$

We remark that $\mathrm{Ex}[Q] = \mathrm{Tr}(R_Q^* Q) =: \|Q\|^2_{\mathrm{Ex}}$.

Moreover we write

$$B_Q := v[\rho_Q - \nu] - R_Q \text{ and } D_Q := \mathcal{D}^0 + \alpha B_Q. \tag{4.19}$$

The Cauchy expansion Let $\gamma' = \gamma + N$ be a minimizer for $E^{\nu}_{\rm BDF}(M)$, the decomposition being that of (4.18).

Notation 4.2. Throughout this paper $n := \rho_N$, moreover we write ρ'_γ for $\rho_{\gamma'}$ and the double prime means $-\nu$ is added :

$$\rho''_\gamma := \rho_\gamma + n - \nu,\ n'' = n - \nu.$$

We also write $B'_\gamma = B_{\gamma'} := \rho''_\gamma * \frac{1}{|\cdot|} - R[\gamma']$.

By functional calculus, we expand $\chi_{(-\infty,0)}(D_Q) - \mathcal{P}^0_-$ in power of α : this is the Cauchy expansion [HLS05a]

$$\begin{cases} \gamma + N &= N - \dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{+\infty} d\eta \Big(\frac{1}{D_{\gamma'} + i\eta} - \frac{1}{\mathcal{D}^0 + i\eta}\Big) = \sum_{j=1}^{+\infty} \alpha^j Q_j(\gamma', \rho''_\gamma), \\ Q_j(\gamma', \rho''_\gamma) &:= -\dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{+\infty} d\eta \frac{1}{\mathcal{D}^0 + i\eta}\Big(B_{\gamma'}\frac{1}{\mathcal{D}^0 + i\eta}\Big)^j. \end{cases} \tag{4.20}$$

We define $Q_{k,l}$ as the part of $Q_{k+l}(Q,\rho)$ which is a homogeneous polynomial of degree k in R_Q and of degree l in ρ ; $\rho_{k,l}(Q,\rho)$ denotes its density. For $\ell \ge 1$ and $(Q,\rho) \in \mathfrak{S}_2(H^{1/2}) \in \mathcal{C}$, $\widetilde{Q}_\ell[Q,\rho]$ is the operator :

$$\widetilde{Q}_\ell[Q,\rho] := \sum_{j=\ell}^{+\infty} \alpha^{j-\ell} Q_j[Q,\rho].$$

As shown in [HLS05a, GLS09] we have

$$\rho_{0,1}[\rho] = -\mathscr{F}^{-1}(B_\Lambda) * \rho \tag{4.21}$$

where $\mathscr{F}^{-1}(B_\Lambda)$ is a radial L^1 function.

In the following Lemma, we refer to the Banach spaces $\mathbf{Q}_w$ and $\mathfrak{C}_w$: they are defined below (4.26). This Lemma is proved in Section 4.4.

Lemma 4.1. *$F_{1,0} : Q \mapsto Q_{1,0}(Q)$ is a bounded linear map of $\mathfrak{S}_p$ for $p = 1$ and $p = 2$ with respective norms $\mathcal{O}(\log(\Lambda))$ and $\mathcal{O}(\sqrt{\log(\Lambda)})$. By interpolation $F_{1,0}$ is in $L(\mathfrak{S}_p)$ for $1 < p = 1+\varepsilon < 2$ with norm $\mathcal{O}((\log(\Lambda))^{1-\frac{\varepsilon}{2}})$.*

Moreover it is also a bounded operator in $L(\mathbf{Q}_w)$ with norm $\mathcal{O}(1)$, and the function

$$\rho F_{1,0} : Q \in \mathbf{Q}_w \mapsto \rho\big(F_{1,0}[Q]\big) \in \mathfrak{C}_w$$

is bounded with norm $\mathcal{O}(\sqrt{\log(\Lambda)})$. Provided that $\alpha \log(\Lambda)$ is sufficiently small, the operator $(Id - \alpha F_{1,0})$ is invertible with inverse $\mathbf{T}$ in all those Banach spaces with norm $\mathcal{O}(1)$. The function $\mathfrak{t} : Q \in \mathbf{Q}_w \mapsto \rho\big(\mathbf{T}[Q] - Q\big) \in \mathfrak{C}_w$ is bounded and

$$\|\mathfrak{t}_Q\|_{\mathfrak{C}_w} \lesssim \sqrt{L\alpha}\|Q\|_{\mathbf{Q}_w}.$$

We write

$$\mathfrak{T} := \mathbf{T} - \mathrm{Id},\ \tau_Q := \rho_{\mathbf{T}(Q)}, \tau_{j,k} := \rho_{\mathbf{T}(Q_{j,k})} \text{ and } \mathfrak{t}_Q := \rho_{\mathfrak{T}(Q)}. \tag{4.22}$$

If $Q \in \mathbf{Q}_{w=1} \cap \mathfrak{S}_1^{P^0_-}$ then $\tau_Q \in \mathcal{C}$ and if $(Q, \rho_Q) \in \mathbf{Q}_w \times \mathfrak{C}_w$ then $\tau_Q \in \mathfrak{C}_w$.

The self-consistent equation (4.18) is rewritten as follows :

$$(\mathrm{Id} - \alpha F_{1,0})(\gamma') = N + \alpha Q_{0,1}(\rho''_\gamma) + \sum_{j=2}^{+\infty} Q_j(\gamma', \rho''_\gamma).$$

Taking the inverse $\mathbf{T}$, we get :

$$\gamma' = \mathbf{T}\Big\{N + \alpha Q_{0,1}(\rho''_\gamma) + \sum_{j=2}^{+\infty} Q_j(\gamma', \rho''_\gamma)\Big\}. \tag{4.23}$$

The important proposition holds :

Proposition 4.1. *For $\rho \in \mathcal{C}$ we have $\alpha\tau_{0,1}(\rho) = -\check{f}_\Lambda * \rho$ where $\check{f}_\Lambda$ is a radial L^1 function whose L^1-norm is $\mathcal{O}(\alpha \log(\Lambda))$.*

Its technical proof is in Appendix 4.C.

There holds a Theorem *à la Furry* [Fur37, HLS05a] :

Theorem 4.1. *There exists $K > 0$ such that for any ρ_0, ρ_1 (say in $\mathcal{C}$) and $\alpha\sqrt{\log(\Lambda)} \le K$ there holds :*

$$\rho\big\{\mathbf{T}(Q_{0,2}(\rho_0))\big\} = \rho\Big\{\mathbf{T}\big(Q_{1,1}(\mathbf{T}Q_{0,1}(\rho_1), \rho_0)\big)\Big\} = 0. \tag{4.24}$$

Remark 4.4. $\mathbf{T}(Q_{0,2}(\rho_0))$ and $\mathbf{T}(Q_{1,1}(\mathbf{T}(Q_{0,1}(\rho_1)), \rho_0))$ may not vanish but their density do due to the fact that the trace $\mathrm{Tr}_{\mathbf{C}^4}$ is taken. The smallness of $\alpha\sqrt{\log(\Lambda)}$ is to ensure the $\mathbf{T}$ operator is well defined on $\mathbf{Q}_1$.

Main Theorems

Theorem 4.2 (Computation of $\int_{\mathbb{R}} \rho_\gamma(x)dx$)**.** *Let M be in $\mathbb{N}$ and $\gamma' = \gamma + N$ be a minimizer of $E^\nu_{BDF}(M)$ and assume $M, \|\nu\|^2_{\mathcal{C}} \lesssim \log(\Lambda)$ and (4.28), the decomposition of γ' is that of (4.18). Then $\rho_\gamma \in L^1$ and*

$$\int \rho_\gamma(x)dx = -\frac{\alpha f_\Lambda(0)}{1 + \alpha f_\Lambda(0)}(M - Z) \tag{4.25}$$

Theorem 4.3 (Existence of minimizers)**.** *There exists $K_0 > 0$ satisfying the following result : for any non-negative function $\nu \in \mathcal{C} \cap L^1$ with $Z = \int \nu$ and $0 < L \le 1/(MK_0)$, there exists $\alpha_1 = \alpha_1(\nu, L) > 0$ such that if $\alpha \le \alpha_1$ then for any integer $0 \le M < Z + 1$ the problem $E^\nu_{BDF}(M)$ admits a minimizer.*

Let $\gamma' = \chi_{(0,\mu]}(D_{\gamma'})$ be a minimizer, decomposed as in (4.18) and let U_α be defined as follows :

$$U_\alpha : \begin{array}{ccc} L^2(\mathbb{R}^3, \mathbf{C}^4) & \to & L^2(\mathbb{R}^3, \mathbf{C}^4) \\ \phi(x) & \mapsto & \alpha^{-3/2}\phi(\frac{x}{\alpha}) \end{array}.$$

We write $\frac{f_\Lambda(0)}{1+f_\Lambda(0)} = a$, then as α tends to 0, $U^*_\alpha \chi_{(0,\mu]}(D_{\gamma'})U_\alpha$ tends to a minimizer of

$$\begin{array}{rl} \mathcal{E}^Z_{nr}(\Gamma) & := \frac{1}{2}\mathrm{Tr}(-\Delta\Gamma) - Z(1-a)\mathrm{Tr}\big(\frac{1}{|\cdot|}\Gamma\big) + \frac{1}{2}(D(\rho_\Gamma, \rho_\Gamma) - \mathrm{Ex}[\Gamma]) - \frac{a}{2}D(\rho_\Gamma, \rho_\Gamma), \\ & \text{for } 0 \le \Gamma \le 1,\ \mathrm{Tr}(\Gamma) = M \text{ and } \frac{1+\beta}{2}\Gamma = 0. \end{array}$$

Remark 4.5. Thanks to Section 4.C and [GLS09] we have

$$\frac{f_\Lambda(0)}{1+f_\Lambda(0)} = \frac{\frac{2}{3\pi}\alpha\log(\Lambda)}{1+\frac{2}{3\pi}\alpha\log(\Lambda)} + \mathcal{O}(\alpha + (\alpha\log(\Lambda))^2).$$

Banach spaces We use several Banach spaces. For $p \in [1,+\infty]$, $s \geq 0$, $\|\cdot\|_{L^p}$ (resp.$\|\cdot\|_{H^s}$) is the norm of the usual L^p (resp. Sobolev) space. We write $\|\cdot\|_{\mathfrak{S}_p}$ for the norm of Schatten class operators $\mathfrak{S}_p$ [Sim79]. The norm of bounded linear operator in $\mathfrak{H}$ is written $\|\cdot\|_{\mathcal{B}}$. We recall $\|\cdot\|_{\mathrm{Ex}}$ and $\|\cdot\|_{\mathcal{C}}$ have already been defined in Sections 1 and 2 and $\|\cdot\|_{\mathbf{Q}_w}, \|\cdot\|_{\mathfrak{C}_w}$ are defined in Remark 4.3.

Notation 4.3. From now on, for any $w : \mathbb{R}^3 \to [1,+\infty)$ satisfying the condition

$$\exists\, K_{(w)} > 0 \mid \forall\, p, q, p_1 \in \mathbb{R}^3,\ w(p-q) \leq K_{(w)}(w(p-p_1) + w(p_1-q)),$$

we define two Hilbert spaces :

$$\begin{aligned} \mathbf{Q}_w \quad &:= \big\{Q \in \mathfrak{S}_2,\ \iint (\sqrt{1+|p|^2} + \sqrt{1+|q|^2}) w(p-q) |\widehat{Q}(p,q)|^2 dp dq < +\infty\big\}, \\ \mathfrak{C}_w \quad &:= \big\{\rho \in \mathcal{S}'(\mathbb{R}^3),\ \int \frac{w(k)}{|k|^2} |\widehat{\rho}(k)|^2 dk < +\infty\big\}. \end{aligned} \tag{4.26}$$

The letter w always refers to a function of this kind. The case $w \equiv 1$ gives the space $\mathbf{Q}_1$ of operators Q with $\mathrm{Tr}(|\mathcal{D}^0||Q|^2 + Q^*|\mathcal{D}^0|Q) < +\infty$ and $\mathfrak{C}_1 = \mathcal{C}$. Typically, we consider $w(p-q) := E(p-q)^a$ for $a > 1$.

By the fixed point method we may estimate together

— $\|F_Q(Q,\rho)\|_{\mathrm{T}}$ and $\|F_\rho(Q,\rho)\|_{\mathcal{C}}$,

— In general $\|F_Q(Q,\rho)\|_{\mathbf{Q}_w}$ and $\|F_\rho(Q,\rho)\|_{\mathfrak{C}_w}$. We define $\mathcal{X}_g := \mathbf{Q}_w \times \mathfrak{C}_w$

Notations

Notation 4.4 (On D_0 and $\mathcal{D}^0$). The operator $\mathrm{sign}(\mathcal{D}^0)$ is a Fourier multiplier that we write $\mathbf{s}_p = \frac{\widehat{\mathcal{D}^0}(p)}{\sqrt{g_0(p)^2+g_1(p)^2}}$. We also write

$$E(p) := \sqrt{1+|p|^2} \text{ and } \widetilde{E}\,(p) := \sqrt{g_0(p)^2 + g_1(p)^2}. \tag{4.27}$$

Remark 4.6 (Regime). We will work in the regime

$$\alpha \leq \alpha_0 \ll 1 \text{ and } L := \alpha\log(\Lambda) \leq L_0 \ll 1. \tag{4.28}$$

We consider systems with M electrons and an external charge density $\nu \geq 0$ with $\|\nu\|_{\mathcal{C}}, Z := \|\nu\|_{L^1} < +\infty$. We will often consider $M = \mathcal{O}(Z)$ and $\|\nu\|_{\mathcal{C}}^2 + M = \mathcal{O}(\log(\Lambda))$.

Throughout this paper the letter K denotes a constant independent of the parameters α, Λ, M, ν. $K(M,\nu)$ is a constant depending on M, ν and so on. The inequality $a \lesssim b$ means that $a \leq Kb$ for $a, b > 0$. When $a > 1$ is some integer, then as in [HLS05a] we write

$$K_a := \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^a} = \underset{a\to+\infty}{\mathcal{O}}(a^{-1/2}). \tag{4.29}$$

Notation 4.5 (On $\widetilde{Q}_{k,\ell}$). For $(\varepsilon_1, \cdots, \varepsilon_{J+1}) \in \{+,-\}^{J+1}$ we define $Q_J^{\varepsilon_1\cdots\varepsilon_{J+1}}$ with the same formula as in (4.20) except that we replace the $J+1$ operators $(\mathcal{D}^0 + i\eta)^{-1}$'s by $P^0_{\varepsilon_j}/(\mathcal{D}^0 + i\eta)$. We define $Q_{k,\ell}^{\varepsilon_1\cdots\varepsilon_{J+1}}$ analogously.

We write $Q_{k,\ell}^{\varepsilon_1 a_1 \varepsilon_2 \cdots a_J \varepsilon_{J+1}}$ with $a_j \in \{v, R\}$ for the operator

$$-\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\eta \frac{P^0_{\varepsilon_1}}{\mathcal{D}^0 + i\eta} A_1 \frac{P^0_{\varepsilon_2}}{\mathcal{D}^0 + i\eta} \cdots A_J \frac{P^0_{\varepsilon_{J+1}}}{\mathcal{D}^0 + i\eta},$$

where $A_j = v = \rho''_\gamma * \frac{1}{|\cdot|}$ if $a_j = v$ or $A_j = -R(\gamma')$ if $a_j = R$.

Notation 4.6 (On f_Λ). We introduce the function $F_\Lambda := \frac{f_\Lambda}{1+f_\Lambda}$, studied in Appendix 4.C. We prove in particular that $\check{F_\Lambda} \in L^1$ and that $\|F_\Lambda\|_{L^1} \lesssim L$.

4.3 Description of minimizers

4.3.1 Minimizers and fixed point schemes

Let $\gamma' = \gamma + N$ be a minimizer for $E^{\nu}_{\mathrm{BDF}}(M)$. From Eq. (4.20) and (4.21), we define a fixed-point scheme :

$$F^{(1)} = F^{(1)}_Q \times F^{(1)}_\rho : \mathcal{X}_1 \to \mathcal{X}_1,$$

$$F^{(1)}_Q(Q', \rho'') = N + \sum_{\ell=1}^{\infty} \alpha^\ell Q_\ell(Q', \rho''), \tag{4.30a}$$

$$\mathscr{F}(F^{(1)}_\rho(Q', \rho''); k) = \frac{1}{1+\alpha B_\Lambda(k)} \widehat{n}''(k) + \frac{1}{1+\alpha B_\Lambda(k)} \Big(\alpha \widehat{\rho}_{1,0}(Q'; k) + \sum_{\ell=2}^{\infty} \alpha^\ell \widehat{\rho}_\ell(Q', \rho''; k) \Big) \tag{4.30b}$$

To prove $F^{(1)}$ is well-defined we use the following Lemma proved in Section 4.5.

Lemma 4.2. *Let w be some function satisfying (4.3), with constant $K_{(w)} > 0$. There exists $C_0 > 0$ such that for any $J \geq 2$, the linear operator :*

$$(Q, \rho) \in \boldsymbol{Q}_w \times \mathfrak{C}_w \mapsto (Q_J(Q, \rho), \rho_J(Q, \rho)) \in \boldsymbol{Q}_w \times \mathfrak{C}_w$$

is bounded with norm lesser than $2K^J_{(w)} C^J_0 J^{1/2}$.

We apply the Banach-Picard Theorem.

Lemma 4.3. *Let $\gamma' = \gamma + N$ be a minimizer for $E^{\nu}_{BDF}(M)$. In the regime of Remark 4.6 the following holds :*

1. *$F^{(1)} : B_{\mathcal{X}_1}(0, R_0) \to B_{\mathcal{X}_1}(0, R_0)$ is well-defined for some $R_0 > 0$ and this restriction is a Lipschitz function with constant lesser than 1.*
2. *(γ', ρ''_γ) is in the previous ball and so is the unique fixed point of $F^{(1)}$, moreover :*

$$\|F^{(1)}(\gamma', \rho''_\gamma) - (N, n'')\|_{\mathcal{X}_1} = o(1).$$

3. *As a consequence $N = \chi_{(0,\mu]}(D_Q)$ has rank $M_0 = M$.*

Proof of part 3. If we assume the first two points, the last one is clear. Indeed on the one hand we have : $|\mathrm{Tr}_0(\gamma)| \lesssim \|\gamma\|^2_{\mathfrak{S}_2} = o(1)$, on the other hand, as γ is a difference of an orthogonal projector and $\mathcal{P}^0_-$, it must be an integer [HLS05a, Lemma 2]. Thus $\mathrm{Tr}_0(\gamma) = 0$ and

$$\mathrm{Tr}(N) = \mathrm{Tr}_0(N) = \mathrm{Tr}_0(\gamma') - \mathrm{Tr}_0(\gamma) = M.$$

□

To prove that ρ_γ is integrable we need another fixed point scheme.

We see ρ''_γ as the fixed point of a function $F^{(2)}$ defined in (a ball of) $\mathcal{C}$ and also in (a ball of) $\mathcal{C} \cap L^1$. We write :

$$\begin{cases} h_2 &= \alpha^2 \tau_{1,1} \Big\{ \mathbf{T}[N] + \alpha^2 \big\{ \alpha \mathbf{T} \widetilde{Q}_3(\gamma', \rho''_\gamma) + \mathbf{T} Q_{2,0}(\gamma', \rho''_\gamma) \big\}, \rho''_\gamma \Big\} + \alpha^2 \tau_{2,0}(\gamma') \\ F^{(2)}_2(\rho'') &= \alpha^2 \big(\tau_{1,1} \big\{ \alpha^2 \big[\mathbf{T} Q_{1,1}(\gamma', \rho'') + \mathbf{T} Q_{0,2}(\rho'') \big], \rho'' \big\} \big) \\ h_3 &= \alpha^4 \tau \big(\widetilde{Q}_4(\gamma', \rho''_\gamma) \big) + \alpha^3 \big\{ \tau_{3,0}(\rho''_\gamma) + \tau_{2,1}(\gamma', \rho''_\gamma) \big\} \\ F^{(2)}_3(\rho'') &= \alpha^3 \tau_{0,3}(\rho'') + \alpha^3 \tau_{1,2}(\gamma', \rho'') \end{cases} \tag{4.31}$$

$$\mathscr{F}\big\{ F^{(2)}(\rho'') \big\} = \frac{1}{1+f_\Lambda(\cdot)} \widehat{n}'' + \frac{1}{1+f_\Lambda(\cdot)} \Big\{ \widehat{h}_2 + \mathscr{F}\big\{F^{(2)}_2\big\} + \widehat{h}_3 + \mathscr{F}\big\{F^{(2)}_3\big\} \Big\}(\rho'') \tag{4.32}$$

Remark 4.7. The definition of $F^{(2)}$ may appear complicated. It is built on the following self-consistent equation :

$$\rho'_\gamma = \tau \Big\{ N + \alpha Q_{0,1}(\rho''_\gamma) + \alpha^2 \big(\widetilde{Q}_2(\gamma', \rho''_\gamma) - Q_{1,1}(\gamma', \rho''_\gamma) \big) \Big\} + \alpha^2 \tau \big[Q_{1,1}(F^{(1)}_Q(\gamma', \rho''_\gamma), \rho''_\gamma) \big].$$

Lemma 4.4. *Let $\gamma' = \gamma + N$ be a minimizer for $E^{\nu}_{BDF}(M)$ and $F^{(2)}$ the function* (4.31)*. In the regime of Remark 4.6, there exists $R_0 > 0$ such that $F^{(2)}$ is well-defined in $B_{\mathcal{C}}(0, R_0)$ and in $B_{\mathcal{C}\cap L^1}(0, R_0)$.*

Furthermore these balls are $F^{(2)}$-invariant and $F^{(2)}$ is a contraction on them; ρ''_{γ} is the only fixed point in both Banach spaces. In particular $\rho_{\gamma} \in L^1$.

Remark 4.8. The *linear* response of the vacuum to the presence of electrons N and the external potential ν is :

$$\begin{cases} \gamma &= \alpha \mathbf{T}[Q_{0,1}((\delta_0 - \check{F}_\Lambda) * (n - \nu + \mathfrak{t}_N))] + \mathfrak{T}_N + \cdots \\ \rho_\gamma &= -\check{F}_\Lambda * (n - \nu) + (\delta_0 - \check{F}_\Lambda) * \mathfrak{t}_N + \cdots \end{cases}$$

4.3.2 *A priori* estimates

Lemma 4.5 (Estimates on the energy)**.** *Let $M \in \mathbb{N}$ and Q a test function for $E^{\nu}_{BDF}(M)$. We assume : $\mathcal{E}^{\nu}_{BDF}(Q) \leq E^{\nu}_{BDF}(M) + \varepsilon$ where $0 < \varepsilon = o(\alpha\|\nu\|^2_{\mathcal{C}})$.*

Then we have $\|Q\|^2_{\mathfrak{S}_2} \lesssim M + \alpha\|\nu\|^2_{\mathcal{C}}$ and

$$\begin{aligned} &\mathrm{Tr}(|\nabla| Q^2) \lesssim \alpha\|\nu\|^2_{\mathcal{C}} + \alpha^{1/2} M + \sqrt{\alpha M}\|\nu\|_{\mathcal{C}}, \\ &\alpha\|\rho_Q - \nu\|^2_{\mathcal{C}} \lesssim \alpha\|\nu\|^2_{\mathcal{C}} + \alpha^{3/2} M + \sqrt{\alpha M}\alpha\|\nu\|_{\mathcal{C}}. \end{aligned}$$

As a corollary we get the following.

Lemma 4.6 (Estimates on the mean-field operator)**.** *In the regime of Remark 4.6 and for Q as in Lemma 4.5 we have in the sense of self-adjoint operator :*

$$(1 - o(1))|\mathcal{D}^0| \leq |\mathcal{D}^0 + \alpha B_Q| \leq (1 + o(1))|\mathcal{D}^0|. \tag{4.33}$$

Both $o(1)$ are $\mathcal{O}\big(\alpha\|\nu\|_{\mathcal{C}} + \alpha^{5/4} M^{1/2} + (\alpha M)^{1/4}\alpha\|\nu\|^{1/2}_{\mathcal{C}}\big)$.

Lemma 4.7 (*A priori estimates of a minimizer*)**.** *Let $\gamma' = \gamma + N$ be a minimizer for $E^{\nu}_{BDF}(M)$, decomposed as in* (4.18)*. Then we have in the regime* (4.28)

$$\begin{array}{rcl|rcl} \mathrm{Tr}(|\mathcal{D}^0| N) & \lesssim & \log(\Lambda), & \|\gamma\|_{\mathrm{T}} & \lesssim & \lesssim L, \\ \|n''\|_{\mathcal{C}} & \lesssim & \sqrt{\log(\Lambda)}, & \|\rho_\gamma\|_{\mathcal{C}} & \lesssim & L\sqrt{\log(\Lambda)}. \end{array}$$

Proof of Lemma 4.5 : It is known that $E^{\nu}_{\mathrm{BDF}}(M) \leq M$ [HLS09]. There holds :

$$\begin{aligned} M + \varepsilon + \tfrac{\alpha}{2}\|\nu\|^2_{\mathcal{C}} &\geq \mathcal{E}^{\nu}_{\mathrm{BDF}}(Q) + \tfrac{\alpha}{2}\|\nu\|^2_{\mathcal{C}} \geq \big(1 - \alpha\tfrac{\pi}{4}\big)\mathrm{Tr}_0(\mathcal{D}^0 Q) + \tfrac{\alpha}{2}\|\rho_Q - \nu\|^2_{\mathcal{C}} \\ &\geq \big(1 - \alpha\tfrac{\pi}{4}\big)\|Q\|^2_{\mathfrak{S}_2} + \tfrac{\alpha}{2}\|\rho_Q - \nu\|^2_{\mathcal{C}}. \end{aligned}$$

Furthermore :

$$\begin{aligned} \mathrm{Tr}_0(\mathcal{D}^0 Q) - M &= \mathrm{Tr}(|\mathcal{D}^0|^{1/2}(Q^{++} - Q^{--})|\mathcal{D}^0|^{1/2}) - \mathrm{Tr}_0(Q) \\ &\geq \mathrm{Tr}(|\mathcal{D}^0|^{1/2} Q^2 |\mathcal{D}^0|^{1/2}) - \mathrm{Tr}(Q^2) \\ &\geq \frac{1}{(2\pi)^3}\iint (\widetilde{E}(p) - 1)|\widehat{Q}(p,q)|^2 dp dq, \end{aligned} \tag{4.34}$$

and $\widetilde{E}(p) - 1 \geq \frac{1}{2}\frac{p^2}{E(p)}$. Then thanks to Kato's inequality (4.61) :
$\mathrm{Tr}(Q R_Q) \leq \frac{\pi}{2}\mathrm{Tr}(|\nabla| Q^2)$ which leads to :

$$\frac{1}{2}\mathrm{Tr}\Big(\frac{-\Delta}{|D_0|}Q^2\Big) + \frac{\alpha}{2}\|\rho_Q - \nu\|^2_{\mathcal{C}} \leq \varepsilon + \alpha\Big(\frac{\|\nu\|^2_{\mathcal{C}}}{2} + \frac{\pi}{4}\mathrm{Tr}(|\nabla| Q^2)\Big).$$

Splitting at level $r_0 = \frac{\alpha\pi}{\sqrt{1-(\alpha\pi)^2}}$ (to get $\alpha\frac{|p|\pi}{4} \leq \frac{1}{4}\frac{|p|^2}{E(p)}$ for $|p| \geq r_0$) we obtain :

$$\mathrm{Tr}\Big(\frac{-\Delta}{|D_0|}Q^2\Big) \lesssim \alpha(\|\nu\|^2_{\mathcal{C}} + M), \tag{4.35}$$

thus by the Cauchy-Schwartz inequality : $\mathrm{Tr}(|\nabla|Q^2) \lesssim \alpha\|\nu\|_{\mathcal{C}}^2 + \sqrt{\alpha}M + \sqrt{\alpha M}\|\nu\|_{\mathcal{C}}$. □

Proof of Lemma 4.6 :

For all $f \in \mathfrak{H}_\Lambda$ we have :

$$\langle\, |\mathcal{D}^0|^2 f\,,\, f\rangle(1-\alpha\||\mathcal{D}^0|^{-1}B\|_{\mathcal{B}})^2 \le \langle|\mathcal{D}^0+\alpha B|^2 f\,,\, f\rangle \le \langle\, |\mathcal{D}^0|^2 f\,,\, f\rangle(1+\alpha\||\mathcal{D}^0|^{-1}B\|_{\mathcal{B}})^2. \tag{4.36}$$

However thanks to Ineq.(4.58) and the second point of Lemma 4.8 :

$$\|R_Q|\nabla|^{-1/2}\|_{\mathcal{B}} \lesssim \sqrt{\mathrm{Tr}(QR_Q)} \text{ and } \|(\rho_Q-\nu)*\tfrac{1}{|\cdot|}|\nabla|^{-1/2}\|_{\mathcal{B}} \lesssim \|(\rho_Q-\nu)*\tfrac{1}{|\cdot|}\|_{L^6} \lesssim \|\rho_Q-\nu\|_{\mathcal{C}}.$$

As the square root is monotone, there holds

$$(1-\alpha\||\mathcal{D}^0|^{-1}B_Q\|_{\mathcal{B}})|\mathcal{D}^0| \le |\mathcal{D}^0+\alpha B_Q| \le (1+\alpha\||\mathcal{D}^0|^{-1}B_Q\|_{\mathcal{B}})|\mathcal{D}^0|, \tag{4.37}$$

and in the regime of Remark 4.6, this gives $(1-o(1))|\mathcal{D}^0| \le |\mathcal{D}^0+\alpha B_Q| \le (1+o(1))|\mathcal{D}^0|$. This $o(1)$ is of order $\mathcal{O}(\alpha(\|\rho_Q-\nu\|_{\mathcal{C}} + \|\,|\nabla|^{1/2}Q\|_{\mathfrak{S}_2}))$, that is of order
$\mathcal{O}\big(\alpha\|\nu\|_{\mathcal{C}} + \alpha^{5/4}M^{1/2} + (\alpha M)^{1/4}\alpha\|\nu\|_{\mathcal{C}}^{1/2}\big)$. □

Proof of Lemma 4.7 : For $E^{\nu}_{\mathrm{BDF}}(M)$ with $M, \|\nu\|_{\mathcal{C}}^2 \lesssim \log(\Lambda)$, we have thanks to Lemma 4.5 :

$$\alpha(\|\rho''_\gamma\|_{\mathcal{C}} + \sqrt{\mathrm{Tr}(|\nabla|\gamma')}) \lesssim \sqrt{\alpha}(\alpha^{1/2}\|\nu\|_{\mathcal{C}} + \alpha^{3/4}M^{1/2} + (\alpha M)^{1/4}\alpha^{1/2}\|\nu\|_{\mathcal{C}}^{1/2}) =: \alpha^{1/2}\ell.$$

We have $\ell = O(\sqrt{L})$. Using Eq. (4.23) and assuming Lemma 4.2 and Proposition 4.1 above we get that :

$$\|\rho_\gamma\|_{\mathcal{C}} \le \|\check{F_\Lambda} * n''\|_{\mathcal{C}} + \|(\delta_0-\check{F_\Lambda})*(\mathfrak{t}_N + \sum_{j\ge 2}\alpha^j\tau_j)\|_{\mathcal{C}} \lesssim L\|n''\|_{\mathcal{C}} + \sqrt{L\alpha}\|N\|_{\mathrm{T}} + O(L\alpha).$$

As $\|n''\|_{\mathcal{C}} \le \|\rho''_\gamma\|_{\mathcal{C}} + \|\rho_\gamma\|_{\mathcal{C}}$ we get

$$\|n''\|_{\mathcal{C}} \lesssim \|\nu\|_{\mathcal{C}} + (\alpha M)^{1/4}(M^{1/4} + \sqrt{\|\nu\|_{\mathcal{C}}}) + \sqrt{L\alpha M} + O(\alpha\ell^2) \lesssim \sqrt{\log(\Lambda)}.$$

Thanks to the equations $\mathcal{D}^0\psi_j = \mu_j\psi_j - B\psi_j$, there holds :

$$\mathrm{Tr}(|\mathcal{D}^0|N) \lesssim M(1+O(\sqrt{\alpha}\ell)) \lesssim \log(\Lambda).$$

Finally we have

$$\begin{aligned} \|\gamma\|_{\mathrm{T}} &\lesssim \sqrt{L\alpha}\|n''\|_{\mathcal{C}} + \alpha\sqrt{\mathrm{Tr}(|\nabla|Q^2)} + O(L\alpha) \lesssim L + O(L\alpha) \lesssim L \\ \|\rho_\gamma\|_{\mathcal{C}} &\lesssim L\|n''\|_{\mathcal{C}} + \sqrt{L\alpha M} + O(L\alpha) \lesssim L\sqrt{\log(\Lambda)}. \end{aligned} \tag{4.38}$$

□

4.4 The operator $F_{1,0}$

Remark 4.9.
- If Q is a nonnegative operator then so is R_Q when it is well defined. Moreover if Q is self-adjoint then so is R_Q.
- The $R.$ operator commutes with Fourier multiplier of the form $g(p-q)$, indeed we have

$$\widehat{R_Q}(p,q) = \frac{1}{2\pi^2}\int \frac{\widehat{Q}(p-l,q-l)}{|l|^2}.$$

In particular there holds :

$$[\partial_j, R_Q] = R([\partial_j, Q]). \tag{4.39}$$

Lemma 4.8. *Let Q be in $\mathcal{S}(\mathbb{R}^3\times\mathbb{R}^3)$ (Schwartz class).*

1. *We have :*
$$\| \, |\nabla|^{-1/2} R_Q \|_{\mathfrak{S}_2} \lesssim \sqrt{\mathrm{Tr}(R_Q^* Q)}.$$
In particular for any $w \geq 1$ there holds :
$$\iint \frac{w(p-q)}{|p|} |\widehat{R}_Q(p,q)|^2 dpdq \lesssim \iint |p+q| w(p-q) |\widehat{Q}(p,q)|^2 dpdq.$$
2. *There exists $K > 0$ such that for all $0 < \epsilon \leq 1$*
$$\begin{aligned} \| \, |D_0|^{-\frac{1+\varepsilon}{2}} R_Q |D_0|^{-\frac{1+\varepsilon}{2}} \|_{\mathfrak{S}_1} &\leq \tfrac{K}{\varepsilon} \|Q\|_{\mathfrak{S}_1}, \\ \| \, |D_0|^{-(1+\varepsilon)} R_Q \|_{\mathfrak{S}_2} &\leq \tfrac{K}{\sqrt{\varepsilon}} \|Q\|_{\mathfrak{S}_2}. \end{aligned}$$

For $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, we can replace $|D_0|^{-(1+\varepsilon)/2}$ by $|\mathcal{D}^0|^{-1/2}$, provided that ε^{-1} is replaced by $\log(\Lambda)$. By density, these inequalities hold for Q in the Banach spaces corresponding to the norms in the r.h.s.

We prove this Lemma in Appendix A.

4.4.1 Proof of Lemma 4.1

In the Schatten norms We recall $F_{1,0}$ is defined as
$$F_{1,0} : Q \mapsto Q_{1,0}(Q) := -\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \frac{1}{\mathcal{D}^0 + i\eta} R_Q \frac{1}{\mathcal{D}^0 + i\eta}. \tag{4.40}$$
The integral kernel of its Fourier transform is [HLS05a] :
$$\widehat{Q}_{1,0}(p,q) = \frac{1}{2} \frac{1}{\widetilde{E}(p) + \widetilde{E}(q)} \left(\widehat{R}(p,q) - \mathbf{s}_p \widehat{R}(p,q) \mathbf{s}_q \right). \tag{4.41}$$
It corresponds to a difference of two operators which are in $\mathfrak{S}_p$ if Q is in $\mathfrak{S}_p$ for both cases $p=1$ and $p=2$ (see below). By interpolation, for $p \in [1,2]$, if $Q \in \mathfrak{S}_p$ then so is $F_{1,0}(Q)$. Let us show the $\mathfrak{S}_1$-norm is $\mathcal{O}(\log(\Lambda))$ while the $\mathfrak{S}_2$-norm is $\mathcal{O}(\sqrt{\log(\Lambda)})$. Indeed
$$\frac{1}{f(p)+f(q)} = \int_{s=0}^{+\infty} e^{-sf(p)-sf(q)} ds,$$
therefore if Q is nonnegative, then so is
$$\int_{s=0}^{+\infty} \tfrac{\mathcal{D}^0}{|\mathcal{D}^0|} \mathscr{F}^{-1}(e^{-s\widetilde{E}(\cdot)}) R_Q \mathscr{F}^{-1}(e^{-s\widetilde{E}(\cdot)}) \tfrac{\mathcal{D}^0}{|\mathcal{D}^0|} ds.$$
Writing $Q = \frac{Q+Q^*}{2} + \frac{Q-Q^*}{2}$ and splitting each self-adjoint operator into nonnegative and nonpositive part, we may assume that $Q \geq 0$. Then from Eq. (4.41), we get :
$$\|F_{1,0}(Q)\|_{\mathfrak{S}_1} \leq K \log(\Lambda) \|Q\|_{\mathfrak{S}_1}.$$
As $(\widetilde{E}(p) + \widetilde{E}(q))^{-1} \leq \widetilde{E}(p)^{-1/2} \widetilde{E}(q)^{-1/2}$, it follows that
$$\begin{aligned} \| \, |\mathcal{D}^0|^{-\frac{1}{2}} R(\mathscr{F}^{-1}(|\widehat{Q}(p,q)|)) |\mathcal{D}^0|^{-\frac{1}{2}} \|_{\mathfrak{S}_2} &\leq K \sqrt{\log(\Lambda)} \| \mathscr{F}^{-1}(|\widehat{Q}(p,q)|) \|_{\mathfrak{S}_2} \\ &= K \sqrt{\log(\Lambda)} \|\widehat{Q}\|_{\mathfrak{S}_2} = K \sqrt{\log(\Lambda)} \|Q\|_{\mathfrak{S}_2}. \end{aligned}$$
By interpolation ($1 < p = 1 - \varepsilon + 2\varepsilon < 2$), there exists $K^{\mathfrak{S}}_{(1,0)} > 0$
$$\|Q_{1,0}(Q)\|_{\mathfrak{S}_p} \leq K^{\mathfrak{S}}_{(1,0)} (\log(\Lambda))^{1-\frac{\varepsilon}{2}} \|Q\|_{\mathfrak{S}_p}, \tag{4.42}$$
Remark 4.10. The operators $Q_{1,0}(Q_0)$ (and $Q_{0,1}(\rho_0)$) can be rewritten as
$$\mathcal{J}_t(x-y) := \mathscr{F}^{-1}(\exp(-t\widetilde{E}(p)))(x-y) \tag{4.43a}$$
$$\begin{cases} Q_{1,0}(Q_0) &= \frac{1}{2} \int_{t=0}^{+\infty} (\mathcal{J}_t R_{Q_0} \mathcal{J}_t - \mathcal{J}_t \frac{\mathcal{D}^0}{|\mathcal{D}^0|} R_{Q_0} \frac{\mathcal{D}^0}{|\mathcal{D}^0|} \mathcal{J}_t) dt \\ Q_{0,1}(\rho_0) &= -\frac{1}{2} \int_{t=0}^{+\infty} \left(\mathcal{J}_t \, v_{\rho_0} \, \mathcal{J}_t - \mathcal{J}_t \frac{\mathcal{D}^0}{|\mathcal{D}^0|} \, v_{\rho_0} \, \frac{\mathcal{D}^0}{|\mathcal{D}^0|} \mathcal{J}_t \right) dt \end{cases} \tag{4.43b}$$

$\rho[Q_{1,0}(\cdot)]$ We show here inequalities needed to estimate $\mathbf{T}(Q_\ell(Q,\rho))$ and $\tau_\ell(Q,\rho)$ in norms $\|\cdot\|_{\mathbf{Q}_w}, \|\cdot\|_{\mathfrak{C}_w}$. There exists a constant C_R (defined in [HLS05a]) such that for any function $w \geq 0$

$$\iint (\widetilde{E}\,(p) + \widetilde{E}\,(q)) w(p-q) |\widehat{Q}_{1,0}(Q,p,q)|^2 dpdq \leq C_R^2 \iint w(p-q) E(p+q) |\widehat{Q}(p,q)|^2 dpdq. \tag{4.44}$$

By Cauchy-Schwartz inequality (*cf* [HLS05a] and inequality (4.98)) :

$$|\widehat{\rho}_{1,0}(Q,k)|^2 \lesssim |k|^2 \int_{B(0,\Lambda)} \frac{|\widehat{R}(u+\frac{k}{2}, u-\frac{k}{2})|^2}{1+\widetilde{E}\,(u,k/2)} du \int_{B(0,\Lambda)} \frac{du}{1+\widetilde{E}\,(u,k/2)} \frac{1}{1+|u|^2+|k|^2/4}, \tag{4.45}$$

where $\widetilde{E}\,(u,k/2) := \max(\widetilde{E}\,(u+k/2)\,, \widetilde{E}\,(u-k/2))$. Thus we have :

$$|\widehat{\rho}_{1,0}(Q,k)|^2 \leq \mathrm{C}_{(1,0)} \int E(2u) |\widehat{Q}(u+\tfrac{k}{2}, u-\tfrac{k}{2})|^2 du, \tag{4.46}$$

where $0 < \mathrm{C}_{(1,0)} = \mathrm{C}_{(1,0)}(\Lambda)$ satisfies $\mathrm{C}_{(1,0)} \lesssim \log(\Lambda)$.

Well-definedness of T and τ Thanks to (4.42) we can prove Lemma 4.1 : for $\alpha\log(\Lambda)$ sufficiently small the function $\mathbf{T}$ is a linear bounded operator in $\mathrm{L}(\mathfrak{S}_p)$ for $1 \leq p = 1+\varepsilon \leq 2$ with norm lesser than

$$\mathrm{C}_{\mathbf{T},\mathfrak{S}}^{(p)} := \sum_{\ell=0}^{+\infty} \big(\alpha K_{(1,0)}^{\mathfrak{S}} (\log(\Lambda))^{1-\frac{\varepsilon}{2}}\big)^\ell = \frac{1}{1-\alpha(\log(\Lambda))^{1-\frac{\varepsilon}{2}} K_{(1,0)}^{\mathfrak{S}}}$$

which is finite as soon as $\alpha\log(\Lambda)$ is sufficiently small. We write $\mathrm{C}_{\mathbf{T},\mathfrak{S}} := \mathrm{C}_{\mathbf{T},\mathfrak{S}}^{(1)}$.

As $\mathbf{T} = (\mathrm{Id} - \alpha F_{1,0})^{-1} = \sum_{\ell=0}^{+\infty} \alpha^\ell F_{1,0}^{\circ(\ell)}$, let us show that $\alpha F_{1,0}$ is a bounded operator in $\mathrm{L}(\mathbf{Q}_w)$ with norm lesser than 1. Thanks to inequality (4.44), $\alpha F_{1,0}$ is bounded with norm lesser than αC_R. Thus $\mathbf{T}$ is a bounded linear operator with norm lesser than

$$\mathrm{C}_{\mathbf{T},\mathbf{Q}_w} := \frac{1}{1-\alpha C_R}. \tag{4.47}$$

Then thanks to Ineq. (4.44) and (4.46), for $\ell \geq 1$ we have :

$$|\widehat{\rho}(F_{1,0}^{\circ(\ell)}(Q);k)|^2 \leq \alpha^{2\ell} \mathrm{C}_{(1,0)}^\ell |k|^2 \int E(2u) |\widehat{Q}(u+\tfrac{k}{2}, u-\tfrac{k}{2})|^2 du$$

Therefore :

$$\int \frac{g(k)}{|k|^2} |\widehat{\rho}(F_{1,0}^{\circ(\ell)};k)|^2 \leq \alpha^{2\ell} \mathrm{C}_{(1,0)}^\ell \iint g(p-q) E(p+q) |\widehat{Q}(p,q)|^2 dpdq \tag{4.48}$$

and $\mathfrak{t}$ is a bounded linear operator in $\mathrm{L}(\mathfrak{C}_w)$ with norm lesser than

$$\mathrm{C}_{\mathfrak{t},\mathfrak{C}} := \sum_{\ell=1}^{+\infty} (\alpha\sqrt{\mathrm{C}_{(1,0)}})^\ell = \mathcal{O}(\alpha\sqrt{\log(\Lambda)}) \tag{4.49}$$

for $\alpha\sqrt{\log(\Lambda)}$ sufficiently small.

Notation 4.7. Let us define for $1 \leq p = 1+\varepsilon \leq 2$:

$$Y_{\alpha,\Lambda}(p) = Y(p) \lesssim \mathrm{C}_{\mathbf{T},\mathfrak{S}}^{(p)}, \tag{4.50}$$

which is an upper bound of the $\mathrm{L}(\mathfrak{S}_p)$-norm of $Q \mapsto |D_0|^{-7/12} R(\mathbf{T}[Q]) |D_0|^{-7/12}$: *cf* Lemma 4.8 in Appendix 4.A.1.

We have thus proved :

$$\begin{cases} \|\mathbf{T}(Q)\|_{\mathbf{Q}_w} & \leq \mathrm{C}_{\mathbf{T},\mathbf{Q}_w} \|Q\|_{\mathbf{Q}_w} = \frac{\|Q\|_{\mathbf{Q}_w}}{1-\alpha C_R}, \\ \|\tau_Q\|_{\mathfrak{C}_w} & \leq \mathrm{C}_{\mathfrak{t},\mathfrak{C}} \|Q\|_{\mathbf{Q}_w}. \end{cases} \tag{4.51}$$

4.4.2 Proof of Theorem 4.1

First we recursively define the function $A_J^{(\ell_j)_{j=1}^J}$ as follows :

$$\left\{\begin{array}{ll} A_1^{\ell_1}\widehat{Q}(p,q) & := \widehat{Q}(p-\ell_1,q-\ell_1) - \mathbf{s}_p\widehat{Q}(p-\ell_1,q-\ell_1)\mathbf{s}_q, \\ A_J^{(\ell_1,\mathbf{L})}\widehat{Q}(p,q) & := A_1^{\ell_1}\big(A_{J-1}^{\mathbf{L}}Q\big)(p,q) \text{ with } J\in\mathbb{N}^*, \ell_j\in\mathbb{R}^3. \end{array}\right. \tag{4.52}$$

These functions appear in the Fourier transform of $Q_{1,0}^{\circ J}[Q]$ (see Appendix 4.C).

Proof : It is based on the following fact :

Lemma 4.9. *The trace $\mathrm{Tr}_{\mathbb{C}^4}$ of the product of an odd number of Dirac matrices (that is $\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3,\beta$) vanishes.*

Writing $\langle a_1,\ldots,a_M\rangle$ the algebra spanned by the a_j's, we define :

$$\left\{\begin{array}{ll} \mathcal{A}_D & := \langle \boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3,\beta\rangle, \\ \mathcal{A}_D^+ & := \langle \mathrm{Id}, (1-\delta_{jk})\boldsymbol{\alpha}_j\boldsymbol{\alpha}_k, \beta\boldsymbol{\alpha}_j\rangle \\ \mathcal{A}_D^- & := \boldsymbol{\alpha}_1\mathcal{A}_D^+ + \boldsymbol{\alpha}_2\mathcal{A}_D^+ + \boldsymbol{\alpha}_3\mathcal{A}_D^+ + \beta\mathcal{A}_D^+ \end{array}\right. \tag{4.53}$$

It is clear that $\mathcal{A}_D = \mathcal{A}_D^+ + \mathcal{A}_D^-$ and Lemma 4.9 just says that

$$\forall M\in\mathcal{A}_D^- : \mathrm{Tr}_{\mathbb{C}^4}(M) = 0.$$

Remark 4.15 and Appendix 4.C implies that for almost all $(p,q)\in\mathbb{R}^3\times\mathbb{R}^3$:

- $\widehat{F_{1,0}^{\circ J}}(Q_{0,1}(\rho);p,q)\in\mathcal{A}_D^+$,
- if $\widehat{Q}(p,q)\in\mathcal{A}_D^\varepsilon$ then so is $\widehat{F_{1,0}^{\circ J}}(Q;p,q)$.

Now let us study $Q_{0,2}(\rho)$:

$$Q_{0,2} = -\frac{1}{2\pi}\int_{\eta=-\infty}^{+\infty}\frac{d\eta}{\mathcal{D}^0+i\eta}v_\rho\frac{1}{\mathcal{D}^0+i\eta}v_\rho\frac{1}{\mathcal{D}^0+i\eta}.$$

where $Q_{0,2}^{\varepsilon_1\,\varepsilon_2\,\varepsilon_3}$ is defined in Notation 4.5 (as $Q_{1,2}^{\varepsilon_1,R,\varepsilon_2,v,\varepsilon_3}$ and so on). By the residuum formula in the case $\varepsilon_1=\varepsilon_2=\varepsilon_3$ the term vanishes. We deal with $Q_{0,2}^{+--}$ and $Q_{0,2}^{-++}$ together, like $Q_{0,2}^{+-+}$ and $Q_{0,2}^{-+-}$, $Q_{0,2}^{--+}$ and $Q_{0,2}^{++-}$. We compute the first couple with $A=Q_{0,2}^{+--}$ and $B=Q_{0,2}^{-++}$:

$$\begin{aligned} A &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}d\eta\int_{p_1}dp_1\frac{P_+^0(p)}{\widetilde{E}(p)+i\eta}\widehat{v}(p-p_1)\frac{P_-^0(p_1)}{-\widetilde{E}(p_1)+i\eta}\widehat{v}(p_1-q)\frac{P_-^0(q)}{-\widetilde{E}(q)+i\eta} \\ &= \int_{p_1}\frac{dp_1}{8}\frac{1}{\widetilde{E}(p)+\widetilde{E}(p_1)}\frac{1}{\widetilde{E}(p)+\widetilde{E}(q)}(1+\mathbf{s}_p)\widehat{v}(p-p_1)(1-\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1-\mathbf{s}_q), \\ B &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}d\eta\int_{p_1}dp_1\frac{P_-^0(p)}{-\widetilde{E}(p)+i\eta}\widehat{v}(p-p_1)\frac{P_+^0(p_1)}{\widetilde{E}(p_1)+i\eta}\widehat{v}(p_1-q)\frac{P_+^0(q)}{\widetilde{E}(q)+i\eta} \\ &= -\int_{p_1}\frac{dp_1}{8}\frac{1}{\widetilde{E}(p)+\widetilde{E}(p_1)}\frac{1}{\widetilde{E}(p)+\widetilde{E}(q)}(1-\mathbf{s}_p)\widehat{v}(p-p_1)(1+\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1+\mathbf{s}_q), \end{aligned}$$

However

$$\begin{aligned} &\tfrac{1}{2}\big((1+\mathbf{s}_p)\widehat{v}(p-p_1)(1-\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1-\mathbf{s}_q) - (1-\mathbf{s}_p)\widehat{v}(p-p_1)(1+\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1+\mathbf{s}_q)\big) \\ &= \mathbf{s}_p\widehat{v}(p-p_1)\mathbf{s}_{p_1}\widehat{v}(p_1-q)\mathbf{s}_q + \mathbf{s}_p\widehat{v}(p-p_1)\widehat{v}(p_1-q) - \widehat{v}(p-p_1)\widehat{v}(p_1-q)\mathbf{s}_q - \widehat{v}(p-p_1)\mathbf{s}_{p_1}\widehat{v}(p_1-q). \end{aligned} \tag{4.54}$$

In (4.54) there only remains matrices in $\mathcal{A}_D^-$. Symmetrically, the other two couples give :

$$\begin{aligned} &\bullet\ \tfrac{1}{2}\big((1+\mathbf{s}_p)\widehat{v}(p-p_1)(1-\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1+\mathbf{s}_q) - (1-\mathbf{s}_p)\widehat{v}(p-p_1)(1+\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1-\mathbf{s}_q)\big) \\ &= -\mathbf{s}_p\widehat{v}(p-p_1)\mathbf{s}_{p_1}\widehat{v}(p_1-q)\mathbf{s}_q + \mathbf{s}_p\widehat{v}(p-p_1)\widehat{v}(p_1-q) + \widehat{v}(p-p_1)\widehat{v}(p_1-q)\mathbf{s}_q - \widehat{v}(p-p_1)\mathbf{s}_{p_1}\widehat{v}(p_1-q), \\ &\bullet\ \tfrac{1}{2}\big((1-\mathbf{s}_p)\widehat{v}(p-p_1)(1-\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1+\mathbf{s}_q) - (1+\mathbf{s}_p)\widehat{v}(p-p_1)(1+\mathbf{s}_{p_1})\widehat{v}(p_1-q)(1-\mathbf{s}_q)\big) \\ &= \mathbf{s}_p\widehat{v}(p-p_1)\mathbf{s}_{p_1}\widehat{v}(p_1-q)\mathbf{s}_q - \mathbf{s}_p\widehat{v}(p-p_1)\widehat{v}(p_1-q) + \widehat{v}(p-p_1)\widehat{v}(p_1-q)\mathbf{s}_q - \widehat{v}(p-p_1)\mathbf{s}_{p_1}\widehat{v}(p_1-q). \end{aligned} \tag{4.55}$$

Therefore for almost all (p,q) : $\widehat{Q}_{0,2}(\rho;p,q)\in\mathcal{A}_D^-$: its trace $\mathrm{Tr}_{\mathbb{C}^4}$ vanishes. Furthermore for all $J\geq 1$:

$$\widehat{\rho}(F_{1,0}^{\circ J}(Q_{0,2}(\rho));k) \quad = \mathrm{Cst}\iint_{u,\ell_1}\cdots\int_{\ell_J}\frac{du d\boldsymbol{\ell}}{\prod_{1\leq j\leq J}|\ell_j|^2}\mathrm{Tr}_{\mathbb{C}^4}\frac{A_J^{(\ell_j)_{j=1}^J}\widehat{Q}_{0,2}(\rho)(u+\frac{k}{2},u-\frac{k}{2})}{\prod_{0\leq j\leq J}(\widetilde{E}\,(u+k/2-L_j)+\widetilde{E}\,(u-k/2-L_j))} \tag{4.56}$$

where for almost all (p,q,ℓ_j) : $\mathrm{Tr}_{\mathbb{C}^4}\Big\{A_J^{(\ell_j)_{j=1}^J}\widehat{Q}_{0,2}(\rho;p,q)\Big\}=0$ because these matrices are in $\mathcal{A}_D^-$. Thus $\widehat{\rho}(F_{1,0}^{\circ J}(Q_{0,2}(\rho));k)=0$ for almost all $k\in\mathbb{R}^3$ and so $\widehat{\tau}_{0,2}(\rho;k)=0$ for almost all $k\in\mathbb{R}^3$. In other words $\widehat{\tau}_{0,2}(\rho)=0$.

There remains to prove that $\tau_{1,1}\Big(\alpha\mathbf{T}(Q_{0,1}(\rho_0)),\rho_1\Big)=0$: it suffices to show that for all $J,J'\geq 0$: $\rho\Big\{F_{1,0}^{\circ J}\big[Q_{1,1}\big(\alpha F_{1,0}^{\circ J'}[Q_{0,1}(\rho_0)],\rho_1\big)\big]\Big\}$ vanishes. As before we treat together

- $Q_{1,1}^{+R-v-}(F_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)),\rho_1)$ and $Q_{1,1}^{-R+v+}(F_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)),\rho_1)$,
- then $Q_{1,1}^{+v-R-}(F_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)),\rho_1)$ and $Q_{1,1}^{-v+R+}(F_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)),\rho_1)$, and so on.

As $\widehat{F_{1,0}^{\circ J'}}(Q_{0,1}(\rho_0);p,q)\in\mathcal{A}_D^+$ for almost all p,q, then $\widehat{Q}_{1,1}^{+R-v-}(F_{1,0}^{\circ J'}(Q_{0,1}(\rho_0);p,q),\rho_1)+\widehat{Q}_{1,1}^{-R+v+}(F_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)),\rho_1;p,q)\in\mathcal{A}_D^-$ for almost all p,q thanks to (4.54) and (4.55). So its trace $\mathrm{Tr}_{\mathbb{C}^4}$ vanishes. The same result holds for the other cases : $Q_{1,1}^{+v-R-}+Q_{1,1}^{-v+R+}$, $Q_{1,1}^{+-+}+Q_{1,1}^{-+-}$ and $Q_{1,1}^{--+}+Q_{1,1}^{++-}$. Finally as in (4.56) we have :

$$\widehat{\rho}(F_{1,0}^{\circ J}(Q_{1,1}(F_{1,0}^{\circ J'}(\rho_0),\rho_1));k)=0 \text{ for almost all } k.$$

□

4.5 The fixed point method

We prove here Lemmas 4.2, 4.3 and 4.4 and start with some inequalities.

4.5.1 Tools

- We recall the following Sobolev inequalities in $\mathbb{R}^3$: for suitable f –say H^1– we have

$$\|f\|_{L^6}\lesssim\|\nabla f\|_{L^2},\quad \|f\|_{L^4}\lesssim\||\nabla|^{3/4}f\|_{L^2},\quad \|f\|_{L^3}\lesssim\||\nabla|^{1/2}f\|_{L^2}. \tag{4.57}$$

We use them to prove the following inequalities : for $\rho\in\mathcal{C}$, $v_\rho:=\rho*\frac{1}{|\cdot|}$ and $\phi\in H^{1/2}$:

$$\|v_\rho\phi\|_{L^2}\lesssim\|v_\rho\|_{L^6}\|\phi\|_{L^3}\lesssim\|\rho\|_{\mathcal{C}}\||\nabla|^{1/2}\phi\|_{L^2}. \tag{4.58}$$

$$\|\rho*\tfrac{1}{|\cdot|}\|_{L^4}\lesssim\||\nabla|^{3/4}\rho*\tfrac{1}{|\cdot|}\|_{L^2}\lesssim\sqrt{\int\frac{|\widehat{\rho}(k)|^2}{|k|^{5/2}}dk}\lesssim\Big(\inf_{\varepsilon>0}\Big\{2\pi\varepsilon^{1/2}\|\widehat{\rho}\|_{L^\infty}^2+\varepsilon^{-1/2}\|\rho\|_{\mathcal{C}}^2\Big\}\Big)^{1/2}. \tag{4.59}$$

With $v_\rho:=\rho*\frac{1}{|\cdot|}$ Eq. (4.59) is used in :

$$\|\tfrac{1}{\mathcal{D}^0+i\eta}v_\rho\|_{\mathfrak{S}_4},\|\tfrac{1}{|\mathcal{D}^0+i\eta|^{1/2}}v_\rho\tfrac{1}{|\mathcal{D}^0+i\eta|^{1/2}}\|_{\mathfrak{S}_4}\leq\frac{K_2^{1/4}}{E(\eta)^{1/4}}\|\rho*\tfrac{1}{|\cdot|}\|_{L^4} \tag{4.60}$$

- We recall Kato's and Hardy's inequalities for $\phi\in L^2(\mathbb{R}^3)$:

$$\begin{cases}\displaystyle\int_{\mathbb{R}^3}\frac{|\varphi(x)|^2}{|x|}dx & \leq\frac{\pi}{2}\langle|\nabla|\varphi\,,\,\varphi\rangle,\\ \displaystyle\int_{\mathbb{R}^3}\frac{|\varphi(x)|^2}{|x|^2}dx & \leq 4\langle(-\Delta)\varphi\,,\,\varphi\rangle,\end{cases} \tag{4.61}$$

and the Kato-Seiler-Simon's inequality (KSS) for compact operators in $\mathcal{B}(L^2(\mathbb{R}^3))$:

$$\forall\,2\leq p\leq+\infty:\ \|f(-i\nabla)g(x)\|_{\mathfrak{S}_p}\leq(2\pi)^{-3/p}\|f\|_{L^p}\|g\|_{L^p}. \tag{4.62}$$

- We recall that for any $p,q\in B(0,\Lambda)$ we have (see [Sok14b].)

$$\big|\widehat{\mathcal{P}^0_-}(p)-\widehat{\mathcal{P}^0_-}(q)\big|=\big|\widehat{\mathcal{P}^0_+}(p)-\widehat{\mathcal{P}^0_+}(q)\big|\lesssim\frac{|p-q|}{\max(\widetilde{E}\,(p)\,,\widetilde{E}\,(q))}. \tag{4.63}$$

By Ineq. (4.63) we get the following.

Lemma 4.10. *Let $\rho\in\mathcal{C}$, then there exists $K>0$ such that for any $a>1/2$ and $\varepsilon\in\{+,-\}$ we have :*

$$\|\mathcal{P}^0_\varepsilon v_\rho\mathcal{P}^0_{-\varepsilon}|D_0|^{-a}\|_{\mathfrak{S}_2}\le\frac{K}{\sqrt{2a-1}}\|\rho\|_{\mathcal{C}}.$$

Proof : It is obvious once we have seen that the norm of the integral kernel of its Fourier transform is lesser than :

$$K\frac{|\widehat{\rho}(p-q)|}{|p-q|}\frac{1}{E(q)^a\max(E(q),E(p))}.$$

□

4.5.2 Estimate on $Q_{0,1}$

We estimate $\|Q_{0,1}\|_{\mathbf{Q}_w}$ as in [HLS05a]. We have

$$\begin{aligned}\int\limits_{B(0,\Lambda)}\frac{du}{E(u+\varepsilon k/2)^2}\frac{\widetilde{E}\,(u+k/2)+\widetilde{E}\,(u-k/2)}{(\widetilde{E}\,(u+k/2)+\widetilde{E}\,(u-k/2))^2}&\le4\pi\int_0^\Lambda\frac{du}{\sqrt{1+r^2}}\\&\le4\pi(1+\log(\Lambda))\lesssim\log(\Lambda),\end{aligned} \tag{4.64}$$

leading to :

$$\iint w(p-q)(\widetilde{E}\,(p)+\widetilde{E}\,(q))|\widehat{Q}_{0,1}(\rho;p,q)|^2dpdq\lesssim(1+\log(\Lambda))\|\rho\|^2_{\mathfrak{C}_w}, \tag{4.65}$$

where we have used (4.63).

4.5.3 Proof of Lemma 4.2

We recall that for $J\ge1$:

$$Q_J(Q,\rho):=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\eta}{\mathcal{D}^0+i\eta}\prod_{1\le j\le J}\Big((v_\rho-R_Q)\frac{1}{\mathcal{D}^0+i\eta}\Big)$$

We write

$$\mathfrak{a}(Q):=\mathscr{F}^{-1}(|\widehat{Q}|)\text{ and }\mathfrak{a}(\rho):=\mathscr{F}^{-1}(|\widehat{\rho}|).$$

It is clear that $|\widehat{Q}_{k,\ell}(p,q)|$ is lesser than the integral kernel of the Fourier transform of

$$\mathfrak{a}(Q_{k,\ell}):=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\eta}{\sqrt{|\mathcal{D}^0|^2+\eta^2}}\Big(\mathfrak{a}(\rho)*\tfrac{1}{|\cdot|}+R[\mathfrak{a}(Q)]\Big)^J.$$

We write $\mathfrak{a}(v_\rho)=v_{\mathfrak{a}(\rho)}$ and $\mathfrak{a}(R_Q):=R_{\mathfrak{a}(Q)}$ and $d_\eta:=\sqrt{|\mathcal{D}^0|^2+\eta^2}$. We have :

$$\left|\begin{array}{lllll}\|\mathfrak{a}(v_\rho)\|_{L^6}&\lesssim&\|\nabla\mathfrak{a}v_\rho\|_{L^2}&\lesssim&\|\mathfrak{a}(\rho)\|_{\mathcal{C}}=\|\rho\|_{\mathcal{C}},\\\|\mathfrak{a}(v_\rho)\|_{L^4}&\lesssim&\|\,|\nabla|^{3/2}\mathfrak{a}(v_\rho)\|_{L^2}&\lesssim&\|\widehat{\mathfrak{a}(\rho)}\|_{L^\infty}+\|\mathfrak{a}(\rho)\|_{\mathcal{C}}=\|\widehat{\rho}\|_{L^\infty}+\|\rho\|_{\mathcal{C}},\\\|\frac{1}{|\cdot|^{1/2}}\mathfrak{a}(R_Q)\|_{\mathfrak{S}_2}&\lesssim&\|\mathfrak{a}(R_Q)\|_{\mathrm{Ex}}&\lesssim&\|\mathfrak{a}(Q)\|_{\mathrm{T}}=\|Q\|_{\mathrm{T}}.\end{array}\right.$$

By the KSS inequality, there exist $\mathrm{C}_6,\mathrm{C}_4>0$ such that :

$$\begin{aligned}\|d_\eta^{-1/2}v_\rho d_\eta^{-1/2}\|_{\mathfrak{S}_6}&\le\mathrm{C}_6E(\eta)^{-1/2}\|\rho\|_{\mathcal{C}},\\\|d_\eta^{-5/12}v_\rho d_\eta^{-7/12}\|_{\mathfrak{S}_4}&\le\mathrm{C}_4E(\eta)^{-1/4}\|v_\rho\|_{L^4}.\end{aligned} \tag{4.66}$$

As w satisfies (4.3), we have :

$$w(p-q)\widehat{\mathfrak{a}}(Q_J(Q,\rho);p,q)\le JK_{(w)}^J\widehat{\mathfrak{a}}\Big(Q_J\big[\mathscr{F}^{-1}(w(p'-q')\widehat{Q}(p',q')),\mathscr{F}^{-1}(\rho)\big];p,q\Big).$$

It suffices to check that for $p_0=p, p_{J+1}=q$ and $p_1,\cdots,p_J\in\mathbb{R}^3$ we have :

$$w(p-q)\le\sum_{j=1}^{J+1}K_{(w)}^j w(p_{j-1}-p_j)\le JK_{(w)}^J\prod_{j=1}^{J+1}w(p_{j-1}-p_j).$$

In the definition of $\|\cdot\|_{\mathbf{Q}_w}$, there remains to multiply by $\widetilde{E}(p)^{1/2}+\widetilde{E}(q)^{1/2}$. We use the first or the last d_η^{-1} to get :

$$\frac{\widetilde{E}(r)^{1/2}}{\sqrt{\widetilde{E}(r)^2+\eta^2}}\le\frac{1}{(\widetilde{E}(r)^2+\eta^2)^{1/4}}\text{ with } r\in\{p,q\}.$$

For the terms $Q_J(Q,\rho)$ with $J\ge 3$ we get that :

$$\|\mathfrak{a}Q_J(Q,\rho)\|_{\mathbf{Q}_w}\le\frac{JK_{(w)}^J}{2\pi}\Big(\|\tfrac{1}{|\cdot|^{1/2}}R[\mathfrak{a}(Q)]\|_{\mathfrak{S}_2}+\mathrm{C}_6\|\rho\|_{\mathcal{C}}\Big)^J\int_{-\infty}^{+\infty}\frac{d\eta}{\widetilde{E}(\eta)^{(J+1)/2}}.$$

For $J=2$, we treat $Q_{0,2}(\rho)$ in another way because the product of two operators in $\mathfrak{S}_6$ is not necessarily Hilbert-Schmidt. By the Cauchy expansion we have [HLS05a]

$$Q_J^{+\cdots+}=Q_J^{-\cdots-}=0.$$

So it suffices to treat $Q_{0,2}^{\varepsilon_1,\varepsilon_2,\varepsilon_3}$ with $(\varepsilon_1,\varepsilon_2,\varepsilon_3)\neq(+++),(---)$. In particular there is a change of sign $+-$ or $-+$. By Hölder inequality and Lemma 4.10 we have for $\varepsilon\in\{+,-\}$:

$$\|d_\eta^{-1/2}v_\rho^{\varepsilon,-\varepsilon}d_\eta^{-1/4}\|_{\mathfrak{S}_2}\lesssim\|\rho\|_{\mathcal{C}}\Big\{\int\frac{dq}{E(q)^{7/2}}\Big\}^{1/2}\lesssim\|\rho\|_{\mathcal{C}}.$$

Hence using the above inequality and (4.66) we get :

$$\|Q_{0,2}(\rho)\|_{\mathbf{Q}_w}\lesssim\|\rho\|_{\mathcal{C}}^2\int_{-\infty}^{+\infty}\frac{d\eta}{E(\eta)^{1+4^{-1}}}.$$

By (4.29), there exists $K>0$ such that

$$\|Q_J(Q,\rho)\|_{\mathbf{Q}_w}\le J^{1/2}\big(K\times K_{(w)}(\|Q\|_{\mathbf{Q}_w}+\|\rho\|_{\mathfrak{C}_w})\big)^J.$$

To deal with ρ_J, we use the same method as in [HLS05a] and estimate $\|\rho_J\|_{\mathcal{C}}$ by duality. We take a Schwartz function $\zeta\in\mathcal{S}(\mathbf{R^3})$ and prove that for any $k,\ell\ge 0$ with $k+\ell\ge 2$ we have :

$$\big|\mathrm{Tr}(Q_{k,\ell}\zeta)\big|\le K(Q,\rho,k,\ell)\sqrt{\int\frac{|p|^2|\widehat{\zeta}(p)|^2}{g(p)^2}dp}=K(Q,\rho,k,\ell)\|\zeta\|_{\mathfrak{C}'_w}.$$

We emphasize that by Furry's Theorem [Fur37, HLS05a] we have $\rho_{0,2J}=0$ for any $J\in\mathbb{N}^*$.

First we must prove that $Q_{k,\ell}\zeta$ is trace-class. We use the same method as in [HLS05a] :

$$\|Q_{k,\ell}\zeta\|_{\mathfrak{S}_1}\le\|Q_{k,\ell}|\mathcal{D}^0|^2\|_{\mathfrak{S}_2}\|\tfrac{1}{|\mathcal{D}^0|^2}\zeta\|_{\mathfrak{S}_2}\lesssim E(\Lambda)^2\|Q_{k,\ell}\|_{\mathfrak{S}_2}\|\zeta\|_{L^2}.$$

It is clear that $|\widehat{Q_{k,\ell}\zeta}(p,p)|\le|\mathfrak{a}\widehat{(Q_{k,\ell})}\zeta|$.

Writing $d_\eta(p):=\sqrt{\widetilde{E}(p)^2+\eta^2}$, $p_0=p$ and $\mathbf{m}=(m_1,\cdots,m_J)\in\{v_\rho,R_Q\}^J$ we have :

$$2\pi|\mathfrak{a}\widehat{(Q_{k,\ell}^{\mathbf{m}})}\zeta(p,p)|\le\int_{\mathbb{R}}\mathrm{d}\eta\int_{(B(0,\Lambda))^J}\frac{\mathrm{d}\mathbf{p}}{d_\eta(p)}\prod_{j=1}^J|\widehat{m_j}(p_j,p_{j-1})|d_\eta(p_j)^{-1}|\widehat{\zeta}(p_J-p)|$$

We replace $|\widehat{\zeta}(p_J-p)|$ by :

$$|\widehat{\zeta}(p_J-p)|\times\frac{w(p_J-p)}{w(p_J-p)}\le JK_{(w)}^J\frac{|\widehat{\zeta}(p_J-p)|}{w(p_J-p)}\prod_{j=1}^J w(p_j-p_{j-1})=:JK_{(w)}^J|\widehat{\zeta'}(p_J-p)|\prod_{j=1}^J w(p_j-p_{j-1}).\tag{4.67}$$

We write $R':=R\big[\mathscr{F}^{-1}(w(p-q)|\widehat{Q}(p,q)|)\big]$ and $V':=v\big[\mathscr{F}^{-1}(w(p)|\widehat{\rho}(p)|)\big]$.
For (k,ℓ) different from $(0,3),(1,1),(0,2J)$ we have :

$$\begin{aligned}|\mathrm{Tr}(Q_{k,\ell}\zeta)| &\le \frac{(k+\ell)K_{(w)}^{k+\ell}}{2\pi}\binom{k+\ell}{k}\int_{\mathbb{R}}d\eta\|d_\eta^{-1/2}\zeta' d_\eta^{-1/2}\|_{\mathfrak{S}_6}\|d_\eta^{-1/2}R'd_\eta^{-1/2}\|_{\mathfrak{S}_2}^k\|d_\eta^{-1/2}V'd_\eta^{-1/2}\|_{\mathfrak{S}_6}^\ell\\ &\lesssim \frac{(k+\ell)K_{(w)}^{k+\ell}}{2\pi}\binom{k+\ell}{k}K^{k+\ell}\int_{\mathbb{R}}\frac{d\eta}{E(\eta)^{(1+j+\ell)/2}}\|Q\|_{\mathbf{Q}_w}^k\|\rho\|_{\mathfrak{C}_w}^\ell.\end{aligned}$$

To deal with $\rho_{1,1},\rho_{0,3}$ we use the same method as the one used for $\|Q_{0,2}\|_{\mathbf{Q}_w}$. We treat the case of $\rho[Q_{1,1}^{+R-v-}]$ as an example and the other cases are similar and left to the reader.

$$|\mathrm{Tr}_{\mathbf{C}^4}(\widehat{Q}_{1,1}^{+R-v-}(p_0,p_2)\widehat{\zeta}(p_2-p_0))|\le\int_{\mathbb{R}}\int_{(B(0,\Lambda))^3}\frac{d\eta dp_1dp_2|\widehat{R}_Q(p_0,p_1)||\widehat{v}(p_1-p_2)|}{d_\eta(p_0)d_\eta(p_1)d_\eta(p_2)}|\widehat{\zeta^{-+}}(p_2-p_0)|.$$

Using Lemma 4.10 and (4.67) we get that :

$$|\mathrm{Tr}(Q_{1,1}^{+R-v-}\zeta)|\lesssim\|Q\|_{\mathbf{Q}_w}\|\rho\|_{\mathfrak{C}_w}K_{5/4}\|\zeta\|_{\mathfrak{C}'_w}.$$

□

4.5.4 Estimates for $F^{(2)}$

We consider $\gamma'=\gamma+N$ a minimizer of $E_{\mathrm{BDF}}^\nu(M)$ and define the function $F^{(2)}$ (4.32). Two Banach spaces will be considered : first $\mathcal{C}$ and then $\mathcal{C}\cap L^1$. We recall that for $\eta\in\mathbb{R}$ we write $d_\eta=\sqrt{|\mathcal{D}^0|^2+\eta^2}$.

Estimates on the $\mathcal{C}$-norm

Thanks to previous estimates (Lemmas 4.5, 4.6, *a priori* estimates (4.38) and estimates in the $\|\cdot\|_{\mathfrak{C}_w}$-norm), in the regime $M,\|\nu\|_{\mathcal{C}}\lesssim\log(\Lambda)$ there hold the following *non-sharp* estimates :

$$\begin{cases}\|h_2\|_{\mathcal{C}} &\lesssim \alpha^2\Big\{\|\rho_\gamma''\|_{\mathcal{C}}\big[\|N\|_{\mathrm{T}}+\alpha^2(\|\gamma'\|_{\mathrm{T}}+\|\rho_\gamma''\|_{\mathcal{C}})^2\big]+\|\gamma'\|_{\mathrm{T}}^2\Big\}\\ &\lesssim \alpha^2\times\log(\Lambda)=L\alpha\\ \|h_3\|_{\mathcal{C}} &\lesssim \alpha^3(\|\gamma'\|_{\mathrm{T}}+\|\rho_\gamma''\|_{\mathcal{C}})^3\lesssim(L\alpha)^{3/2}.\end{cases}\tag{4.68}$$

Then $F_2^{(2)}(\rho'')$ and $F_3^{(2)}(\rho'')$ are at most cubic in ρ'' :

$$\begin{cases}\|F_2^{(2)}(\rho')\|_{\mathcal{C}} &\lesssim \alpha^4(\|\gamma'\|_{\mathrm{T}}+\|\rho''\|_{\mathcal{C}})\|\rho''\|_{\mathcal{C}}^2\\ \|F_3^{(2)}(\rho')\|_{\mathcal{C}} &\lesssim \alpha^3(\|\rho''\|_{\mathcal{C}}+\|\gamma'\|_{\mathrm{T}})\|\rho''\|_{\mathcal{C}}^2\\ \|\mathrm{d}F_2^{(2)}(\rho')\|_{\mathrm{L}(\mathcal{C})} &\lesssim \alpha^4(\|\gamma'\|_{\mathrm{T}}\|\rho''\|_{\mathcal{C}}+\|\rho''\|_{\mathcal{C}}^2)\\ \|\mathrm{d}F_3^{(2)}(\rho')\|_{\mathrm{L}(\mathcal{C})} &\lesssim \alpha^3(\|\gamma'\|_{\mathrm{T}}\|\rho''\|_{\mathcal{C}}+\|\rho''\|_{\mathcal{C}}^2).\end{cases}\tag{4.69}$$

Estimates on the L^1-norm

Our aim in this part is to prove Lemma 4.11 below which states that $F^{(2)}$ is a well-defined $\mathscr{C}^1$ function of $\mathcal{C}\cap L^1$ (differentiable with a continuous differential).
• We first prove that $h_2,h_3\in L^1$ (we recall they are defined in (4.31)). In fact they are densities of trace-class operators : to see this we use the methods of the proof of Lemma 4.2.

1. $N = \sum_j |\psi_j\rangle\langle\psi_j| \in \mathfrak{S}_1$ so $\mathbf{T}[N] \in \mathfrak{S}_1$ and
$$\|\tau_N\|_{L^1} \leq \|\mathbf{T}[N]\|_{\mathfrak{S}_1} \leq \mathrm{C}_{\mathbf{T},\mathfrak{S}}\|N\|_{\mathfrak{S}_1}. \tag{4.70}$$
2. $Q_{2,0}(\gamma') \in \mathfrak{S}_1$: We have :
$$\|Q_{2,0}(\gamma')\|_{\mathfrak{S}_1} \lesssim \|\gamma'\|^2_{\mathrm{Ex}} K_2. \tag{4.71}$$
3. $Q_{0,\ell}(\rho''_\gamma)$ with $\ell \geq 4$. As $Q_{0,\ell}^{+\cdots+} = Q_{0,\ell}^{-\cdots-} = 0$ there is at least one change of sign $+-$ or $-+$. Then with the help of Lemma 4.10 and Estimates (4.66) we have
$$\|Q_{0,\ell}(\rho''_\gamma)\|_{\mathfrak{S}_1} \lesssim \|\rho''_\gamma\|^\ell_{\mathcal{C}} K_{\frac{\ell+1}{2}+\frac{1}{4}},$$
the product of $\ell-1$ operators in $\mathfrak{S}_6$ and one in $\mathfrak{S}_2$ is trace-class.
4. Similarly $Q_{k,\ell}(\gamma', \rho''_\gamma) \in \mathfrak{S}_1$ with $k \geq 2$ or $k \geq 1$ and $\ell \geq 3$:
$$\|Q_{k,\ell}(\gamma', \rho''_\gamma)\|_{\mathfrak{S}_1} \lesssim \binom{k+\ell}{k} (K\|\gamma'\|_{\mathrm{T}})^k (K\|\rho''_\gamma\|_{\mathcal{C}})^\ell K_{1+(k+\ell)/2}. \tag{4.72}$$
5. Thanks to Furry's Theorem and Theorem 4.1 :
$$\tau\big\{Q_{0,2}(\rho''_\gamma)\big\} = \tau_{1,1}\big\{\mathbf{T}[Q_{0,1}(\rho''_\gamma)], \rho''_\gamma\big\} = 0. \tag{4.73}$$
6. By the same methods as before we have $Q_{0,3}(\rho''_\gamma), Q_{1,2}(\gamma', \rho''_\gamma) \in \mathfrak{S}_{6/5}$ with :
$$\|Q_{0,3}(\rho''_\gamma)\|_{\mathfrak{S}_{6/5}} \lesssim \|\rho''_\gamma\|^3_{\mathcal{C}} K_{2+1/4} \text{ and } \|Q_{1,2}(\gamma', \rho''_\gamma)\|_{\mathfrak{S}_{6/5}} \lesssim \|\gamma'\|_{\mathrm{T}} \|\rho''_\gamma\|^2_{\mathcal{C}} K_{1+3/2}.$$
Furthermore the following inequalities hold (we recall that Y is defined in (4.50)) :
$$\|d_\eta^{-3/8} v_\rho d_\eta^{-5/8}\|_{\mathfrak{S}_6} \lesssim E(\eta)^{-1/2}\|\rho\|_{\mathcal{C}} \text{ and } \|d_\eta^{-5/8} R\big(\mathbf{T}[Q]\big) d_\eta^{-5/8}\|_{\mathfrak{S}_{6/5}} \lesssim Y(\tfrac{6}{5})\|Q\|_{\mathfrak{S}_{6/5}}.$$
Thus
$$\left\{\begin{array}{rl} \|\mathbf{T}_{1,1}\big\{\mathbf{T}Q_{0,3}(\rho''_\gamma), \rho''_\gamma\big\}\|_{\mathfrak{S}_1} & \lesssim 2\mathrm{C}_{\mathbf{T},\mathfrak{S}} K_{5/4}\|\rho''_\gamma\|_{\mathcal{C}}\big(Y(\tfrac{6}{5})\|\rho''_\gamma\|^3_{\mathcal{C}} K_{2+1/4}\big), \\ \|\mathbf{T}_{1,1}\big\{\mathbf{T}Q_{1,2}(\gamma', \rho''_\gamma), \rho''_\gamma\big\}\|_{\mathfrak{S}_1} & \leq 2\mathrm{C}_{\mathbf{T},\mathfrak{S}} K_{5/4}\|\rho''_\gamma\|_{\mathcal{C}}\big(3Y(\tfrac{6}{5})\|\gamma'\|_{\mathrm{T}}\|\rho''_\gamma\|^2_{\mathcal{C}} K_{1+3/2}\big) \\ \|\mathbf{T}_{1,1}\big\{\mathbf{T}N, \rho''_\gamma\big\}\|_{\mathfrak{S}_1} & \lesssim 2\mathrm{C}_{\mathbf{T},\mathfrak{S}} K_{5/4}\|\rho''_\gamma\|_{\mathcal{C}} Y(\tfrac{6}{5})M. \end{array}\right. \tag{4.74}$$
7. We apply $\mathbf{T}$, h_2 (resp. h_3) is the density of $Q(h_2)$ (resp. $Q(h_3)$) with
$$\left\{\begin{array}{rl} Q(h_2) & = \alpha^2\Big\{\mathbf{T}Q1,1\big[\mathbf{T}N + \alpha^2\mathbf{T}[Q_{2,0}(\gamma') + \widetilde{Q}_3(\gamma', \rho''_\gamma)]; \rho''_\gamma\big] + \mathbf{T}Q_{2,0}(\gamma')\Big\} \\ Q(h_3) & = \alpha^3\Big\{\mathbf{T}Q_{3,0}(\gamma') + \mathbf{T}Q_{2,1}(\gamma', \rho''_\gamma) + \alpha\widetilde{Q}_4(\gamma', \rho''_\gamma)\Big\} \end{array}\right.$$
The previous estimates lead to a sequence of numbers $(b_\ell)_{\ell\geq 2}$ with the following asymptotic behaviour :
$$b_\ell = \mathcal{O}_{\ell\to+\infty}(\ell^{1/2}) \tag{4.75}$$
and a constant $\mathrm{C}_0 > 0$ such that :
$$\begin{aligned} &\Big\|\alpha^2 Q_{2,0}(\gamma') + \alpha^3[Q_{3,0} + Q_{2,1}](\gamma', \rho''_\gamma) + \alpha^4\widetilde{Q}_4(\gamma', \rho''_\gamma)\Big\|_{\mathfrak{S}_1} \\ &+\alpha^3\Big\|Q_{0,3}(\rho''_\gamma) + Q_{1,2}(\gamma', \rho''_\gamma)\Big\|_{\mathfrak{S}_{6/5}} \leq \sum_{\ell=2}^{+\infty} b_\ell(\alpha\mathrm{C}_0)^\ell(\|\rho''_\gamma\|_{\mathcal{C}} + \|\gamma'\|_{\mathrm{T}})^\ell =: \mathrm{A}_{h,\mathfrak{S}}. \end{aligned} \tag{4.76}$$
We have :
$$\|Q(h_2)\|_{\mathfrak{S}_1} \lesssim \alpha^2\mathrm{C}_{\mathbf{T},\mathfrak{S}}\big(2K_{5/4}Y(\tfrac{6}{5})(M + \mathrm{A}_{h,\mathfrak{S}}) + \|\gamma'\|^2_{\mathbf{Q}_w}\big) \tag{4.77}$$
and write $B_{h_2,\mathfrak{S}}$ this upper bound. Similarly :
$$\|Q(h_3)\|_{\mathfrak{S}_1} \leq \mathrm{C}_{\mathbf{T},\mathfrak{S}} \sum_{\ell=3}^{+\infty} b_\ell(\alpha\mathrm{C}_0)^\ell(\|\rho''_\gamma\|_{\mathcal{C}} + \|\gamma'\|_{\mathrm{T}})^\ell =: \mathrm{B}_{h_3,\mathfrak{S}_1}. \tag{4.78}$$

Remark 4.11. The introduced numbers $\mathrm{A}_{h,\mathfrak{S}}, \mathrm{B}_{h_2,\mathfrak{S}_1}, \mathrm{B}_{h_3,\mathfrak{S}}$ are *not* constants : they all depend on α and the minimizer γ'. As *a priori* estimates hold(Lemma 4.5), these upper bounds are small provided that we are in the regime of Remark 4.6. Indeed we have

$$\big(1-\frac{\alpha\pi}{4}\big)\|\gamma'\|_{\mathrm{T}}^2+\frac{\alpha}{2}\|\rho''_\gamma\|_{\mathcal{C}}^2\le\frac{\alpha}{2}\|\nu\|_{\mathcal{C}}^2+M,$$

so $\alpha(\|\gamma'\|_{\mathrm{T}}+\|\rho''_\gamma\|_{\mathcal{C}})\lesssim\alpha\|\nu\|_{\mathcal{C}}+\sqrt{\alpha M}=\mathcal{O}((L\alpha)^{1/4})$. In particular those upper bounds are $o(1)$.

• Let us estimate the L^1-norm of $F_2^{(2)}(\rho'')$ and $F_3^{(2)}(\rho'')$ with $\rho''\in\mathcal{C}\cap L^1$. To this end we use (4.60) and (4.59) at level $\varepsilon=1$ for instance : there exists $K_{L^4}^{(v)}>0$ such that :

$$\|v_{\rho''}\|_{L^4}\le K_{L^4}^{(v)}\{\|\rho''\|_{L^1}+\|\rho''\|_{\mathcal{C}}\}. \tag{4.79}$$

We use the second inequality of (4.66) and Lemma 4.10 with $a=7/12$. Using the method of the proof of Lemma 4.2, we obtain the following.

Lemma 4.11. *Let ρ'' be in $\mathcal{C}\cap L^1$ and γ' a minimizer for $E_{BDF}^\nu(M)$ with density ρ'_γ. We have :*

$$\begin{array}{rcl}
\|\mathbf{T}Q_{0,3}(\rho'')\|_{\mathfrak{S}_1} & \lesssim & 6K_{13/12}C_{\mathbf{T},\mathfrak{S}}\{\|\rho''\|_{L^1}+\|\rho''\|_{\mathcal{C}}\}^2\|\rho''\|_{\mathcal{C}}\\
\|\mathbf{T}Q_{1,2}(\gamma',\rho'')\|_{\mathfrak{S}_1} & \lesssim & \binom{3}{1}K_2C_{\mathbf{T},\mathfrak{S}}\|\gamma'\|_{\mathrm{T}}\{\|\rho''\|_{L^1}+\|\rho''\|_{\mathcal{C}}\}^2\\
\|Q_{0,2}(\rho'')\|_{\mathfrak{S}_{4/3}} & \lesssim & 4K_{7/3}\|\rho''\|_{\mathcal{C}}\{\|\rho''\|_{L^1}+\|\rho''\|_{\mathcal{C}}\}\\
\|Q_{1,1}(\gamma',\rho'')\|_{\mathfrak{S}_{4/3}} & \lesssim & 2K_{7/4}\|\gamma'\|_{\mathrm{T}}\{\|\rho''\|_{L^1}+\|\rho''\|_{\mathcal{C}}\}\\
\|\mathbf{T}Q_{1,1}\big\{\mathbf{T}Q_{0,2}(\rho''),\rho''\big\}\|_{\mathfrak{S}_1} & \lesssim & 2K_{13/12}Y(\tfrac{4}{3})C_{\mathbf{T},\mathfrak{S}}\|Q_{0,2}(\rho'')\|_{\mathfrak{S}_{4/3}}\{\|\rho''\|_{L^1}+\|\rho''\|_{\mathcal{C}}\}\\
\|\mathbf{T}Q_{1,1}\big\{\mathbf{T}Q_{1,1}(\gamma',\rho''),\rho''\big\}\|_{\mathfrak{S}_1} & \lesssim & 2K_{13/12}Y(\tfrac{4}{3})C_{\mathbf{T},\mathfrak{S}}\|Q_{1,1}(\gamma',\rho'')\|_{\mathfrak{S}_{4/3}}K_{L^4}^{(v)}\{\|\rho''\|_{L^1}+\|\rho''\|_{\mathcal{C}}\}
\end{array} \tag{4.80}$$

Similarly we can estimate $\|dF_j^{(2)}\|_{\mathrm{L}(\mathcal{C}\cap L^1)}$. As $\|\gamma'\|_{\mathrm{T}}\lesssim\sqrt{\log(\Lambda)}$ we have :

$$\left\{\begin{array}{lcl}
\|F_2^{(2)}(\rho'')\|_{\mathcal{C}\cap L^1} & \lesssim & \alpha^4\|\rho''\|_{\mathcal{C}\cap L^1}^2\big\{\sqrt{\log(\Lambda)}+\|\rho''\|_{\mathcal{C}\cap L^1}\big\}\\
\|F_3^{(2)}(\rho'')\|_{\mathcal{C}\cap L^1} & \lesssim & \alpha^3\|\rho''\|_{\mathcal{C}\cap L^1}^2\big\{\sqrt{\log(\Lambda)}+\|\rho''\|_{\mathcal{C}\cap L^1}\big\},\\
\|dF_2^{(2)}(\rho'')\|_{\mathrm{L}(\mathcal{C}\cap L^1)} & \lesssim & \alpha^4\|\rho''\|_{\mathcal{C}\cap L^1}^2\big\{\sqrt{\log(\Lambda)}+\|\rho''\|_{\mathcal{C}\cap L^1}\big\},\\
\|dF_2^{(2)}(\rho'')\|_{\mathrm{L}(\mathcal{C}\cap L^1)} & \lesssim & \alpha^3\|\rho''\|_{\mathcal{C}\cap L^1}^2\big\{\sqrt{\log(\Lambda)}+\|\rho''\|_{\mathcal{C}\cap L^1}\big\}.
\end{array}\right. \tag{4.81}$$

4.5.5 Application of the Banach fixed point theorem

$F^{(1)}$

With *exactly* the same method of [HLS05a] let us apply the Banach fixed point theorem to $F^{(1)}$ with the help of estimates of the previous subsections. We recall the different steps.
We define (where $K_{(w)}>0$ is defined in (4.3) and $\mathrm{C}_0>0$ is the constant of Lemma 4.2)

$$\mathcal{X}_w:=\mathbf{Q}_w\times\mathfrak{C}_w,\quad\text{with }\|(Q,\rho)\|_{\mathcal{X}_w}:=K_{(w)}\mathrm{C}_0(\|Q\|_{\mathbf{Q}}+\|\rho\|_{\mathfrak{C}_w}). \tag{4.82}$$

Thanks to the previous estimates we can say that the function $F^{(1)}$ is well defined in a ball $B_{\mathcal{X}_g}(0,\overline{R})$ with $\overline{R}=O(\sqrt{\log(\Lambda)})$, say $\overline{R}=K_0\sqrt{\log(\Lambda)}$. Indeed :

$$\|F^{(1)}(Q',\rho'')\|_{\mathcal{X}_w}\le\|(N,n'')\|_{\mathcal{X}_w}+\alpha\boldsymbol{\kappa}_1(\Lambda)\|(Q',\rho'')\|_{\mathcal{X}_w}+\sum_{\ell=2}^{+\infty}\alpha^\ell\boldsymbol{\kappa}_\ell\|(Q',\rho'')\|_{\mathcal{X}_w}^\ell, \tag{4.83}$$

where

$$\left\{\begin{array}{ll}
\boldsymbol{\kappa}_1(\Lambda) & =\mathcal{O}_{\Lambda\to+\infty}(\sqrt{\log(\Lambda)})\\
\boldsymbol{\kappa}_\ell & =\mathcal{O}_{\ell\to+\infty}(\ell^{1/2}).
\end{array}\right. \tag{4.84}$$

In particular the radius of convergence of the power series $f(x)=\sum_{\ell=2}^{+\infty}\boldsymbol{\kappa}_\ell x^\ell$ is 1 and :

$$\|\mathrm{d}F^{(1)}(Q',\rho'')\|_{\mathrm{L}(\mathcal{X}_g)}\le \alpha\boldsymbol{\kappa}_1(\Lambda)+\alpha f'(\alpha\|(Q',\rho'')\|_{\mathcal{X}_w}). \tag{4.85}$$

For$\|(N,n'')\|_{\mathcal{X}_w}\neq(0,0)$ it is clear that $F^{(1)}(0,0)=(N,\mathscr{F}^{-1}(-\frac{1}{1+\alpha B_\Lambda(\cdot)}\widehat{n}''))\neq 0$. So

$$\sup_{(Q',\rho'')\in B_{\mathcal{X}_g}(0,\overline{R})}\|\mathrm{d}F^{(1)}(Q',\rho'')\|_{\mathrm{L}(\mathcal{X}_g)}\le \alpha\boldsymbol{\kappa}_1(\Lambda)+\alpha f'(\alpha\overline{R})=:\nu(\overline{R}). \tag{4.86}$$

For $(Q',\rho'')\in B_{\mathcal{X}_g}(0,\overline{R})$ we have

$$\begin{aligned}\|F^{(1)}(Q',\rho'')\|_{\mathcal{X}_w} &\le \|F^{(1)}(Q',\rho'')-F^{(1)}(0,0)\|_{\mathcal{X}_w}+\|F^{(1)}(0,0)\|_{\mathcal{X}_w}\\ &\le \nu(\overline{R})\|(Q',\rho'')\|_{\mathcal{X}_w}+\|F^{(1)}(0,0)\|_{\mathcal{X}_w}.\end{aligned}$$

Thus $B_{\mathcal{X}_g}(0,\overline{R})$ is invariant under $F^{(1)}$ provided that :

$$\|F^{(1)}(0,0)\|_{\mathcal{X}_w}\le(1-\nu(\overline{R}))\overline{R}. \tag{4.87}$$

As $F^{(1)}(0,0)\neq 0$ this gives $\nu(\overline{R})<1$.

Let us say that $\|(N,n'')\|_{\mathcal{X}_w}=\varepsilon_0\overline{R}=\varepsilon_0K_0\sqrt{\log(\Lambda)}$, $\varepsilon_0<1$. We have :

$$\|F^{(1)}(0,0)\|_{\mathcal{X}_w}\le\varepsilon_0\overline{R}, \tag{4.88}$$

it suffices to take $\alpha>0$ such that $\sqrt{L\alpha}K_0\ll 1$ and then take $\overline{R}$ accordingly. The constant K_0 depends on the constants in the conditions $M,\|\nu\|_{\mathcal{C}}\lesssim\sqrt{\log(\Lambda)}$: we get $\overline{R}=K_0\sqrt{\log(\Lambda)}$ and for sufficiently small α the Theorem can be applied on that ball.

$F^{(2)}$

We work with $(\mathcal{C},\|\cdot\|_{\mathcal{C}})$ and $(\mathcal{C}\cap L^1,\max(\|\cdot\|_{\mathcal{C}},\|\cdot\|_{L^1}))$. In Appendix 4.C it is proved that $\|\check{f}_\Lambda\|_{L^1}\le K\alpha B_\Lambda(0)$ where we can choose $K=2$ for $\alpha\log(\Lambda)$ sufficiently small. Thus :

$$\mathscr{F}^{-1}(F_\Lambda)=\mathscr{F}^{-1}\left\{\frac{f_\Lambda}{1+f_\Lambda}\right\}=\sum_{\ell=1}^{+\infty}(-1)^{\ell+1}\check{f}_\Lambda^{*\ell}\in L^1$$

and its L^1-norm is lesser than $\frac{2\alpha B_\Lambda(0)}{1-2\alpha B_\Lambda(0)}\le 4\alpha B_\Lambda(0)$ as soon as $\alpha B_\Lambda(0)\le 4^{-1}$. Moreover we can write

$$\frac{1}{1+f_\Lambda}=1-\frac{f_\Lambda}{1+f_\Lambda};$$

therefore if $\rho\in L^1$ then $\mathscr{F}^{-1}\{\frac{1}{1+f_\Lambda}\widehat{\rho}\}^{-1}\in L^1$ and its L^1-norm is lesser than

$$(1+4\alpha B_\Lambda(0))\|\rho\|_{L^1}\le 2\|\rho\|_{L^1}.$$

In particular :

$$\|\mathscr{F}^{-1}(\tfrac{1}{1+f_\Lambda}\widehat{n}'')\|_{L^1}\le 2(M+Z).$$

So we have :

$$\begin{cases}\|F^{(2)}(\rho'')\|_{\mathcal{C}\cap L^1} &\le 2(M+Z)+\|h_2+h_3\|_{\mathcal{C}\cap L^1}+K\alpha^3(\sqrt{\log(\Lambda)}+\|\rho''\|_{\mathcal{C}\cap L^1})\|\rho''\|^2_{\mathcal{C}\cap L^1}\\ \|\mathrm{d}F^{(2)}(\rho'')\|_{\mathrm{L}(\mathcal{C}\cap L^1)} &\le K\alpha^3\|\rho''\|_{\mathcal{C}\cap L^1}(2\sqrt{\log(\Lambda)}+3\|\rho''\|_{\mathcal{C}\cap L^1}).\end{cases} \tag{4.89}$$

where the constants K can be chosen indepently of $\alpha\le\alpha_0$ and $\alpha\log(\Lambda)\le L_0$ for α_0,L_0 sufficiently small. The term $\sqrt{\log(\Lambda)}$ is due to $\|\gamma'\|_{\mathrm{T}}\lesssim\sqrt{\log(\Lambda)}$ (see Lemma 4.5 and the regime of Remark 4.6). We get similar estimates for $F^{(2)}$ defined in $\mathcal{C}$. So it suffices to take $\overline{R}>2$ sufficiently large so that $B_{\mathcal{C}\cap L^1}(0,\overline{R})$ is invariant under $F^{(2)}$. This function is a contraction and we can apply the fixed point theorem. To end the proof we remark :

— There is only one fixed point of $F^{(2)}$ in $B_{\mathcal{C}}(0,\overline{R})$ by the Banach-Picard Theorem and $\rho_\gamma+n-\nu$ is a fixed point. Indeed by Section 4.3.2, $(\gamma+N,\rho_\gamma+n-\nu)$ has norm $\mathbf{Q}_1\times\mathcal{C}$ bounded by $K\sqrt{\log(\Lambda)}$ in the regime of Remark 4.6 and is a fixed point of $F^{(1)}$. So it is a fixed point of $F^{(2)}$.

— There is only one fixed point of $F^{(2)}$ in $B_{\mathcal{C}\cap L^1}(0,\overline{R})$ by the same theorem. In particular it is also a fixed point of $F^{(2)}$ in $B_{\mathcal{C}}(0,\overline{R})$ as $B_{\mathcal{C}\cap L^1}(0,\overline{R})\subset B_{\mathcal{C}}(0,\overline{R})$. By unicity $\rho_\gamma\in L^1$.

4.6 Proofs of Theorems 4.2 and 4.3

4.6.1 Proof of Theorem 4.2

Proof : The fact that $\rho_\gamma \in L^1$ is a result of Section 4.5.5. We recall that if $Q \in \mathfrak{S}_1$, then $\int \rho_Q = \mathrm{Tr}(Q) = \mathrm{Tr}_{P^0_-}(Q)$. Writing

$$\begin{array}{ll|ll} A & := \alpha \mathbf{T}[Q_{0,1}(\rho''_\gamma)] & C & := \alpha^3 \mathbf{T}\Big\{Q_{1,1}\big[\mathbf{T}[Q_{0,1}(\rho''_\gamma)], \rho''_\gamma\big]\Big\} \\ B & := \alpha^2 \mathbf{T}(Q_{0,2}(\rho''_\gamma)) & S & := \gamma - (A + B + C) \end{array} \tag{4.90}$$

it has been shown in Section 4.5 that $S \in \mathfrak{S}_1$. Theorem 4.1 says $\rho_B = \rho_C = 0$.

Let us show that $B^{++}, B^{--}, C^{++}, C^{--}$ are trace-class. First for any Q in $\mathfrak{S}_2$, we have

$$\mathcal{P}^0_- Q_{1,0}(Q) \mathcal{P}^0_- = \mathcal{P}^0_+ Q_{1,0}(Q) \mathcal{P}^0_+ = 0.$$

It follows that $B^{\pm\pm} = \alpha^2 Q_{0,2}(\rho''_\gamma)^{\pm\pm}$ and $C^{\pm\pm} = \alpha^3 Q_{1,1}\big(\mathbf{T}Q_{0,1}(\rho''_\gamma), \rho''_\gamma\big)^{\pm\pm}$. And as

$$Q^{+++}_{0,2} = Q^{---}_{0,2} = Q^{+++}_{1,1} = Q^{---}_{1,1} = 0$$

there only remain $Q^{+-+}_{0,2}, Q^{-+-}_{0,2}, Q^{+-+}_{1,1}, Q^{-+-}_{1,1}$. Using Lemma 4.10 with $a = \frac{3}{4}$ and Cauchy-Schwartz inequality we have

$$\|\tfrac{1}{|D_0|^{3/8}} \mathcal{P}^0_\pm v_\rho \mathcal{P}^0_\mp \tfrac{1}{|D_0|^{3/8}}\|_{\mathfrak{S}_2} \lesssim \|\rho\|_{\mathcal{C}} \lesssim \|\rho\|_{\mathcal{C}} \tag{4.91}$$

We recall that $\|\frac{1}{|\nabla|^{1/2}} R_Q\|_{\mathfrak{S}_2} \lesssim \|Q\|_{\mathrm{Ex}}$: these two estimates enables us to prove the following :

$$\begin{array}{rcl} \|Q^{\pm\mp\pm}_{0,2}(\rho''_\gamma)\|_{\mathfrak{S}_1} & \lesssim & K_{3/2}\|\rho''_\gamma\|^2_{\mathcal{C}}, \\ \|Q^{\pm\mp\pm}_{1,1}(\gamma', \rho''_\gamma)\|_{\mathfrak{S}_1} & \lesssim & K_{7/4}\|\gamma'\|_{\mathrm{Ex}}\|\rho''_\gamma\|_{\mathcal{C}}. \end{array}$$

As shown in Sections 4.5 and 4.C we have $Q^{++}_{0,1} = Q^{--}_{0,1} = 0$ and $\rho_A = -\check{f}_\Lambda * (\rho'_\gamma) \in L^1$.

$$\begin{aligned} \int \rho_\gamma &= \int (\rho_{\gamma^{++}} + \rho_{\gamma^{--}}) + \int \{\rho_{A^{+-}} + \rho_{A^{-+}} + \rho_{B^{+-}} + \rho_{B^{-+}} + \rho_{C^{+-}} + \rho_{C^{-+}}\} \\ &= \mathrm{Tr}_{P^0_-}(\gamma) - \alpha f_\Lambda(0) \int \{\rho_\gamma + n - \nu\} - \int \{\rho_{B^{++}} + \rho_{B^{--}} + \rho_{C^{--}} + \rho_{C^{++}}\} \\ &= 0 - \alpha f_\Lambda(0) \Big\{ \int \rho_\gamma + M - Z \Big\} - \mathrm{Tr}_{P^0_-}(B) - \mathrm{Tr}_{P^0_-}(C). \end{aligned}$$

To end the proof we have to show that $\mathrm{Tr}(B^{++} + B^{--}) = \mathrm{Tr}(C^{++} + C^{--}) = 0$: this is straightforward when written in Fourier space (see [HLS05a] for formulae). □

4.6.2 Proof of Theorem 4.3

We follow the method of [HLS09]. We apply a Lemma of Borwein and Preiss [HLS09, Theorem 4] and consider an approximate minimizer $\gamma'_0 = \gamma_0 + N_0$ of $E^\nu(M)$.

Indeed, we can extend $\mathcal{E}^\nu_{BDF}$ to $\mathfrak{K} = \cap\{Q \in \mathfrak{S}_2 : Q^* = Q,\ 0 \le Q + P^0_- \le 1\}$ by setting $\mathcal{E}^\nu_{BDF}(Q) := +\infty$ whenever $Q \notin \mathcal{K}$. This extension is lower semi-continuous and bounded from below in the $\mathfrak{S}_2$-topology and the set

$$\mathcal{M} := \{Q \in \mathfrak{K}, (Q + P^0_-)^2 = Q + P^0_-, \mathrm{Tr}_0(Q) = M\}$$

is closed in the same topology. Its convex closure in $\mathfrak{S}_2$ is

$$\mathfrak{K}(M) := \{Q \in \mathfrak{K},\ \mathrm{Tr}_0(Q) = M\}.$$

Applying the lemma, for each $\varepsilon > 0$ there exists a projector P and $A \in \mathfrak{K}(M)$ such that $\gamma'_0 := P - P^0_-$ minimizes the functional $\mathcal{E}^\nu_{\mathrm{BDF}} + \varepsilon \mathrm{Tr}((A - \cdot)^2)$ on $\mathcal{M}$ and

$$\mathcal{E}^\nu_{\mathrm{BDF}}(\gamma'_0) \le E^\nu_{\mathrm{BDF}}(M) + \varepsilon^2,\ \|\gamma'_0 - A\|_{\mathfrak{S}_2} \le \sqrt{\varepsilon}.$$

As in [HLS09], γ_0' satisfies the self-consistent equation

$$\begin{aligned}\gamma_0' + P_-^0 &= \chi_{(-\infty,\mu_0]}(D_{\gamma_0'} + 2\varepsilon(\mathrm{sgn}(D_0) - A)) \\ &= \chi_{(-\infty,\mu_0]}(\widetilde{D} + \alpha B_{\gamma_0'} - 2\varepsilon A)\end{aligned} \tag{4.92}$$

where $\mu_0 \in \mathbb{R}$ and $\widetilde{D} := \mathcal{D}^0 + D_0 \frac{2\varepsilon}{|D_0|}$. We choose $\varepsilon = \lambda^{-1}$ small *e.g.* $\varepsilon = \Gamma(\frac{\Lambda}{\alpha})^{-1}$. Using the proof of Lemma 4.5 we show that the following *a priori* estimate holds for γ_0' :

$$\mathrm{Tr}(|\nabla|(\gamma_0')^2) + \alpha\|\rho''_{\gamma_0}\|_{\mathcal{C}}^2 \lesssim \alpha\|\nu\|_{\mathcal{C}}^2 + \sqrt{\alpha}M + \sqrt{\alpha M}\|\nu\|_{\mathcal{C}}.$$

Using the Cauchy expansion, we can write

$$\gamma_0 = \sum_{j=0}^{+\infty} \alpha^j O_j(\rho''_{\gamma_0}, \gamma_0') + \frac{2}{\lambda} W_\lambda(A, \alpha B(\gamma_0')),$$

where the O_j's are defined as the Q_j's with $\widetilde{D}$ replacing $\mathcal{D}^0$ (see (4.20)). By the same method as in Section 4.5 we have :

$$\|\,|\mathcal{D}^0|^{1/2} W_\lambda\|_{\mathfrak{S}_2} + \|\rho[W_\lambda]\|_{\mathcal{C}} \lesssim \|A\|_{\mathfrak{S}_2}\big(1 + \alpha[\|\rho''_{\gamma_0}\|_{\mathcal{C}} + \|\,|\nabla|^{1/2}\gamma_0'\|_{\mathfrak{S}_2}]\big).$$

Indeed it suffices to replace one $R[\gamma_0']$ in the O_j's by A and remark that $A \in \mathfrak{S}_2$. Replacing $\mathcal{D}^0$ by $\widetilde{D}$ is harmless; as before, by defining some function $\widetilde{F}^{(1)}$ we can show that
$\mathrm{Tr}_0(\gamma_0) = 0$ (but with an alternative B_Λ *cf* Section 4.C).

In particular we can write

$$\rho_{\gamma_0} := -\mathscr{F}^{-1}(\widetilde{F}_\Lambda) * n_0'' + (\delta_0 - \mathscr{F}^{-1}(\widetilde{F}_\Lambda)) * \tau_{\mathrm{rem}} \in \mathcal{C}$$

where $\|\tau_{\mathrm{rem}}\|_{\mathcal{C}} \lesssim \|\mathfrak{t}[N_0]\|_{\mathcal{C}} + \alpha^2\|\widetilde{\tau}_2\|_{\mathcal{C}} + \|A\|_{\mathfrak{S}_2}/\lambda$ and $\widetilde{F}_\Lambda$ is defined in Section 4.C. We write $\mathfrak{f}_\Lambda := \mathscr{F}^{-1}(\widetilde{F}_\Lambda)$ for short. As in Section 4.5 we get :

$$\left|\begin{array}{l}\|\gamma_0\|_{\mathfrak{S}_2} \lesssim \alpha(\|\rho''_\gamma\|_{\mathcal{C}} + \|\gamma_0'\|_{\mathrm{T}}) \\ \|\rho_{\gamma_0} + \mathfrak{f}_\Lambda * n_0'' - (\delta_0 - \mathfrak{f}_\Lambda) * \mathfrak{t}[N_0]\|_{\mathcal{C}} \lesssim \alpha^2(\|\gamma_0'\|_{\mathrm{T}} + \|\rho''_{\gamma_0}\|_{\mathcal{C}})^2. \\ \|-\mathfrak{f}_\Lambda * n_0'' + (\delta_0 - \mathfrak{f}_\Lambda) * \mathfrak{t}[N_0]\|_{L^1} \lesssim L(Z+M).\end{array}\right. \tag{4.93}$$

Let $(\psi_j)_{1\le j\le M}$ be an orthonormal family of eigenvectors of $\widetilde{D} + \alpha B_{\gamma_0'} + 2/\varepsilon(1 - P_-^0 - A)$ spanning $\mathrm{Ran}(N_0)$ (with eigenvalues (μ_j)).

We then scale γ_0' by α^{-1} (this procedure is emphasized by an underline) as in [HLS09] we get :

$$\Big[\big(\frac{g_0(-i\alpha\nabla)\beta}{\alpha^2} - \frac{ig_1(-i\alpha\nabla)}{\alpha^2}\boldsymbol{\alpha}\cdot\nabla\big) + \rho[\underline{\gamma_0'}] * \frac{1}{|\cdot|} - R[\underline{\gamma_0'}] + \frac{2}{\alpha^2\lambda}(\tfrac{1}{2} - \underline{\mathcal{P}_-^0} - \underline{A})\Big]\underline{\psi_j} = \frac{\mu_j}{\alpha^2}\underline{\psi_j}. \tag{4.94}$$

Remark 4.12. We have $U_\alpha\underline{\psi}(x) = \alpha^{\frac{3}{2}}\underline{\psi}(\alpha x) = \psi(x)$ and for an operator S we define :

$$\underline{S} := U_\alpha^* S U_\alpha.$$

This mean-field operator $H_{\alpha^{-1}}$ is decomposed as follows : $H_{\alpha^{-1}} = H_{\alpha^{-1}}^{(1)} + h_{\mathrm{rem}}$ where

$$H_{\alpha^{-1}}^{(1)} := \frac{\mathcal{D}^0}{\alpha^2} + (\delta_0 - \underline{\mathfrak{f}_\Lambda}) * \underline{n_0''} - R[\underline{N_0}],\ \underline{n_0''}(x) = \alpha^{-3}n''(x/\alpha), \underline{\widetilde{F}_\Lambda}(k) = \widetilde{F}_\Lambda(\alpha k).$$

As in the Lemma 13 and 14 of [HLS09] we can show that there exists $\varepsilon > 0$ such that
$\limsup_{\alpha\to 0}(\alpha^{-2}(\mu_j - 1)) < -\varepsilon < 0$ for all $1 \le j \le M$ and that $(\underline{\psi_j})_j$ is bounded in $H^1(\mathbb{R}^3, \mathbf{C}^4)^M$ (as α tends to 0). Lemma 13 is based on a min-max description of eigenvalues in the gap of the mean-field operator $H_{\alpha^{-1}}$. We refer to this paper for the proofs. The only difference lies in the presence of $-\underline{\mathfrak{f}_\Lambda} * (\underline{n_0}'') * \frac{1}{|\cdot|}$ and $(\delta_0 - \underline{\mathfrak{f}_\Lambda}) * \mathfrak{t}_{\underline{N_0}}$: we deal with these terms in the following lemma, proved below.

Lemma 4.12. *Let χ be a Schwartz function and for $R>0$: $\chi_R(x) := R^{-3/2}\chi(x/R)$. Then there holds :*

$$\Big|\langle \underline{\mathfrak{f}_\Lambda} * (\underline{n_0}'') * \tfrac{1}{|\cdot|}\chi_R - Z\widetilde{F}_\Lambda(0)\tfrac{\chi_R}{|\cdot|}\,,\,\chi_R\rangle\Big| \lesssim \tfrac{ZL}{R^2}\|\nabla\chi\|_{L^2}^2 + \tfrac{1}{R}\|\nabla\chi\|_{L^2}\|\chi\|_{L^2}\Big(L\int_{|y|>\frac{1}{\alpha}}\nu(y)dy + Z\int_{|y|>\frac{1}{\alpha}}|\mathfrak{f}_\Lambda(y)|dy\Big),$$

and $\int_{|y|>\frac{1}{\alpha}}|\mathfrak{f}_\Lambda(y)|dy \lesssim L\alpha^{1/2}$. *Moreover for $r_0>0$ we have*

$$R\Big|\langle(\delta_0-\underline{\mathfrak{f}_\Lambda}) * \underline{\mathfrak{t}_{N_0}} * \tfrac{1}{|\cdot|}\chi_R\,,\,\chi_R\rangle\Big| \lesssim \tfrac{\alpha\|\mathfrak{t}_{N_0}\|_{L^1}}{R}\int\frac{|\mathscr{F}(|\chi|^2;k)|}{|k|}dk + \int_{|y|\geq r_0}|\underline{\mathfrak{t}_{N_0}}(y)|dy\int\frac{|\chi(x)|^2}{|x|}dx + \|\mathfrak{t}_{N_0}\|_{L^1}\int_{|x|\leq\frac{r_0}{R}}\tfrac{|\chi(x)|^2}{|x|}dx.$$

Remark 4.13. This is because of the last term that the bound on L depends on M. If we could prove that $\int_{|x|\geq r_0}|\mathfrak{t}_{N_0}(y)|dy$ tends to 0 as $r_0\to+\infty$ *uniformly in* ε (the parameter of Borwein and Preiss's Lemma), then we could take $L\leq L_0$ instead of $L\leq 1/(K_0M)$ in Theorem 4.3.

To prove $(\underline{\psi_j})_j$ is H^1-bounded we show that :

$$\frac{M}{\alpha^4}+\frac{\mathrm{Tr}(-\Delta\underline{N_0})}{\alpha^2}\leq\frac{\mathrm{Tr}(\underline{\mathcal{D}^0}^2\underline{N_0})}{\alpha^4}\leq\frac{M}{\alpha^4}+K(M,\nu)\Big\{\mathrm{Tr}(-\Delta\underline{N_0})+\frac{\|\nabla\underline{N_0}\|_{\mathfrak{S}_2}}{\alpha^2}\Big\}. \tag{4.95}$$

The lower bound is clear and the upper bound follows from Eq. (4.94), Lemma 4.5 and Proposition 4.5 (for estimations of $g_\star(\alpha p)^2$, $\star\in\{0,1\}$). We get :

$$\begin{aligned}\Big\|\rho[\underline{\gamma_0}]+\rho[\underline{\mathfrak{f}_\Lambda}*\underline{n_0''}-(\delta_0-\underline{\mathfrak{f}_\Lambda})*\underline{\mathfrak{t}_{N_0}}]\underline{\psi_j}\Big\|_{L^2} &\lesssim \alpha^{3/2}(\|\rho''_{\gamma_0}\|_{\mathcal{C}}+\|\gamma_0'\|_{\mathrm{T}})^2\|\,|\nabla|^{1/2}\underline{\psi_j}\|_{L^2}\\ &\lesssim K(M,\nu)\|\,|\nabla|^{1/2}\underline{\psi_j}\|_{L^2}.\end{aligned}$$

Moreover :

$$\left|\begin{aligned}&\|R[\underline{\gamma_0}]\underline{\psi_j}\|_{L^2}\lesssim\|\gamma_0\|_{\mathfrak{S}_2}\|\nabla\underline{\psi_j}\|_{L^2}\lesssim\alpha^{3/4}K(M,\nu)\|\nabla\underline{\psi_j}\|_{L^2}\\ &\|v\big[\underline{\mathfrak{f}_\Lambda}*\underline{n_0''}-(\delta_0-\underline{\mathfrak{f}_\Lambda})*\underline{\mathfrak{t}_{N_0}}\big]\underline{\psi_j}\|_{L^2}^2\leq 4\|\nabla\underline{\psi_j}\|_{L^2}^2\|\rho[\underline{\mathfrak{f}_\Lambda}*\underline{n_0''}-(\delta_0-\underline{\mathfrak{f}_\Lambda})*\underline{\mathfrak{t}_{N_0}}]\|_{L^1}^2\\ &\qquad\lesssim L^2(Z+M)^2\|\nabla\underline{\psi_j}\|_{L^2}^2\\ &\big|\langle v\big[\underline{\mathfrak{f}_\Lambda}*\underline{n_0''}-(\delta_0-\underline{\mathfrak{f}_\Lambda})*\underline{\mathfrak{t}_{N_0}}\big]\underline{\psi_j}\,,\,\underline{\psi_j}\rangle\big|\leq\big|D(\rho\big[\underline{\mathfrak{f}_\Lambda}*\underline{n_0''}-(\delta_0-\underline{\mathfrak{f}_\Lambda})*\underline{\mathfrak{t}_{N_0}}\big],|\underline{\psi_j}|^2)\big|\\ &\qquad\lesssim L(Z+M)\langle|\nabla|\underline{\psi_j}\,,\,\underline{\psi_j}\rangle.\end{aligned}\right. \tag{4.96}$$

Summing over $1\leq j\leq M$ the inequalities (4.96) we get (4.95) because

$$\sum_{j=1}^M\|\nabla\underline{\psi_j}\|_{L^2},\mathrm{Tr}(|\nabla|\overline{N}_0)\leq\sqrt{M}\sqrt{\mathrm{Tr}(-\Delta\underline{N_0})}.$$

We conclude as in [HLS09] (the proof uses [Lio87]) provided that there hold binding inequalities for the non-relativistic limit : this is the result of Proposition 4.2 in Appendix 4.B.

In particular there holds

$$\lim_{\alpha\to0}\alpha^{-2}\big(E^\nu_{BDF}(M)-M+\frac{\alpha}{2}D(\check{F}_\Lambda*\nu,\nu)\big)=E_{nr}(M), \tag{4.97}$$

where E_{nr} is the non-relativistic energy *cf* Appendix 4.B.

Proof of Lemma 4.12 With $f(x)=|\chi_R|^2*\mathscr{F}^{-1}(\underline{\widetilde{F}_\Lambda})$, we first estimate $|\iint f(x)\nu(y)(1/|x-\alpha y|-1/|x|)dxdy|$: it is lesser than

$$\iint|f(x)|\nu(y)|\alpha y|\frac{dxdy}{|x||x-\alpha y|}.$$

Splitting at level α^{-1} for y, we use Hardy's and Kato's inequalities :

$$\begin{cases} \displaystyle\int_{|y|\le\frac{1}{\alpha}} \nu(y)dy \int \frac{|f(x)|dx}{|x||x-\alpha y|} & \le (4Z\|\widetilde{F}_\Lambda\|_{L^1}) \frac{\|\nabla\chi\|_{L^2}^2}{R^2} \\ \displaystyle\int_{|y|>\frac{1}{\alpha}} \nu(y)dy \int |\alpha y| \frac{dx}{|x||x-\alpha y|}|f(x)| & \le \frac{2\pi}{2} \displaystyle\int_{|y|>\frac{1}{\alpha}} \nu(y)dy \|\widetilde{F}_\Lambda\|_{L^1} \frac{\|\nabla\chi\|_{L^2}\|\chi\|_{L^2}}{R}. \end{cases}$$

We estimate $Z\big|\iint |\chi_R(x)|^2 \mathfrak{f}_\Lambda(y)(1/|x-\alpha y| - 1/|x|)dxdy\big|$ analogously, with the help of Lemma 4.15. To treat the terms with $\underline{\mathfrak{t}_{N_0}}$ we use the fact that :

$$\|\underline{\mathfrak{t}_{N_0}}\|_{L^1} = \|\mathfrak{t}_{N_0}\|_{L^1} \lesssim LM \text{ and } \int \underline{\mathfrak{t}_{N_0}} = \int \mathfrak{t}_{N_0} = 0.$$

The first term in the upper bound corresponds to the error term that we get when we replace $\mathscr{F}^{-1}(\widetilde{F}_\Lambda) * \frac{1}{|\cdot|}$ by $\widetilde{F}_\Lambda(0)$. To see this, we write $a := \widehat{\underline{\mathfrak{t}_{N_0}}}$ and $b := \widehat{|\chi|^2}$: we have

$$\begin{array}{rcl} \displaystyle\int \frac{a^*(k)b(Rk)}{|k|^2}(\widetilde{F}_\Lambda(\alpha k) - \widetilde{F}_\Lambda(0)) & = & \displaystyle\int \frac{a^*\big(\frac{k}{R}\big)b(k)}{|k|^2}(\widetilde{F}_\Lambda(\frac{\alpha k}{R}) - \widetilde{F}_\Lambda(0)), \\ \Big|\displaystyle\int \frac{a^*(k)b(Rk)}{|k|^2}(\widetilde{F}_\Lambda(\alpha k) - \widetilde{F}_\Lambda(0))\Big| & \lesssim & \frac{\alpha\|\mathfrak{t}_{N_0}\|_{L^1}}{R} \displaystyle\int \frac{|b(k)|}{|k|}dk. \end{array}$$

Let ϱ be in L^1. Thanks to Newton's Theorem (for radial functions) we have

$$\begin{array}{rcl} R \times D\big(|\chi_R|^2, \varrho\big) & = & \displaystyle\int \varrho(y)\Big(\frac{R}{|y|}\int_{|x|\le\frac{|y|}{R}} |\chi(x)|^2dx + \int_{|x|\ge\frac{|y|}{R}} \frac{|\chi(x)|^2}{|x|}dx\Big) \\ & = & \displaystyle\int_{|y|>r_0} \varrho(y)\int_{|x|\le\frac{|y|}{R}} |\chi(x)|^2\big(\frac{R}{|y|} - \frac{1}{|x|}\big)dx + \int_{|y|\le r_0} \varrho(y)\Big(\int_{|x|\le\frac{|y|}{R}} |\chi(x)|^2\big(\frac{R}{|y|} - \frac{1}{|x|}\big)dx\Big) \\ & \lesssim & \| \, |\nabla|^{1/2}\chi\|_{L^2} \displaystyle\int_{|y|>r_0} |\varrho(y)|dy + \|\varrho\|_{L^1} \int_{|x|\le\frac{r_0}{R}} \frac{|\chi(x)|^2}{|x|}. \end{array}$$

□

4.A Estimates and inequalities

Notation 4.8. In Section 4.A and 4.C, $\mathbf{e}$ refers to any unitary vector in $\mathbb{R}^3$ and for $p \in \mathbb{R}^3$, we write $\omega_p := \frac{p}{|p|}$.

We recall that $\mathbf{s}_p = \mathscr{F}(\text{sign}(\mathcal{D}^0); p)$. There exists $C_s > 0$ such that :

$$\left| \begin{array}{l} \text{Id} - \mathbf{s}_p\mathbf{s}_q = \mathbf{s}_p(\mathbf{s}_p - \mathbf{s}_q) = (\mathbf{s}_p - \mathbf{s}_q)\mathbf{s}_q \\ |\text{Id} - \mathbf{s}_p\mathbf{s}_q| \le |\mathbf{s}_p - \mathbf{s}_q| = \Big|\widehat{\mathcal{P}^0_-}(p) - \widehat{\mathcal{P}^0_-}(q)\Big| \le C_s \frac{|p-q|}{\max(\widetilde{E}(p), \widetilde{E}(q))}. \end{array} \right. \tag{4.98}$$

4.A.1 Proof of Lemma 4.8

We have [LL97] $\frac{1}{|\nabla|}(x-y) = \text{Cst}/|x-y|^2$. By Cauchy-Schwartz inequality there holds :

$$\begin{array}{rcl} \text{Tr}(R_Q^*|\nabla|^{-1}R_Q) & = & \displaystyle\iiint \text{Tr}_{\mathbf{C}^4} \frac{{}^t\overline{Q}(x,y)}{|x-y|}\frac{\text{Cst}}{|y-z|^2}\frac{Q(z,x)}{|z-x|}dxdydz \\ & \lesssim & \displaystyle\iiint |Q(x,y)|^2 \frac{1}{|y-z|^2}\frac{dxdydz}{|z-x|^2} \\ & \lesssim & \displaystyle\iint \frac{|Q(x,y)|^2}{|x-y|} = \text{Tr}(R_Q^*Q). \end{array}$$

We write $m(|p+q|)$ the multiplication in Fourier space by $|p+q|$: the operators $R.$ and $\frac{1}{|\nabla|^{1/2}}$ commute with the multiplication in Fourier space by $w(p-q)$ (written $m(w)$). By Kato's inequality we have

$$\|m(w) \cdot \tfrac{1}{|\nabla|^{1/2}}R[Q]\|_{\mathfrak{S}_2} = \|\tfrac{1}{|\nabla|^{1/2}}R[m(w)\cdot Q]\|_{\mathfrak{S}_2} \lesssim \|m(|p+q|)m(w)\cdot Q\|_{\mathfrak{S}_2}.$$

Similarly for $a > 0$ the operator $|D_0|^{-a}$ is a convolution operator associated to a *positive* function ϕ_a. Indeed there holds [LL97] : $\frac{1}{\omega^2-\Delta}(x-y) = \dfrac{e^{-\omega|x-y|}}{4\pi|x-y|}, \omega \geq 0$ and for any $0 < \varepsilon < 1$ (see [LS10, footnote p. 87]) :

$$\frac{1}{|D_0|^{2\varepsilon}} = \frac{\sin(\varepsilon\pi)}{\pi} \int_0^{+\infty} t^{p-1} \frac{1-\Delta}{t+1-\Delta} dt.$$

Thus for $a = 1+\varepsilon > 1$ we have by Cauchy-Schwarz inequality :

$$\begin{aligned} \mathrm{Tr}(R_Q^* \tfrac{1}{|D_0|^{2a}} R_Q) &\leq \iint |Q(x,y)|^2 \tfrac{1}{|\cdot|^2} * \phi_{2a}(x-y) dx dy, \\ &\leq \iint |Q(x,y)|^2 \| \tfrac{1}{|\cdot|^2} * \phi_{2a} \|_{L^\infty} \\ &\lesssim \iint |Q(x,y)|^2 dx dy \int \frac{dp}{|p| E(p)^{2a}} \lesssim \frac{\|Q\|_{\mathfrak{S}_2}^2}{2(a-1)}. \end{aligned}$$

Let us consider a finite rank operator $Q(x,y)$. As $Q = \frac{Q+Q^*}{2} + \frac{Q-Q^*}{2}$ one may suppose it is self-adjoint, writing $Q = Q_+ - Q_-$ one may suppose it is nonnegative : then so is R_Q and $|D_0|^{-a/2} R_Q |D_0|^{-a/2}$. We have

$$\begin{aligned} \int \frac{\mathrm{Tr}_{\mathbf{C}^4}(\widehat{R}(p,p))}{E(p)^{2a}} dp &= \frac{1}{2\pi^2} \iint \frac{d\ell}{|\ell|^2} \mathrm{Tr}(\widehat{Q}(p-\ell, p-\ell)) \frac{dp}{E(p)^{2a}} \\ &= \frac{1}{2\pi^2} \int dp \mathrm{Tr}(\widehat{Q}(p,p)) \int \frac{d\ell}{|\ell|^2} \frac{1}{E(p+\ell)^{2a}} \\ &\lesssim \frac{\|\widehat{Q}\|_{\mathfrak{S}_1}}{2a-2}. \end{aligned}$$

In Fourier space we have : $\mathscr{F}\big(|\mathcal{D}^0|^{-1/2}\big) : f(p) \mapsto \chi_{|p|<\Lambda} \frac{f(p)}{E(p)^{1/2}}$. Thus writing Π_A the projection onto $\{f \in L^2,\ \mathrm{supp}\,\widehat{f} \subset B(0,A)\}$ we get

$$\|\,|\mathcal{D}^0|^{1/2} R_Q \|_{\mathfrak{S}_2} \leq \|\,|\mathcal{D}^0|^{1/2} \Pi_{2\Lambda} R_Q \Pi_{3\Lambda} \|_{\mathfrak{S}_2}.$$

As $|\mathcal{D}^0|^{-1/2} \Pi_{2\Lambda} \leq e |D_0|^{-\frac{1}{2} - \frac{1}{2\log(\Lambda)}}$ for $\Lambda \geq e$ we finally have :

$$\mathrm{Tr}\big(\Pi_{3\Lambda} R_{Q*} \frac{\Pi_{2\Lambda}}{|\mathcal{D}^0|} R_Q \Pi_{3\Lambda}\big) \leq \mathrm{Tr}\big(R_{Q*} \frac{e}{|\mathcal{D}^0|^{\frac{1}{2} + \frac{1}{2\log(\Lambda)}}} R_Q\big) \lesssim \log(\Lambda) \|Q\|_{\mathrm{Ex}}^2.$$

4.B The non relativistic limit

We fix the value $F_\Lambda(0) = a$. For any trace-class operator $0 \leq \Gamma \leq 1$ with density ρ_Γ the non-relativistic energy is

$$\begin{aligned} \mathcal{E}_{nr}^Z(\Gamma) &:= \tfrac{1}{2} \mathrm{Tr}(-\Delta\Gamma) - Z(1-a) \mathrm{Tr}\big(\tfrac{1}{|\cdot|}\Gamma\big) \\ &\quad + \tfrac{1}{2}(D(\rho_\Gamma, \rho_\Gamma) - \mathrm{Ex}[\Gamma]) - \tfrac{a}{2} D(\rho_\Gamma, \rho_\Gamma). \end{aligned} \tag{4.99}$$

If we drop the last term, this is exactly the Hartree-Fock energy $\mathcal{E}_{\mathrm{HF}}$ with a nucleus of charge $Z_0 := Z(1-a)$ and if we drop $\mathrm{Tr}(\frac{1}{|\cdot|} Q)$ we get the Pekar-Tomasevitch energy $\mathcal{E}_{nr}^0 = \mathcal{E}_{\mathrm{PT}}[\frac{a}{2}, U = \frac{1}{2}]$ (*cf* [FLST11]).

Remark 4.14. We can easily show stability of matter of the second kind for $a \leq a_0$ by splitting the energy in two : a Hartree-Fock one and a Pekar-Tomasevitch one,

$$\begin{aligned} \mathcal{E}_{nr}^Z(\Gamma) &= \tfrac{x^2}{2} \mathrm{Tr}(-\Delta\Gamma) + \tfrac{y^2}{2}(D(\rho_\Gamma, \rho_\Gamma) - \mathrm{Ex}[\Gamma]) - Z(1-a) \mathrm{Tr}\big(\tfrac{1}{|\cdot|}\Gamma\big) \\ &+ \tfrac{1-x^2}{2} \mathrm{Tr}(-\Delta\Gamma) + \tfrac{1-y^2}{2}(D(\rho_\Gamma, \rho_\Gamma) - \mathrm{Ex}[\Gamma]) - \tfrac{a}{2} D(\rho_\Gamma, \rho_\Gamma) \text{ with } 0 < x, y < 1. \end{aligned}$$

Optimizing in x and y we get a lower bound $\mathcal{O}(K(a)M)$ for $M \geq 2Z_0 + 1$.

We define

$$\mathcal{G}(x) = \{\Gamma \in \mathfrak{S}_1 : \Gamma^* = \Gamma,\ 0 \leq \Gamma \leq 1, \sqrt{-\Delta}\Gamma \in \mathfrak{S}_2 \text{ and } \mathrm{Tr}(\Gamma) = x\} \text{ with } x \in \mathbb{R}_+^*.$$

$E_{nr}(M)$ corresponds to the infimum over $\mathcal{G}(M)$. We want to prove :

Proposition 4.2. *For any $M < Z+1$, the variational problem $E^Z_{nr}(M)$ admits a minimizer.*

By Lieb's method in [Lie77], it is easy to see that there is a minimizer for $E^Z_{nr}(1)$.To prove binding for $2 \leq M \leq Z(1-a)$ we can follow Lieb's and Simon's method [LS77, Lio87]. We will however prove it with the method of concentration-compactness. We prove the problem $E^Z_{nr}(M)$ admits a minimizer by induction over M by using :

Proposition 4.3. *For each $\ell > 0$ the following assertions are equivalent*

- $\forall 0 < k < \ell :\ E^Z_{nr}(\ell) < E^Z_{nr}(\ell - k) + E^0_{nr}(k)$.
- *Each minimizing sequence for $E^Z_{nr}(\ell)$ is precompact in $H^1(\mathbb{R}^3 \times \mathbb{R}^3)$.*

In the case $\ell \in \mathbb{N}^*$, it suffices to prove binding inequalities for $K \in (0, \ell) \cap \mathbb{N}$.

This proposition is standard and we will not give the proof here but refer to [Lew11, LL10, Lio87]. In [FLST11] Frank *et al.* prove that $E^0_{nr}(M_0) = M_0 E^0_{nr}(1)$ for $M_0 \in \mathbb{N}^*$ provided that a is sufficiently small. Thus we just have to show

$$E^Z_{nr}(M) < E^Z_{nr}(M-1) + E^0_{nr}(1).$$

To this end, we exhibit a test function Q whose energy is lesser than $E^Z_{nr}(M-1) + E^0_{nr}(1)$.

Lieb's variational principle still holds (*cf* [HLS09, Proposition 3]). In fact for any orthonormal family (ϕ_1, ϕ_2) , with $P_\phi := |\phi\rangle\langle\phi|$ and $0 < t < 1$, we have

$$\begin{array}{l}\mathcal{E}^Z_{nr}(\Gamma + t(P_{\phi_1} - P_{\phi_2})) - \mathcal{E}^Z_{nr}(\Gamma) = \frac{t}{2}(\|\nabla\phi_1\|^2_{L^2} - \|\nabla\phi_2\|^2_{L^2} + 2(1-a)D(\rho_\Gamma, |\phi_1|^2 - |\phi_2|^2)) \\ -t\Re[\mathrm{Tr}(\Gamma R[P_{\phi_1} - P_{\phi_2}])] - t^2\big\{D(|\phi_1|^2, |\phi_2|^2) - D(\phi_1^*\phi_2, \phi_1^*\phi_2) + \frac{a}{2}\||\phi_1|^2 - |\phi_2|^2\|^2_{\mathcal{C}}\big\}.\end{array} \tag{4.100}$$

This shows that $E^Z_{nr}(m)$ is also the infimum of $\mathcal{E}^Z_{nr}$ over

$$\{\Gamma \in \mathcal{G}(m) :\ \Gamma = P + (m - [m])|\phi\rangle\langle\phi|, P^2 = P = P^*, \phi \in \mathrm{Ker}(P)\}.$$

Taking $\phi_2 = 0$ in (4.100) shows that $E^Z_{nr}(\cdot)$ is concave in $[M_0, M_0+1]$ with $M_0 \in \mathbb{N}$. It is also clear that E^Z_{nr} is decreasing since large binding inequalities hold.

We consider a minimizer of $E^Z_{nr}(M-1)$ of the form $\Gamma = \sum_{1\leq j\leq M-1} |\psi_j\rangle\langle\psi_j|$, each ψ_j satisfying

$$\frac{-\Delta}{2}\psi_j - \frac{Z_0}{|\cdot|}\psi_j + (1-a)\rho[\Gamma] * \frac{1}{|\cdot|}\psi_j - R[\Gamma]\psi_j + \varepsilon_j\psi_j = 0, \text{ with } \varepsilon_j > 0.$$

In particular we can easily show the ψ_j's are in $H^2(\mathbb{R}^3)$ and fast decaying.

We also consider a minimizer for $E^0_{nr}(1)$: this is a minimizer ϕ_{CP} of $E_{\mathrm{PT}}(1)$ scaled by $a : \phi_0(x) = a^{3/2}\phi_{\mathrm{CP}}(ax)$, we chose it to be radial [Lie77]. Following [LL10], we take a Schwartz function $0 \leq \chi \leq 1$ that satisfies $\chi(x) = 1$ for $|x| \leq 1$ and $\chi(x) = 0$ for $|x| \geq 2$ and $\chi_R(x) = \chi(x/R)$ with $R > 0$ to be chosen.

We define the trial state as follows : for some $\mathbf{e} \in \mathbb{S}^2$ we write

$$\Gamma' := \chi_R\Gamma\chi_R + \tau_{-5R\mathbf{e}}|\chi_R\phi_0\rangle\langle\chi_R\phi_0|\tau_{5R\mathbf{e}}$$

where $\tau_{x_0}\psi(x) := \psi(x - x_0)$. We have $0 \leq \Gamma' \leq 1$ and $\mathrm{Tr}(\Gamma') \leq M$, so
$\mathcal{E}_{nr}(\Gamma') \geq E_{nr}(M)$. As the wave functions (ψ_j)'s and ϕ_0 are fast decaying, the following holds :

$$\begin{array}{c}\mathcal{E}^Z_{nr}(\Gamma') = \mathcal{E}^Z_{nr}(\Gamma) + \mathcal{E}^0_{nr}(\phi_0) + \displaystyle\int \big(\rho[\Gamma] * \frac{1}{|\cdot|}(x) - \frac{Z_0}{|x|}\big)|\tau_{5R\mathbf{e}}\phi_0(x)|^2 dx \\ -aD(\rho[\Gamma], |\tau_{5R\mathbf{e}}\phi_0|^2) + o(R^{-1}).\end{array}$$

As R tends to infinity we get :

$$\mathcal{E}^Z_{nr}(\Gamma') \leq E^Z_{nr}(M-1) + E^0_{nr}(1) + \frac{(M-1)(1-a) - Z_0}{5R} + o(R^{-1}) < E_{nr}(M-1) + E^0_{nr}(1).$$

4.C Proof of Proposition 4.1

Notation 4.9. We write :

$$E(u,k/2) := \max\big(E(u+k/2), E(u-k/2)\big) \geq \sqrt{1+|u|^2+\tfrac{|k|^2}{4}},$$
$$\widetilde{E}\,(u,k/2) := \max\big(\widetilde{E}\,(u+k/2)\,,\widetilde{E}\,(u-k/2)\,\big) \geq E(u,k/2).$$

Our aim is to prove Proposition 4.4 below.

Proposition 4.4. *Let $\rho_0 \in \mathcal{C}$. Then we have :*

$$\alpha\rho(\mathbf{T}[Q_{0,1}(\rho_0)]) = -\check{f}_\Lambda * \rho_0$$

where $\check{f}_\Lambda \in L^1$ is a radial function. Moreover

$$f_\Lambda = \sum_{J=0}^{+\infty} \alpha^J f_{\Lambda,J}, \quad f_{\Lambda,0} = \alpha B_\Lambda \quad \text{and} \quad g_\Lambda := \sum_{J=1}^{+\infty} \alpha^J f_{\Lambda,J},$$

with

$$\|\check{f}_\Lambda\|_{L^1} \lesssim L \text{ and } \|\check{\gamma}_\Lambda\|_{L^1} \lesssim L\alpha.$$

In particular $\check{F}_\Lambda := \mathscr{F}^{-1}\big(\frac{f_\Lambda}{1+f_\Lambda}\big) \in L^1$.

We also study an alternative function F_Λ, needed for the proof of Theorem 4.3, at the end of this section. We need the following proposition.

Proposition 4.5. *The function $\widehat{\mathcal{D}^0} : \overline{B(0,\Lambda)} \to \mathbb{R}^3$ is infinitely differentiable. In particular so is $\widetilde{E}\,(\cdot)$ and there exists $L_0 \geq 0$ such that if $L := \alpha\log(\Lambda) \leq L_0$ then for any $J \geq 1$ there exists $C_J > 0$ such that :*

$$\|d^J g_0\|_{L^\infty} \leq \alpha C_J \text{ and } \|d^J \mathbf{g}_1\|_{L^\infty} \leq \chi_{J=1} + LC_J.$$

Proof : In the spirit of [Sok14b], we can prove it by induction over J : in [HLS07] Hainzl *et al.* proved that $\widehat{\mathcal{D}^0}$ is infinitely differentiable. Thus the function

$$|\widehat{\mathcal{D}^0}(p)| = \sqrt{g_0(p)^2 + \mathbf{g}_1(p)\cdot\mathbf{g}_1(p)},$$

is infinitely differentiable and does not vanish on $\overline{B(0,\Lambda)}$. Thanks to the self-consistent equation one has :

$$\mathrm{d}^J\widehat{\mathcal{D}^0}(p) = \mathrm{d}^J\widehat{D_0}(p) + \frac{\alpha}{4\pi^2}\frac{1}{|\cdot|^2} * \mathrm{d}^J\Big(\frac{\mathcal{D}^0}{|\mathcal{D}^0|}\Big)(p).$$

□

Proof of Proposition 4.4 : Throughout this proof we write $k := r\mathbf{e}$.
1. Let us first prove the following :

$$\widehat{\tau}_{1,0}(\rho) = -f_\Lambda(\cdot)\widehat{\rho}(\cdot),$$

We recall that for any $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ we have (4.41) :

$$\widehat{Q}_{1,0}(Q,p,q) = \frac{1}{4\pi^2}\frac{1}{\widetilde{E}\,(p)+\widetilde{E}\,(q)}\int_\ell \frac{d\ell}{|\ell|^2}\big(\widehat{Q}(p-\ell,q-\ell) - \mathbf{s}_p\widehat{Q}(p-\ell,q-\ell)\mathbf{s}_q\big),$$

and (*cf* [HLS05a])

$$\widehat{Q}_{0,1}(\rho;p,q) = \frac{4\pi}{2^{5/2}\pi^{3/2}}\frac{\widehat{\rho}(p-q)}{|p-q|^2}\frac{1}{\widetilde{E}\,(p)+\widetilde{E}\,(q)}(\mathbf{s}_p\mathbf{s}_q - 1). \tag{4.101}$$

The functions $A_J^{(\ell_j)_{j=1}^J}$ are defined recursively in (4.52). We have for instance :

$$\begin{aligned} A_2^{(\ell_1,\ell_2)}\widehat{Q}(p,q) &= A_1^{\ell_1}\big(\widehat{Q}(\cdot_p-\ell_2,\cdot_q-\ell_2)-\mathbf{s}_{\cdot_p}\widehat{Q}(\cdot_p-\ell_2,\cdot_q-\ell_2)\mathbf{s}_{\cdot_q}\big)(p,q)\\ &= \Big\{\widehat{Q}(p-\ell_1-\ell_2,q-\ell_1-\ell_2)-\mathbf{s}_{p-\ell_1}\widehat{Q}(p-\ell_1-\ell_2,q-\ell_1-\ell_2)\mathbf{s}_{q-\ell_1}\Big\}\\ &\quad -\mathbf{s}_p\Big\{\widehat{Q}(p-\ell_1-\ell_2,q-\ell_1-\ell_2)-\mathbf{s}_{p-\ell_1}\widehat{Q}(p-\ell_1-\ell_2,q-\ell_1-\ell_2)\mathbf{s}_{q-\ell_1}\Big\}\mathbf{s}_q. \end{aligned}$$

Writing $L_J := \sum_{j=1}^J \ell_j$ with $L_0 := 0 \in \mathbb{R}^3$ we have :

$$\widehat{F_{1,0}^{\circ J}}(Q;p,q) = \frac{\alpha^J}{(4\pi^2)^J}\int_{\ell_1}\cdots\int_{\ell_J}\frac{d\boldsymbol{\ell}}{\prod\limits_{1\le j\le J}|\ell_j|^2}\frac{A_J^{(\ell_j)_{j=1}^J}\widehat{Q}(p,q)}{\prod\limits_{0\le j\le J-1}(\widetilde{E}\,(p-L_j)+\widetilde{E}\,(q-L_j))}. \tag{4.102}$$

In particular the Fourier transform of the density $\rho\big(F_{1,0}^{\circ J}(Q)\big)$ is

$$\begin{aligned} \widehat{\rho}(F_{1,0}^{\circ J}(Q);k) &= \frac{1}{(2\pi)^{3/2}}\int_u \mathrm{Tr}_{\mathbb{C}^4}\widehat{F_{1,0}^{\circ J}}(Q;u+\tfrac{k}{2},u-\tfrac{k}{2})du\\ &= \frac{\alpha^J}{(2\pi)^{3/2}(4\pi^2)^J}\iint\limits_{u,\ell_1}\cdots\int\limits_{\ell_J}\mathrm{Tr}_{\mathbb{C}^4}\frac{dud\boldsymbol{\ell}}{\prod\limits_{1\le j\le J}|\ell_j|^2}\frac{A_J^{(\ell_j)_{j=1}^J}\widehat{Q}(u+\frac{k}{2},u-\frac{k}{2})}{\prod\limits_{0\le j\le J-1}(\widetilde{E}\,\big(u+\frac{k}{2}-L_j\big)+\widetilde{E}\,\big(u-\frac{k}{2}-L_j\big))}\\ &= \frac{\alpha^J}{(2\pi)^{3/2}(4\pi^2)^J}\iint\limits_{u,\ell_1}\cdots\int\limits_{\ell_J}\frac{dud\boldsymbol{\ell}}{\prod\limits_{1\le j\le J}|\ell_j|^2}\frac{\mathrm{Tr}_{\mathbb{C}^4}\big\{(1-\mathbf{s}_{u-\frac{k}{2}}\mathbf{s}_{u+\frac{k}{2}})A_J^{(\ell_j)_{j=2}^{J-1}}\widehat{Q}(u+\frac{k}{2},u-\frac{k}{2})\big\}}{\prod\limits_{0\le j\le J-1}(\widetilde{E}\,\big(u+\frac{k}{2}-L_j\big)+\widetilde{E}\,\big(u-\frac{k}{2}-L_j\big))}. \end{aligned} \tag{4.103}$$

Above the domain of ℓ_j is :

$$\widetilde{B}_j(r) := \big\{\ell_j,\ \big|u-L_j\pm\tfrac{r}{2}\mathbf{e}\big|<\Lambda\big\},$$

and the domain of u is $\widetilde{B}_0(r) := \big\{u,\ \big|u\pm\frac{r}{2}\mathbf{e}\big|<\Lambda\big\}$. In particular

$$\mathrm{supp}\,\widehat{\rho}(F_{1,0}^{\circ J}(Q))\subset B(0,2\Lambda).$$

Remark 4.15. We would like to apply (4.103) to the operator $Q_{0,1}(\rho)$. From (4.101) we realize that $\widehat{Q}_{0,1}(p,q)$ is not a scalar matrix because of the term $\mathbf{s}_p\mathbf{s}_q-\mathrm{Id}$. Yet it is in the algebra spanned by the Dirac matrices $\boldsymbol{\alpha}_1,\boldsymbol{\alpha}_2,\boldsymbol{\alpha}_3,\beta$ as a sum of *even* products of Dirac matrices. The form of $\widehat{Q}_{1,0}(Q)$ is similar to $\widehat{Q}_{0,1}$: it only adds an *even* number of Dirac matrices to $\widehat{Q}$. This is an important remark to be done to prove Theorem 4.1.

For any $J\ge 1$ and $\rho\in\mathcal{C}$, the density $\widehat{\rho}(F_{1,0}^{\circ J}(Q_{0,1}[\rho]);k)$ is equal to :

$$\begin{aligned} &\frac{4\pi\alpha^J\widehat{\rho}(k)}{(2^5\pi^3)^{\frac12}(2\pi)^{3/2}(4\pi^2)^J}\int\limits_{\prod_{0\le j\le J}\widetilde{B}_j(r)}\frac{dud\boldsymbol{\ell}}{|k|^2\prod\limits_{1\le j\le J}|\ell_j|^2}\frac{\mathrm{Tr}_{\mathbb{C}^4}\big\{(1-\mathbf{s}_{u-\frac{k}{2}}\mathbf{s}_{u+\frac{k}{2}})A_{J-1}^{(\ell_j)_{j=2}^J}(\mathbf{s}_{u-\frac{k}{2}}\mathbf{s}_{u+\frac{k}{2}}-1)\big\}}{\prod\limits_{0\le j\le J}(\widetilde{E}\,\big(u+\frac{k}{2}-L_j\big)+\widetilde{E}\,\big(u-\frac{k}{2}-L_j\big))}\\ &=\widehat{\rho}(k)\int\limits_{\prod_{0\le j\le J}\widetilde{B}_j(r)}dud\boldsymbol{\ell}\ S_J(u-L_j\pm\tfrac{k}{2})T_J(u-L_j\pm\tfrac{k}{2}) \end{aligned} \tag{4.104}$$

where $S_J(u-L_j\pm\frac{k}{2})$ is a scalar which is a function of $|u-L_j\pm\frac{k}{2}|$ while $T_J(u-L_j\pm\frac{k}{2})$ is the trace $\mathrm{Tr}_{\mathbf{C}^4}$ of a sum of products of $\mathbf{s}_{u-L_j-\frac{k}{2}}$.

We have to deal with $\frac{1}{|k|^2}$ and we must show that this integral is well defined. The first problem is easy, the quantity

$$\frac{1}{|k|^2}(\mathbf{s}_{u-L_J+k/2}\mathbf{s}_{u-L_J-k/2}-1)(1-\mathbf{s}_{u-k/2}\mathbf{s}_{u+k/2}) = \frac{(\mathbf{s}_{u-L_J+k/2}\mathbf{s}_{u-L_J-k/2}-1)}{|k|}\frac{(1-\mathbf{s}_{u-k/2}\mathbf{s}_{u+k/2})}{|k|}$$

defines a smooth function by Taylor's formula (for $|k|$ or for k in $\mathbb{R}^3\backslash\{0\}$). Moreover from (4.98), we get the estimates :

$$\begin{aligned}\left|\frac{\mathbf{s}_{u-L_J+k/2}\mathbf{s}_{u-L_J-k/2}-1}{|k|}\frac{1-\mathbf{s}_{u-k/2}\mathbf{s}_{u+k/2}}{|k|}\right| &\le \frac{4C_s^2}{E(u-L_J,k/2)}\\ &\le \tfrac{4C_s^2}{|u-L_J|E(u,k/2)}.\end{aligned}$$

For any U, we have :

$$\begin{aligned}\int_\ell \frac{d\ell}{|\ell|^2}\frac{1}{|U-\ell|\widetilde{E}\,(U-\ell,k/2)} &\le \int_\ell \frac{d\ell}{|\ell|^2}\frac{1}{|U-\ell|^2},\\ &\le \tfrac{1}{|U|}\int\frac{d\ell}{|\ell|^2|\mathbf{e}-\ell|^2}.\end{aligned}$$

Integrating over the ℓ_{j+1}'s one after the other from from $\ell=J-1$ down to $j=1$ as above with $U=U_j=u-L_j$, there remains but the integral over u :

$$\begin{aligned}\int\limits_{u\in\widetilde{B}_0(k)}\frac{2C_s^2du}{\widetilde{E}\,(u,k/2)}\tfrac{1}{|u|\widetilde{E}(u,k/2)} &\times\left\{2\int\frac{d\ell}{|\ell|^2|\mathbf{e}-\ell|^2}\right\}^J\\ &\le\left\{2\int\frac{d\ell}{|\ell|^2|\mathbf{e}-\ell|^2}\right\}^J\int\limits_{u\in\widetilde{B}_0(r)}\frac{2C_s^2du}{|u|^2\widetilde{E}\,(u,k/2)}\\ &=(K\log(\Lambda))\times\left(C'_{1,0}\right)^J.\end{aligned}$$

At last we have :

$$\begin{aligned}\alpha|\widehat{\rho}(F_{1,0}^{\circ J}(Q_{0,1}(\rho));k)| &\le \tfrac{\alpha^{J+1}}{(2\pi)^{3/2}(4\pi^2)^J}2^{J+1}C_s^2\left\{\int\frac{d\ell}{|\ell|^2|\mathbf{e}-\ell|^2}\right\}^J\int\limits_{u\in\widetilde{B}_0(r)}\tfrac{du}{|u|^2\widetilde{E}(u)}|\widehat{\rho}(k)|\\ &\lesssim C_{1,0}\left(\alpha C'_{1,0}\right)^J\alpha\log(\Lambda)|\widehat{\rho}(k)|.\end{aligned}\tag{4.105}$$

As a consequence there holds $\alpha\widehat{\rho}(F_{1,0}^{\circ J}(Q_{0,1}(\rho));k)=-g_{\Lambda;J}(k)\widehat{\rho}(k)$, and $\sum_{J=0}^\infty f_{\Lambda,J}$ is well defined (at least in $L^\infty\cap L^2$) as soon as α is sufficiently small. We have

$$\alpha\widehat{\tau_{0,1}}(\rho,k)=-\left(\alpha B_\Lambda(k)+\sum_{J=1}^{+\infty}g_{\Lambda;J}(k)\right)\widehat{\rho}(k)=:-f_\Lambda(k)\widehat{\rho}(k),\tag{4.106}$$

with

$$|f_\Lambda(k)|\le\alpha B_\Lambda(k)+\alpha^2\log(\Lambda)K=\mathcal{O}(\alpha\log(\Lambda)).\tag{4.107}$$

2. Let us prove this function is radial. Let $\mathbf{e}_1$ and $\mathbf{e}_2$ in $\mathbb{S}^2$ and $r>0$. We must show that $f_\Lambda(r\mathbf{e}_1)=f_\Lambda(r\mathbf{e}_2)$. There exists $\mathcal{R}\in\mathrm{SO}_3(\mathbb{R})$ such that $\mathbf{e}_2=\mathcal{R}\mathbf{e}_1$. In (4.104) for $k=r\mathbf{e}_2$, we change variables in the integrals : $v=\mathcal{R}^{-1}u$ and $m_j=\mathcal{R}^{-1}\ell_j$. Writing $M_j=m_1+\cdots+m_j$, we get : $S_J(\mathcal{R}(v-M_J\pm\frac{r}{2}\mathbf{e}_1))=S_J(v-M_J\pm\frac{r}{2}\mathbf{e}_1)$. We must show the same holds for T_J. Let $\mathbf{b}=(b_1,b_2,b_3)$ be the canonical base of $\mathbb{R}^3$. We define

$$\alpha'_j:=\boldsymbol{\alpha}\cdot\mathcal{R}b_j.$$

These new matrices satisfy the same relation as the α's :

$$\{\alpha'_j,\alpha'_k\}=2\delta_{jk}\text{ and }\{\alpha'_j,\beta\}=0.$$

Thus we have $T_J(\mathcal{R}(v-M_J\pm\frac{r}{2}\mathbf{e}_1))=T_J(v-M_J\pm\frac{r}{2}\mathbf{e}_1)$ and f_Λ is radial.

From now on we change variables :

$$\begin{cases}u_0:=u\text{ and for }1\le j\le J,\ u_j:=u-L_j,\ l_j=u_j-u_{j-1},\\ u_j\in B(|k|):=\left\{v\in B(0,\Lambda),\ \left|v\pm\frac{|k|}{2}\mathbf{e}\right|<\Lambda\right\}.\end{cases}\tag{4.108}$$

3. Our purpose is to show that f_Λ is in $\mathscr{F}(L^1)$ with a (rather) precise bound on $\|\check{f}_\Lambda\|_{L^1}$. We already know : $f_\Lambda(k) = \alpha B_\Lambda(k) + \mathcal{O}_{L^\infty}(\alpha^2 \log(\Lambda)) = \mathcal{O}(\alpha \log(\Lambda))$.

As f_Λ is radial we take a fixed vector $\mathbf{e} \in \mathbb{S}^2$ and study $f_\Lambda(k) = f_\Lambda(|k|)$ with the help of the integral formulae where k is replaced by $|k|\mathbf{e}$.

The strategy is to differentiate f_Λ and prove that its Sobolev norms $\|-\Delta f_\Lambda\|_{L^2}$ and $\|-\Delta f_\Lambda\|_{L^p}$ are "small" where $p < 2$ is some constant to be chosen later. By Cauchy-Schwartz inequality in Direct space, we obtain an upper bound of $\|\check{f}_\Lambda\|_{L^1}$. We will use the *co-area formula* [EG92].

We show that $\check{f}_\Lambda \in L^1$ with L^1-norm lesser than 1 in order to give a meaning to $\sum_{\ell=1}^{\infty}(-1)^\ell\{\check{f}_\Lambda\}^{*\ell}$.

Remark 4.16. 1. As f_Λ is radial we have :

$$(-\Delta) f_\Lambda \quad = (-\Delta_r) f_\Lambda \quad = -\big(\partial_r^2 + \tfrac{2}{r}\partial_r\big) f_\Lambda. \tag{4.109}$$

2. For any $u \in \mathbb{R}^3$ and $r \geq 0$ Taylor's formula gives :

$$\begin{cases} (1 - \mathbf{s}_{u+2^{-1}r\mathbf{e}}\mathbf{s}_{u-2^{-1}r\mathbf{e}}) & = r\{\mathbf{s}_u m_1(-\frac{r}{2}) - m_1(\frac{r}{2})\mathbf{s}_u\} \\ \text{with } m_1(\frac{x}{2}) & := \displaystyle\int_{t=0}^{1} d\mathbf{s}_{u+tx\mathbf{e}/2} \cdot \big(\frac{\mathbf{e}}{2}\big) dt. \end{cases} \tag{4.110}$$

We write $\mathbf{g}(p) := \begin{pmatrix} g_0(p) \\ \mathbf{g}_1(p) \end{pmatrix} \in \mathbb{R}^4$ and $\sigma(p) := \frac{\mathbf{g}(p)}{\widetilde{E}(p)}$.

As we have $\langle \sigma(u)\,,\, \mathrm{d}\sigma(u)\rangle = 0$, Taylor's Formula at order 2 gives

$$\begin{cases} \dfrac{1 - \langle \sigma(u + r\frac{\mathbf{e}}{2})\,,\, \sigma(u - r\frac{\mathbf{e}}{2}\rangle)}{r^2} := \langle a(u)\,,\, a(u)\rangle + \langle \sigma(u)\,,\, m_2(r) + m_2(-r)\rangle \\ \qquad +r\langle a(u)\,,\, m_2(r) - m_2(-r)\rangle + r^2\langle m_2(r)\,,\, m_2(-r)\rangle, \\ a(u) := \mathrm{d}\sigma(u)\cdot\frac{\mathbf{e}}{2} \text{ and } m_2(\frac{x}{2}) := \displaystyle\iint_{[0,1]^2} \mathrm{d}^2\sigma u + stx\mathbf{e}/2 \cdot \big(\tfrac{\mathbf{e}}{2}, \tfrac{\mathbf{e}}{2}\big) t ds dt. \end{cases} \tag{4.111}$$

3. For any $-\frac{1}{2} \leq x \leq \frac{1}{2}$:

$$\widetilde{E}\,(u + x\mathbf{e}) \geq E(u + x\mathbf{e}) \geq \frac{E(u)}{2}. \tag{4.112}$$

In particular if one takes the modulus of the derivative over r in (4.110) or (4.111) for $0 \leq r \leq 1$, we get the following upper bounds :

(a) $K/\widetilde{E}\,(u)$ for the first derivative,

(b) $K/\widetilde{E}\,(u)^2$ for the second.

Lemma 4.13. *The functions $\partial_r f_\Lambda$ and $\partial_r^2 f_\Lambda$ are well defined in $\mathbb{R}^3$ with support in $\overline{B}(0, 2\Lambda)$. Furthermore for $J \in \mathbb{N}$ we have :*

$$\left\{ \begin{array}{ll|ll} |\partial_r f_{\Lambda,J}(p)| & \lesssim J\frac{\alpha^{J+1}\log(\Lambda)K^{J+1}}{E(p)}\chi_{|p|<2\Lambda} & |\partial_r f_\Lambda(p)| & \lesssim \frac{L}{E(p)}\chi_{|p|<2\Lambda}, \\ |\partial_r^2 f_{\Lambda,J}(p)| & \lesssim J\frac{\alpha^{J+1}\log(\Lambda)K^{J+1}}{E(p)^2}\chi_{|p|<2\Lambda} & |\partial_r^2 g_\Lambda| & \lesssim \frac{\alpha^2\log(\Lambda)}{E(r)^2}\chi_{r<2\Lambda}. \end{array} \right. \tag{4.113}$$

As a consequence :

Lemma 4.14. *For α sufficiently small, $\check{g}_\Lambda \in L^1$ and*

$$\|\check{g}_\Lambda\|_{L^1} \lesssim (\alpha\log(\Lambda))^2. \tag{4.114}$$

Remark 4.17. At the very end of the proof of Lemma 4.13, we refer the reader to the thesis of the author for a (last) technical assumption : proving that $\lim\limits_{|x|\to 2\Lambda^-} \partial_r^2 f_\Lambda(x) = 0$.

Proof of Lemma 4.14

We assume Lemma 4.13. As $(-\Delta_r) = -(\partial_r^2 + \frac{2}{r}\partial_r)$ we have $f_\Lambda \in H^2(\mathbb{R}^3)$ with :

$$|\Delta f_\Lambda(p)| \lesssim \tfrac{L}{|p|E(p)}. \tag{4.115}$$

Proof of $\int_{B(0,1)} |\check{f}_\Lambda(x)|dx \lesssim L$: The function $-\Delta f_\Lambda$ has a singularity at $r=0$ due to the term $\frac{2\partial f_\Lambda(r)}{r}$. We split $-\Delta f_\Lambda$ w.r.t. $\chi_{|x|\le 1} + \chi_{|x|>1}$. We have

$$I_\Lambda^{(2)} := -\Delta f_\Lambda \chi_{|x|\le 1} \in L^{p_1} \cap L^3_w, \text{ and } E_\Lambda^{(2)} := -\Delta f_\Lambda \chi_{|x|>1} \in L^{3/2}_w \cap L^{p_2},\ |p_2| > \frac{3}{2}, 1 \le p_1 < 3. \tag{4.116}$$

The corresponding norms are respectively $\mathcal{O}(LK(p_1))$ and $\mathcal{O}(LK(p_2))$. We use the Hausdorff-Young inequality and the generalized Young inequality [RS75, Vol. II]. The decomposition (4.116) implies the decomposition $f_\Lambda = I_\Lambda^{(0)} + E_\Lambda^{(0)}$ by multiplication by $\frac{1}{-\Delta}$.

For $p=1, a=\frac{1}{2}, q=2$ and $q'=\frac{q}{q-1}$ we have

$$\begin{aligned}\int_{|x|\le 1} \big|\check{I}_\Lambda^{(0)}(x)\big|dx &\le \Big(\int |x|^{aq'}\big|\check{I}_\Lambda^{(0)}(x)\big|^{q'}dx\Big)^{1-1/q}\Big(\int_{|x|\le 1}\frac{dx}{|x|^{aq}}\Big)^{1/q},\\ &\lesssim \| \, |\nabla|^a I_\Lambda^{(0)}\|_{L^q} \lesssim \|\tfrac{1}{|\cdot|^{1+a}} * I_\Lambda^{(2)}\|_{L^q},\\ &\lesssim \|I_\Lambda^{(0)}\|_{L^p}\|\frac{1}{|\cdot|^{1+a}}\|_{L_w^{\frac{3}{1+a}}} \lesssim L.\end{aligned}$$

Similarly let $0<\varepsilon<1$ to be chosen : we have $|\nabla|^{2-\varepsilon}E_\Lambda^{(0)} = \frac{K(\varepsilon)}{|\cdot|^{3-\varepsilon}} * E_\Lambda^{(2)}$. This last function is in L^2 provided that $E_\Lambda^{(2)} \in L^{\frac{6}{3-2\varepsilon}}$. We choose $\varepsilon = 3/4$ for instance : this gives

$$\int_{B(0,1)} |E_\Lambda^{(0)}(x)|dx \le \sqrt{\int |x|^{5/2}|E_\Lambda^{(0)}(x)|^2dx \int_{B(0,1)}\frac{dx}{|x|^{5/2}}} \lesssim \|E_\Lambda^{(2)}\|_{L^4}\Big|\Big|\frac{1}{|\cdot|^{9/4}}\Big|\Big|_{L_w^{4/3}} \lesssim L.$$

Proof of $\int_{|x|\ge 1} |\check{f}_\Lambda(x)|dx \lesssim L$: Then it is clear that

$$\int_{|x|\ge 1} |\check{f}_\Lambda(x)| \le \|-\Delta f_\Lambda\|_{L^2}\sqrt{\int_{|x|\ge 1}\frac{dx}{|x|^4}} \lesssim L.$$

□

Proof of Lemma 4.13 The idea of the proof is that each time we differentiate with respect with the radius $r>0$, it leads to an additional term $\frac{1}{E(U)}$ in the integrand or a change of the domains and so a better upper bound of the integral.

We will often use the following inequality :

$$\int_{B(0,\Lambda)} \frac{dv}{|u-v|^2(\widetilde{E}\left(v+\frac{k}{2}\right)+\widetilde{E}\left(v-\frac{k}{2}\right))|u+\varepsilon\frac{k}{2}|} \le \frac{1}{|u+\varepsilon\frac{k}{2}|}\int\frac{dv}{|v|^2|v-\mathbf{e}|^2}, \tag{4.117}$$

and for convenience we write :

$$u^\varepsilon := u + \varepsilon\frac{k}{2},\ \varepsilon \in \{1,-1\}. \tag{4.118}$$

That the function (and its derivatives) has an extension in 0 is clear from (4.110) and (4.112) : differentiating under the integral sign of the Taylor's formula, we get :

$$\Big|d^{J+1}\mathbf{s}_{u+tr\mathbf{e}/2}\cdot\big((t\mathbf{e}/2)^J,\frac{\mathbf{e}}{2}\big)\Big| \le K^J\frac{1}{E(u)^{J+1}},\ 0<r,t<1, \tag{4.119}$$

thus the problem of singularity at $r=0$ drops thanks to (4.112).

More generally the variable r appears

1. either in the domains $B(r)^{J+1}$,

2. or in a function of $v_j \pm r\frac{e}{2}$.

One may write :

$$\begin{aligned} f_{\Lambda,J}(r) &=: \int_{B(r)^{J+1}} G_J(u_0 \pm r\tfrac{\mathbf{e}}{2}, \cdots, u_J \pm r\tfrac{\mathbf{e}}{2}) d\mathbf{u}, \\ G_J &=: G_J^0(u_0 \pm r\tfrac{\mathbf{e}}{2}, \cdots, u_J \pm r\tfrac{\mathbf{e}}{2}) \prod_{1\le j\le J} \frac{1}{|u_j - u_{j-1}|^2}. \end{aligned} \tag{4.120}$$

It is easy to see that $G_J^0 : (\mathbb{R}^3)^{2J+2} \to \mathbb{R}$ is a differentiable function and that each time we take $\partial_{u_j + r\frac{\mathbf{e}}{2}} - \partial_{u_j - r\frac{\mathbf{e}}{2}}$ we get a term $K(r^{-1} + \widetilde{E}\left(u \pm \frac{k}{2}\right)^{-1})$ for $r > 1$ or $K\widetilde{E}\left(u\right)^{-1}$ for $r \le 1$ (see Remark 4.16). This enables us to get upper bounds of the terms of $\partial_r^j f_{\Lambda,J}$ corresponding to derivatives of G_J^0. Indeed for the first derivative : for $\varepsilon, \varepsilon' \in \{+,-\}$ one has for $1 < |k| < 2\Lambda$:

$$\begin{cases} \displaystyle\int \frac{du_j}{|u_j - u_{j-1}|^2 \widetilde{E}\left(u_j + \varepsilon k/2\right)^2} \le \frac{1}{|u_{j-1} + \varepsilon k/2|} \int_{\mathbb{R}^3} \frac{du_j}{|u_j|^2 |u_j - \mathbf{e}|^2}, \\ \displaystyle\int \frac{du_i}{|u_i - u_{i-1}|^2 |u_i + \varepsilon k/2| \widetilde{E}\left(u_i, k/2\right) \widetilde{E}\left(u_i + \varepsilon' k/2\right)} \lesssim \frac{1}{|k|}\Big(\frac{1}{|u_{i-1} + k/2|} + \frac{1}{|u_i - k/2|}\Big) \\ \qquad\qquad \times \displaystyle\int_{(\mathbb{R})^3} \frac{du_i}{|u_i - \mathbf{e}|^2 |u_i|^2}. \end{cases} \tag{4.121}$$

For the term $(\partial_{u_0 + k/2} - \partial_{u_0 - k/2}) G_0$ we have :

$$\int_{B(r)} \frac{du_0}{|u_0 - \varepsilon k/2| \widetilde{E}\left(u + \varepsilon k/2\right)} \Big(\frac{1}{\widetilde{E}\left(u + \varepsilon k/2\right)^2} + \frac{1}{\widetilde{E}\left(u - \varepsilon k/2\right)^2}\Big) \lesssim \frac{2}{|k|} \int_{B(0,2\Lambda)} \frac{du_0}{\widetilde{E}\left(u_0\right)^2 |u_0|} \lesssim \frac{\log(\Lambda)}{|k|}. \tag{4.122}$$

If $r \le 1$, Remark 4.16 enables us to say that

$$\int_{B(r)^{J+1}} \frac{|\partial_r G_J^0(u_j \pm r\mathbf{e}/2)|}{\prod_{1\le j\le J} |u_j - u_{j-1}|^2} \lesssim \alpha^{J+1} J \Big(K \int \frac{du}{|u|^2 |u - \mathbf{e}|^2}\Big)^J \log(\Lambda).$$

– In the case of the terms corresponding to $\partial_{v_1}\partial_{v_2} G_J^0$ with $v_a = u_{i(a)} + \varepsilon(a)\frac{k}{2}$, the above upper bounds enable us to say that if $i(1) \ne i(2)$ then it suffices to apply twice (4.121),(4.122) and we get an upper bound of the form :

$$K J^2 \big(\chi_{|k|\le 1} + \frac{\chi_{1<|k|<2\Lambda}}{|k|^2}\big) \alpha^{J+1} \Big(K \int \frac{du}{|u|^2 |u - \mathbf{e}|^2}\Big)^J \log(\Lambda),$$

If $i(1) = i(2)$, then as :

$$\int \frac{du}{|u - v|^2 |u| \widetilde{E}\left(u, \frac{k}{2}\right)} \Big(\frac{1}{\widetilde{E}\left(u + k/2\right)^2} + \frac{1}{\widetilde{E}\left(u - k/2\right)^2}\Big) \lesssim \frac{1}{|k|^2 |u|}, \tag{4.123}$$

we obtain an upper bound of the form

$$K J (\chi_{|k|\le 1} + \frac{\chi_{1<|k|<2\Lambda}}{|k|^2}) \alpha^{J+1} \Big(K \int \frac{du}{|u|^2 |u - \mathbf{e}|^2}\Big)^J \log(\Lambda).$$

If $i(1) = i(2) = 0$, we integrate first over u_0, then over $u_1, u_2, \cdots, u_J$ and use (4.123) with $u = u_0$, $v = u_1$: this gives

$$\text{for } 1 < r < 2\Lambda,\ \Big|\partial_r^2 \frac{1 - \mathbf{s}_{u_0 + \frac{k}{2}} \mathbf{s}_{u_0 - \frac{k}{2}}}{r(\widetilde{E}\left(u_0 + \frac{k}{2}\right) + \widetilde{E}\left(u_0 - \frac{k}{2}\right))}\Big| \lesssim \frac{r^{-2} + \widetilde{E}\left(u_0 + \frac{k}{2}\right)^{-2} + \widetilde{E}\left(u_0 - \frac{k}{2}\right)^{-2}}{|u| \widetilde{E}\left(u, \frac{k}{2}\right)}.$$

If $r \le 1$ we use Remark 4.16 as before.

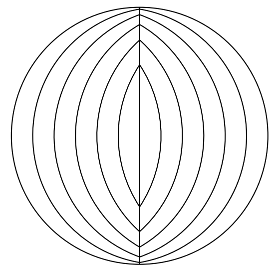

FIGURE 4.2 – Level sets of the z function

– There remains to deal with the terms corresponding to differentiation over r in the domain $B(r)^{J+1}$. We rewrite (4.120) using the *co-area formula*. Indeed, let us write for $\varepsilon \in \{1,-1\}$ and $r \in [0,2\Lambda]$:

$$B_\varepsilon(r) := \{p,\ |p + \tfrac{\varepsilon r}{2}\mathbf{e}| < \Lambda,\ \langle p\,,\, \varepsilon\mathbf{e}\rangle > 0\} \text{ and } B(r) := B_1(r) \cup B_{-1}(r) \subset B(0,\Lambda).$$

In particular $B(\Lambda) = \{p \in B(0,\Lambda),\ \langle p\,,\,\mathbf{e}\rangle \neq 0\}$. We define the level function :

$$z : \begin{array}{rcl} B(\Lambda) & \to & [0,2\Lambda] \\ p \in B_\varepsilon(\Lambda) & \mapsto & r \text{ such that } \left|u + \dfrac{r\varepsilon\mathbf{e}}{2}\right| = \Lambda. \end{array}$$

We apply the co-area formula with respect to z. If $p \in B_{\varepsilon_0}$, we write $\varepsilon(p) := \varepsilon_0$ and

$$n(p) := \frac{p + \varepsilon(p)z(p)\frac{\mathbf{e}}{2}}{\left|p + \varepsilon(p)z(p)\frac{\mathbf{e}}{2}\right|} = \Lambda^{-1}(p + \varepsilon(p)z(p)\tfrac{\mathbf{e}}{2}).$$

For $0 \le r < 2\Lambda$ we write $S(r) := \{p \in B,\ z(p) = r\}$ and $S_\varepsilon(r) := S \cap B_\varepsilon$; each $S_\varepsilon(r)$ is a spherical cap of $S(-\frac{r\varepsilon\mathbf{e}}{2},\Lambda)$. The measure of $B(0,\Lambda)\backslash B(\Lambda)$ is zero and the function z is differentiable with

$$\nabla z(p) = \frac{-2\varepsilon(p)}{\langle n(p)\,,\,\mathbf{e}\rangle} n(p).$$

Thus for any integrable function $F : B(0,\Lambda) \to \mathbb{R}$ and $0 \le r < 2\Lambda$ we have :

$$\int\limits_{B(r)} F(p)\big|\nabla z(p)\big| dp = \int_{t=r}^{2\Lambda} dt \int\limits_{S(t)} F(p) d\mathcal{H}_2(p), \tag{4.124}$$

where $d\mathcal{H}_2(p)$ is the Hausdorff measure on $S(r)$. If we take spherical coordinates with axis $\mathbb{R}\mathbf{e}$ in $S_\varepsilon(r)$ there holds $d\mathcal{H}_2(p) = \Lambda^2 \sin(\theta) d\theta d\phi$ in the domain :

$$M_\pm(r) = \{(\theta,\phi) \in (\tfrac{\pi}{2}, \tfrac{\pi}{2} \mp \tfrac{\pi}{2}) \times (-\pi,\pi),\ \cos(\theta) \ge \frac{r}{2\Lambda}\}.$$

Notation 4.10. For convenience we write du for both $d\mathcal{H}_2(u)$ (integration over a spherical cap) or $d\mathcal{H}_1(u)$ (integration over a curve).

– For each u_j we rewrite the integration over $u_i \in B(r)$. For each $0 \le j \le J$ we need to estimate

$$\int\limits_{B(r)^{j-1}\times S(r) \times B(r)^{J-j}} \frac{du_0 \cdots \widehat{du_j} \cdots du_J d\mathcal{H}_2(u_j)}{\prod\limits_{1\le j\le J} |u_j - u_{j-1}|^2} |G_J^0(u_i \pm \tfrac{k}{2})|.$$

In $S_\varepsilon(r)$ we take spherical coordinates and write $v = u_{j-1} + \frac{\varepsilon r}{2}\mathbf{e}$, if $j = 0$ we replace u_{j-1} by u_2 and integrate over $u_1, u_2, \cdots u_J$. Using (4.121) we have :

$$\begin{aligned} \int\limits_{M_\varepsilon(r)} \frac{\Lambda^2 \sin(\theta) d\theta d\phi}{|v - \Lambda n|^2} \frac{1}{|\Lambda n|(\widetilde{E}\,(\Lambda n) + \widetilde{E}\,(\Lambda n - k))} &\le \int\limits_{\mathbb{S}^2} \frac{\sin(\theta) d\theta d\phi}{|v - \Lambda n|^2} \\ &\le \tfrac{2\pi}{\Lambda|v|} \log\left(\tfrac{\Lambda + |v|}{\Lambda - |v|}\right). \end{aligned}$$

Then writing $v := u_{i-1} + \varepsilon\frac{k}{2}$ we have :

$$\begin{aligned}
&\int\limits_{B(r)} \frac{du_i}{|u_i-u_{i-1}|^2|u_i+\varepsilon\frac{k}{2}|}\log\Big(\tfrac{\Lambda+|u_i+\varepsilon\frac{k}{2}|}{\Lambda-|u_i+\varepsilon\frac{k}{2}|}\Big)\frac{1}{\widetilde{E}\,(u_i,k/2)} = \int\limits_{B(r)+\frac{\varepsilon k}{2}} \frac{du_i}{|u_i-v|^2|u_i|\widetilde{E}\,(u_i)}\log\Big(\tfrac{\Lambda+|u_i|}{\Lambda-|u_i|}\Big)\\
&\le \int\limits_{B(0,1)} \frac{du}{|u-v\Lambda^{-1}|^2|u|\widetilde{E}\,(\Lambda u)}\log\Big(\frac{1+|u|}{1-|u|}\Big) \le 2\pi\int_{r=0}^1 \frac{\Lambda dr}{|v|\widetilde{E}\,(\Lambda r)}\log\Big(\frac{1+r}{1-r}\Big)\log\Big|\frac{\Lambda^{-1}|v|+r}{\Lambda^{-1}|v|-r}\Big|\\
&\le 2\pi\int_0^1 \frac{\Lambda dr}{|v|\widetilde{E}\,(\Lambda r)}\Big(\log^2\Big(\frac{1+r}{1-r}\Big)+\log^2\Big|\frac{\Lambda^{-1}|v|+r}{\Lambda^{-1}|v|-r}\Big|\Big) \lesssim |v|^{-1}.
\end{aligned}$$

Finally for sufficiently small α, we have

$$|\partial_r f_{\Lambda,J}(r)| \le KL(\alpha K)^J\big(\chi_{r\le 1} + \tfrac{\chi_{1<r<2\Lambda}}{r}\big).$$

So by dominated convergence, as r tends to $(2\Lambda)^-$, $\partial_r f_{\Lambda,J}$ tends to 0 and $g_\Lambda \in H^1(\mathbb{R}^3)$.

– Let us deal with the second derivative. There remains the three cases :

1. One derivative in $B(r)$ and one derivative in the integrand.
2. Two derivatives in two different $B(r)$.
3. Two derivatives in the same $B(r)$.

In fact, we have to deal with the last two cases together because each term alone is not well defined but the sum gives a finite term. Seeing the second derivative as the coefficient of the second term in the Taylor series of $g_{\Lambda,J}(r+\delta r)$, each term is $\underset{\delta r\to 0}{\mathcal{O}}(-\delta r\log(\delta r))$ but the sum is $\mathcal{O}(\delta r)$ due to some cancellation.

1.

1.1. One derivative in $u_{i_1} \pm \frac{r}{2}\mathbf{e}$ and one in the domain of u_{i_2} with $i_1 \neq i_2$. Up to integrating over u_j from $j=0$ to $j=J$, we can suppose that $i_1 < i_2$. We split $S(r)$ between $S_+(r)$ and $S_-(r)$. In $S_\varepsilon(r)$, we use (4.117) (and (4.98) at the beginning), this gives :

$$\begin{aligned}
&\int\limits_{S_\varepsilon(r)} \frac{du_{i_2}}{|u_{i_2-1}-u_{i_2}|^2\widetilde{E}\,\big(u_{i_2}+\varepsilon\frac{k}{2}\big)\,|u_{i_2}+\varepsilon\frac{k}{2}|} \le \int\limits_{\mathbb{S}^2}\frac{du_{i_2}}{\Lambda^2|\frac{|u^\varepsilon_{i_2-1}|}{\Lambda}-u_{i_2}|^2}\\
&\lesssim \frac{1}{\Lambda|u^\varepsilon_{i_2-1}|}\log\Big(\frac{1+\frac{|u^\varepsilon_{i_2-1}|}{\Lambda}}{\Lambda-|u^\varepsilon_{i_2-1}|}\Big).
\end{aligned}$$

We take spherical coordinates with respect to $-\varepsilon\frac{k}{2}$: for any $v \in B = B_+\cup B_-$ we have

$$\begin{aligned}
\int\limits_{B(0,\Lambda)} \frac{du}{|u_{i_2-1}-v^\varepsilon|^2|u_{i_2-1}|\widetilde{E}\,(u_{i_2-1})}\log\Big(\frac{1+\frac{|u_{i_2-1}|}{\Lambda}}{1-\frac{|u_{i_2-1}|}{\Lambda}}\Big) &\lesssim \frac{1}{|v|}\int_0^1 dz\log\Big(\frac{1+z}{1-z}\Big)\log\Big(\frac{\frac{|v^\varepsilon|}{\Lambda}+z}{\frac{|v^\varepsilon|}{\Lambda}-z}\Big)\\
&\lesssim \frac{1}{|v^\varepsilon|}\int_0^2\log\Big(\frac{1+z}{1-z}\Big)^2,\\
\int\limits_{B(0,\Lambda)} \frac{du}{|u_{i_2-1}|\widetilde{E}\,\big(u^2_{i_2-1}\big)}\log\Big(\frac{1+\frac{|u_{i_2-1}|}{\Lambda}}{1-\frac{|u_{i_2-1}|}{\Lambda}}\Big) &\lesssim \int_0^\Lambda\frac{dz}{E(z)}\log\Big(\frac{1+\frac{z}{\Lambda}}{1-\frac{z}{\Lambda}}\Big)\\
&\lesssim 1+\Lambda^{-1}.
\end{aligned}$$

Then we use the same method as for the first derivative : when integrating over u_{i_1}, we use $(\widetilde{E}\,\big(u_{i_1}+\frac{k}{2}\big)+\widetilde{E}\,\big(u_{i_1}-\frac{k}{2}\big))^{-1} \le \widetilde{E}\,\big(\frac{k}{2}\big)^{-1}$. In this first subcase, we get an upper bound of the form :

$$\frac{J^2(K\alpha)^{J+1}\log(\Lambda)}{\Lambda E(k)}.$$

1.2. One derivative in $u_i \pm \frac{r}{2}\mathbf{e}$ and one in the domain of u_i. Splitting the integration over $S_+(r)$ and $S_-(r)$, and using (4.117), we have to estimate

$$\int\limits_{S_\varepsilon(r)} \frac{du_i}{|u_i - v|^2 |u_i + \varepsilon\frac{k}{2}| \widetilde{E}\left(u_i, k/2\right) \widetilde{E}\left(u_i + \varepsilon' \frac{k}{2}\right)} \leq \int\limits_{S_\varepsilon(r)} \frac{du_i}{|u_i - v|^2 |u_i + \varepsilon\frac{k}{2}| \widetilde{E}\left(u_i, k/2\right) \widetilde{E}\left(u_i - \varepsilon \frac{k}{2}\right)}. \tag{4.125}$$

Above v is either u_{i+1} or u_{i-1} depending on the order of integration (from u_J to u_0 or from u_0 to u_J if the derivatives act on $u_0 + \frac{k}{2}$). Moreover $\varepsilon, \varepsilon' \in \{1, -1\}$ and the term with ε' comes from the derivative in the integrand. By using (4.117) several times (starting with (4.98)) we get the term $|u_i + \varepsilon\frac{k}{2}| = |u_i^\varepsilon|$ in (4.125).

In (4.125), we use spherical coordinates to obtain the following upper bound :

$$\int\limits_{\mathbb{S}^2} \frac{\Lambda^2 du}{\Lambda^2} \frac{1}{|\Lambda u - v^\varepsilon|^2 \widetilde{E}\left(\Lambda u - r\mathbf{e}\right)} \leq 2 \int\limits_{\mathbb{S}^2} \frac{du}{\left|\Lambda u - |v^\varepsilon| \mathbf{e}\right|^2 E(u - r\mathbf{e})}. \tag{4.126}$$

Let us assume for the moment that this integral is lesser than :

$$\frac{K}{\Lambda^2 |v^\varepsilon|}\Big(1 - \chi_{|v^\varepsilon| > (2-\sqrt{3})\Lambda} \log\big(1 - \frac{|v^\varepsilon|}{\Lambda}\big)\Big). \tag{4.127}$$

In the process of integrating over the u_i's, we have to integrate over v with this upper bound. Taking spherical coordinates with respect to $-\frac{\varepsilon r}{2}\mathbf{e}$, we have :

$$\begin{cases} \displaystyle\int\limits_{B(0,\Lambda)} \frac{dv}{|v' - v|^2 \widetilde{E}(v) |v|} \lesssim \frac{1}{|v'|} \int \frac{dv}{|v|^2 |v - \mathbf{e}|^2} \\ \displaystyle\int\limits_{B(0,\Lambda)} \frac{dv}{|v| \widetilde{E}(v)^2} \lesssim \log(\Lambda). \end{cases}$$

Moreover, writing $A_\Lambda := A(0, (2 - \sqrt{3})\Lambda, \Lambda)$ the annulus, we have :

$$\begin{cases} \displaystyle\int\limits_{A_\Lambda} \frac{\log(1 - \frac{|v|}{\Lambda}) dv}{|v' - v|^2 |v| \widetilde{E}(v) (\Lambda^2 + |v|^2)} & \lesssim \displaystyle\frac{1}{\Lambda^2 |v'|} \int_{2-\sqrt{3}}^1 \frac{-\log(1 - z) dz}{z(1 + z^2)} \log\Big|\frac{\frac{|v'|}{\Lambda} + z}{\frac{|v'|}{\Lambda} - z}\Big| \\ & \lesssim \displaystyle\frac{1}{\Lambda^2 |v'|}, \\ \displaystyle\int\limits_{A_\Lambda} \frac{\log(1 - \frac{|v|}{\Lambda}) dv}{|v| \widetilde{E}(v)^2 (\Lambda^2 + |v|^2)} & \lesssim \displaystyle\frac{1}{\Lambda^2} \int_{2-\sqrt{3}}^1 \frac{-\log(1 - z) dz}{z^3}. \end{cases}$$

Proof of (4.126)≤(4.127) We write

$$x := |v^\varepsilon|,\ A := \Lambda^2 + x^2,\ B := \sqrt{1 + \Lambda^2 + r^2},\ a := \frac{2x\Lambda}{x^2 + \Lambda^2} \text{ and } b := \frac{2\Lambda r}{1 + \Lambda^2 + r^2}.$$

The upper bound (4.126) is equal to

$$\frac{4\pi}{AB} \int_{-1}^1 \frac{dy}{(1 - ay)\sqrt{1 - by}} = \frac{4\pi}{ABa} \int\limits_0^{\frac{2b}{\sqrt{1+b} + \sqrt{1-b}}} \frac{dz}{z^2 + 2z\sqrt{1 - b} + b(\frac{1}{a} - 1)}. \tag{4.128}$$

If $a \leq \frac{1}{2}$, then this integral is $\mathcal{O}\left(\frac{1}{AB} \int_{-1}^1 \frac{dy}{\sqrt{1 - by}}\right) = \mathcal{O}\left(\frac{1}{\Lambda^2 E(v^\varepsilon)}\right)$.

Similarly, if $b \leq \frac{1}{2}$, we get : $\mathcal{O}\left(\frac{1}{AB} \int_{-1}^1 \frac{dy}{1 - ay}\right) = \mathcal{O}\left(\frac{1}{\Lambda^2 E(v^\varepsilon)}\right)$.

If $\frac{1}{2} < a, b \leq 1$, we consider formula (4.128).
We have $z^2 \geq 2z\sqrt{1-b}$ for $z \geq 2\sqrt{1-b}$ and $2\sqrt{1-b} < \frac{2b}{\sqrt{1+b}+\sqrt{1-b}}$ *iff* $b > \frac{4}{5}$.

For $\frac{1}{2} < b \leq \frac{4}{5}, a > \frac{1}{2}$ we get the upper bound :

$$\frac{20\pi}{AB}\int_{-1}^{1}\frac{dy}{1-ay} \lesssim \frac{1}{\Lambda^2|v^\varepsilon|}.$$

For $b > \frac{4}{5}, a > \frac{1}{2}$, we have the upper bound

$$\frac{4\pi}{AaB}\left(\int_{0}^{2\sqrt{1-b}}\frac{dz}{2z\sqrt{1-b}+b(\frac{1}{a}-1)} + \int_{2\sqrt{1-b}}^{\frac{2b}{\sqrt{1+b}+\sqrt{1-b}}}\frac{dz}{z^2+b(\frac{1}{a}-1)}.\right) \tag{4.129}$$

The first integral of (4.129) gives (without $4\pi/(AB)$)

$$\frac{1}{2a\sqrt{1-b}}\log\left(1+\frac{4(1-b)}{b(\frac{1}{a}-1)}\right) \leq \frac{1}{\sqrt{1-b}}\log\left(1+5\frac{1-b}{1-a}\right).$$

If $1-b \leq 1-a$, then this gives $\mathcal{O}((1-b)^{-1/2})$, else this gives $\mathcal{O}(\frac{\log(1-a)}{\sqrt{1-b}})$.

The second integral of (4.129) gives (without $4\pi/(AaB)$ and writing $X := (a^{-1}-1)^{-1}$) :

$$\begin{aligned}\sqrt{\frac{X}{b}}\int_{2\sqrt{\frac{1-b}{b}}X}^{\frac{2\sqrt{bX}}{\sqrt{1-b}+\sqrt{1+b}}}\frac{dz}{z^2+1} &\lesssim \int_{2\sqrt{1-b}}^{2}\frac{Xz^2}{1+Xz^2}\frac{dz}{z^2}\\ &\lesssim \frac{1}{\sqrt{1-b}} = \frac{\sqrt{1+\Lambda^2+r^2}}{\sqrt{1+(\Lambda-r)^2}}.\end{aligned}$$

We have : $\dfrac{\log(1-a)}{AB\sqrt{1-b}} = 2\dfrac{\log\left|\frac{\sqrt{\Lambda^2+x^2}}{\Lambda-x}\right|}{(\Lambda^2+x^2)\sqrt{1+(\Lambda-x)^2}} \lesssim \dfrac{1+\log(1-\frac{|v^\varepsilon|}{\Lambda})}{(\Lambda^2+|v^\varepsilon|^2)\sqrt{1+(\Lambda-|v^\varepsilon|)^2}}.$

Let us emphasize that the condition $a > 2^{-1}$ is equivalent to $\frac{|v^\varepsilon|}{\Lambda} \geq 2-\sqrt{3}$.

Bringing all those estimates together ends the proof of (4.126)≤(4.127).

2.

2.1. One derivative in the domain of u_j and one in the domain of u_i with $i-j \geq 2$. We integrate over $u_{j'}$ from $j'=0$ to $j'=j$ and from $j'=J$ to $j'=i$ using the method for the first derivative. The integration over u with u either u_j or u_i (resp. with v either u_{j+1} or u_{i-1}) gives :

$$\begin{aligned}\sum_{\varepsilon\in\{1,-1\}}\int_{S_\varepsilon(r)}\frac{du}{|u-v|^2}\frac{1}{|u+\varepsilon\frac{k}{2}|\widetilde{E}\left(u+\varepsilon\frac{k}{2}\right)} &\lesssim \frac{1}{\Lambda^2}\sum_\varepsilon\int_{\frac{r}{2\Lambda}}^{1}\frac{dy}{\Lambda^2+|v^\varepsilon|^2-2\Lambda|v^\varepsilon|y}\\ &\lesssim \sum_\varepsilon\frac{1}{\Lambda|v^\varepsilon|}\log\left(\frac{\Lambda+|v^\varepsilon|}{\Lambda-|v^\varepsilon|}\right).\end{aligned} \tag{4.130}$$

If $j+2 \leq i$, then by integrating over u_{j+1} we have :

$$\begin{aligned}&\int_{B(r)}\frac{du_{j+1}}{|u_{j+1}-u_{j+2}|^2}\frac{1}{|u_{j+1}^\varepsilon|(\widetilde{E}\left(u_{j+1}^+\right)+\widetilde{E}\left(u_{j+1}^-\right))}\log\left(\frac{\Lambda+|u_{j+1}^\varepsilon|}{\Lambda-|u_{j+1}^\varepsilon|}\right)\\ &\quad\lesssim \frac{1}{\Lambda}\int_{B(0,1)}\frac{du}{|u|^2|u-\Lambda^{-1}u_{j+2}^\varepsilon|^2}\log\left(\frac{1+|u|}{1-|u|}\right)\\ &\quad\lesssim \int_0^1\frac{dr}{|u_{j+2}^\varepsilon|}\log\left(\frac{1+r}{1-r}\right)\log\left(\frac{r+\frac{|u_{j+2}^\varepsilon|}{\Lambda}}{r-\frac{|v^\varepsilon|}{\Lambda}}\right) \lesssim \frac{1}{|u_{j+2}^\varepsilon|},\end{aligned}$$

and we conclude as before. Else $j+1=i$ and we have :

$$\int\limits_{B(r)} \frac{du_{j+1}}{|u^\varepsilon_{j+1}|^2}\frac{1}{\widetilde{E}\left(u^+_{j+1}\right)+\widetilde{E}\left(u^-_{j+1}\right)}\log\left(\frac{\Lambda+|u^\varepsilon_{j+1}|}{\Lambda-|u^\varepsilon_{j+1}|}\right)^2 \lesssim \frac{1}{\Lambda}\int_{z=0}^{\Lambda}\frac{dz}{\widetilde{E}\left(z\right)}\log\left(\frac{1+\frac{z}{\Lambda}}{1-\frac{z}{\Lambda}}\right)^2(1-\tfrac{r}{2\Lambda})$$
$$\lesssim (1-\tfrac{r}{2\Lambda})(\log(\Lambda)+1).$$

2.2. One derivative in the domain of u_j and one in the domain of u_{j+1}. We only look at the corresponding coefficient in the Taylor series of $g_{\Lambda,J}(r+\delta r)$ with $r'=r+\delta r$. Indeed, let us treat for instance

$$\iint\limits_{(u_j,u_{j+1})\in B(r')\times S(r)} \tfrac{du_j du_{j+1}}{|u_j-u_{j+1}|^2}\frac{|\langle n(u_{j+1})\,,\,\mathbf{e}\rangle|}{2}\int\limits_{B(r)^{J-1}}\frac{G^0_J(u_\ell\pm\frac{k}{2})}{\prod_{a\neq j+1}|u_a-u_{a+1}|^2}$$
$$=:\iint\limits_{(u_j,u_{j+1})\in B(r')\times S(r)} \tfrac{du_j du_{j+1}}{|u_j-u_{j+1}|^2}\frac{|\langle n(u_{j+1})\,,\,\mathbf{e}\rangle|}{2}G_{J,j}(u_j,u_{j+1}).$$

We substract the integral of the same function but over $(u_j,u_{j+1},\mathbf{u'})$ in $B(r)\times S(r)\times B(r)^{J-1}$ where $\mathbf{u'}=(u_0,\cdots,\widehat{u}_j,\widehat{u}_{j+1},\cdots)$ and use the co-area formula. This gives

$$\int_{r+\delta r}^{r}dt\int\limits_{S(t)}\int\limits_{S(r)}\frac{du_j du_{j+1}}{|u_j-u_{j+1}|^2}\frac{|\langle n(u_j)\,,\,\mathbf{e}\rangle|}{2}\frac{|\langle n(u_{j+1})\,,\,\mathbf{e}\rangle|}{2}G_{J,j}(u_j,u_{j+1}). \tag{4.131}$$

We deal with $G_{J,j}(u_j,u_{j+1})$ as in the case 2.1. Let us say for instance $0<\delta r\ll 1$, then for any $(u_{j+1},t)\in S(r)\times(r,r')$ we have :

$$\mathrm{dist}(u_{j+1},S(t))\geq\Lambda\Big|\sqrt{1+\tfrac{\langle n_u\,,\,\mathbf{e}\rangle}{\Lambda}\delta r+(\tfrac{(t-r)}{2})^2}-1\Big|=\underset{\delta r\to 0}{\mathcal{O}}(\Lambda|(t-r)\langle n_u\,,\,\mathbf{e}\rangle|).$$

By the Theorem of projection onto a closed convex $\mathbb{R}^3$, we have

$$|u_{j+1}-u_j|^2\geq|u_{j+1}-\Pi_{S(t)}u_{j+1}|^2+|\Pi_{S(t)}u_{j+1}-u_j|^2.$$

If $r'<r$, then we consider instead the projection of $u_j\in S(r)$ onto $B(t)$. Anyway the quantity in (4.131) is

$$\underset{\delta r\to 0}{\mathcal{O}}\left(\frac{(\alpha K)^J}{\Lambda^2}\int_r^{r+\delta r}dt\int\limits_{\mathbb{S}^2}da|\langle a\,,\,\mathbf{e}\rangle|\log\left(1+\frac{1}{|t-r|^2|\langle a\,,\,\mathbf{e}\rangle|^2}\right)=\frac{(\alpha K)^J}{\Lambda^2}\delta r(1-\log(\delta r))\right).$$

The corresponding term is not Lipschitz because of the term $-\delta_r\log(\delta_r)$.

3. Let us write the expansion of

$$\int\limits_{B(r')}\frac{|\langle n_{u_j}\,,\,\mathbf{e}\rangle|du_j}{2}\int\limits_{B(r)^J}du_0\cdots\widehat{du_j}\cdots du_J G_J(u_\ell\pm\tfrac{k}{2})=:\int\limits_{B(r')}\widetilde{G}_{J,j}(u_j)du_j. \tag{4.132}$$

We substract $\int\limits_{B(r)}\widetilde{G}_{J,j}(u_j)du_j$ in (4.132) and get

$$\int_{r+\delta r}^{r}dt\int\limits_{S(t)}du_j\widetilde{G}_{J,j}(u_j). \tag{4.133}$$

We split (4.133) between integration over $S_+(t)$ and $S_-(t)$. For any $t\in(r,r']$, we write $s:=t-r$ and :

$$\Phi_t:\begin{array}{ccl} S(t) & \to & S(r)\\ u\in S_\varepsilon(t) & \mapsto & v(u):=u+z_t(u)n_u\in S_\varepsilon(r)\text{ where }|z(u)|=\underset{\delta r\to 0}{\mathcal{O}}(\delta r)\end{array}. \tag{4.134}$$

From now on we assume $v \in S(r)$ and $u \in S(t)$ and write $\overline{n}_u$ instead of n_u to emphasize this is a function of $u \in S(t)$ and not of $v \in S(r)$. The function $z_t : S(t) \to \mathbb{R}$ satisfies the equation

$$\Big| u + z_t(u)\overline{n}_u + \varepsilon\frac{r}{2}\mathbf{e}\Big|^2 = \Lambda^2 \text{ that is } z_t\big(1 + \frac{z_t}{2\Lambda} - \tfrac{\varepsilon s\langle \overline{n}_u\,,\,\mathbf{e}\rangle}{2\Lambda}\big) = \frac{\varepsilon s\langle \overline{n}_u\,,\,\mathbf{e}\rangle}{2} - \frac{s^2}{8\Lambda}. \tag{4.135}$$

Changing variables in the integration over $S(t)$ we have :

$$\int\limits_{S(t)} du_j \widetilde{G}_{J,j}(u_j) = \int\limits_{\Phi_t(S(t))} dv \widetilde{G}_{J,j}(\Phi_t^{-1}(v))\mathrm{J}(\Phi_t;\Phi_t^{-1}(v))^{-1}dv.$$

– We need to compute $\Phi_t^{-1}(v)$ and $\mathrm{J}(\Phi_t;\Phi_t^{-1}(v))$. First we have :

$$\overline{n}_u = \frac{v - z_t\overline{n}_u + \varepsilon\frac{r+s}{2}\mathbf{e}}{\Lambda} = n_v + \varepsilon\frac{s}{2\Lambda}\mathbf{e} - \frac{z_t}{\Lambda}\overline{n}_u,$$

thus

$$\overline{n}_u = \frac{1}{1 + \frac{z_t}{\Lambda}}(n_v + \varepsilon\tfrac{s}{2\Lambda}\mathbf{e}), \tag{4.136}$$

and

$$n_v = \big(1 + \frac{z_t}{\Lambda}\big)\overline{n}_u - \frac{\varepsilon s}{2\Lambda}\mathbf{e}. \tag{4.137}$$

Using the formula (4.136) in (4.135), we obtain the following equation satisfied by z_t :

$$z_t\Big(1 + \frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda(1+\frac{z_t}{\Lambda})}\big(\langle n_v\,,\,\mathbf{e}\rangle + \frac{\varepsilon s}{2\Lambda}\big)\Big) = \frac{\varepsilon s}{2(1+\frac{z}{\Lambda})}\Big(\langle n_v\,,\,\mathbf{e}\rangle + \frac{\varepsilon s}{2\Lambda}\Big) - \frac{s^2}{8\Lambda}. \tag{4.138}$$

In particular there holds :

$$z_t(u) = \frac{\varepsilon s}{2\Lambda}\langle n_v\,,\,\mathbf{e}\rangle + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2). \tag{4.139}$$

We differentiate z_t in (4.135) and get :

$$\mathrm{d}z_t(u) : \begin{array}{ccc} \mathrm{T}_u S_\varepsilon(t) & \to & \mathbb{R} \\ h & \mapsto & \dfrac{\varepsilon s}{2\Lambda}\dfrac{\langle h\,,\,\mathbf{e}\rangle\big(1+\frac{z_t}{\Lambda}\big)}{1+\frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda}\langle \overline{n}_u\,,\,\mathbf{e}\rangle}. \end{array} \tag{4.140}$$

Thus differentiating in (4.134) and using (4.136) in (4.140) give

$$\mathrm{d}\Phi_t(u) : \begin{array}{ccc} \mathrm{T}_u S_\varepsilon(t) & \to & \mathrm{T}_v S_\varepsilon(r) \\ h & \mapsto & \big(1+\frac{z_t}{\Lambda}\big)h + \dfrac{\varepsilon s}{2\Lambda}\dfrac{\langle h\,,\,\mathbf{e}\rangle\big(1+\frac{z_t}{\Lambda}\big)}{1+\frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda(1+\frac{z_t}{\Lambda})}\big(\langle n_v\,,\,\mathbf{e}\rangle + \frac{\varepsilon s}{2\Lambda}\big)}\dfrac{n_v + \frac{s}{2\Lambda}\mathbf{e}}{1+\frac{z}{\Lambda}} \end{array} \tag{4.141}$$

Let (a,b) be an orthonormal basis of $\mathrm{T}_u S_\varepsilon(t)$ with $b \times \overline{n}_u = a$, then we have :

$$\begin{aligned}
\mathrm{J}(\Phi_t;u) &= \langle \mathrm{d}\Phi_t(u)a \times \mathrm{d}\Phi_t(u)b\,,\,n_v\rangle \\
&= \langle \big(\big[1+\tfrac{z_t}{\Lambda}\big]a + \overline{n}_u\mathrm{d}z_t(u)a\big) \times \big(\big[1+\tfrac{z_t}{\Lambda}\big]b + \overline{n}_u\mathrm{d}z_t(u)b\big)\times\,,\,n_v\rangle \\
&= \big(1+\tfrac{z_t}{\Lambda}\big)^2\langle \overline{n}_u\,,\,n_v\rangle - \big(1+\tfrac{z_t}{\Lambda}\big)\big[\langle a\,,\,n_v\rangle\mathrm{d}z_t(u)a + \langle b\,,\,n_v\rangle\mathrm{d}z_t(u)b\big] \\
&= \big(1+\tfrac{z_t}{\Lambda}\big)(1+\tfrac{\varepsilon s}{2\Lambda}\langle n_v\,,\,\mathbf{e}\rangle) + \frac{\varepsilon s}{2\Lambda}\big(1+\tfrac{z_t}{\Lambda}\big)\big(\langle a\,,\,\mathbf{e}\rangle\mathrm{d}z_t(u)a + \langle b\,,\,\mathbf{e}\rangle\mathrm{d}z_t(u)b\big) \\
&= \big(1+\tfrac{z_t}{\Lambda}\big)(1+\tfrac{\varepsilon s}{2\Lambda}\langle n_v\,,\,\mathbf{e}\rangle) + \tfrac{\varepsilon s}{2\Lambda}\Big(1 - \frac{(\langle n_v\,,\,\mathbf{e}\rangle + \frac{\varepsilon s}{2\Lambda})^2}{(1+\frac{z_t}{\Lambda})^2}\Big)\times \\
&\qquad \frac{1+\frac{z_t}{\Lambda}}{1+\frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda(1+\frac{z_t}{\Lambda})}\big(\langle n_v\,,\,\mathbf{e}\rangle + \frac{\varepsilon s}{2\Lambda}\big)} \\
&= 1 + \frac{\varepsilon s}{2\Lambda}\Big[1 - \tfrac{(\langle n_v\,,\,\mathbf{e}\rangle + \frac{\varepsilon s}{2\Lambda})^2}{(1+\frac{z_t}{\Lambda})^2} + \langle n_v\,,\,\mathbf{e}\rangle\big(\tfrac{1}{\Lambda}+1\big)\Big] + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2).
\end{aligned}$$

– As $u = v - z_t\overline{n}_u = v + \frac{\varepsilon s}{2}\langle n_v\,,\,\mathbf{e}\rangle n_{v_j} + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2)$, we get :

$$\int\limits_{S_\varepsilon(t)} du_j \widetilde{G}_{J,j}(u_j) r \;=\; \int\limits_{\Phi_t(S_\varepsilon(t))} dv_j \widetilde{G}_{J,j}(v_j + \tfrac{\varepsilon s}{2}\langle n_{v_j}\,,\,\mathbf{e}\rangle n_{v_j} + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2))\times \Big(1 - \frac{\varepsilon s}{2\Lambda}\Big[1 - \frac{(\langle n_v\,,\,\mathbf{e}\rangle + \frac{\varepsilon s}{2\Lambda})^2}{(1+\frac{z_t}{\Lambda})^2} + \langle n_v\,,\,\mathbf{e}\rangle\big(\tfrac{1}{\Lambda}+1\big)\Big] + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2)\Big) dv. \tag{4.142}$$

We have $\Phi_t(S_\varepsilon(t)) \neq S(r)$. In spherical coordinates (r,θ,ϕ) with respect to $-\varepsilon\frac{r}{2}\mathbf{e}$ and positive vertical half-line $\mathbb{R}^3_+\varepsilon\mathbf{e}$ we have

$$\Phi_t(S_\varepsilon(t)) \simeq \Big\{(\Lambda,\theta,\phi),\ \frac{rs}{2\Lambda\sqrt{1-\frac{rs}{2\Lambda^2}+\frac{s^2}{4\Lambda^2}}} = \cos(\theta_t) \le \cos(\theta) \le 1\Big\}, \tag{4.143}$$

and $\cos(\theta_t) = \frac{r}{2\Lambda} - \frac{r^2}{8\Lambda^2}s + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2)$.

At this point, we need to differentiate $\widetilde{G}_{J,j}$: we have

$$\widetilde{G}_{J,j}(u_j) = \frac{|\langle n_{u_j}\,,\,\mathbf{e}\rangle|}{2}\int\limits_{B(r)^J} du_0\cdots\widehat{du_j}\cdots du_J \frac{G^0_J(u_\ell \pm \frac{k}{2})}{\prod\limits_{1\le i\le J}|u_i-u_{i-1}|^2}.$$

We change variables as follows : $v_i := u_i - u_j$, this enables us to remove u_j from the term $|u_j - u_{j\pm 1}|^{-2}$. Writing $B_\varepsilon(r,u_j) := \{v :\ |v + u_j + \varepsilon\frac{k}{2}| < \Lambda\}$, $B(r;u_j) = B_+(r;u_j)\cup B_-(r;u_j)$ and $S_\varepsilon(r,u_j) := \partial B_\varepsilon(r,u_j)$, we have

$$\widetilde{G}_{J,j}(u_j) = \frac{|\langle n_{u_j}\,,\,\mathbf{e}\rangle|}{2}\int\limits_{B(r;u_j)^J} dv_0\cdots\widehat{dv_j}\cdots dv_J \frac{G^0_J(v_\ell + u_j \pm \frac{k}{2})}{\prod\limits_{1\le i\le J}|v_i - v_{i+1}|^2}, \tag{4.144}$$

with the convention $v_j = 0$. We differentiate the formula (4.144) : u_j appears in the integrand and in the domains $B(r;u_j)$. We deal with the terms corresponding to differentiation of the integrand as before. Then we have for any integrable function F and small displacement $\delta u \in \mathbb{R}^3$:

$$\int\limits_{B_\varepsilon(r,u_j+\delta u)} \mathrm{F}(v)dv - \int\limits_{B_\varepsilon(r,u_j)} \mathrm{F}(v)dv = \int\limits_{S_\varepsilon(r;u_j)} \mathrm{F}(v)(\langle n(v-u_j)\,,\,\delta u\rangle + \underset{\delta u\to 0}{\mathcal{O}}(|\delta u|^2))dv, \tag{4.145}$$

where $n(v-u_j)$ is the outward normal of $S_\varepsilon(r,u_j)$ at v. Substituting in (4.142), as in the case 2.2. we get terms which are $\underset{\delta u\to 0}{\mathcal{O}}\Big(|\delta u|(1-\log|\delta u|)\Big)$. Writing $u_j = u$ we have

$$\begin{aligned}&\widetilde{G}_{J,j}(v - \tfrac{\varepsilon s}{2}\langle n_v\,,\,\mathbf{e}\rangle n_v + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2)) = \underset{\delta r\to 0}{\mathcal{O}}(-(\delta r)^2\log(\delta r))\\ &+\widetilde{G}_{J,j}(v) - \tfrac{\varepsilon s\langle n_v\,,\,\mathbf{e}\rangle}{2}\sum_{i\neq j}\int\limits_{\substack{v_i\,\in\, S(r;v)\\ \mathbf{v}'_i\,\in\, B(r,v)^J}} \frac{du_i d\mathbf{v}'_i}{\prod\limits_{1\le\ell\le J}|v_\ell - v_{\ell-1}|^2} G^0_J(v_\ell \pm \tfrac{r}{2}\mathbf{e})\langle n(v_i - u_j)\,,\,n_v\rangle.\end{aligned} \tag{4.146}$$

We write $\mathcal{C}(r) := S_+(r)\cap S_-(r)$ (this is a curve) : the integration of $\widetilde{G}_{J,j}(v_j)$ over $S_\varepsilon(r)\Delta\Phi_{\delta r}(S_\varepsilon(\delta r))$ gives rise to a term :

$$-\frac{2r^2}{8\Lambda^2}\int\limits_{u_j\in\mathcal{C}(r),(u_i)_{i\neq j}\in B(r)^J} \frac{r}{4\Lambda} du_0\cdots du_J G_J(u_\ell \pm \tfrac{k}{2}) + \underset{\delta r\to 0}{\mathcal{O}}((\delta r)^2).$$

Thus we get a term of order

$$-\frac{2r^2}{8\Lambda^2}\int\limits_{u_j\in\mathcal{C}(r),(u_i)_{i\neq j}\in B(r)^J} \frac{r}{4\Lambda} du_0\cdots du_J G_J(u_\ell \pm \tfrac{k}{2}) = \mathcal{O}\Big(\frac{(\alpha K)^{J+1}}{\Lambda^2}\Big).$$

By integrating the term $\widetilde{G}_{J,j}(v)\times(\mathrm{J}(\Phi_t;u_j)^{-1}-1)$, we get a well defined number in the limit $\delta r\to 0$. Furthermore this term is

$$\mathcal{O}\Big(\frac{1}{\Lambda}\int\limits_{u_j\in S(r)}\int\cdots\int\limits_{(u_0,\cdots,\widehat{u_j},\cdots,u_J)\in B(r)^J} du_0\cdots du_J |G_J(u_\ell\pm\tfrac{k}{2})|\Big)=\mathcal{O}\Big(\frac{(\alpha K)^{J+1}\log(\Lambda)}{\Lambda^2}\chi_{r<2\Lambda}\Big).$$

– To conclude, we consider $\widetilde{G}_{J,j}(\Phi_t^{-1}(v))-\widetilde{G}_{J,j}(v)$ to deal with the problem of case 2.2.

Up to a term $-\delta^2\log(\delta r)=\underset{\delta r\to 0}{o}(\delta r)$, we can take $S(r)$ instead of $\Phi_t(S_\varepsilon(t))$ and 1 instead of the full jacobian $\mathrm{J}(\Phi_t;u)$. We have $\varepsilon\langle n_v\,,\,\mathbf{e}\rangle=|\langle n_v\,,\,\mathbf{e}\rangle|$. In (4.146) we take back the previous variables $u_i=v+v_j$, this gives

$$\delta r\int\limits_{v\in S_\varepsilon(r)}\sum_{i\neq j}\int\limits_{(u_i,\mathbf{u}')\in S(r)\times B(r)^{J-1}} du_0\cdots du_J\frac{|\langle n_v\,,\,\mathbf{e}\rangle|}{2}\left(-\frac{|\langle n_v\,,\,\mathbf{e}\rangle|\langle n_v\,,\,n_{u_i}\rangle}{2}\right)G_J(u_\ell\pm\tfrac{k}{2}).$$

When we sum this term with that of (4.131), for each $i\neq j$ we have

$$\begin{aligned}\Big||\langle n_{u_i}\,,\,\mathbf{e}\rangle|-|\langle n_v\,,\,\mathbf{e}\rangle|\langle n_v\,,\,n_{u_i}\rangle\Big| &= \Big|\varepsilon(u_i)\langle n_{u_i}\,,\,\mathbf{e}\rangle-\varepsilon(v)\langle n_v\,,\,\mathbf{e}\rangle\times\varepsilon(v)\varepsilon(u_i)\langle n_v\,,\,n_{u_i}\rangle\Big|,\\ &\le \min(\sqrt{2}|n_{u_i}-n_v|,2).\end{aligned}$$

Thus there is no more logarithmic divergence : for $u=u_j$ and $v=u_{j-1}$ or $v=u_{j+1}$, we use the same method as that for (4.131) and get

$$\iint\limits_{S(r)\times S(r)}\frac{|n_u-n_v||\langle n_u\,,\,\mathbf{e}\rangle|du dv}{|u-v|^2}\frac{1}{\widetilde{E}(\Lambda)^2\Lambda^2}.$$

We split the domain in 4 : $S_\varepsilon(r)\times S_{\varepsilon'}(r)$: the case $\varepsilon=\varepsilon'$ gives finite number. Indeed if we use spherical coordinates with respect to $-\frac{\varepsilon r}{2}\mathbf{e}$, we have $|n_u-n_v|\le\frac{|u-v|}{\Lambda}$, and the integral is

$$\mathcal{O}\left(\int\limits_{\mathbb{S}^2}\frac{du}{\Lambda^2|u-\mathbf{e}|}\right)=\mathcal{O}\left(\frac{1}{\Lambda^2}\right).$$

The integration over $S_+(r)\times S_-(r)$ is also finite. To see this we proceed as follows.

For convenience we write $x:=\frac{r}{2\Lambda}$, $\theta_1^0=\arccos(x)$, $\theta_{-1}^0=\arccos(-x)$ and $s(\cdot)$ (resp. $c(\cdot)$) for sin (resp. cos). We take spherical coordinates with respect to $-\varepsilon\frac{r}{2}\mathbf{e}$ for any $S_\varepsilon(r)$ and obtain :

$$\begin{aligned}&\frac{2\pi}{\Lambda^2}\iiint\limits_{(\theta_1,\theta_{-1},\phi)\in(0,\theta_1^0)\times(-\pi,\theta_{-1}^0)\times(-\pi,\pi)}\frac{s(\theta_1)s(\theta_{-1})d\theta_1 d\theta_{-1}d\phi}{(c(\theta_1)-c(\theta_{-1})-2x)^2+s(\theta_{-1})^2s_\phi^2+(s(\theta_1)-s(\theta_{-1})c_\phi)^2}\\ &\lesssim\frac{1}{\Lambda^2}\iiint\limits_{(\theta_1,\theta_{-1},\phi)\in(0,\theta_1^0)\times(-\pi,\theta_{-1}^0)\times(-\pi,\pi)}\frac{s(\theta_1)s(\theta_{-1})d\theta_1 d\theta_{-1}d\phi}{(c(\theta_1)-c(\theta_{-1})-2x)^2+c(\theta_{-1})^2\phi^2}=:\frac{A}{\Lambda^2}.\end{aligned}$$

We write $\theta_\varepsilon=\theta_\varepsilon^0-\varepsilon\phi_\varepsilon$: there holds

$$\begin{aligned}\varepsilon c(\theta_\varepsilon)-x &= x(c(\phi_\varepsilon)-1)+\sqrt{1-x^2}s(\phi_\varepsilon),\\ x(c(\phi_\varepsilon)-1)+\sqrt{1-x^2}s(\phi_\varepsilon) &\ge \phi_\varepsilon\Big(\frac{2}{\pi}\sqrt{1-x^2}-x\frac{\phi_\varepsilon}{2}\Big),\\ &\ge \frac{2\phi_\varepsilon}{\pi}\Big(\sqrt{1-x^2}-\frac{\pi}{4}x\arccos(x)\Big)\ge\frac{2\phi_\varepsilon\sqrt{1-x}}{\pi}\Big(1-\frac{x\pi}{4}\Big)\\ &\ge \frac{2\phi_\varepsilon\sqrt{1-x}}{\pi}\Big(1-\frac{\pi}{4}\Big)\ge\frac{\sqrt{1-x^2}\phi_\varepsilon}{\pi}\Big(1-\frac{\pi}{4}\Big).\end{aligned}$$

Thus we have

$$\begin{aligned} A &\lesssim \iint_{\phi_1,\phi_{-1}\in(0,\theta_1^0)} \frac{\sin(\theta_1)d\phi_1 d\phi_{-1}}{\sqrt{1-x^2}\sqrt{\phi_1^2+\phi_{-1}^2}} \\ &\lesssim \int_{\phi_1\in(0,\theta_1^0)} \frac{d\phi_1}{\sqrt{1-x^2}} \log\Big(1+\frac{\arccos(x)}{\phi_1}\Big) \\ &\lesssim \int_{\phi\in(0,1)} \log(1+\phi^{-1})d\phi. \end{aligned}$$

Conclusion We obtain at last the following upper bound for the terms of cases 2. and 3. :

$$J^2 \frac{(\alpha K)^{J+1}\log(\Lambda)}{\Lambda^2}.$$

It is possible to show that the function $\partial_r^2 f_\Lambda(x)$ tends to zero as $|x|$ tends to 2Λ, this is proved in the thesis of the author (to appear in 2014).

□

Alternative F_Λ In the proof of Theorem 4.3, one is lead to consider a pertubative self-consistent equation with $\mathcal{D}^0$ replaced by $\mathcal{D}^0 + \frac{2}{\lambda}\frac{\mathcal{D}^0}{|\mathcal{D}^0|}$. In particular we need Lemma 4.15 below for the proof of Lemma 4.12. We can write

$$\mathcal{D}^0 + \frac{2}{\lambda}\frac{\mathcal{D}^0}{|\mathcal{D}^0|} = \beta\widetilde{w}_0(-i\nabla) + \boldsymbol{\alpha}\cdot\frac{-i\nabla}{|-i\nabla|}\widetilde{w}_1(-i\nabla).$$

The formulae are the same with g_0, g_1 replaced by $\widetilde{w}_0, \widetilde{w}_1$, estimates of the same kind hold. The alternative functions are marked with a tilde : $\widetilde{B}_\Lambda$ and $\widetilde{g}_\Lambda$.

We can easily estimate $\int_{|x|\geq R} |\mathscr{F}^{-1}(\widetilde{F}_\Lambda)(x)|dx$ for $R \geq 1$: writing $\mathfrak{f}_\Lambda := \mathscr{F}^{-1}(\widetilde{F}_\Lambda)$ we have the following Lemma :

Lemma 4.15. *For $\lambda, \Lambda \gg 1$ we have :*

$$\alpha\int_{|x|\geq R} |\mathfrak{f}_\Lambda(x)|dx \leq \|-\Delta\widetilde{F}_\Lambda\|_{L^2}\sqrt{4\pi R^{-1}} = \mathcal{O}(LR^{-1/2}). \tag{4.147}$$

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Chapitre 5

Sur deux électrons dans le vide

Absence of binding in a mean-field approximation of quantum electrodynamics

Abstract

We study the Bogoliubov-Dirac-Fock model which is a mean-field approximation of QED. It allows to consider relativistic electrons interacting with the Dirac sea. We study the system of two electrons in the vacuum : it has been shown in a previous paper [Sok14b] that an electron alone can bind due to the vacuum polarization, under some technical assumptions. Here we prove the absence of binding for the system of two electrons :the response of the vacuum is not sufficient to counterbalance the repulsion of the electrons.

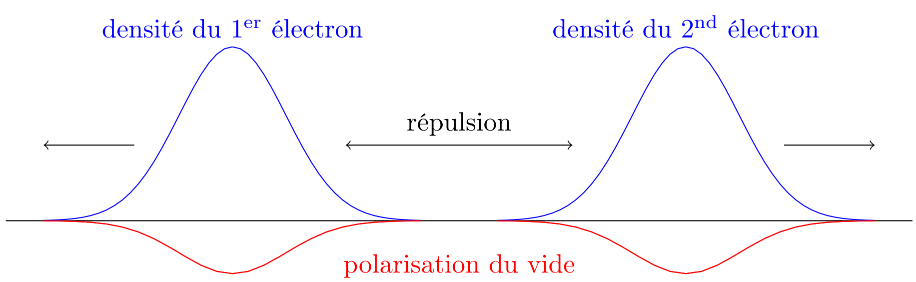

FIGURE 5.1 – Absence d'état fondamental pour le système $\{2\,\text{électrons} + \text{vide}\}$

Contents

Absence of Binding in the BDF Approximation

Abstract

We study the Bogoliubov-Dirac-Fock model which is a mean-field approximation of QED. It allows to consider relativistic electrons interacting with the Dirac sea. We study the system of two electrons in the vacuum : it has been shown in a previous paper [Sok14b] that an electron alone can bind due to the vacuum polarization, under some technical assumptions. Here we prove the absence of binding for the system of two electrons :the response of the vacuum is not sufficient to counterbalance the repulsion of the electrons.

5.1 Introduction and main results

The Dirac operator

The theory of relativistic quantum mechanics is based on the Dirac operator D_0, that describes the kinetic energy of a relativistic electron. To simplify formulae, we take relativistic units $\hbar = c = 4\pi\varepsilon_0 = 1$ and set the bare particle mass equal to 1.

In this case, the Dirac operator is defined by [Tha92] : $D^0 = -i\boldsymbol{\alpha}\cdot\nabla + \beta$ where $\beta, \alpha_j \in \mathcal{M}_4(\mathbf{C})$ are the Dirac matrices :

$$\beta = \begin{pmatrix} \mathrm{Id}_2 & 0 \\ 0 & -\mathrm{Id}_2 \end{pmatrix}, \qquad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, j = 1,2,3 \tag{5.1a}$$

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{5.1b}$$

It acts on the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$. Its spectrum is not bounded from below : $\sigma(D_0) = (-\infty, -1] \cup [1, +\infty)$, which implies the existence of states with arbitrarily small negative energy. Dirac postulated that all the negative energy states are already occupied by "virtual" electrons forming the so-called Dirac sea : by Pauli principle a real electron can only have positive energy.

According to this interpretation, the vacuum, filled by the Dirac sea, is a polarizable medium that reacts to the presence of an electromagnetic field.

BDF model

In this paper we study the Bogoliubov-Dirac-Fock (BDF) model which is a no-photon, mean-field approximation of Quantum Electrodynamics (QED) which was introduced by Chaix and Iracane [CI89]. It enables us to consider a system of relativistic electrons interacting with the vacuum in the presence of an electrostatic field. This paper is a continuation of previous works by Hainzl, Gravejat, Lewin, Séré, Siedentop [HS03, HLS05a, HLS05b, HLS09, GLS09] and Sok [Sok14b, Sok13].

The derivation of the BDF model from QED is explained in [CI89] and [HLS05a, Appendix] : we refer the reader to these papers for full details.

In QED, an electronic system is described by a state in the fermionic Fock space $\mathcal{F}_{el}$ [Tha92, Chapter 10] on which (formally) acts the Hamiltonian $\mathbb{H}_{\mathrm{QED}}$ [HLS05a, Appendix]. The mean-field approximation consists to restricting the study to Hartree-Fock type states, called BDF states. They are fully characterized by their one-body density matrix (1pdm) which are orthogonal projectors of $\mathfrak{H}$.

For instance, the projector $P^0_- := \chi_{(-\infty,0)}(D_0)$ is the 1pdm of the vacuum state $\Omega_0 \in \mathcal{F}_{el}$: it must be thought of as the infiniter Slater determinant $f_1 \wedge f_2 \wedge \cdots$ where $(f_i)_{i\geq 1}$ is an orthonormal basis (BON) of $\mathrm{Ran}(P^0_-)$. A projector P defines a BDF state *iff* $P - P^0_-$ is Hilbert-Schmidt (*i.e.* its integral kernel is square integrable).

The (formal) difference of the energy $\mathcal{E}_{\mathrm{QED}}(P)$ of a state P with that of P^0_- considered as a reference state turns out to be a function of the reduced density matrix (r1pdm) $Q := P - P^0_-$. Formally this function is

$$\widetilde{\mathcal{E}}^{\nu}_{\mathrm{BDF}}(Q) := \mathrm{Tr}\big(D_0 Q\big) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2}\big(D(\rho_Q, \rho_Q) - \|Q\|^2_{\mathrm{Ex}}\big), \tag{5.2}$$

where $\alpha > 0$ is the fine structure constant, ν is the external density of charge, $\rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big)$ is the density of Q, with $Q(x,y)$ the integral kernel of Q, and :

$$D(\nu,\nu) = \|\nu\|^2_{\mathcal{C}} := 4\pi \int_{\mathbb{R}^3} \frac{|\widehat{\nu}(k)|^2}{|k|^2} dk \text{ and } \|Q\|^2_{\mathrm{Ex}} := \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|Q(x,y)|^2}{|x-y|} dx dy. \tag{5.3}$$

The hat in $\widehat{\nu}$ denotes the Fourier transform and $D(\nu,\nu) < +\infty$ is the Coulomb energy of ν : it coincides with $\iint \frac{\nu(x)^*\nu(y)}{|x-y|}dxdy$ whenever this integral makes sense.

In (5.2) we recognize the kinetic energy, the interaction energy with ν, the direct term $\frac{\alpha}{2}D(\rho_Q,\rho_Q)$ and the exchange term $-\frac{\alpha}{2}\|Q\|^2_{\mathrm{Ex}}$. *A priori* this formula makes sense only when Q and D_0Q are trace-class and the variational problem is ill-defined.

An ultraviolet cut-off $\Lambda > 0$ is necessary. Following [GLS09], we replace D_0 by

$$\mathbf{D} := D_0\big(1 - \frac{\Delta}{\Lambda^2}\big) \text{ with domain } H^{3/2}(\mathbf{R}^3, \mathbf{C}^4),$$

and only consider states Q such that $\mathrm{Tr}\big(|\mathbf{D}|\,|Q|^2\big) < +\infty$.

By adapting (5.2), we get a well-defined energy $\mathcal{E}^\nu_{\mathrm{BDF}}$ (defined in the next section).

Remark 5.1. Other choices of cut-off are possible. This one, the *smooth* cut-off, is convenient for the study in Direct space of functions. In [HLS05a, HLS05b, HLS09] Hainzl *et al.* have chosen the *sharp* cut-off, replacing $L^2(\mathbb{R}^3,\mathbb{C}^4)$ by its subspace $\mathfrak{H}_\Lambda$ made of square-integrable functions whose Fourier transform vanishes outside the ball $B_{\mathbb{R}^3}(0,\Lambda)$.

Remark 5.2. We still have $\chi_{(-\infty,0)}(\mathbf{D}) = P^0_-$. We also write $P^0_+ := \chi_{(-\infty,0)}(D^0) = \mathrm{Id} - P^0_-$ the projector on its positive spectral subspace.

Notation 5.1. For an operator Q, we define R_Q by its integral kernel :

$$R_Q(x,y) := \frac{Q(x,y)}{|x-y|},\ x,y \in \mathbb{R}^3 \times \mathbb{R}^3. \tag{5.4}$$

Moreover for any $\rho \in \mathcal{C}$ we write

$$v_\rho := \rho * \tfrac{1}{|\cdot|}. \tag{5.5}$$

Existence of minimizers

For a r1pdm $Q = P - P^0_-$, the charge of the system is given by its so-called P^0_--trace $\mathrm{Tr}_{P^0_-}(Q)$, defined by

$$\mathrm{Tr}_{P^0_-}(Q) := \mathrm{Tr}\big(P^0_- Q P^0_-\big) + \mathrm{Tr}\big(P^0_+ Q P^0_+\big). \tag{5.6}$$

It coincides with the usual trace for trace-class operators and is well-defined for r1pdm because of their structure. Indeed as a difference of orthogonal projectors Q satisfies :

$$P^0_+(P - P^0_-)P^0_+ - P^0_-(P - P^0_-)P^0_- = (P - P^0_-)^2. \tag{5.7}$$

A minimizer for $\mathcal{E}^\nu_{\mathrm{BDF}}$ among states with charge $M \in \mathbb{N}$ is interpreted as a ground state of the system with M electrons in the presence of ν. For $q \in \mathbb{R}$, the infimum of the BDF energy on the charge sector $\mathcal{Q}_\Lambda(q) := \{Q : \mathrm{Tr}_{P^0_-}(Q) = q\}$ is written $E^\nu(q)$.

A sufficient condition for the existence of a minimizer for $E^\nu(q)$ is the validity of binding inequalities at level q [HLS09, Theorem 1]. This result is stated for the *sharp* cut-off, however it is possible to adapt its proof to get this Theorem :

Theorem 5.1. *Let $0 \le \alpha < \frac{4}{\pi}$, $\Lambda > 0$, $\nu \in \mathcal{C}$ and $q \in \mathbb{R}$. Then the following assertions are equivalent :*

1. *the binding inequalities hold : $\forall\, k \in \mathbb{R}\backslash\{0\},\ E^\nu(q) < E^\nu(q-k) + E^0(k)$,*
2. *each minimizing sequence $(Q_n)_{n\ge1}$ for $E^\nu(q)$ is precompact in $\mathcal{Q}_\Lambda(q)$ and converges, up to a subsequence, to a minimizer for $E^\nu(q)$. If $\nu = 0$, this result holds up to translation.*

If q is an integer, then we can only consider $k \in \mathbb{Z}\backslash\{0\}$ in the first assertion.

Checking binding inequalities is a difficult task. Hainzl *et al.* checked them in some cases with non-vanishing ν [HLS09, Theorems 2 and 3]. [HLS09, Theorem 3] states that for $\nu \in L^1(\mathbb{R}^3,\mathbb{R}_+) \cap \mathcal{C}$, there exists a minimizer for $E^\nu(M)$ provided that $M - 1 < \int \nu$ under technical assumptions on α, Λ.

In [Sok14b], the existence of a ground state for $E^0(1)$ is proved, still under technical assumptions on α, Λ. It is remarkable that an electron can bind alone without any external potential : this is due to the vacuum polarization. The electron creates a hole in the Dirac sea that allows it to bind. This effect causes a charge screening : from far away the charge of the electron appears smaller as it is surrounded by the hole.

Let Q be a minimizer for $E^0(1)$, then its density ρ_Q is integrable [Sok13], and we have the *charge renormalisation formula* :

$$\int \rho_Q = 1 \times Z_3 \approx 1 \times \frac{1}{1 + \frac{2}{3\pi}\alpha \log(\Lambda)} \neq 1. \tag{5.8}$$

Here Z_3 is the *renormalisation constant*. This inadequacy is possible because the minimizer is *not* trace-class (hence the mere fact that ρ_Q is integrable is non-trivial).

We emphasize that these results were proved with the *sharp* cut-off, but the proofs can be adapted in the present case.

Our purpose in this paper is to study the variational problem $E^0(2)$, that is two electrons in the vacuum. We recall that an electron does not see its own field, but in the case of two electrons any electron feel the field induced by the other resulting to a repulsive force. If the vacuum polarization is not strong enough to counterbalance this repulsion, then there is no minimizer for $E^0(2)$. This constitutes our main Theorem.

Theorem 5.2. *There exist α_0, Λ_0, L_0 such that if $\alpha \leq \alpha_0$, $\Lambda \geq \Lambda_0$ and $\alpha \log(\Lambda) \leq L_0$, then there is no minimizer for $E^0(2)$.*

Remark 5.3. This result is proved in the case of the *smooth* cut-off, and we expect it to be true for the *sharp* one but we were unable to show it.

We prove it *ad absurdum*. Let us give the main ideas.

Along this paper we suppose that there exists a minimizer Q for $E^0(2)$. Such a minimizer satisfies a self-consistent equation [HLS09, Proposition 1], [GLS09] and can be decomposed as follows :

$$Q = |\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + \gamma, \tag{5.9}$$

where the ψ_j's are eigenvectors of the so-called mean-field operator :

$$D_Q := \mathbf{D} + \alpha\big(v_{\rho_Q} - R_Q\big), \tag{5.10}$$

where for a density $\rho \in \mathcal{C}$ and an operator Q, we define

$$R_Q(x, y) := \frac{Q(x, y)}{|x - y|},\ x, y \in \mathbb{R}^3 \text{ and } v_\rho := \rho * \tfrac{1}{|\cdot|}. \tag{5.11}$$

For short we will also write

$$B_Q := v_{\rho_Q} - R_Q. \tag{5.12}$$

By studying $E^0(2) \leq 2E^0(1)$, we get *a priori* information on the ψ_j's. In particular we show that the subspace $\mathrm{Span}(\psi_1, \psi_2)$ splits as follows

$$\mathrm{Span}(\psi_1, \psi_2) = \mathbb{C}h_1 \overset{\perp}{\oplus} \mathbb{C}h_2,\ \ \|h_j\|_{L^2} = 1,$$

where h_1 and h_2 are essentially two bump functions which are some distance R_g away from each other. The operator γ is also localised around each h_j such that the energy $\mathcal{E}^0_{\mathrm{BDF}}(Q)$ can be written

$$\mathcal{E}^0_{\mathrm{BDF}}(Q) = 2E^0(1) + \theta_{12},$$

where $\theta_{12} > 0$ in our range of parameters (α, Λ).

Roughly speaking the BDF energy should be the sum of the BDF energy of these two parts plus the interaction energy. This interaction energy is too big to ensure $E^0(2)$ is attained.

Remark 5.4. Throughout this paper, we work in the regime $\alpha \leq \alpha_0, \alpha\log(\Lambda) := L \leq L_0$ and $\Lambda \geq \Lambda_0 > 0$ for small constants $\alpha_0, L_0, \Lambda_0^{-1}$. K is some constant independent of those numbers while $K(\lambda)$ means a constant depending on the quantity λ. Symbols $o(\cdot)$,$\mathcal{O}(\cdot)$ and $\Theta(\cdot)$ are to be understood in this regime.

The paper is organized as follows. In the next Section we properly define our model and give *a priori* estimates about $E^0(2)$ and its hypothetical minimizer in Lemma 5.1. This Lemma is proved in Section 5.5.

Then in Section 5.3, we study the Pekar-Tomasevitch functional to exploit these results (Propositions 5.3, 5.4 and 5.5). These Propositions are proved in Appendix 5.B.

Section 5.4 is devoted to introduce important tools of the proof : the Cauchy expansion (part 5.4.1) and useful inequalities (part 5.4.3). We recall in part 5.4.2 the form of the density of a minimizer.

Section 5.6 is dedicated to prove Theorem 5.2. We show how the energy is distributed in Direct space (Proposition 5.6). This enables us to prove Theorem 5.2 (part 5.6.3). To this end we first study the localisation of the "real" electrons' wave functions (Lemma 5.7, proved in Appendix 5.C). We then show how this enables us to get localisation of the energy of a minimizer (Lemma 5.8, proved in this Section but using Appendix 5.D). For the sake of clarity we explain in Remark 5.15 how Appendix 5.D is used to prove Lemma 5.8.

We have postponed the most technical proofs in the Appendices. In Appendix 5.A, we prove Proposition 5.1 and Lemma 5.6. This last Lemma shows estimates on a minimizer by bootstrap arguments. Maybe the most difficult results lie in Appendices 5.C and 5.D, dedicated to prove localisation estimates in Direct space.
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5.2 Presentation of the model

Remark 5.5 (Fourier transform). In this paper, the Fourier transform is defined on $L^1(\mathbb{R}^3)$ by the formula :

$$\forall\, f \in L^1(\mathbb{R}^3),\ \widehat{f}(p) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} f(x) e^{-ip\cdot x} dx.$$

Notation 5.2 (Splitting w.r.t. $P^0_\pm$). For an operator Q and $e_1, e_2 \in \{+,-\}$ we write $Q^{e_1\, e_2} := P^0_{e_1} Q P^0_{e_2}$.

Notation 5.3 (Schatten classes). We recall that for $1 \le p \le \infty$, the set of compact operators whose singular values form a sequence in ℓ^p is written $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ [Sim79, Sim79]. The case $p = 2$ (resp. $p = 1$) corresponds to Hilbert-Schmidt operators (resp. trace-class operators).

Those Banach spaces satisfy Hölder-type inequalities [RS75]. We also recall the Kato-Seiler-Simon inequalities [Sim79] :

$$\forall\, 2 \le p \le \infty,\ \forall\, f, g \in\ L^p(\mathbb{R}^3),\ \|f(x)g(-i\nabla)\|_{\mathfrak{S}_p} \le (2\pi)^{-3/p} \|f\|_{L^p} \|g\|_{L^p}. \tag{5.13}$$

Furthermore we write $\mathcal{B}(\mathfrak{H}_\Lambda)$, the set of bounded linear endomorphisms on $\mathfrak{H}_\Lambda$.

Notation 5.4 (On D_0 and $\mathbf{D}$). We write $\mathbf{s}_p$ for $\frac{\widehat{D_0}(p)}{\sqrt{1+|p|^2}}$ the action of $\mathrm{sign}(D_0)$ in the Fourier space. The function $\sqrt{1+|p|^2}$ is also written $E(p)$ and $\overline{E}_p := \sqrt{1+|p|^1}(1+|p|^2/\Lambda^2)$.

Throughout this paper

$$\varepsilon[\Lambda] = \varepsilon_\Lambda := \frac{1}{\log(\Lambda)} \text{ and } a[\Lambda] := \frac{1+\varepsilon[\Lambda]}{2}. \tag{5.14}$$

We have

$$|D_0|^{1+\varepsilon_\Lambda} \le E(\Lambda)^\varepsilon |\mathbf{D}| \le (1+e)|\mathbf{D}|,\ \Lambda \ge e = \exp(1). \tag{5.15}$$

5.2.1 The BDF energy

Let ν be an external charge density in $\mathcal{C}$ and $\alpha, \Lambda > 0$ be given. We want to extend (5.2) : the result is the BDF energy (5.23) below.

Following [GLS09] we define the set :

$$\mathcal{Q}_{\mathrm{Kin}} := \big\{Q \in \mathfrak{S}_2, |\mathbf{D}|^{1/2} Q, Q|\mathbf{D}|^{1/2} \in \mathfrak{S}_2, |\mathbf{D}|^{1/2} Q^{++} |\mathbf{D}|^{1/2}, |\mathbf{D}|^{1/2} Q^{--} |\mathbf{D}|^{1/2} \in \mathfrak{S}_1\big\}. \tag{5.16}$$

The kinetic energy functional is defined on $\mathcal{Q}_{\mathrm{Kin}}$ by the following formula

$$\mathrm{Tr}_{P^0_-}(\mathbf{D}Q) := \mathrm{Tr}(|\mathbf{D}|^{1/2}(Q^{++} - Q^{--})|\mathbf{D}|^{1/2}). \tag{5.17}$$

It coincides with $\mathrm{Tr}(\mathbf{D}Q)$ when $\mathbf{D}Q$ is trace-class. We will work in the subset of this space defined by :

$$\mathcal{K} := \{Q \in \mathcal{Q}_{\mathrm{Kin}},\ -P_-^0 \le Q \le P_+^0\} \subset \big\{Q \in \mathcal{Q}_{\mathrm{Kin}},\ Q^* = Q\big\}, \tag{5.18}$$

the closed convex hull (under that norm) of the difference of two orthogonal projectors : $P - P_-^0$.

We also define $\mathbf{Q_1}$ the Hilbert space of $Q(x,y) \in L^2(\mathbf{R}^3 \times \mathbf{R}^3, \mathbf{C}^4)$ such that

$$\|Q\|_{\mathbf{Q_1}}^2 := \iint (\overline{E}_p + \overline{E}_q)|\widehat{Q}(p,q)|^2 dpdq < +\infty. \tag{5.19}$$

The definition of the density ρ_Q must coincide with the usual one when Q is (locally) trace-class and ρ_Q must be of finite Coulomb norm : $\|\rho_Q\|_{\mathcal{C}} < +\infty$. For Q in $\mathfrak{S}_1^{P_-^0}$, ρ_Q is defined by duality :

$$\forall\ V \in \mathcal{C}',\ QV \in \mathfrak{S}_1^{P_-^0} \text{ and } \mathrm{Tr}_{P_-^0}(QV) = \langle V\ ,\ \rho_Q\rangle_{\mathcal{C}'\times\mathcal{C}}. \tag{5.20}$$

We have the following proposition (proved in Appendix 5.A).

Proposition 5.1. *The map $Q \in \mathfrak{S}_1^{P_-^0} \mapsto \rho_Q \in \mathcal{C}$ is continuous and :*

$$\begin{aligned}\|\rho_Q\|_{\mathcal{C}} &\lesssim \||D_0|^{a[\Lambda]}Q^{++}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1} + \||D_0|^{a[\Lambda]}Q^{--}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1}\\ &\quad + \sqrt{\log(\Lambda)}\||D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2}.\end{aligned} \tag{5.21}$$

Thanks to Kato's inequality (5.59), the exchange term is well-defined [BBHS98a]

$$\begin{aligned}\frac{2}{\pi}\iint \frac{|Q(x,y)|^2}{|x-y|}dxdy &\le \mathrm{Tr}(|D_0|Q^2) = \mathrm{Tr}\{|D_0|^{1/2}Q^2|D_0|^{1/2}\}\\ \text{and for } Q\in\mathcal{K}: &\le \mathrm{Tr}\{|D_0|^{1/2}(Q^{++}-Q^{--})|D_0|^{1/2}\} \le \mathrm{Tr}_{P_-^0}(\mathbf{D}Q),\end{aligned} \tag{5.22}$$

The BDF energy is defined as follows :

$$\mathcal{E}_{\mathrm{BDF}}^{\nu}(Q) := \mathrm{Tr}_{P_-^0}(\mathbf{D}Q) - \alpha D(\nu,\rho_Q) + \frac{\alpha}{2}\Big(D(\rho_Q,\rho_Q) - \iint \frac{|Q(x,y)|^2}{|x-y|}dxdy\Big),\ Q\in\mathcal{K}. \tag{5.23}$$

Any charge sector $\mathcal{Q}(q) := \{Q \in \mathcal{K},\ \mathrm{Tr}_{P_-^0}(Q) = q\}$ leads to a variational problem

$$E_{\mathrm{BDF}}^{\nu}(q) := \inf_{Q\in\mathcal{Q}(q)} \mathcal{E}_{\mathrm{BDF}}(Q). \tag{5.24}$$

By Lieb's variational principle [HLS09, Proposition 3], a minimizer Q for $E^{\nu}(M)$ with $M \in \mathbb{Z}$ is necessarily a difference of two projectors $P - P_-^0$.

5.2.2 Form of a minimizer

To simplify, from this point we assume that $\nu = 0$. For an integer $M \in \mathbb{N}$, let Q be a ground state for $E^0(M)$, then necessarily $Q = \overline{P} - P_-^0$, where $\overline{P}$ is an orthogonal projector.

The study of the first and second derivative gives more information : we have $\big[D_Q, \overline{P}\big] = 0$, and [HLS09, Proposition 1]

$$\overline{P} = \chi_{(-\infty,\mu]}\big(D_Q\big),\ 0 < \mu < 1, \tag{5.25}$$

where we recall the mean-field operator is defined in (5.10). We decompose Q with respect to the positive and negative spectrum :

$$N := \chi_{(0,\mu]}(D_Q) \text{ and } \boldsymbol{\pi}_{\mathrm{vac}} = \gamma + P_-^0 := \chi_{(-\infty,0)}(D_Q), \tag{5.26}$$

where $\boldsymbol{\pi}_{\mathrm{vac}}$ (resp. n) is interpreted as the polarized vacuum (resp. as the real electrons). If αM is small enough, then we can show that $\mathrm{Tr}_{P_-^0}(\gamma) = 0$ and thus N has rank M [HLS09, Sok13]. We will recall the proof below.

In the present case, a minimizer for $E^0(2)$ can be written as in (5.25)-(5.26). For small enough α, we have

$$N = |\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|,\ D_Q\psi_j = \mu_j\psi_j,\ 0 < \mu_2 \le \mu_1 = \mu < 1,\ j \in \{1,2\}. \tag{5.27}$$

These equations constitutes the starting point of our proof : they enable us to get estimates on the Sobolev norms of the ψ_j's. More precisely we will prove Lemma 5.1.

Before stating it, let us recall the Pekar-Tomasevitch functional :

$$\mathcal{E}_{\rm PT}(\psi) := \|\nabla\psi\|_{L^2}^2 - \iint \frac{|\psi(x)|^2|\psi(y)|^2}{|x-y|}dxdy,\ \forall\,\psi\in H^1.$$

It describes the energy of a single electron in its own hole. In the case of M electrons, the energy is [FLST11] :

$$\forall\, 0\le\Gamma\le 1,\ \operatorname{Tr}\Gamma = M,\ \mathcal{E}_{\rm PT}^U(\Gamma) := \operatorname{Tr}\big(-\Delta\big) - \|\rho_\Gamma\|_{\mathcal{C}}^2 + U\Big(\|\rho_\Gamma\|_{\mathcal{C}}^2 - \|\Gamma\|_{\rm Ex}^2\Big), \tag{5.28}$$

where $U>0$ is some number. By scaling we can assume $U=1$ but $-\|\rho_\Gamma\|_{\mathcal{C}}^2$ has to be replaced by U^{-1} : this last number measures the strength of the polarization.

In this paper, a specific value $U=U_0(\alpha,\Lambda)$ is considered : $U_0^{-1} = 1-Z_3(\alpha,\Lambda)$ where Z_3 is the renormalisation constant that we have mentionned in the introduction. Its precise expression is given below (5.56).

We write $E_{\rm PT}^U(M)$ the infimum of the Pekar-Tomasevitch energy on the set $\{0\le\Gamma\le 1,\ \operatorname{Tr}\Gamma = M\}$, with $U=U_0$.

Remark 5.6. We assume that $U_0>2U_{\rm c}$, where $U_{\rm c}$ is the critical value above which, there is no minimizer for $E_{\rm PT}^U(M)$ for any integer $M\ge 2$. This important result is proved in [FLST11].

For unitary wave functions $\phi_1\perp\phi_2$, we also write

$$\mathcal{E}_{\rm PT}^U(\phi_1\wedge\phi_2) := \mathcal{E}_{\rm PT}^U\Big(\sum_{j=1}^2 |\phi_j\rangle\langle\phi_j|\Big).$$

Lemma 5.1. *In the regime of Remark 5.4, let $Q=N+\gamma$ be a minimizer for $E^0(2)$, decomposed as in* (5.25)-(5.27)*.*

Let c be $\big\{\alpha(1-Z_3(\alpha,\Lambda))\big\}^{-1}$ where Z_3 is defined in (5.56)*. We write $\underline{\psi_j}$ the scaling of ψ_j by c :*

$$\underline{\psi_j}(x) := c^{3/2}\psi_j(cx),\ x\in\mathbb{R}^3,$$

Then we have the following :

$$\left\{\begin{array}{rcl} E_{BDF}^0(1) &=& 1+\frac{1}{2c^2}E_{PT}(1)+\mathcal{O}(\alpha c^{-2}),\\ E_{BDF}^0(2)=\mathcal{E}_{BDF}^0(Q) &=& 2+\frac{1}{2c^2}\mathcal{E}_{PT,U_0}(\underline{\psi_1}\wedge\underline{\psi_2})+\mathcal{O}(\alpha c^{-2}). \end{array}\right. \tag{5.29}$$

We split each ψ_j into an upper spinor φ_j and a lower one χ_j, both in $L^2(\mathbb{R}^3,\mathbb{C}^2)$. We write $n_j=|\psi_j|^2$ (resp $\underline{n_j}=|\underline{\psi_j}|^2$) and $n=n_1+n_2$ (resp $\underline{n}=\underline{n_1}+\underline{n_2}$). Then we have

$$\mu_j = 1+\frac{\|\nabla\underline{\varphi_j}\|_{L^2}^2}{2c^2} - \frac{1}{c^2}D(\underline{n_j},\underline{n})+\mathcal{O}(\alpha c^{-2}), \tag{5.30}$$

in particular :

$$(1-\mu_j)c^2\gtrsim 1. \tag{5.31}$$

Estimate (5.31) follows from (5.46)-(5.47). This quantitative error $\mathcal{O}(\alpha c^{-2})$ gives *a priori* information about the $\underline{\psi_j}$'s thanks to [Lie77, FLST11] (see the next Section).

Notation 5.5. Throughout this paper, we will use the following notations.

$$\begin{array}{rcl|rcl} N_j &=& |\psi_j\rangle\langle\psi_j| & N &=& N_1+N_2,\\ n_j &=& |\psi_j|^2 & n &=& n_1+n_2,\\ \gamma'=Q &=& =\gamma+N, & \rho_\gamma' &=& \rho_\gamma+n. \end{array} \tag{5.32}$$

When we add an underline $\underline{N_j}$ etc. we mean the scaled object by $c=(\alpha(1-Z_3))^{-1}$. Writing

$$O_c : \phi(x)\in L^2\mapsto c^{3/2}\phi(cx),$$

we have $\underline{\psi_j}=O_c\psi_j$, $\underline{N_j}:=O_cN_jO_c^{-1}$, $\underline{\gamma}=O_c\gamma O_c^{-1}$.

5.3 The Pekar-Tomasevitch functional

5.3.1 Decoupling of almost minimizers for $E^{U_0}_{\mathbf{PT}}(2)$

Thanks to [Lie77], one knows that there exists but one minimizer for $E_{\rm PT}(1)$ up to a phase and to translation in $L^2(\mathbb{R}^3,\mathbb{C})$. This minimizer can be chosen positive radially symmetric and decreasing. It is also smooth and with exponential falloff. As $\int \big|\nabla|\phi|\big|^2 \le \int |\nabla\phi|^2$ [LL97], there holds the same in $L^2(\mathbb{R}^3,\mathbb{C}^4)$. The set of minimizers is a manifold $\mathscr{P}\simeq \mathbb{S}^7\times\mathbb{R}^3$ where $\mathbb{S}^7$ is the unit sphere of $\mathbb{C}^4$. There also holds coercivity inequality [Len09] :

Proposition 5.2. *Let $\phi\in H^1$ with $\|\phi\|_{L^2}=1$ and let $\overline{\phi}\in\mathscr{P}$ such that :*
$\|\phi-\overline{\phi}\|_{H^1}=\inf_{f\in\mathscr{P}}\|\phi-f\|_{H^1}$, then there exists $\kappa>0$ such that (at least in a neighborhood of $\mathscr{P}$) :

$$\mathcal{E}_{PT}(\phi)-E_{PT}(1)\ge\kappa\|\phi-\overline{\phi}\|^2_{H^1}.$$

Notation 5.6. We write $\mathscr{P}_0\subset\mathscr{P}$ the submanifold of $\mathscr{P}$ made of minimizers with center $0\in\mathbb{R}^3$: it is isomorphic to $\mathbb{S}^7$.

We are interested in $E^{U}_{\rm PT}(2)$, with $U=U_0>2U_{\rm c}$, where $U_{\rm c}$ is the critical value above which there is no mminimizers for $E_{\rm PT}(2)$ [FLST11] : in particular $E_{\rm PT}(2)=2E_{\rm PT}(1)$ (the proof of [FLST11] also applies for spinor-valued functions). If we *choose* $U_0>2\mathrm{U}_c$:

$$\forall\Psi\in L^2_a(\mathbb{R}^3\times\mathbb{R}^3),\ \|\Psi\|_{L^2}=1:\ \mathcal{E}_{\rm PT}(\Psi)-2E_{\rm PT}(1)\ge\frac{U_0}{2}(D(\rho_\Psi,\rho_\Psi)-\mathrm{Tr}(\gamma_\Psi R[\gamma_\psi]))\tag{5.33}$$

where we recall ρ_Ψ is the density of Ψ and γ_Ψ is its one-body density matrix.

There holds Lieb's variational principle : $E^U_{\rm PT}(2)$ is also the infimum of $\mathcal{E}^U_{\rm PT}$ over Slater determinant $h_1\wedge h_2$ with $h_j\in H^1$ and $\langle h_j\,,\,h_k\rangle=\delta_{jk}$.

Let us consider such a state $\Psi=h_1\wedge h_2$. The plane $\mathrm{Span}(h_1,h_2)$ can be defined with other orthonormal families : $\mathbf{U}(2)$ acts on the set $\mathrm{S}[\Psi]$ of those families :

$$\left(\begin{pmatrix}a & c\\ b & d\end{pmatrix},\begin{pmatrix}h_1\\ h_2\end{pmatrix}\right)\in\mathbf{U}(2)\times\mathrm{S}[\Psi]\mapsto\begin{pmatrix}ah_1+bh_2\\ ch_1+dh_2\end{pmatrix}\in\mathrm{S}[\Psi],\tag{5.34}$$

The first vector is written $(\mathbf{m}\cdot\mathbf{h})_1$ and the second is written $(\mathbf{m}\cdot\mathbf{h})_2$.

Characteristic length For $\Psi=h_1\wedge h_2$ we define the inverse d_Ψ of the *characteristic length* $R_{12}(\Psi)$:

$$d_\Psi:=\inf_{\mathbf{m}\in\mathbf{SU}(2)}D(|(\mathbf{m}\cdot\mathbf{h})_1|^2,|(\mathbf{m}\cdot\mathbf{h})_2|^2)=R_{12}(\Psi)^{-1}.\tag{5.35}$$

Let $\phi_0\in\mathscr{P}_0$ be the radially symmetric and positive function (with $\phi_0(x)$ parallel to $(1\ \ 0\ \ 0\ \ 0)^*$ for instance). Let $\phi_{\mathbf{x}_0}=\tau_{\mathbf{x}_0}\phi_0$ be its translation by $\mathbf{x}_0\in\mathbb{R}^3$. We have :

$$\forall x_0,\ |\mathbf{x}_0|\ge 1:\ \ |\mathbf{x}_0|\times D(|\phi_0|^2,|\phi_{\mathbf{x}_0}|^2)\le\sup_{|\mathbf{z}|\ge1}|\mathbf{z}|\sqrt{\iint\frac{|\phi_0(x)|^2|\phi_{\mathbf{z}}(y)|^2}{|x-y|^2}dxdy}:=\mathrm{Y}_0<+\infty.\tag{5.36}$$

Geometric length For a Slater determinant $\Psi=h_1\wedge h_2$ where h_1 and h_2 satisfy $D(|h_1|^2,|h_2|^2)=d_\Psi$, we define the *geometric length* R_g as follows.

Let $\phi_{(j)}\in\mathscr{P}$ be the closest function of $\mathscr{P}$ to h_j in H^1. Each $\phi_{(j)}$ is radial with respect to some vector $z_j\in\mathbb{R}^3$, we set $\mathrm{R}_g(\Psi):=|z_1-z_2|$ (or the smallest of such $|z_1-z_2|$) : it should be seen as the *interparticle distance.*

Remark 5.7. The geometric length R_g does not appear in the energy and $R_{12}=d_\Psi^{-1}$ may be much smaller.

Proposition 5.3. *There exist $a_0>0$ and $b=b(a_0)>0$ such that*

$$\forall\Psi=h_1\wedge h_2:\ \ \Delta_2\mathcal{E}=\mathcal{E}^U_{PT}(\Psi)-2E_{PT}(1)<a_0\ \Rightarrow\ \frac{\Delta_2\mathcal{E}}{d_\Psi}\ge b.\tag{5.37}$$

Proposition 5.4. *There exist $a_0' > 0$ and $b' > 0$ such that :*

$$\forall \Psi = h_1 \wedge h_2 : \ \Delta_2 \mathcal{E} < a_0' \ \Rightarrow \iint \frac{|\Psi(x,y)|^2}{|x-y|} dxdy \geq \frac{b'}{R_g}. \tag{5.38}$$

More precisely :

For any $0 < \lambda$ let B_j^λ be $B(z_j, \lambda R_g)$ and $\mathcal{B}^\lambda := B_1^\lambda \times B_2^\lambda \cup B_2^\lambda \cup B_1^\lambda$. Then there exist $a_\lambda > 0, k_\lambda > 0$ such that

$$\forall \Psi = h_1 \wedge h_2 : \ \Delta_2 \mathcal{E} < a_\lambda \ \Rightarrow \iint_{(x,y)\in \mathcal{B}^\lambda} \frac{|\Psi(x,y)|^2}{|x-y|} dxdy \geq \frac{k_\lambda}{R_g} \tag{5.39}$$

Remark 5.8. It is not possible to replace R_g^{-1} by d_Ψ.

To prove Proposition 5.4, we need to compare $R_{12}(\Psi)$ and R_g.

5.3.2 On the relation between $R_{12}(\Psi)$ and $\mathbf{R}_g$

Let us consider an almost minimizer for $E^U_{\mathrm{PT}}(2)$:

$$\Psi = h_1 \wedge h_2, \ \mathcal{E}^U_{\mathrm{PT}}(2) - E^U_{\mathrm{PT}}(2) \lesssim a_0 \ll 1, U \text{ big enough.} \tag{5.40}$$

We suppose that $D(|h_1|^2, |h_2|^2) = d_\Psi$ and write ϕ_j the closest function to h_j in $\mathscr{P}$. We write $\delta_j = h_j - \phi_j$. By Propositions 5.2 and 5.3 we have :

$$d_\Psi = \tfrac{1}{R_{12}} \quad \lesssim \varepsilon_0 \quad \text{and} \quad \|\delta_1\|^2_{H^1} + \|\delta_2\|^2_{H^1} \lesssim a_0.$$

We will here compare R_{12} and R_g (defined as $|z_1 - z_2|$ where z_j is the center of ϕ_j).

As $\phi_j(\cdot - z_j)$ is radial and smooth then :

$$0 < \inf_{x\in\mathbb{R}^3} \frac{(|\phi_j|^2 * \frac{1}{|\cdot|})(x)}{\big((|\phi_j|^2 * \frac{1}{|\cdot|^2})(x)\big)^{1/2}} \leq \sup_{x\in\mathbb{R}^3} \frac{(|\phi_j|^2 * \frac{1}{|\cdot|})(x)}{\big((|\phi_j|^2 * \frac{1}{|\cdot|^2})(x)\big)^{1/2}} < +\infty. \tag{5.41}$$

By Newton's Theorem [LL97], writing $|\phi_0|^2 = |\phi_j(\cdot - z_j)|^2$ we have :

$$\forall\, x \in \mathbb{R}^3, \ (|\phi_0|^2 * \tfrac{1}{|\cdot|})(x) = \frac{1}{|x|}\int_{|y|\leq|x|} |\phi_0(y)|dy + \int_{|y|\geq|x|} \frac{|\phi_0(y)|^2}{|y|}dy \leq \frac{1}{|x|}. \tag{5.42}$$

As a consequence, for sufficiently small a_0 :

$$|D(\mathfrak{Re}(\delta_1^*\phi_1), |\delta_2|^2)| \quad \lesssim \|\delta_1\|_{L^2} D(|\phi_1|^2, |\delta_2|^2), \quad |D(\mathfrak{Re}(\delta_1^*\phi_1), |\phi_2|^2)| \quad \lesssim \tfrac{\|\delta_1\|_{L^2}}{\mathrm{R}_g}, \tag{5.43}$$

where we used Cauchy-Schwarz inequality :

$$\int_x |\delta_1(x)^*\phi_1(x)| \tfrac{dx}{|x-y|} \leq \|\delta_1\|_{L^2} \{\int_x |\phi_1(x)|^2 \tfrac{dx}{|x-y|^2}\}^{1/2}.$$

Thus there holds the following.

Proposition 5.5. *Let Ψ be as in* (5.40)*. We write $\|\delta\| = \sum_j \|\delta_j\|$: there exists $\kappa > 0$ such that for sufficiently small $a_0 > 0$:*

$$\begin{aligned} &d_\Psi \geq (1 - \kappa\sqrt{a_0})\big(D(|\phi_1|^2, |\phi_2|^2) + D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2)\big) + D(|\delta_1|^2, |\delta_2|^2), \\ &\iint \tfrac{|h_1(x)|^2|h_2(y)|^2}{|x-y|^2} dxdy \lesssim \frac{1}{R_g^2} + \frac{\|\delta\|_{L^2}\|\delta\|_{H^1}}{R_g} + \|\delta\|^2_{L^2}\|\delta\|_{H^1}, \end{aligned} \tag{5.44}$$

Remark 5.9. In particular $R_{12} = \mathcal{O}(\mathrm{R}_g)$. Moreover for sufficiently small a_0, we have

$$\Delta_1 \mathcal{E} := \sum_j \big(\mathcal{E}_{\mathrm{PT}}(h_j) - E_{\mathrm{PT}}(1)\big) = \Theta(\|\delta\|^2_{H^1}).$$

With the help of Proposition 5.3, we get the following estimates :

$$\iint \frac{|h_1(x)|^2|h_2(y)|^2}{|x-y|^2} dxdy \lesssim a_0^3. \tag{5.45}$$

5.3.3 On the decomposition of $\underline{\psi_1} \wedge \underline{\psi_2}$

In our problem, we consider a couple (a_0, b) described in Lemma 5.3, and we *choose* (α, Λ) such that $U_0 \geq (2+1)U_{\rm c}$.

We consider $\underline{\Psi} = \underline{\psi_1} \wedge \underline{\psi_2}$ of Lemma 5.1. We have : $\mathcal{E}_{\rm PT}^U(\underline{\psi_1} \wedge \underline{\psi_2}) \lesssim \alpha$ and $d_\Psi \lesssim \alpha$.

This result and the estimate of Remark 5.9 lead to the following Lemma.

Lemma 5.2. *For* $(k, k') = (1,2)$ *or* $(2,1)$ *and* $\psi_k(x) = c^{-3/2}\underline{\psi_k}(x/c)$, *we have*

$$\||\psi_{k'}|^2 * \tfrac{1}{|\cdot|} \times \psi_k - (\psi_{k'}^* \psi_k) * \tfrac{1}{|\cdot|} \times \psi_{k'}\|_{L^2}^2 \lesssim \frac{1}{c^2} \iint \frac{|h_1(x)|^2 |h_2(y)|^2}{|x-y|^2} dxdy \lesssim \frac{\alpha^3}{c^2}.$$

Proof : Indeed the quantity in the l.h.s. of (5.2) corresponds to the squared L^2-norm of $(\rho_\Psi * \frac{1}{|\cdot|}\psi_k - R[\gamma_\Psi]\psi_k)$ where $\Psi := \psi_1 \wedge \psi_2$. Then we decompose ψ_k with respect to an orthonormal family (h_1, h_2) with $h_1 \wedge h_2 = \Psi$ and $D(|h_1|^2, |h_2|^2) = d_\Psi$. □

We recall that ψ_1 and ψ_2 are eigenvectors of the mean-field operator with eigenvalues μ_1 and μ_2. In the case $\mu_1 \neq \mu_2$ we cannot choose $\underline{\psi_1} = h_1$ and $\underline{\psi_2} = h_2$.

From the estimation of the μ_j's (5.30) we may ask whether the quantity

$$F_{\mathcal{E}}(\underline{\psi_k}) := \mathcal{E}_{\rm PT}(\underline{\psi_k}) - D(|\underline{\psi_k}|^2, |\underline{\psi_{k'}}|^2) \tag{5.46}$$

is negative and away from 0 or not. As $h_k = \phi_k + \delta_k$ with $\phi_k \in \mathscr{P}$ and $\|\delta_k\|_{H^1} = \mathcal{O}(\sqrt{\Delta_2 \mathcal{E}})$ a simple computation shows that :

$$\forall (a,b) \in \mathbb{C}^2 \cap \mathbb{S}^3 : \ F_{\mathcal{E}}(ah_1 + bh_2) = \frac{3}{2} E_{\rm PT}(1) + \mathcal{O}((\Delta_2 \mathcal{E})^{1/4}). \tag{5.47}$$

5.4 Technical tools

5.4.1 The Cauchy expansion

In this part we use the functions $\mathbf{s}.$, $E(\cdot)$ and $\overline{E}.$ and numbers $\varepsilon_\lambda, a[\Lambda]$ defined in Notation 5.4. We recall Ineq. (5.15). The results stated here follow from [Sok14b, Sok13].

Let $\widetilde{\gamma}$ be the operator defined by :

$$\widetilde{\gamma} = \chi_{(-\infty,0)}(\mathbf{D} + \alpha(v_{\widetilde{\rho}} - R_{\widetilde{Q}})) - P_-^0, \ (\widetilde{Q}, \widetilde{\rho}) \in \mathbf{Q}_1 \times \mathcal{C}.$$

For instance we can take γ of (5.26). Provided that $\|\widetilde{Q}\|_{\rm Kin}, \|\widetilde{\rho}\|_{\mathcal{C}}$ are small enough, by Lemma 5.3 we have

$$|D + \alpha(v_{\widetilde{\rho}} - R_{\widetilde{Q}})| \geq |\mathbf{D}|\big(1 - \alpha(\|\rho_Q\|_{\mathcal{C}} + \|Q\|_{\rm Ex})\big) = |\mathbf{D}|(1 + o(1)).$$

As a result we can expand $\widetilde{g}$ in power of α, this is the Cauchy expansion [HLS05a] :

$$\begin{cases} \widetilde{\gamma} & = & \displaystyle\sum_{j=1}^{+\infty} \alpha^j Q_j[\widetilde{Q}, \widetilde{\rho}], \\ Q_j[\widetilde{Q}, \widetilde{\rho}] & := & -\frac{1}{2\pi} \displaystyle\int_{-\infty}^{\infty} \frac{d\omega}{\mathbf{D} + i\omega} \Big((R_{\widetilde{Q}} - v[\widetilde{\rho}]) \frac{1}{\mathbf{D} + i\omega} \Big)^j. \end{cases} \tag{5.48}$$

We can further expand each Q_j into $\sum_{j=0}^{j} Q_{k,j-k}[\widetilde{Q}, \rho_{\widetilde{Q}}]$ where each $Q_{k,j-k}$ is polynomial in $R_{\widetilde{Q}}$ (resp. $v[\rho_{\widetilde{Q}}]$) of degree k (resp. $j-k$).

The respective densities of $Q_{k,j-k}$ and Q_j are written $\rho_{k,j-k}$ and ρ_j.

Convergence of the series (5.48) In [HLS05a, GLS09], Hainzl *et al.* proved that this series is well-defined and in [Sok14b, Sok13] the functions $(Q_{k,j-k}, \rho_{k,j-k})[\cdot,\cdot]$ are studied in several norms.

It is possible to adapt the proofs to show that these functions are multilinear continuous in $\mathbf{Q}_1 \times \mathcal{C}$ or more generally in the banach spaces $\mathcal{X}_w = \mathbf{Q}_w \times \mathfrak{C}_w$, defined by the following norms :

$$\|Q\|^2_{\mathbf{Q}_w} := \iint (\overline{E}_p + \overline{E}_q) w(p-q) |\widehat{Q}(p,q)|^2 dpdq \text{ and } \|\rho\|^2_{\mathfrak{C}_w} := \iint \frac{w(k)}{|k|^2} |\widehat{\rho}(k)|^2 dk, \tag{5.49}$$

where $\sqrt{w} : \mathbb{R}^3 \to [1, +\infty)$ is a weight function satisfying some sub-additive assumptions.

Furthermore the growth of the norms $\|(Q_{k,j-k}, \rho_{k,j-k})\|_{\mathcal{B}(\mathcal{X}_w)}$ is also polynomial : it follows that there exists some radius $A(\alpha, \Lambda, w)$ such that

$$(\widetilde{Q}, \widetilde{\rho}) \in B_{\mathcal{X}_w}(0, A) \mapsto \Big(\widetilde{\gamma} := \sum_{j=1}^{+\infty} \alpha^j Q_j \big[\widetilde{Q}, \widetilde{\rho}\big], \rho_{\widetilde{\gamma}} \Big) \in B_{\mathcal{X}_g}(0, A),$$

is well-defined and contractant.

The main ingredients of the proof are the following inequalities :

$$\begin{array}{rcl|rcl} \|P^0_{\pm} v_{\widetilde{\rho}} P^0_{\mp} \frac{1}{|D_0|^{a[\Lambda]}}\|_{\mathfrak{S}_2} & \lesssim & \sqrt{\log(\Lambda)} \|\widetilde{\rho}\|_{\mathcal{C}} & \|R_{\widetilde{Q}} \frac{1}{|\nabla|^{1/2}}\|_{\mathfrak{S}_2} & \lesssim & \|\widetilde{Q}\|_{\mathrm{Ex}}, \\ \|v_{\widetilde{\rho}} \frac{1}{|D_0|^{a[\Lambda]}}\|_{\mathfrak{S}_6} & \lesssim & \|\widetilde{\rho}\|_{\mathcal{C}} & \|v_{\widetilde{\rho}} \frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} & \lesssim & \|\widetilde{\rho}\|_{\mathcal{C}} \end{array} \tag{5.50}$$

In the l.h.s. the first estimate follows from a simple computation in Fourier space [HLS05a, Sok14b], and the second one is an application of the KSS inequality (5.13).

In the r.h.s. the first is proved below (Lemma 5.3) and the last follows from an homogeneous Sobolev inequality (5.58). We will say no more about these results and refer the reader to the cited articles and to [Sok14c].

5.4.2 On the minimizers : equation and density

The results of this part are proved in [Sok13].

Let $Q = \gamma + N$ be a minimizer for $E^0(M)$ with $M \in \{1, 2\}$. It satisfies Eq. (5.25)-(5.26) and $\operatorname{rank} N = M$ for α sufficiently small. We recall :

$$\gamma = \chi_{(-\infty,0)}(D_Q) - P^0_-. \tag{5.51}$$

In [HLS05a, Sok14b, Sok13], a fixed-point scheme is used to see γ as a fixed point of some function $F^{(1)}$ (with parameter N). This scheme enables us to get estimates on γ and N. By the Cauchy expansion, Eq. (5.51) is rewritten as follows :

$$\big(\mathrm{Id} - \alpha Q_{1,0}[\cdot]\big)\big[\gamma'\big] = N + \alpha Q_{0,1}\big[\rho'_\gamma\big] + \sum_{j=2}^{+\infty} \alpha^j Q_j \big[\gamma', \rho'_\gamma\big].$$

In [Sok13], it is proved that the linear operator $\big(\mathrm{Id} - \alpha Q_{1,0}[\cdot]\big)$ is a continuous endomorphism for $\mathbf{Q}_g$ and $\mathfrak{S}_p$ $(1 \le p \le 2)$ provided that $\alpha \log(\Lambda) \le L_0$ is small enough.

Its inverse $\mathbf{T}$ is written and it has a uniform bound for all those Banach spaces.

This gives

$$\gamma = \alpha \mathbf{T}[Q_{1,0}(N)] + \alpha \mathbf{T}[Q_{0,1}(\rho'_\gamma)] + \sum_{j=2}^{+\infty} \alpha^j \mathbf{T}\big[Q_j[\gamma', \rho'_\gamma]\big]. \tag{5.52}$$

In [Sok13], the density $\alpha \rho\big[Q_{0,1}(\rho'_\gamma)\big]$ is computed and we have :

$$\alpha \rho\big[Q_{0,1}(\rho'_\gamma)\big] = -\check{f}_\Lambda * \rho'_\gamma,$$

where $\check{f}_\Lambda \in L^1$ with norm $\|\check{f}_\lambda\|_{L^1} \lesssim L$.

Remark 5.10. For the *smooth* cut-off, the same proof applies for $|\cdot|^\ell \check{f}_\Lambda$. For any fixed integer ℓ, there exists $K(\ell) > 0$ such that, if $\alpha \le K(\ell)$ then

$$\begin{aligned} \| |\cdot|^\ell \check{f}_\Lambda \|_{L^1} &\le \Big\{ \int |x|^{2(1+\ell)} (1+|x|^2) |\check{f}_\Lambda(x)|^2 dx \int \frac{dx}{|x|^2(1+|x|^2)} \Big\}^{1/2}, \\ &\lesssim \alpha. \end{aligned} \tag{5.53}$$

The same results hold for

$$\check{F}_\Lambda := \mathscr{F}^{-1}\Big(\frac{f_\Lambda}{1+f_\Lambda}\Big) = \sum_{j=1}^{+\infty}(-1)^{j+1}\check{f}_\Lambda^{*j} \tag{5.54}$$

provided that $\alpha \le K'(\ell)$ with a smaller bound $K'(\ell) \le K(\ell)$.

We write $\tau_j[\cdot] := \rho\big[\mathbf{T}Q_j[\cdot]\big]$ and $\tau_{k,j-k}[\cdot] := \rho\big[\mathbf{T}Q_{k,j-k}[\cdot]\big]$. There holds :

$$\begin{aligned} \rho_\gamma &= -\check{F}_\Lambda * n + (\delta_0 - \check{F}_\Lambda) * \big(\alpha\tau_{1,0}[N] + \sum_{j=2}^{+\infty}\alpha^j\tau_j[\gamma', \rho'_\gamma]\big), \\ &= -\check{F}_\Lambda * n + (\delta_0 - \check{F}_\Lambda) * \big(\alpha\tau_{1,0}[N] + \alpha^2\widetilde{\tau}_2[\gamma', \rho'_\gamma]\big). \end{aligned} \tag{5.55}$$

We have $\rho_\gamma \in L^1$ with $\int \rho_\gamma = -F_\Lambda(0) \times M$. The renormalisation constant Z_3 is

$$Z_3 := 1 - F_\Lambda(0) = \frac{1}{1+f_\Lambda(0)} \approx \frac{1}{1+\frac{2}{3\pi}\alpha\log(\Lambda)} \text{ and } U_0 := \frac{1}{F_\Lambda(0)}. \tag{5.56}$$

We also recall [Sok13]

$$\forall\, k, k' \in B_{\mathbb{R}^3}(0,2) :\ |F_\Lambda(k) - F_\Lambda(k')| \lesssim \alpha|k-k'| \tag{5.57}$$

we will use below with $k' = 0$.

5.4.3 Some inequalities

– Let us recall some Sobolev inequalities in $\mathbb{R}^3$:

$$\|f\|_{L^6} \lesssim \|\nabla f\|_{L^2}, \quad \|f\|_{L^4} \lesssim \||\nabla|^{3/4} f\|_{L^2}, \quad \|f\|_{L^3} \lesssim \||\nabla|^{1/2} f\|_{L^2} \tag{5.58}$$

The last one gives $\|v_{\widetilde{\rho}}\frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} \lesssim \|\widetilde{\rho}\|_{\mathcal{C}}$ for $\widetilde{\rho} \in \mathcal{C}$.

– We also recall Kato's inequality and Hardy's inequality :

$$\left\{\begin{aligned} \int_{\mathbb{R}^3}\frac{|\phi(x)|^2}{|x|}dx &\le \tfrac{\pi}{2}\langle|\nabla|\phi\,,\,\phi\rangle, \\ \int_{\mathbb{R}^3}\frac{|\phi(x)|^2}{|x|^2}dx &\le 4\langle(-\Delta)\phi\,,\,\phi\rangle. \end{aligned}\right. \tag{5.59}$$

– The following Lemma gives estimates about the operator R_Q.

Lemma 5.3. *Let $Q(x,y)$ be an operator of finite exchange term and ρ of finite Coulomb energy, then :*

$$\left\{\begin{aligned} \|\tfrac{1}{|\nabla|^{1/2}}R_Q\|_{\mathfrak{S}_2} &= \mathrm{Tr}(R_Q^*\tfrac{1}{|\nabla|}R_Q) \le \Big(\int\frac{dy}{|y|^2|y-\mathbf{e}|^2}\Big)^2\mathrm{Tr}(Q^*R_Q), \\ \iint\frac{|Q(x,y)|^2}{|x-y|}dxdy &= \mathrm{Tr}(Q^*R_Q) \le \tfrac{\pi}{2(2\pi)^3}\iint|u||\widehat{Q}(u+k/2, u-k/2)|^2dudk, \\ \|v_\rho\tfrac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} &\lesssim \|\rho\|_{\mathcal{C}}. \end{aligned}\right.$$

In particular $\|(v_\rho - R_Q)f\|_{L^2} \lesssim (\|\rho\|_{\mathcal{C}} + \|Q\|_{\mathrm{Ex}})\||\nabla|^{1/2}f\|_{L^2}$.

Proof : The proof for $\|\frac{1}{|\nabla|^{1/2}}R_Q\|_{\mathfrak{S}_2}$ is just an application of the Cauchy-Schwarz inequality once we remark that $|\nabla|^{-1}$ is the convolution by Const$/|\cdot|^2$ [LL97]. For the last inequality we write $s = \frac{x+y}{2}$ and $t = x-y$ and $A(s,t) := Q(s+t/2, s-t/2)$ *a.e.* By Kato's inequality :

$$\begin{aligned} \iint\frac{|Q(x,y)|^2}{|x-y|}dxdy &= \iint\frac{|A(s,t)|^2}{|t|}dsdt \\ &\le \frac{\pi}{2}\int ds\langle|\nabla|A(s,\cdot)\,,\,A(s,\cdot)\rangle \\ &\le \frac{\pi}{2}\iint|u||\widehat{Q}(u+k/2, u-k/2)|dudk. \end{aligned}$$

Those inequalities are true at least for $Q(x,y)$ in the Schwartz class $\mathcal{S}(\mathbb{R}^3\times\mathbb{R}^3)$, we conclude by density. □

– To end this part we give estimates about $\mathbf{D}$.

We have

$$\mathrm{Id}-\mathbf{s}_p\mathbf{s}_q=\mathbf{s}_p(\mathbf{s}_p-\mathbf{s}_q)=(\mathbf{s}_p-\mathbf{s}_q)\mathbf{s}_q$$

and

$$|\mathrm{Id}-\mathbf{s}_p\mathbf{s}_q|\le|\mathbf{s}_p-\mathbf{s}_q|=\Big|\frac{\widehat{D_0}(p)}{E(p)}-\frac{\widehat{D_0}(p)}{E(q)}+\frac{\widehat{D_0}(p)-\widehat{D_0}(q)}{E(q)}\Big|\le\frac{2|p-q|}{\max(E(p),E(q))}. \tag{5.60}$$

Notation 5.7. The symbol $\mathbf{e}$ will always stand for any unitary vector in $\mathbb{R}^3$.

Remark 5.11. There holds (*cf* [LL97] for the expression of $(a^2-\Delta)^{-1}$) :

$$\begin{aligned}\frac{1}{|D_0|}(x-y)&=\frac{2}{\pi}\int_0^{+\infty}\frac{d\omega}{|D_0|^2+\omega^2}(x-y)\\&=\sqrt{\frac{2}{\pi}}\int_0^{+\infty}\frac{e^{-E_\omega|x-y|}}{|x-y|}d\omega\\&=\mathrm{Cnst}\tfrac{\mathrm{K}_1(|x-y|)}{|x-y|}\end{aligned}$$

where K_1 is the modified Bessel function [Wat22].

5.5 Proof of Proposition 5.1

5.5.1 *A priori* estimates on a minimizer for $E^0(2)$

This part is devoted to prove (5.62).

Let us say $\gamma'=\gamma+N$ is a minimizer for $E^0(2)$ written as in (5.25)-(5.26).

First we prove (5.27). There holds *a priori* estimates [Sok13] :

$$\frac{1}{2}\mathrm{Tr}\big(\frac{-\Delta(1-\frac{\Delta}{\Lambda^2})}{|D_0|}(\gamma')^2\big)+\frac{\alpha}{2}\|\rho'_\gamma\|_{\mathcal{C}}^2\le\mathcal{E}(\gamma')-2+\frac{\alpha}{2}\mathrm{Tr}(\gamma' R[\gamma'])\le\frac{\alpha\pi}{4}\mathrm{Tr}(|\nabla|(\gamma')^2)$$

where we have used $|\mathbf{D}|-1\ge\frac{1}{2}\frac{-\Delta\left(1-\frac{\Delta}{\Lambda^2}\right)}{|D_0|}$. It follows that :

$$\mathrm{Tr}\big(\frac{-\Delta(1-\frac{\Delta}{\Lambda^2})}{|D_0|}(\gamma')^2\big)+\alpha\|\rho'_\gamma\|_{\mathcal{C}}^2\le K\alpha.$$

As in [Sok13], we can apply a fixed point scheme on (γ,ρ_γ) with the help of the self-consistent equation (in $\mathbf{Q}_1\times\mathcal{C}$ for instance). This gives :

$$\|\gamma\|_{\mathbf{Q}_1}\lesssim\sqrt{L\alpha}\|\rho'_\gamma\|_{\mathcal{C}}+\alpha\||\nabla|^{1/2}\gamma'\|_{\mathfrak{S}_2}\text{ and }\|\rho_\gamma\|_{\mathcal{C}}\lesssim L\|\rho'_\gamma\|_{\mathcal{C}}+\sqrt{L\alpha}\||\nabla|^{1/2}\gamma'\|_{\mathfrak{S}_2}.$$

Hence $|\mathrm{Tr}_0(\gamma)|\le\|\gamma\|_{\mathfrak{S}_2}<1$ and $\mathrm{Tr}_0(\gamma)=0$ as shown in [HLS05a]. This proves $\mathrm{Tr}(N)=\mathrm{Tr}_0(N)=\mathrm{Tr}_0(\gamma')-\mathrm{Tr}_0(\gamma)=2$.

Let $(\psi_i)_{1\le i\le 2}$ be a basis of orthonormal eigenvectors of $\chi_{0,\mu}(D_{\gamma'})$ with eigenvalues $0<\mu_1\le\mu_2<1$. We write $N_j:=|\psi_j\rangle\langle\psi_j|$ and $|n_j:=\psi_j|^2$. From the equation satisfied by ψ_j

$$(\mathbf{D}+\alpha(v[\rho_\gamma+n]-R[\gamma+N]))\psi_j=\mu_j\psi_j \tag{5.61}$$

we get the following.

Lemma 5.4. *Let γ' and $(\psi_j)_j$ be as above in the regime of Remark 5.4. Then there holds :*

$$\begin{cases}\frac{1}{(2\pi)^3}\displaystyle\int|p|^2\big(\Lambda^{-2}(2+\tfrac{|p|^2}{\Lambda^2})+(1+\tfrac{|p|^2}{\Lambda^2})\big)|\widehat{\psi}_j(p)|^2dp\le\|\mathbf{D}\psi_j\|_{L^2}^2-1\text{ and}\\\|\mathbf{D}\psi_j\|_{L^2}^2-1\le\alpha\|\rho_\gamma\|_{\mathcal{C}}\|n_j\|_{\mathcal{C}}+\alpha\|\gamma\|_{\mathfrak{S}_2}\|R[N_j]\|_{\mathfrak{S}_2}+\big(\alpha\|B_{\gamma'}\frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}}\||\nabla|^{1/2}\psi_j\|_{L^2}\big)^2.\end{cases}$$

As a consequence we also have :

$$\mathrm{Tr}(-\Delta(1-\tfrac{\Delta}{\Lambda^2}+\tfrac{\Delta^2}{\Lambda^4})N)\lesssim c^{-2}. \tag{5.62}$$

It suffices to use the inequalities in the r.h.s. of (5.50) in Eq. (5.61).

Remark 5.12. Compared to the case of $E^0(1)$ there is an additional term $(v_n - R_N)\psi_j$ that has been neglected in $-2\alpha\mathfrak{Re}\langle B_N\psi_j\,,\,\psi_j\rangle$: this term is non-positive.

Notation 5.8. From now on, we write $v_{jk} = (\psi_j^*\psi_k) * \frac{1}{|\cdot|}$ and $v_j := v_{jj}$ and define $a_{jk} := \|v_k\psi_j - v_{kj}\psi_k\|_{L^2}$.

5.5.2 Proof of Lemma 5.1 : estimate of $E^0(1)$

We compute the energy of a particular test function $Q_0' = Q_0 + N_0$, defined as follows [Sok14b]. First, we take $\phi_{\rm CP} = \phi_1$ a minimizer for $E_{\rm PT}(1)$ in $L^2(\mathbb{R}^3,\mathbb{C})$ (*e.g.* real-valued and positive centered in 0, *cf* [Lie77]). Then let ψ_1 be :

$$\psi_1 := {}^t(\,\phi_1\ \ 0\ \ 0\ \ 0\,) \in L^2(\mathbb{R}^3,\mathbb{C}^4). \tag{5.63}$$

Then, we define $\psi_{\frac{1}{c}} := c^{-3/2}\psi_1(c^{-1}(\cdot))$ where $c^{-1} := \alpha^2 F_\Lambda(0)$ and

$$\begin{array}{ll|ll} \overline{N}_0 & := |\psi_{\frac{1}{c}}\rangle\langle\psi_{\frac{1}{c}}|, & Q_0 + P_-^0 = \Pi_0 & := \chi_{-\infty,0}\big\{\mathbf{D} + \alpha\big((\rho_{Q_0} + \overline{n}_0) * \frac{1}{|\cdot|} - (R_{Q_0} + R_{\overline{N}_0})\big)\big\}, \\ \overline{n}_0 & := |\psi_{\frac{1}{c}}|^2, & \psi_0 & := \frac{1}{\sqrt{1 - \|\Pi_0\psi_{\frac{1}{c}}\|_{L^2}^2}}(\psi_{\frac{1}{c}} - \Pi_0\psi_{\frac{1}{c}}). \end{array}$$

We have used the fixed point scheme of Section 5.4.1 to define Q_0. We also write

$$\begin{array}{ll|ll} N_0 & := |\psi_0\rangle\langle\psi_0|, & Q_0' & := Q_0 + N_0, \\ B_0 & := (\rho_{Q_0} + \overline{n}_0) * \frac{1}{|\cdot|} - \alpha(R_{Q_0} + R_{\overline{N}_0}), & \mathbf{D}_{Q_0} & := \mathbf{D} + \alpha B_0. \end{array}$$

The test function Q_0' is the difference between the orthogonal projections $\Pi_0 + N_0$ and P_-^0. Following the same method as in [Sok14b], the following estimates hold.

$$\begin{array}{ll|ll} \|Q_0\|_{\mathbf{Q}_{w_2}} & \lesssim \alpha & \|\overline{n}_0\|_{\mathfrak{C}_{w_2}} & \lesssim c^{-1/2} \\ \|Q_0\|_{\mathbf{Q}_{w_1}} & \lesssim c^{-1} & \|\rho_{Q_0}\|_{\mathfrak{C}_{w_2}} & \lesssim Lc^{-1/2} \\ \|Q_0\|_{\mathfrak{S}_2} & \lesssim \alpha c^{-1/2} & \|R_{\overline{N}_0}\|_{\mathfrak{S}_2} & \lesssim c^{-1} \end{array} \tag{5.64}$$

where $w_1(p-q) = E(p-q)$ and $w_2(p-q) = E(p-q)^2$.

As shown previously in [Sok14b, Sok13] there holds

$$\begin{array}{rl} \mathcal{E}_{\rm BDF}(Q_0') = & \langle \mathbf{D}\psi_0\,,\,\psi_0\rangle - \frac{\alpha}{2}\mathrm{Tr}_0(B[Q_0]Q_0) - \frac{1}{2}(\mathrm{Tr}(|\mathbf{D} + \alpha B_0|Q_0^2) - \mathrm{Tr}(|\mathbf{D}|Q_0^2)) \\ & + \frac{\alpha}{2}\big(D(\rho[Q_0] + n_0, \rho[Q_0] + n_0) - \mathrm{Tr}(Q_0'R[Q_0'])\big) \end{array} \tag{5.65}$$

Estimate of the density ρ_{Q_0} By Section 5.4.2, we write

$$\rho_{Q_0'} = (\delta_0 - \check{F}_\Lambda) * (\overline{n}_0 + \mathfrak{t}[\overline{N}_0] + \alpha^2\widetilde{\tau}_2), \tag{5.66}$$

$$= (\delta_0 - \check{F}_\Lambda) * \overline{n}_0 + \tau_{rem}. \tag{5.67}$$

We have

$$\|(\delta_0 - \check{F}_\Lambda) * \overline{n}_0 * \tfrac{1}{|\cdot|}\|_{L^\infty} \le \frac{\pi}{2}(1 + \|\check{F}_\Lambda\|_{L^1})\langle|\nabla|\psi_{\frac{1}{c}}\,,\,\psi_{\frac{1}{c}}\rangle \lesssim \|\nabla\psi_{\frac{1}{c}}\|_{L^2} = \mathcal{O}(c^{-1}).$$

We use Ineq. (5.50) to estimate the norm $\|\tau_{rem}\|_{\mathcal{C}}$ of the remainder τ_{rem}.

The traces in (5.65) By Lemma 5.3, we can estimate $\big|\mathbf{D} + \alpha B_0\big| - \big|\mathbf{D}\big|$ and get the following [Sok14b].

Lemma 5.5. *There holds :*

$$\begin{array}{rl} |\delta\mathrm{Tr}| & := \Big|\mathrm{Tr}\big\{|\mathbf{D} + \alpha B[Q_0']|\gamma_0^2 - |\mathbf{D}|Q_0^2\big\}\Big| \\ & \lesssim \{\|Q_0\|_{\mathcal{B}}^2 + \alpha(\|Q_0\|_{Kin} + \|\tau_{rem}\|_{\mathcal{C}})\}\|Q_0\|_{Kin}^2 + \alpha\{\|\tau_{rem}\|_{\mathcal{C}} + \|\nabla\psi_{\frac{1}{c}}\|_{L^2}\}\|Q_0\|_{\mathfrak{S}_2}^2 \\ & \lesssim \alpha c^{-3} + \alpha c^{-1} \times \alpha^2 c^{-1} \lesssim \alpha c^{-3}. \end{array} \tag{5.68}$$

$\langle \mathbf{D}\psi_0 \,,\, \psi_0\rangle$ **in** (5.65) There holds $(1-\Pi_0)\psi_{\frac{1}{c}} = -Q_0\psi_{\frac{1}{c}} + P^0_+\psi_{\frac{1}{c}}$. Then

$$\begin{aligned}
\langle \mathbf{D}\psi_{\frac{1}{c}} \,,\, \psi_{\frac{1}{c}}\rangle &= \langle \mathbf{D}Q_0\psi_{\frac{1}{c}} \,,\, Q_0\psi_{\frac{1}{c}}\rangle - 2\mathfrak{Re}\langle P^0_+Q_0\psi_{\frac{1}{c}} \,,\, P^0_+\psi_{\frac{1}{c}}\rangle + \langle |\mathbf{D}|P^0_+\psi_{\frac{1}{c}} \,,\, \psi_{\frac{1}{c}}\rangle \\
\langle |\mathbf{D}|P^0_+\psi_{\frac{1}{c}} \,,\, \psi_{\frac{1}{c}}\rangle &= 1 + \tfrac{1}{2}\|\nabla\psi_{\frac{1}{c}}\|^2_{L^2} + \mathcal{O}(c^{-4}).
\end{aligned}$$

Then thanks to Lemma 5.3 : $\||\mathbf{D}|^{1/2}Q_0\psi_{\frac{1}{c}}\|_{L^2} \le \||\mathbf{D}|^{1/2}Q_0\frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}}\||\nabla|^{1/2}\psi_{\frac{1}{c}}\|_{L^2}$ and

$$\||\mathbf{D}|^{1/2}Q_0\psi_{\frac{1}{c}}\|_{L^2} \lesssim \alpha c^{-1}.$$

As $Q_0 = \alpha Q_1[Q_0', \rho'_{Q_0}] + \alpha^2\widetilde{Q}_2[Q_0', \rho'_{Q_0}]$ and that $Q_1 = Q_1^{+-} + Q_1^{-+}$:

$$P^0_+Q_0\psi_{\frac{1}{c}} = \alpha Q_1^{+-}P^0_-\psi_{\frac{1}{c}} + \alpha^2 P^0 + \widetilde{Q}_2\psi_{\frac{1}{c}}.$$

Therefore :

$$\begin{aligned}
\alpha^2\langle |\mathbf{D}|\widetilde{Q}_2\psi_{\frac{1}{c}} \,,\, P^0 + \psi_{\frac{1}{c}}\rangle &\le \alpha^2\||\nabla|^{1/2}\psi_{\frac{1}{c}}\|^2_{L^2}\|\tfrac{|\mathbf{D}|}{|\nabla|^{1/2}}\widetilde{Q}_2\tfrac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} \\
&\lesssim \alpha^2c^{-1}\times c^{-1} = \mathcal{O}(\alpha^2c^{-2}) \\
\alpha\langle |\mathbf{D}|Q_1^{+-}P^0_-\psi_{\frac{1}{c}} \,,\, P^0_+\psi_{\frac{1}{c}}\rangle &\le \alpha\||\mathbf{D}|^{1/2}Q_1^{+-}\tfrac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}}\||\nabla|^{1/2}P^0_-\psi_{\frac{1}{c}}\|_{L^2}\||\mathbf{D}|^{1/2}\psi_{\frac{1}{c}}\|_{L^2} \\
&\lesssim \alpha c^{-1/2}\times c^{-3/2} = \mathcal{O}(\alpha c^{-2}).
\end{aligned}$$

Hence :

$$\langle \mathbf{D}(1-\Pi_0)\psi_{\frac{1}{c}} \,,\, (1-\Pi_0)\psi_{\frac{1}{c}}\rangle/(1-\|\Pi_0\psi_{\frac{1}{c}}\|^2_{L^2}) = 1 + \frac{1}{2}\|\nabla\psi_{\frac{1}{c}}\|^2_{L^2} + \mathcal{O}(\alpha c^{-2}). \tag{5.69}$$

The potential energy in (5.65) By the same methods we prove :

$$\begin{aligned}
&\tfrac{\alpha}{2}\big(2D(\rho[Q_0], n_0) - D(\rho[Q_0], \overline{n}_0) - \mathfrak{Re}(2\mathrm{Tr}(Q_0R[N_0]) - \mathrm{Tr}(Q_0R[\overline{N}_0]))\big) \\
&\quad = -\tfrac{\alpha}{2}D(\check{F}_\Lambda * \overline{n}_0, \overline{n}_0) + \mathcal{O}(\alpha^2c^{-3/2}).
\end{aligned} \tag{5.70}$$

For instance by Cauchy-Schwarz inequality followed by Hardy inequality :

$$\big|D\big(\rho[Q_0], (P^0_+\psi_{\frac{1}{c}})^*(Q_0\psi_{\frac{1}{c}})\big)\big| \le \|\rho[Q_0]\|_{\mathcal{C}} \times 4^{1/4}\|\nabla\psi_{\frac{1}{c}}\|^{1/2}_{L^2}\|Q_0\psi\|_{L^2} = \mathcal{O}(c^{-3}).$$

By Ineq. (5.57), there holds :

$$-\frac{\alpha}{2}D(\check{F}_\Lambda * \overline{n}_0, \overline{n}_0) = -\frac{1}{2c}D(\overline{n}_0, \overline{n}_0) + \mathcal{O}(\alpha^2c^{-2} + c^{-1}\|\overline{n}_0\|^2_{L^2}) = \mathcal{O}(\alpha^2c^{-2});$$

indeed : $\|\overline{n}_0\|_{L^2} = \|\psi_{\frac{1}{c}}\|^2_{L^4} \lesssim \||\nabla|^{3/4}\psi_{\frac{1}{c}}\|^2_{L^2}$. As a consequence :

$$E^0_{\mathrm{BDF}}(1) \le \mathcal{E}_{\mathrm{BDF}}(Q_0 + N_0) = 1 + \frac{\mathcal{E}_{\mathrm{PT}}(\phi_1)}{2c^2} + \mathcal{O}(\alpha c^{-2}). \tag{5.71}$$

We have proved the inequality the $\le$ part. For the $\ge$ part, it suffices to take a *real* minimizer and with the same estimates as above and [Sok14b] we prove similar estimates.

That there exists a minimizer for $E^0(1)$ follows from Theorem 5.1, using the same method as in [Sok14b]. We have proved $E^0(1) < 1$, then by Lieb's variational principle we get that for any $0 < q < 1$, $E^0(q) > qE^0(1)$, hence the binding inequalities holds for $0 < q < 1$. For $q \in [0,1]^c$, binding inequalities hold for sufficiently small α. We refer to [Sok14b] for more details.

Similar estimates apply for $E^0(2)$, in particular we have $E^0(2) \le 2E^0(1) \le 2 + \frac{\mathcal{E}_{\mathrm{PT}}(\phi_1)}{2c^2} + \mathcal{O}(\alpha c^{-2})$.

5.5.3 Study of a minimizer γ' for $E^0(2)$

Bootstrap argument We write $x^2 := \mathrm{Tr}(-\Delta(1 - \frac{\Delta}{\Lambda^2} + \frac{\Delta^2}{\Lambda^4})N)$. By Lemma 5.4, we have $x^2 \lesssim c^{-2}$. This fact enables us to use the method of [ES01, Sok14b].

We scale ψ_j by c : $\underline{\psi_j}(x) = c^{3/2}\psi_j(cx)$ and scale γ accordingly : $\underline{\gamma}(x,y) = c^3\gamma(cx,cy)$. Then writing $\mathcal{L}_A := (1 - \Delta/A^2)$, the wave function $\underline{\psi_j}$ satisfies :

$$(c^2\beta - ic\boldsymbol{\alpha}\cdot\nabla)\underline{\psi_j} + \alpha c\mathcal{L}_{c\Lambda}^{-1}(v[\rho[\underline{\gamma}] + \underline{n}] - R[\underline{g} + \underline{N}])\underline{\psi_j} = c^2\mu_j\mathcal{L}_{c\Lambda}^{-1}\underline{\psi_j}. \tag{5.72}$$

Splitting $\underline{\psi_j}$ between upper spinor $\underline{\varphi_j}$ and lower spinor $\underline{\chi_j}$ both in $L^2(\mathbb{R}^3, \mathbb{C}^2)$, this gives :

$$\|\underline{\chi_1}\|_{L^2} + \|\underline{\chi_2}\|_{L^2} \lesssim c^{-1}.$$

Going back to ψ_j one gets $\langle \mathbf{D}\psi_j\,,\,\psi_j\rangle = 1 + \mathcal{O}(c^{-2})$ and it shows that for $j = 1,2 : 0 < (1-\mu_j)c^2 \le K$ thanks to the equation (5.27). As

$$0 \le c^2(1 - \mathcal{L}_{c\Lambda}^{-1}) = \frac{-c^2\Delta}{c^2\Lambda^2 - \Delta} \le \frac{-\Delta}{\Lambda^2},\ \text{then} \tag{5.73}$$

$$\begin{aligned} c^2(\mu_j\mathcal{L}_{c\Lambda} - 1)\underline{\varphi_j} &= c^2(\mu_j - 1)\underline{\varphi_j} + \tfrac{c^2\Delta}{c^2\Lambda^2 - \Delta}\underline{\varphi_j} \\ &= c^2(\mu_j - 1)\underline{\varphi_j} + \mathcal{O}_{L^2}\big(\tfrac{c}{\Lambda}\big) \end{aligned}$$

thanks to Lemma 5.1 ($\mathcal{O}_{L^2}$ means in L^2-norm). We can get another estimate : in the spirit of [Sok14b, Sok13] we can use bootstrap argument with the norms

$$\|Q\|^2_{\mathbf{Q}_w} = \iint E(p-q)^{2k}(E(p+q))|\widehat{Q}(p,q)|^2 dp dq \text{ and } \|\rho\|^2_{\mathfrak{C}_w} = \int \frac{E(k)^2|\widehat{\rho}(k)|^2}{|k|^2}dk,$$

to get the following statement :

Lemma 5.6. *For any fixed $k \in \mathbb{N}^*$, there exists $\alpha_{(k)} > 0$ such that for $\alpha \le \alpha_{(k)}$, ψ_j with $j = 0,1,2$ is in $H^{k/2}$ with norms $\mathcal{O}(1)$ and*

$$\|\gamma_0\|_{\mathbf{Q}_w}, \|\gamma\|_{\mathbf{Q}_w}, \|\rho[\gamma]\|_{\mathfrak{C}_w}, \|\rho[\gamma_0]\|_{\mathfrak{C}_w} \lesssim 1.$$

It is supposed $\alpha\log(\Lambda) \le L_0$. There also holds :

$$\|\Delta\psi\|_{L^2} \lesssim \min(c^{-1}(c^{-1} + \Lambda^{-1}), c^{-3/2}),\ \|\underline{\chi}\|_{L^2} \lesssim c^{-1} \text{ and } \|\nabla\underline{\chi}\|_{L^2} \lesssim c^{-1},$$

The estimation of $\mathcal{E}_{\mathrm{BDF}}(\gamma')$ is proven with the help of the estimate $\|\Delta\psi\|_{L^2} \lesssim c^{-3/2}$ as shown in the (technical) proof of Lemma 5.6 in Appendix 5.A.2.

Remark 5.13. By Estimate (5.62) we can prove that n, γ, ρ_γ have estimates of the same kind of those stated in (5.64) [Sok14b, Sok13] : we have

$$\|n\|_{\mathcal{C}} \lesssim c^{-1/2},\ \|\rho_\gamma\|_{\mathcal{C}} \lesssim Lc^{-1/2},\ \|R_{N_j}\|_{\mathfrak{S}_2} \lesssim c^{-1}, \||\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2} \lesssim c^{-1}, \|\gamma\|_{\mathfrak{S}_2} \lesssim \alpha c^{-1/2}. \tag{5.74}$$

There also holds $\|n_j\|_{L^2} \lesssim c^{-3/2}$.

By Lemma 5.6, we get :

$$\|\rho_\gamma\|_{L^2} \lesssim Lc^{-3/2}.$$

Following [Sok13] we can prove $\rho_\gamma \in L^1$ and $\|\rho_\gamma\|_{L^1} \lesssim L$.

Estimate on $c^2(1-\mu_j)$ Using estimates on $\nabla\varphi_j$ and $\nabla\chi_j$ (Lemma 5.6) together with Ineq. (5.57), we get the following estimate from (5.27) :

$$\mu_j = 1 + \frac{\|\nabla\underline{\varphi_j}\|^2_{L^2}}{2c^2} - \frac{1}{c^2}D(\underline{n_j}, \underline{n}) + \mathcal{O}(\alpha c^{-2}). \tag{5.75}$$

With (5.46)-(5.47), we get :

$$(1-\mu_j)c^2 \le -\tfrac{3}{2}E_{\mathrm{PT}}(1) + \mathcal{O}(\alpha^{1/4}) \gtrsim 1. \tag{5.76}$$

5.6 Localisation of minimizers in Direct space

5.6.1 Decay estimates on the $\underline{\psi_j}$'s

It is known $\underline{\psi_1} \wedge \underline{\psi_2}$ can be split into two almost minimizers of Choquard-Pekar energy h_1 and h_2 : $h_1 \wedge h_2 = \underline{\psi_1} \wedge \underline{\psi_2}$. For $j \in \{1, 2\}$, we write $\phi_j \in \mathscr{P}$ the closest Pekar minimizer to h_j and its center is written z_j. We write

$$\mathrm{R}_g := |z_1 - z_2|. \tag{5.77}$$

By Section 5.3, we have :

$$M^2(\underline{\psi_1} \wedge \underline{\psi_2}) := \iint \frac{|\underline{\psi_1} \wedge \underline{\psi_2}(x, y)|^2}{|x - y|} dxdy \gtrsim \frac{1}{\mathrm{R}_g}. \tag{5.78}$$

Our aim is to show decay estimates far away from z_1 and z_2. Up to translations, we assume the mean $z_m = \frac{z_1+z_2}{2}$ is 0.

Localisation functions Let $\xi_1 \geq 0$ be some *radial* Schwartz function in $\mathcal{S}(\mathbb{R}^3)$ satisfying

$$|x| \leq 1 \Rightarrow \xi_1(x) = 1 \text{ and } |x| \geq 2 \Rightarrow \xi_1(x) = 0.$$

We define $\xi_A(x) := \xi_1(\frac{x}{A})$ for any $A > 0$ and $\theta_A := \sqrt{1 - \xi_A^2}$. For any $x \in \mathbb{R}^3$ we write

$$d(x) := \min\{|x - z_1|, |x - z_2|\}. \tag{5.79}$$

Let H be the plane $\{x : \ |x - z_1| = |x - z_2|\}$; the function $d(\cdot)$ is differentiable in $\mathbb{R}^3 \backslash \big(\{z_1, z_2\} \cup H\big)$. For any $A \gg \mathrm{R}_g$ and $0 < \lambda < 2$ we define

$$\boldsymbol{\eta}^{\lambda}_{\mathrm{R}_g}(x) := \big(1 - \xi^2_{\lambda \mathrm{R}_g}(x - z_1) - \xi^2_{\lambda \mathrm{R}_g}(x - z_2)\big)^{1/2}. \tag{5.80}$$

We define $\lambda_0 > 0$, defined by the formula

$$\lambda_0 \mathrm{R}_g = \tfrac{C_0}{L} \text{ where } C_0(L, \mathrm{R}_g) > 1 \text{ is chosen large.} \tag{5.81}$$

The function $\boldsymbol{\eta}^{\lambda}_{\mathrm{R}_g}$ can be seen as the dilation of $\boldsymbol{\eta}^{\lambda}_1 := \sqrt{1 - \xi^2_{\lambda}(\cdot - e_1) - \xi^2_{\lambda}(\cdot - e_2)}$ by R_g where $e_j := \frac{z_j - z_m}{\mathrm{R}_g}$.

At last we define :

$$\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(x) := \sqrt{1 - \xi^2_{c\lambda \mathrm{R}_g}(x - cz_1) - \xi^2_{c\lambda \mathrm{R}_g}(x - cz_2)}, \tag{5.82}$$

we use it in Section 5.D.2.

Lemma 5.7. • *For each $\lambda_0 \leq \lambda < 2^{-1}$, there exists K_λ such that :*

$$\forall A > 0, \ \int d(x)^2 \xi_A^2(x) (\boldsymbol{\eta}^{\lambda}_{R_g}(x))^2 \Big(\big||D_0|^{1/2} \underline{\psi_1}(x)\big|^2 + \big||D_0|^{1/2} \underline{\psi_2}(x)\big|^2 \Big) dx \quad \leq K_\lambda \tag{5.83}$$

Moreover we can choose $(K_\lambda)_\lambda$ to be nonincreasing and K_{λ_0} is (uniformly) bounded in the regime α, L, Λ^{-1} small.

• *For any $2\lambda_0 \leq \lambda < 2^{-1}$ the same holds for $d^{(2)}_{A,\lambda} := d(x)^2 \xi_A \boldsymbol{\eta}^{(\lambda)}_{cR_g}$:*

$$\int d(x)^4 \xi_A^2(x) (\boldsymbol{\eta}^{(\lambda)}_{cR_g})^2(x) \Big(\big||D_0|^{1/2} \underline{\psi_1}(x)\big|^2 + \big||D_0|^{1/2} \underline{\psi_2}(x)\big|^2 \Big) dx \leq K'_\lambda, \tag{5.84}$$

where $K'_\lambda > K_\lambda$ depends on $\lambda, K_\lambda, \xi_1$.

• *We can replace $|D_0|^{1/2} \underline{\psi_j}$ by $\underline{\psi_j}$ above.*

Remark 5.14. This is a weak estimate due to the presence of $\underline{v}_k \underline{\psi_j} - \underline{v}_{kj} \underline{\psi_k}$.

This proposition is proved in Appendix 5.C.1.

5.6.2 Localisation operators

We want to prove that minimizers are localised in space around the centers z_1, z_2 of the electrons. To this end we use localisation operators of [HLS09, LR12] with respect to the functions $\xi_{c\lambda\mathrm{R}_g}$ and $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}$ introduced in the previous Section (5.6.1).

By Lemma 5.7 we know that the wave functions $\underline{\psi_1}$ and $\underline{\psi_2}$ are localized near z_1 and z_2. By scaling, it follows that ψ_1 and ψ_2 are localized near cz_1 and cz_2. We consider :

$$\begin{aligned} \xi_1^{(\lambda)}(x) &:= \xi_{c\lambda\mathrm{R}_g}(x - cz_1) \qquad \text{and} \qquad \xi_2^{(\lambda)}(x) := \xi_{c\lambda\mathrm{R}_g}(x - cz_2), \\ X_1^{(\lambda)} &:= (\xi_1^{(\lambda)})^{++} + (\xi_1^{(\lambda)})^{--} \qquad \text{and} \qquad X_2^{(\lambda)} := (\xi_2^{(\lambda)})^{++} + (\xi_2^{(\lambda)})^{--}, \end{aligned}$$

and localise γ' :

$$\xi_1^{(\lambda)} \cdot [\gamma'] := X_1^{(\lambda)}(\gamma')X_1^{(\lambda)},\ \xi_2^{(\lambda)} \cdot [\gamma'] = X_2^{(\lambda)}(\gamma')X_2^{(\lambda)}.$$

We define the set

$$B_\lambda := \big\{B(cz_1, c\lambda\mathrm{R}_g) \times B(cz_2, c\lambda\mathrm{R}_g)\big\} \cup \big\{B(cz_2, c\lambda\mathrm{R}_g) \times B(cz_2, c\lambda\mathrm{R}_g)\big\} \subset \mathbb{R}^3 \times \mathbb{R}^3. \tag{5.85}$$

Our aim in this section is to prove :

Proposition 5.6. *If γ' is a minimizer of $E^0(2)$ in the regime α, L, Λ^{-1} small then :*

$$\mathcal{E}^0_{BDF}(\gamma') = \mathcal{E}^0_{BDF}(\xi_1^{3^{-1}} \cdot [\gamma']) + \mathcal{E}^0_{BDF}(\xi_2^{3^{-1}} \cdot [\gamma']) + \frac{\alpha}{2}\iint_{(x,y)\in B_{3^{-1}}} \frac{|\psi_1 \wedge \psi_2(x,y)|^2}{|x-y|}dxdy + \mathcal{O}\Big(\frac{1}{c^2 R_g}\Big). \tag{5.86}$$

Moreover :

$$\begin{cases} \mathrm{Tr}_0(\xi_j^{(\frac{1}{3})} \cdot [\gamma']) = 1 + \varepsilon_j,\ \varepsilon_j = o(1), j = 1,2, \\ \mathrm{Tr}_0(\xi_1^{(\frac{1}{3})} \cdot [\gamma']) + \mathrm{Tr}_0(\xi_2^{(\frac{1}{3})} \cdot [\gamma']) = 2 + \mathcal{O}\Big(\dfrac{1}{c^2 R_g}\Big). \end{cases} \tag{5.87}$$

Assuming this Proposition – proved in Subsection (5.6.5) – we can prove Theorem 5.2.

5.6.3 Proof of Theorem 5.2

By Proposition 5.4, for sufficiently small α, L, there holds :

$$\frac{\alpha}{2}\iint_{(x,y)\in B_{3^{-1}}} \frac{|\psi_1 \wedge \psi_2(x,y)|^2}{|x-y|}dxdy \geq \frac{L^{-1}}{c^2 K_{\mathrm{g}} \mathrm{R}_g},$$

for some constant $K_{\mathrm{g}} > 1$ independent of α, Λ in the regime of Remark 5.4. This gives :

$$\mathcal{E}_{\mathrm{BDF}}(\gamma') \geq E^0_{\mathrm{BDF}}(1 + \varepsilon_1) + E^0_{\mathrm{BDF}}(1 + \varepsilon_2) + \frac{L^{-1}}{K_{\mathrm{g}} c^2 \mathrm{R}_g} + \mathcal{O}\Big(\frac{1}{c^2 \mathrm{R}_g}\Big).$$

We know that the function $E^0_{\mathrm{BDF}}(\cdot) : \mathbb{R} \mapsto \mathbb{R}$ is uniformly Lipschitz with constants 1 and this function is concave on each interval $[M, M+1]$ where $M \in \mathbf{Z}$ [HLS09, Corollary 3 *mutatis mutandis*]. Furthermore we may assume $\varepsilon_1 = -\varepsilon_2 > 0$ up to an error $\mathcal{O}\Big(\frac{1}{c^2 \mathrm{R}_g}\Big)$. The case $\varepsilon_1, \varepsilon_2 < 0$ is easily excluded by concavity of E^0_{BDF} in $[0,1]$ because $E^0_{\mathrm{BDF}}(0) = 0$ and $2E^0_{\mathrm{BDF}}(1) \geq E^0_{\mathrm{BDF}}(2)$. Then :

$$\begin{aligned} E^0_{\mathrm{BDF}}(1+\varepsilon_1) + E^0_{\mathrm{BDF}}(1-\varepsilon_1) &\geq \varepsilon_1 E^0_{\mathrm{BDF}}(2) + (1-\varepsilon_1)E_{\mathrm{BDF}}(1) + (1-\varepsilon_1)E_{\mathrm{BDF}}(1) \\ &\geq \varepsilon_1 E^0_{\mathrm{BDF}}(2) + (1-\varepsilon_1)(2E^0_{\mathrm{BDF}}(1)) \geq (1 - \varepsilon_1 + \varepsilon_1)E^0_{\mathrm{BDF}}(2) = E^0_{\mathrm{BDF}}(2). \end{aligned}$$

Thus taking $F_\Lambda(0) = \Theta(\alpha \log(\Lambda))$ sufficiently small, the quantity L^{-1} is big enough to compensate the error term $\mathcal{O}\Big(\frac{1}{c^2 \mathrm{R}_g}\Big)$. We get the desired contradiction :

$$E^0_{\mathrm{BDF}}(2) = \mathcal{E}_{\mathrm{BDF}}(\gamma') \geq E^0_{\mathrm{BDF}}(2) + \frac{1}{c^2 \mathrm{R}_g K'_{\mathrm{g}}} > E^0_{\mathrm{BDF}}(2).$$

5.6.4 Localisation of the energy of the vacuum γ

Lemma 5.8. *For $\lambda_0 \le \lambda < 2^{-1}$ big enough (*e.g. $\lambda = \frac{1}{12}, \frac{1}{6}, \frac{1}{3}$*) there holds :*

$$\|\boldsymbol{\eta}^{(\lambda)}_{cR_g}\rho_\gamma\|_{\mathcal{C}} \lesssim \frac{L}{\sqrt{c\lambda R_g}} \text{ and } \|\boldsymbol{\eta}^{(\lambda)}_{cR_g}|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}, \|\boldsymbol{\eta}^{(\lambda)}_{cR_g}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2} \lesssim \frac{1}{c\sqrt{\lambda R_g}}. \tag{5.88}$$

This part comes after lots of technicalities : we put together results of Lemma 5.7, Propositions 5.7, 5.8, 5.9, Remark 5.17 and the known estimates of Remark 5.13. We refer the reader to Remark 5.15 for explanation.

Here we assume that L is small enough in such a way that $\lambda_0\mathrm{R}_g = \mathcal{O}(L^{-1})$ is big enough. Lemma 5.8 gives that for all $\lambda_0 \le \lambda < 2^{-1}$:

$$\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\rho_\gamma\|_{\mathcal{C}} \le \frac{\epsilon_1}{\sqrt{c\lambda\mathrm{R}_g}} + \epsilon_2\|\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g}\rho_\gamma\|_{\mathcal{C}},\ \epsilon_1,\epsilon_2 = \mathcal{O}(L). \tag{5.89}$$

We recall that $\lambda_0\mathrm{R}_g := \frac{C_0}{L}$ with $C_0(L,\mathrm{R}_g) > 1$ to be chosen. Up to taking a bigger C_0 : $C_0 \le \widetilde{C}_0 < 6C_0$ we assume $\lambda_0 = 2^{-J_0}, J_0 \in \mathbb{N}$. Taking $\ell_0 := c\frac{\widetilde{C}_0}{3L}$ as unity of length, we define the sequences $(u_m),(v_m),(w_m)$ by the formulae :

$$\begin{cases} u_0 = v_0 = w_0 = \|\boldsymbol{\eta}^{(\lambda_0)}_{c\mathrm{R}_g}\rho_\gamma\|_{\mathcal{C}}, \\ u_m := \|\boldsymbol{\eta}^{(2^m\lambda_0)}_{c\mathrm{R}_g}\rho_\gamma\|_{\mathcal{C}},\ v_m = 2^{m/2}u_m, \\ w_{m+1} := \epsilon_1\sqrt{\dfrac{2}{\ell_0}} + \epsilon_2\sqrt{2}w_m \end{cases} \tag{5.90}$$

It is clear from (5.89) that $v_{m+1} \le \epsilon_1\sqrt{\dfrac{2}{\ell_0}} + \epsilon_2\sqrt{2}v_m$. Thus we have :

$$\forall m \in \mathbb{N}^* :\ v_m \le w_m = w_\infty + (2^{1/2}\epsilon_2)^m(w_0 - w_\infty)$$

where $w_\infty = \epsilon_1(2/\ell_0)^{1/2}(1-\epsilon_2\sqrt{2})^{-1/2}$ is well defined provided $\epsilon_2 < 2^{-1/2}$. In particular :

$$\forall m \in \mathbb{N}^* :\ u_m \le \frac{\epsilon_1\sqrt{2}}{\sqrt{2^m\ell_0}} + \frac{(\sqrt{2}\epsilon_2)^m}{\sqrt{2^m}}\Big\{\|\boldsymbol{\eta}^{(\lambda_0)}_{c\mathrm{R}_g}\rho_\gamma\|_{\mathcal{C}} - \frac{\epsilon_1\sqrt{2}}{\sqrt{\ell_0}(1-\epsilon_2\sqrt{2})}\Big\}$$

It remains to evaluate at $m = J_0$: this gives $\|\boldsymbol{\eta}^{(3^{-1})}_{c\mathrm{R}_g}\rho_\gamma\|_{\mathcal{C}}$. Similarly the case $m = J_0 - 1$ corresponds to 6^{-1} etc. By Hardy-Littlewood-Sobolev inequality [LL97, Theorem 4.3] :

$$\|\boldsymbol{\eta}^{(\lambda_0)}_{c\mathrm{R}_g}\rho_\gamma\|_{\mathcal{C}} \le \||\rho_\gamma|\|_{\mathcal{C}} \lesssim \|\rho_\gamma\|_{L^{6/5}} \lesssim \|\rho_\gamma\|_{L^1}^{\frac{2}{3}}\|\rho_\gamma\|_{L^2}^{\frac{1}{3}} \lesssim Lc^{-1/2}.$$

For $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}$ it suffices to use this result, Proposition 5.8 with Lemma 5.7.

Remark 5.15. The following holds.

1. Lemma 5.7 states that each ψ_j is localized around its center cz_j,
2. we give in Remark 5.13 estimates on the norms of γ,N, ρ_γ and n. In particular the densities have the "correct behaviour" in L^1, L^2 and Coulomb norms. We call these estimates : "non-localized estimates".

The other cited results are used of as follows. We remark that $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} = \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\boldsymbol{\eta}^{(\frac{\lambda}{2})}_{c\mathrm{R}_g}$.

Proposition 5.8 gives an estimate of $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}$ and $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|D_0|^{\widetilde{a}}\gamma\|_{\mathfrak{S}_2}$ (where $\widetilde{a} \in \{2^{-1}, a[\Lambda]\}$) in terms of

$$\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}v[\rho'_\gamma]\|_{L^2}, \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\gamma\|_{\mathrm{Ex}}, \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}R_N\|_{\mathfrak{S}_2} \text{ and } \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}v[\rho'_\gamma]\|_{L^6},$$

and in terms of the non-localized estimates (with the "correct behaviour" with respect to $c\lambda\mathrm{R}_g$, that is as in (5.88)). In short we write : non. loc. est. w. the c. b.

Proposition 5.9 gives an estimate of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\nabla v[\rho_\gamma]\|_{L^2}$ in terms of

$$\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2} \text{ and } \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\rho_\gamma\|_{\mathcal{C}} = \|\rho[\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{\lambda}{2})}]\|_{\mathcal{C}},$$

and in terms of the non. loc. est. w. the c. b.

Furthermore, it gives an estimate of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}v_{\rho_\gamma}\|_{L^6}$ in terms of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\nabla v_{\rho_\gamma}\|_{L^2}$ and of the non. loc. est. w. the c. b. The term $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\|_{\mathrm{Ex}}$ is controlled by $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}$ and by the non. loc. est. w. the c. b.

Thanks to Lemma 5.7, the term $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}R_N\|_{\mathrm{Ex}}$ (resp. $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}n\|_{\mathcal{C}}$) is proved to be of order $(c^2\lambda\mathrm{R}_g)^{-1}$ (resp. $(c\lambda\mathrm{R}_g)^{-1/2}$).

Finally Proposition 5.7 together with Remark 5.17 gives an estimate of $\|\rho[\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{\lambda}{2})}]\|_{\mathcal{C}}$ in terms of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{\lambda}{2})}P_\pm^0\gamma\|_{\mathfrak{S}_2}$, $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}P_\pm^0$ and in terms of the non. loc. est. w. the c. b. The presence of $P_\pm^0$ is harmless as we can check from the proofs.

5.6.5 Proof of Proposition 5.6

We consider each term of the BDF energy and write $1 = (\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2 + (\xi_1^{(\frac{1}{3})})^2 + (\xi_2^{(\frac{1}{3})})^2$.

We use once again Lemma 5.7, Proposition 5.8 and Remark 5.13. We treat one after the other the case of N and γ. We write

$$(\xi^{(\lambda)})^2 := (\xi_1^{(\lambda)})^2 + (\xi_2^{(\lambda)})^2.$$

The function ζ refers to $\xi^{(\lambda)}$ or $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$.

Kinetic energy

Kinetic energy for γ :

$$\begin{aligned}\mathrm{Tr}\big((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})|\mathbf{D}|^{1/2}\gamma^2|\mathbf{D}|^{1/2}\big) &\leq \|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}^2 \lesssim \tfrac{1}{c^2\mathrm{R}_g}\\ \mathrm{Tr}\big(\zeta^{\pm\mp}|\mathbf{D}|^{1/2}\gamma^2|\mathbf{D}|^{1/2}\big) &\leq \|\zeta^{\pm\mp}\|_{\mathcal{B}}\||\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}^2 \lesssim \tfrac{1}{c^3\lambda\mathrm{R}_g}\end{aligned}$$

Kinetic energy for N : We recall the following equalities : $\mathbf{D}\psi_j = \mu_j - \alpha B\psi_j$ and $(v_n - R_N)\psi_1 = v_2\psi_1 - v_{21}\psi_2 = \mathcal{O}_{L^2}(\alpha^{3/2}c^{-1})$. Thus, we have :

$$\begin{aligned}\langle\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\mathbf{D}\psi_j\,,\,\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\rangle &= \langle\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}(\mu_j-\alpha B)\psi_j\,,\,\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\rangle\\ |\langle\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\mathbf{D}\psi_j\,,\,\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\rangle| &\leq (1+\alpha\|v[\rho_\gamma']\|_{L^\infty})\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\|_{L^2}^2 + \alpha\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\|_{L^2}(\|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})R_\gamma\psi_j\|_{L^2}\\ &\quad +\alpha\|v_{kj}\|_{L^\infty}\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_k\|_{L^2}) \lesssim \tfrac{1}{\mathrm{R}_g^4} + \tfrac{\alpha\|\gamma\|_{\mathrm{Ex}}}{c\mathrm{R}_g^3} = o(c^{-2}\mathrm{R}_g^{-1}).\end{aligned}$$

We write :

$$(\xi^{(\frac{1}{3})})^2 = (P_+^0+P_-^0)(\xi^{(\frac{1}{3})})(P_+^0+P_-^0)(\xi^{(\frac{1}{3})})(P_+^0+P_-^0),$$

we have to show that $\langle\xi^{\varepsilon_1\varepsilon_2}\xi^{\varepsilon_2\varepsilon_3}\mathbf{D}\psi_j\,,\,\psi_j\rangle$ is $\mathcal{O}(c^{-2}\mathrm{R}_g^{-1})$ whenever $\varepsilon_1\neq\varepsilon_2$ or $\varepsilon_2\neq\varepsilon_3$.

We recall that $\|P_-^0\psi_j\|_{L^2}$ and $\alpha\|B\psi_j\|_{L^2}$ are $\mathcal{O}(c^{-1})$.

The operator $(\xi^{(\frac{1}{3})})^{+-}(\xi^{(\frac{1}{3})})^{-+}$ is $\mathcal{O}(c^{-2}\mathrm{R}_g^{-2})$ in $\|\cdot\|_{\mathcal{B}}$-norm. Except for the corresponding term, we have $\varepsilon_1 = -$ or $\varepsilon_3 = -$, leading to an upper bound :

$$\mathcal{O}\big(\|(\xi^{(\frac{1}{3})})^{+-}\|_{\mathcal{B}}(\|P_-^0\psi_j\|_{L^2}+\alpha\|B\psi_j\|_{L^2})\big) = \mathcal{O}\Big(\frac{1}{c^2\mathrm{R}_g}\Big).$$

Similar estimates lead to (5.87). The estimates $\varepsilon_1,\varepsilon_2 = o(1)$ follow from the fact that $n = |\underline{\psi_1}|^2 + |\underline{\psi_2}|^2 = |h_1|^2+|h_2|^2$, where the h_j's satisfy $h_1\wedge h_2 = \underline{\psi_1}\wedge\underline{\psi_2} = \underline{\Psi}$ and

$$D\big(|h_1|^2,|h_2|^2\big) = d_{\underline{\Psi}}.$$

In fact, this $o(1)$ is an $\mathcal{O}(\alpha + e^{-K\mathrm{R}_g})$.

Direct term

On the outside : $\boldsymbol{\eta}^{(\lambda)}_{c\mathbf{R}_g}$. By Lemma 5.7 and Kato's inequality (Appendix 5.A) :

$$\|(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g})^2 n\|_{\mathcal{C}} \lesssim \frac{1}{c^{1/2}\lambda^2 \mathrm{R}_g^2}.$$

On the inside : $\xi^{(\frac{1}{3})}$. We remark the following :

$$\begin{aligned}(\xi^{(\frac{1}{3})})^2 &= (\xi^{(\frac{1}{3})})^2\big((\boldsymbol{\eta}^{(\frac{1}{12})}_{c\mathrm{R}_g})^2+(\xi^{(\frac{1}{12})})^2\big) = (\boldsymbol{\eta}^{(\frac{1}{12})}_{c\mathrm{R}_g})^2 - (\boldsymbol{\eta}^{(\frac{1}{12})}_{c\mathrm{R}_g})^2(\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g})^2 + (\xi^{(\frac{1}{12})})^2(\xi^{(\frac{1}{3})})^2\\ &= (\boldsymbol{\eta}^{(\frac{1}{12})}_{c\mathrm{R}_g})^2 - (\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g})^2 + (\xi^{(\frac{1}{12})})^2.\end{aligned} \tag{5.91}$$

Thus :

$$\begin{aligned}\Big|D\big((\xi^{(\frac{1}{3})})^2\rho_\gamma,(\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g})^2\rho'_\gamma\big)\Big| &\le \|(\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g})^2\rho_\gamma\|_{\mathcal{C}}(\|(\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g})^2\rho_\gamma\|_{\mathcal{C}} + \|(\boldsymbol{\eta}^{(\frac{1}{12})}_{c\mathrm{R}_g})^2\rho'_\gamma\|_{\mathcal{C}})\\ &+|D((\xi^{(\frac{1}{12})})^2\rho_\gamma,(\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g})^2\rho'_\gamma)| \lesssim \frac{\|\rho_\gamma\|_{L^1}\|\rho'_\gamma\|_{L^1}}{c\mathrm{R}_g} + o\big(\tfrac{L}{c\mathrm{R}_g}\big).\end{aligned}$$

We treat $D\big((\xi_1^{(\frac{1}{3})})^2\rho_\gamma,(\xi_1^{(\frac{1}{3})})^2\rho'_\gamma\big)$ in a similar way : it is $\mathcal{O}\big(\frac{L}{c\mathrm{R}_g}\big)$. We have proved so far :

$$\begin{aligned}D(\rho'_\gamma,\rho'_\gamma) &= D((\xi_1^{(\frac{1}{3})})^2\rho'_\gamma,(\xi_1^{(\frac{1}{3})})^2\rho'_\gamma) + D((\xi_2^{(\frac{1}{3})})^2\rho'_\gamma,(\xi_2^{(\frac{1}{3})})^2\rho'_\gamma)\\ &+2D((\xi_1^{(\frac{1}{3})})^2 n,(\xi_2^{(\frac{1}{3})})^2 n) + \mathcal{O}\big(\frac{L}{c\mathrm{R}_g}\big).\end{aligned}$$

In appendix 5.D we prove the following Lemma.

Lemma 5.9. *For $j=1,2$, we have :*

$$D\big((\xi_1^{(\frac{1}{3})})^2\rho'_\gamma,(\xi_1^{(\frac{1}{3})})^2\rho'_\gamma\big) = D\Big(\rho\Big[\xi_j^{(\frac{1}{3})}\cdot[\gamma']\Big],\rho\Big[\xi_j^{(\frac{1}{3})}\cdot[\gamma']\Big]\Big) + \mathcal{O}\big(\frac{L}{cR_g}\big).$$

Exchange term

By Lemma 5.7 and Kato's inequality (5.59) :

$$\mathrm{Tr}\Big((\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g})^2 N R_N\Big) \lesssim \sum_j \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\psi_j\|^2_{L^2}\mathrm{Tr}\big(|\nabla|N\big) \lesssim \frac{1}{c(\lambda\mathrm{R}_g)^2} = o\big(\frac{\alpha}{\lambda^2 cR_g}\big).$$

With the same trick used before, we have :

$$\iint \frac{|\gamma'(x,y)|^2}{|x-y|}dxdy = \iint ((\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g}(x))^2 + (\xi^{\frac{1}{3}}(x))^2)\frac{|\gamma'(x,y)|^2}{|x-y|}((\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g}(y))^2 + (\xi^{\frac{1}{3}}(y))^2)dxdy.$$

We use Kato's inequality as usual to get :

$$\begin{aligned}\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\gamma'\|_{\mathrm{Ex}} \lesssim \||D_0|^{1/2}\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\gamma'\|_{\mathfrak{S}_2} &\le \|[|D_0|^{1/2},\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}]\tfrac{1}{|D_0|^{1/2}}\|_{\mathcal{B}}\||D_0|^{1/2}\gamma'\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|D_0|^{1/2}\gamma'\|_{\mathfrak{S}_2},\\ &\lesssim \frac{1}{c\sqrt{\lambda\mathrm{R}_g}}.\end{aligned}$$

Using trick (5.91), we get

$$\begin{aligned}\iint \frac{|\gamma'(x,y)|^2}{|x-y|}dxdy &= \|\xi_1^{\frac{1}{3}}\gamma'\|^2_{\mathrm{Ex}} + \|\xi_2^{\frac{1}{3}}\gamma'\|^2_{\mathrm{Ex}} + 2\iint(\xi_1^{\frac{1}{3}}(x))^2\frac{|\gamma'(x,y)|^2}{|x-y|}(\xi_2^{\frac{1}{3}}(y))^2dxdy\\ &+\mathcal{O}\Big(\frac{\|\gamma\|^2_{\mathfrak{S}_2}}{c\mathrm{R}_g} + \mathrm{Tr}\Big((\boldsymbol{\eta}^{(\frac{1}{3})}_{c\mathrm{R}_g})^2NR_N\Big) + \|\boldsymbol{\eta}^{(\frac{1}{12})}_{c\mathrm{R}_g}\gamma'\|^2_{\mathrm{Ex}}\Big).\end{aligned}$$

Now let us show that for $j=1,2$:

$$\|\xi_j^{\frac{1}{3}}\gamma'\|_{\mathrm{Ex}}^2 = \|\xi_j^{\frac{1}{3}}\cdot[\gamma']\|_{\mathrm{Ex}}^2 + \mathcal{O}\big(\frac{1}{(c\mathrm{R}_g)^2}\big). \tag{5.92}$$

It suffices to use Kato's inequality and Eq. (5.93), we have :

$$\begin{aligned}\||D_0|^{1/2}\xi^{+-}Q\|_{\mathfrak{S}_2} &\leq \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \Big\|\frac{|D_0|^{1/2}}{D_0+i\omega}\boldsymbol{\alpha}\cdot\nabla\xi\frac{1}{D_0+i\omega}Q\Big\|_{\mathfrak{S}_2}\\ &\lesssim \|\nabla(\xi_{c\lambda\mathrm{R}_g})\|_{L^\infty}\|Q\|_{\mathfrak{S}_2}\int_{-\infty}^{+\infty}\frac{d\omega}{E(\omega)^{3/2}} \lesssim \frac{\|Q\|_{\mathfrak{S}_2}}{c\lambda\mathrm{R}_g}.\end{aligned}$$

5.A Estimates

5.A.1 $[V,P_-^0]$ and proof of Proposition 5.1

For any smooth complex valued function V, there holds [GLS09] :

$$[V,P_-^0] = -\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{D_0+i\eta}\boldsymbol{\alpha}\cdot\nabla V\frac{d\eta}{D_0+i\eta}. \tag{5.93}$$

Thanks to the KSS inequality as shown in [CDL08], provided smoothness of V ($\nabla V\in L^p$) then this operator is $\mathfrak{S}_p(L^2(\mathfrak{R}^3,\mathfrak{C}^4))$ for $p>3$.

The integral kernel of its Fourier transform [HLS05a] is :

$$\mathscr{F}\big([V,P_-^0];p,q\big) = \frac{i}{2(2\pi)^{3/2}}\frac{1}{E(p)+E(q)}(\alpha_j\widehat{\partial_j V}(p-q) - \mathbf{s}_p\alpha_j\widehat{\partial_j V}(p-q)\mathbf{s}_q). \tag{5.94}$$

We prove Proposition 5.1 by duality, following [GLS09]. Let V be in $\mathcal{S}(\mathbb{R}^3)$, $Q\in\mathfrak{S}_1^{P_-^0}$ (we recall that $2a[\Lambda]=1+\frac{1}{\log(\Lambda)}$), then

$$\mathrm{Tr}_0(QV) = \mathrm{Tr}(P_+^0Q(P_+^0+P_-^0)VP_+^0) + \mathrm{Tr}(P_-^0Q(P_+^0+P_-^0)VP_-^0).$$

The operator $Q^{+-}|D_0|^{a[\Lambda]}\frac{1}{|D_0|^{a[\Lambda]}}[P_-^0,V]$ is in $\mathfrak{S}_1$: indeed thanks to (5.94) we have

$$\iint\frac{|\widehat{V}(p-q)|^2|p-q|^2dpdq}{E(p)^{1+\frac{1}{\log(\Lambda)}}(E(p)+E(q))} \lesssim \log(\Lambda)\|\nabla V\|_{L^2}^2$$

showing $\|\frac{1}{|D_0|^{a[\Lambda]}}[P_-^0,V]\|_{\mathfrak{S}_2}\lesssim\sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}$. This also treats the case $Q^{-+}V^{+-}\in\mathfrak{S}_1$. Then we have $Q^{++}V^{++} = Q^{++}|D_0|^{a[\Lambda]}\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\in\mathfrak{S}_1$.

Indeed $|D_0|^{a[\Lambda]}Q^{++}|D_0|^{a[\Lambda]}\in\mathfrak{S}_1$ and $\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\in\mathfrak{S}_6$ with norm $\mathcal{O}((\log(\Lambda))^{1/6}\|\nabla V\|_{L^2})$.

Then $\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\frac{1}{|D_0|^{a[\Lambda]}}\in\mathfrak{S}_6$ with norm $\mathcal{O}(\|\nabla V\|_{L^2})$. So :

$$\begin{aligned}\mathrm{Tr}(Q^{++}V^{++}) &= \mathrm{Tr}\big(\frac{|D_0|^{a[\Lambda]}}{|D_0|^{a[\Lambda]}}Q^{++}\frac{|D_0|^{a[\Lambda]}}{|D_0|^{a[\Lambda]}}V^{++}\big)\\ &= \mathrm{Tr}\big(\{|D_0|^{a[\Lambda]}Q^{++}|D_0|^{a[\Lambda]}\}\{\tfrac{1}{|D_0|^{a[\Lambda]}}\}V^{++}\tfrac{1}{|D_0|^{a[\Lambda]}}\big)\\ &= \mathcal{O}\big(\||D_0|^{a[\Lambda]}Q^{++}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1}\|\nabla V\|_{L^2}\big).\end{aligned}$$

The same holds for $Q^{--}V^{--}$. This ends the proof.

Remark 5.16. In Appendix 5.D we do analogous estimates but with an additional localisation operator.

We adapt [CDL08, Lemma 5] :

Lemma 5.10. *Let p be in $(3,+\infty]$ and V a smooth function with $\nabla V\in L^p$. Then for any $0<a<1$:*

$$[|D_0|^a,V]\tfrac{1}{|D_0|^a}\in\mathfrak{S}_p. \tag{5.95}$$

To prove it we use [LS10, p. 87]

$$\forall\, x>0,\ 0<a<1:\ x^a = \frac{\sin(a\pi)}{\pi}\int_0^{+\infty}\frac{ds}{s^{1-a}}\frac{x}{x+s}. \tag{5.96}$$

5.A.2 Proof of Lemma 5.6

Proof : Let us explain the bootstrap argument.
– We show that $\mathrm{Tr}((-\Delta)^{a+1}N)\lesssim 1$. As a consequence :

$$\begin{aligned}\||\nabla|^a n_j\|_{L^2} &\le \sum_{\ell=0}^a K(\ell,a)\||\nabla|^\ell \mathscr{F}^{-1}(|\widehat{\psi}_j|)\|_{L^4}\||\nabla|^{a-\ell}\mathscr{F}^{-1}(|\widehat{\psi}_j|)\|_{L^4}\\ &\lesssim \sum_{\ell=0}^a K(\ell,a)\||\nabla|^{\ell+3/4}\mathscr{F}^{-1}(|\widehat{\psi}_j|)\|_{L^2}\||\nabla|^{a-\ell+3/4}\mathscr{F}^{-1}(|\widehat{\psi}_j|)\|_{L^2}\\ &\lesssim K(a).\end{aligned}$$

– As shown in [Sok13], (γ',ρ'_γ) is the fixed point of some function $F^{(1)}$ in a ball of $\widetilde{\mathcal{X}}_a$:

$$\widetilde{\mathcal{X}}_a=\{(Q,\rho)\in\mathfrak{S}_2\times\mathcal{S}' : \iint E(p-q)^{2a}E(p+q)|\widehat{Q}(p,q)|^2<+\infty \text{ and } \int\frac{E(k)^a}{|k|^2}|\widehat{\rho}(k)|^2<+\infty\}.$$

– We multiply by $|D_0|^{(a+3)/2}$ the equation $D_0\psi_j=\mathcal{L}_\Lambda^{-1}(\mu_j\psi_j-\alpha B_{\gamma'}\psi_j)$ and we show that $\mathrm{Tr}((-\Delta)^{a+2}N)\lesssim 1$. We have to deal with $[|D_0|^{(a+3)/2},v]\psi_j$ and $[|D_0|^{(a+3)/2},R]\psi_j$: it suffices to compute in Fourier space and to use Taylor's formula on the function $E(\cdot)^{(a+3)/2}$.

Proof of the estimates Here as $\mathrm{Tr}(-\Delta N)\lesssim 1$, the fixed point method can be applied on $\widetilde{\mathcal{X}}_{a=1}$. Indeed $\|n\|_{L^2}\lesssim\||\nabla|^{3/2}\sqrt{n}\|_{L^2}\lesssim 1$. We get that

$$\iint|p-q|E(p+q)|\widehat{\gamma}(p,q)|^2dpdq\lesssim 1.$$

Let us show the assumption on the H^2-norm of ψ_j.
There holds $f(-i\nabla)\mathbf{D}\psi_j=f(-i\nabla)(\mu_j-\alpha B[\gamma])\psi_j$ for any $f\ge 0$. Taking the L^2-norm we have to deal with $[f(-i\nabla),R_{\gamma'}]$ and $[f(-i\nabla),v[\rho(\gamma')]]$. For $f(-i\nabla)=|\nabla|^{1/2}$ there holds

$$\begin{aligned}\|[|\nabla|^{1/2},v_\rho]\psi\|_{L^2}^2 &\lesssim \iint\frac{|\widehat{\rho}(p-q)|^2}{|p-q|^2}\frac{dpdq}{|q|^2E(q)^2}\int dqE(q)^2|q||\widehat{\psi}(q)|^2\\ \|[|\nabla|^{1/2},R_Q]\psi\|_{L^2}^2 &\lesssim \iint|p-q||\widehat{Q}(p,q)|^2dpdq\,\||\nabla|^{1/2}\psi\|_{L^2}^2\\ |\nabla|^{1/2}D_0\psi &=\mu\frac{|\nabla|^{1/2}}{\mathcal{L}_\Lambda}\psi-\alpha\frac{|\nabla|^{1/2}}{\mathcal{L}_\Lambda}B\psi=\mathcal{O}_{L^2}(1)\text{ a priori}\\ |\nabla|^{1/2}B\psi &=[|\nabla|^{1/2},B]\psi+B\frac{1}{|\nabla|^{1/2}}|\nabla|\psi\text{ and :}\end{aligned}$$

$$\langle|\nabla|(1-\Delta)\psi_1\,,\,\psi_1\rangle-\langle|\nabla|\psi_1\,,\,\psi_1\rangle\lesssim\alpha c^{-1}\|v_2\psi_1-v_{21}\psi_2\|_{L^2}+c^{-3}+\alpha^2c^{-2}=\mathcal{O}(c^{-3}+\alpha c^{-1}a_{12}).$$

We get $\mathrm{Tr}(|D_0|^3N)\lesssim 1$ and by the fixed-point Theorem :

$$\|\gamma\|_{\mathbf{Q}}^2=\iint E(p-q)^2E(p+q)|\widehat{\gamma}(p,q)|^2dpdq\lesssim 1.$$

Notation 5.9. The star in $\|\cdot\|_{\mathbf{Q}}^*$ means that we replace $E(p-q)^2E(p+q)$ by $|p-q|^2|p+q|$.

Using the methods of [HLS05a, Sok14b] we have :

$$\begin{cases}\|\gamma\|_{\mathbf{Q}}^* &\lesssim c^{-1/2}\|\rho'_\gamma\|_{L^2}+\alpha(\|\gamma'\|_{\mathbf{Q}}^*)+\alpha(\|\rho'_\gamma\|_{L^2}+\|\gamma'\|_{\mathbf{Q}}^*)\sum_{k=1}^{+\infty}\sqrt{k}(\alpha K(\|\rho'_\gamma\|_{\mathcal{C}}+\|\gamma'\|_{\mathbf{Q}_1}))^k,\\ \|[\nabla,\gamma]\|_{\mathfrak{S}_2} &\lesssim \alpha(\|\rho'_\gamma\|_{L^2}+\|N\|_{\mathbf{Q}}^*)+\alpha(\|\rho'_\gamma\|_{L^2}+\|\gamma'\|_{\mathbf{Q}}^*)\sum_{k=1}^{+\infty}\sqrt{k}(\alpha K(\|\rho'_\gamma\|_{\mathcal{C}}+\|\gamma'\|_{\mathbf{Q}_1}))^k,\\ \|\rho_\gamma\|_{L^2} &\lesssim L\|n\|_{L^2}+c^{-1/2}\|\gamma'\|_{\mathbf{Q}}^*+\alpha(\|\rho'_\gamma\|_{L^2}+\|\gamma'\|_{\mathbf{Q}}^*)\sum_{k=1}^{+\infty}\sqrt{k}(\alpha K(\|\rho'_\gamma\|_{\mathcal{C}}+\|\gamma'\|_{\mathbf{Q}_1}))^k.\end{cases}$$

Therefore

$$\|\gamma'\|_{\mathbf{Q}}^*=\mathcal{O}(c^{-2}),\ \|[\nabla,\gamma]\|_{\mathfrak{S}_2}=\mathcal{O}(\alpha c^{-3/2})\text{ and }\|\rho_\gamma\|_{L^2}=\mathcal{O}(Lc^{-3/2}+c^{-2}+c^{-1}(\sqrt{\alpha a_{12}})).$$

For $f(-i\nabla)=\partial_k$ with $k=1,2,3$ we have :

$$\begin{aligned}
\partial_k R_Q\psi &= [\partial_k, R[Q]]\psi + R_Q\partial_k\psi \text{ and } \partial_k v\psi = (\partial_k v)\psi + v(\partial_k\psi)\\
\|[\partial_k, R_Q]\psi\|_{L^2} &= \|R([\partial_k, Q])\psi\|_{L^2} \le \|[\partial_k, Q]\|_{\mathfrak{S}_2}\|\nabla\psi\|_{L^2} \text{ and } \|R_Q\partial_k\psi\|_{L^2} \le \|Q\|_{\mathfrak{S}_2}\|\Delta\psi\|_{L^2}\\
\|v_\rho(\partial_k\psi)\|_{L^2} &\le \|v_\rho\|_{L^6}\|\partial_k\psi\|_{L^3} \lesssim \|\rho\|_{\mathcal{C}}\||\nabla|^{3/2}\psi\|_{L^2} \le \|\rho\|_{\mathcal{C}}\sqrt{\|\nabla\psi\|_{L^2}\|\Delta\psi\|_{L^2}}\\
\|(\partial_k v_\rho)\psi\|_{L^2}^2 &\lesssim \iint \frac{|\widehat{\rho}(k)|^2}{|k|^2}\frac{dkdq}{|q|^2(1+|q|^2)}[\|\nabla\psi\|_{L^2}^2 + \|\Delta\psi\|_{L^2}^2]
\end{aligned}$$

$$\begin{aligned}
\sum_{k=1}^{3}(\|\partial_k\mathbf{D}\psi\|_{L^2}^2) - \|\nabla\psi\|_{L^2}^2 &\le (\mu^2-1)\|\nabla\psi\|_{L^2}^2 + 6\alpha\mu\|\nabla\psi\|_{L^2}\|B[\gamma']\psi\|_{L^2} + \alpha^2\|\nabla B[\gamma']\psi\|_{L^2}^2\\
\mathrm{Tr}(\Delta^2(1-\tfrac{\Delta}{\Lambda^2}+\tfrac{\Delta^2}{\Lambda^4})N) &\lesssim \alpha a_{12}c^{-1} + c^{-3}.
\end{aligned}$$

This gives $\|\Delta\psi_j\|_{L^2}^2 \lesssim \alpha c^{-2}$ and in particular :

$$\|c^2(1-\mathcal{L}_{c\Lambda}^{-1})\underline{\psi_j}\|_{L^2} = \mathcal{O}\big(\frac{\sqrt{\alpha}c}{\Lambda^2}\big).$$

As a consequence we have :

$$\|\nabla\underline{\chi_j}\|_{L^2} = \|i\boldsymbol{\sigma}\cdot\nabla\underline{\chi_j}\|_{L^2} = \mathcal{O}(c^{-1}). \tag{5.97}$$

□

Thanks to those estimates, we get :

$$\mathcal{E}_{\mathrm{BDF}}(\gamma+N) = 2 + \frac{\mathcal{E}_{\mathrm{PT}}(\underline{\psi_1}\wedge\underline{\psi_2})}{2c^2} + \mathcal{O}(\alpha^2c^{-3/2}+c^{-3}). \tag{5.98}$$

We recall that $1-\mathcal{L}_\Lambda^{-1} = \frac{-\Delta}{\Lambda^2-\Delta}$.

Thanks to Section 5.B there holds

$$D(\underline{n}_1,\underline{n}_2) - D(\underline{\psi_1}^*\underline{\psi_2},\underline{\psi_1}^*\underline{\psi_2}) \lesssim c^{-1} \text{ and } a_{12}\lesssim \alpha^{3/2}c^{-1}.$$

From this point we get better estimate on $\|\Delta\psi\|_{L^2}^2 \lesssim c^{-3}$ but this is still unsatisfactory. Let us be more precise about $\mu = \langle(\mathbf{D}+\alpha B)\psi\,,\,\psi\rangle$ and χ :

$$\begin{aligned}
(1+\mu_1)\chi_1 &= -i\sigma\cdot\nabla\phi_1 - \tfrac{\mu\Delta}{\Lambda^2-\Delta}\chi_1 + \tfrac{\alpha}{\mathcal{L}_\Lambda}(v_{\rho_\gamma}\chi_1 + (v_2\chi_1 - v_{21}\chi_2) - (R_\gamma\psi_1)_\downarrow)\\
&= \tfrac{1}{1+\mu}(-i\sigma\cdot\nabla\phi_1 + X_1^{(r)}) = \frac{-i\sigma\cdot\nabla}{2}\phi_1 + \mathcal{O}_{L^2}(c^{-2}/\Lambda + c^{-2})\\
\langle\mathbf{D}\psi\,,\,\psi\rangle &= \langle D_0\psi\,,\,\psi\rangle - \langle\tfrac{\Delta}{\Lambda^2}\beta\psi\,,\,\psi\rangle + \langle\tfrac{\Delta}{\Lambda^2} - i\boldsymbol{\alpha}\cdot\nabla\psi\,,\,\psi\rangle\\
&= 1 - 2\|\chi\|_{L^2}^2 + 2\mathfrak{Re}\langle -i\sigma\cdot\nabla\varphi\,,\,\chi\rangle + \mathcal{O}\big(\tfrac{\|\nabla\psi\|_{L^2}^2}{\Lambda^2} + \|\Delta\varphi\|_{L^2}\tfrac{\|\nabla\chi\|_{L^2}}{\Lambda^2}\big)\\
&= 1 + \tfrac{2}{1+\mu}\big(1-\tfrac{1}{1+\mu}\big)\|\nabla\varphi\|_{L^2}^2 + \mathfrak{Re}\tfrac{2}{1+\mu}\big(1-\tfrac{2}{1+\mu}\big)\mathfrak{Re}\langle -i\sigma\cdot\nabla\varphi\,,\,X^{(r)}\rangle + \mathcal{O}\big(\tfrac{1+\|\Delta\varphi\|_{L^2}}{c^2\Lambda^2}\big)\\
&= 1 + \tfrac{1}{2}\|\nabla\varphi\|_{L^2}^2 + \mathcal{O}(c^{-4} + c^{-2}\Lambda^{-2}(1+\|\Delta\varphi\|_{L^2})).
\end{aligned}$$

Then :

$$\begin{aligned}
\|\mathcal{L}_\Lambda^{-1}\psi\|_{L^2}^2 &= 1 + \mathcal{O}(c^{-2}\Lambda^{-2} + \|\Delta\psi\|_{L^2}^2/\Lambda^4)\\
\|\nabla\mathcal{L}_\Lambda^{-1}\psi\|_{L^2}^2 &= \|\nabla\psi\|_{L^2}^2 + \mathcal{O}(\|\Delta\psi\|_{L^2}/(c\Lambda^2) + \|\Delta\psi\|_{L^2}^2/\Lambda^2)\\
-2\alpha\mu\mathfrak{Re}\langle\tfrac{1-\Delta}{\mathcal{L}_\Lambda}B\psi\,,\,\psi\rangle &= -2\alpha\mu\langle B\psi\,,\,\psi\rangle + \mathcal{O}(\alpha\|B\psi\|_{L^2}\|\Delta\psi\|_{L^2}/\Lambda^2)\\
\|-i\boldsymbol{\alpha}\nabla B\psi\|_{L^2} &\lesssim \|[\nabla,B]\psi\|_{L^2} + \|B\nabla\psi\|_{L^2} = \mathcal{O}(c^{-3/2} + \|\Delta\psi\|_{L^2}^{1/2}c^{-1} + \|\Delta\psi\|_{L^2}c^{-1/2}).
\end{aligned}$$

and thus :

$$\begin{aligned}
\langle(1-\Delta)\psi\,,\,(1-\Delta)\psi\rangle &= \mu^2\langle\tfrac{1-\Delta}{\mathcal{L}_\Lambda^2}\psi\,,\,\psi\rangle - 2\alpha\mu\mathfrak{Re}\langle\tfrac{1-\Delta}{\mathcal{L}_\Lambda}B\psi\,,\,\psi\rangle + \|\tfrac{D_0}{\mathcal{L}_\Lambda}B\psi\|_{L^2}^2\\
&= 1 + 2(\mu - 1 - \alpha\langle B\psi\,,\,\psi\rangle) + \|\nabla\psi\|_{L^2}^2\\
&\quad + \mathcal{O}(c^{-2}(c^{-2}+\Lambda^{-2}) + \tfrac{\|\Delta\psi\|_{L^2}}{c^2\Lambda^2} + \|\Delta\psi\|_{L^2}^2(\Lambda^{-2}+\alpha^2c^{-1})).
\end{aligned}$$

From (5.61) and the expression of $D_0\psi_j$, we have $\|\nabla\psi_j\|_{L^2}^2 = -2\alpha\mathfrak{Re}\langle B\psi_j\,,\,\psi_j\rangle$. We conclude $\|\Delta\psi\|_{L^2}^2 \lesssim c^{-2}(c^{-2}+\Lambda^{-2})$ and

$$\|\Delta\psi\|_{L^2}^2 \lesssim \min\big(c^{-3}, c^{-2}(c^{-2}+\Lambda^{-2})\big).$$

5.B Proofs of Section 5.3

5.B.1 Proof of Proposition 5.3

Reductio ad absurdum.

We assume this is false and take a non-increasing sequence $(a_j)_{j\geq 0}$ tending to 0 such that there exists Ψ_j that does not satisfy (5.37) with $\mathrm{b} = a_j$: $\Delta_2\mathcal{E} < a_j$ and $\frac{\Delta_2\mathcal{E}}{d_\Psi} < a_j$. In particular $(\Psi_j)_j$ is a minimizing sequence for $E_{\mathrm{PT}}(2)$. By geometrical methods [Lew11] we see that Ψ_j can be decomposed in two pieces of mass one, each piece tending to a minimizer for $E_{\mathrm{PT}}(1)$. Indeed it is clear that $(\mathrm{Tr}(-\Delta\gamma_{\Psi_j}))_j$ is bounded and that there is no vanishing for $(\rho_{\Psi_j})_{j\geq 0}$. If we follow a bubble [LR11] of ρ_{Ψ_j} (one of the biggest) let us show its mass is 1 at the limit.

By scaling, for any $0 < \lambda < 1$ we have $E_{\mathrm{PT}}(\lambda) \geq \lambda^3 E_{\mathrm{PT}}(1)$, where $E_{\mathrm{PT}}(\lambda)$ is defined as the infimum of $\mathcal{E}_{\mathrm{PT}}$ over non-negative one-body density matrix whose trace is λ.

Up to following a bubble and extracting a subsequence there holds with $\Psi_j = h_{1,j} \wedge h_{2,j}$:

$$|h_{1,j} \wedge h_{2,j}\rangle\langle h_{1,j} \wedge h_{2,j}| \rightharpoonup_g G_{00} \oplus G_{11} \oplus G_{22},\ \sum_{j=0}^{2} \mathrm{Tr}(G_{jj}) = 1 \text{ and } \mathrm{Tr}(G_{00}) < 1.$$

We recall that each G_{jj} is a density matrix in $(L^2)^{\wedge(j)}$. Following [Lew11, part 5] :
$G_{jj} = \mathrm{Tr}(G_{jj})\widetilde{G}_{jj}$

$$\begin{aligned}\liminf_{j\to+\infty} \mathcal{E}^U_{\mathrm{PT}}(\Psi_j) &= E^U_{\mathrm{PT}}(2) \geq \sum_{j=0}^{2}(\mathcal{E}^U_{\mathrm{PT}}(G_{jj}) + \mathrm{Tr}(G_{jj})E^U_{\mathrm{PT}}(2-j)) \\ &\geq \sum_{j=0}^{2} \mathrm{Tr}(G_{jj})(\mathcal{E}^U_{\mathrm{PT}}(\widetilde{G}_{jj}) + E^U_{\mathrm{PT}}(2-j)) \geq E^U_{\mathrm{PT}}(2).\end{aligned}$$

As not all particles are lost (we follow a bubble) either $G_{11} \neq 0$ or $G_{22} \neq 0$. In the case $G_{2,2} \neq 0$, [FLST11] enables us to say $\mathcal{E}^U_{\mathrm{PT}}(\widetilde{G}_{22}) > E_{\mathrm{PT}}(2)$. So $G_{22} = 0$ and $G_{11} \neq 0$. Thanks to [Lie77] and Lieb's variational principle (we may assume $G_{11} = \mathrm{Tr}(G_{11})|\phi\rangle\langle\phi|$) there holds

$$\mathcal{E}_{\mathrm{PT}}(G_{11}) \geq (\mathrm{Tr}(G_{11}))^3 E_{\mathrm{PT}}(1),$$

then necessarily $\mathrm{Tr}(G_{11}) = 1$.

As a consequence there is exactly two bubbles in $(\rho_{\Psi_j})_j$, there exist a decomposition $\Psi_j = \underline{h_{1,j}} \wedge \underline{h_{2,j}}$ and a sequence $(z_{1,j}; z_{2,j})_j$ of $(\mathbb{R}^3)^2$ such that (up to extraction)

1. $\langle \underline{h_{k,j}}, \underline{h_{\ell,j}}\rangle = \delta_{k\ell}$ and $|z_{1,j} - z_{2,j}| \underset{j\to\infty}{\to} +\infty$,
2. $\underline{h_{k,j}}(\cdot - z_{k,j}) \underset{j\to\infty}{\overset{H^1}{\to}} \phi_{j,\infty}$ where $\phi_{j,\infty} \in \mathscr{P}$ is radial.

Then it suffices to compute : $\mathcal{E}^U_{\mathrm{PT}}(\Psi_j)$ with this decomposition :

$$\begin{aligned}\mathcal{E}^U_{\mathrm{PT}}(\Psi_j) &= \mathcal{E}^U_{\mathrm{PT}}(\underline{h_{1,j}}) + \mathcal{E}^U_{\mathrm{PT}}(\underline{h_{2,j}}) - D(|\underline{h_{1,j}}|^2, |\underline{h_{2,j}}|^2) + \tfrac{U}{2}\iint |\underline{h_{1,j}} \wedge \underline{h_{2,j}}(x,y)|^2 \frac{dxdy}{|x-y|} \\ &= \mathcal{E}_1 + \mathcal{E}_2 + \tfrac{U}{2}W_{12} - \underline{D_{12}} \geq \tfrac{U}{4}W_{12} + 2E_{\mathrm{PT}}(1).\end{aligned}$$

The last equality holds because we have $U > 2\mathrm{U}_c$. Let us write

$$\Delta_1\mathcal{E} := \mathcal{E}_{\mathrm{PT}}(\underline{h_{1,j}}) + \mathcal{E}_{\mathrm{PT}}(\underline{h_{2,j}}) - 2E_{\mathrm{PT}}(1).$$

Then :

$$-a_j < \Delta_1\mathcal{E} - \underline{D_{12}} < a_j \text{ and } \Delta_1\mathcal{E} \geq \kappa \sum_{k=1}^{2} \|\underline{h_{k,j}} - \phi_{k,j}\|^2_{H^1}$$

where $\phi_{k,j} \in \mathscr{P}$ is the closest function to $\underline{h_{k,j}}$ in H^1 (Proposition 5.2). We may assume that $\underline{D_{12}} = d_{\Psi_j}$ because minimizing this quantity corresponds to minimizing $\Delta_1\mathcal{E}$. In particular :

$$|\Delta_1\mathcal{E} - \underline{D_{12}}| < a_j = \underset{j\to+\infty}{o}(\underline{D_{12}}) \;\Rightarrow\; \Delta_1\mathcal{E} \underset{j\to+\infty}{\sim} \underline{D_{12}} \gg a_j.$$

Indeed, let us say that $\underline{D_{12}} > d_{\Psi_j}$, then $(\underline{f_{k,j}}(\cdot - z_k))_j$ still converges to $\phi_{j,\infty}$, in particular $(\Delta_1\mathcal{E})_j$ converges to 0. But if $(\underline{f'_{1,j}}, \underline{f'_{2,j}})_j$ is a decomposition with $\underline{D'_{12}} = d_{\Psi_j}$, then $\Delta'_1\mathcal{E} \le \Delta_1\mathcal{E}$ and

$$\mathrm{dist}(\underline{f'_{k,j}}, \mathscr{P}) \underset{j\to+\infty}{\to} 0.$$

From now we will drop the subscript j for convenience and suppose $\underline{D_{12}} = d_{\Psi_j}$.

Notation 5.10. We introduce $\underline{h_k} = (\underline{h_k} - \phi_k) + \phi_k = \delta_k - \phi_k$ in $|\underline{h_k}|^2$ and in $\underline{h_1}^*\underline{h_2}$. We use the convention

$$\|\delta\|_{L^2} := \|\delta_1\|_{L^2} + \|\delta_2\|_{L^2},\ \|\delta\|_{H^1} := \|\delta_1\|_{H^1} + \|\delta_2\|_{H^1}.$$

We recall that an element of $\mathscr{P}$ has an exponential falloff with respect to its center. For some constant $\overline{\varepsilon} > 0$, there holds :

$$\begin{aligned}
|\underline{h_k}|^2 &= |\delta_k|^2 + |\phi_k|^2 + 2\mathfrak{Re}(\delta_k^*\phi_k)\\
\underline{h_1}^*\underline{h_2}^* &= \delta_1^*\delta_2 + \phi_1^*\phi_2 + \delta_1^*\phi_2 + \phi_1^*\delta_2\\
\|\underline{h_1}^*\underline{h_2}\|_{\mathcal{C}}^2 &= \|\delta_1^*\phi_2\|_{\mathcal{C}}^2 + \|\phi_1^*\delta_2\|_{\mathcal{C}}^2 + \mathcal{O}\big((\|\delta_1\|_{L^2}\|\delta_2\|_{L^2})(\mathrm{R}_g^{-1} + \|\delta\|_{L^2}(1 + \|\nabla\delta\|_{L^2}) + e^{-\overline{\varepsilon}\mathrm{R}_g})\big)\\
\underline{D_{12}} &= D(|\phi_1|^2, |\phi_2|^2) + D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2)\\
&\quad + \mathcal{O}\big(\tfrac{\|\delta\|_{L^2}}{\mathrm{R}_g} + \|\delta_1\|_{L^2}\|\delta_2\|_{L^2}(\|\delta\|_{L^2}(1 + \|\nabla\delta\|_{L^2}) + e^{-\overline{\varepsilon}\mathrm{R}_g})\big)
\end{aligned}$$

$$\text{Thus :}\quad a_jU^{-1} \gtrsim \underline{D_{12}} - \|\underline{h_1}^*\underline{h_2}\|_{\mathcal{C}}^2 \gtrsim \frac{1}{\mathrm{R}_g} + \underset{j\to+\infty}{\mathcal{O}}(\|\delta\|_{L^2}^3)$$

$$\text{and}\quad \tfrac{1}{\mathrm{R}_g} = \underset{j\to+\infty}{\mathcal{O}}(a_jU^{-1} + \|\delta\|_{L^2}^3).$$

As $j \to +\infty$, thanks to the coercivity inequality (5.2) there holds

$$\underline{D_{12}} \sim \Delta_1\mathcal{E} = \Theta(\|\delta_1\|_{H^1}^2 + \|\delta_2\|_{H^1}^2) \text{ and } \frac{1}{\mathrm{R}_g} = \underset{j\to+\infty}{o}(\underline{D_{12}}).$$

Studying more precisely $M^2(\underline{h_1} \wedge \underline{h_2}) := \iint |\underline{h_1} \wedge \underline{h_2}(x,y)|^2 \frac{dxdy}{|x-y|}$:

$$\begin{aligned}
M^2(\underline{h_1} \wedge \underline{h_2}) &= M^2(\delta_1 \wedge \phi_2) + M^2(\phi_1 \wedge \delta_2) + \underset{j\to+\infty}{\mathcal{O}}(\mathrm{R}_g^{-1} + \|\delta\|_{L^2}^3) = \underset{j\to+\infty}{o}(\underline{D_{12}})\\
\underline{D_{12}} &= D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2) + \underset{j\to+\infty}{o}(\underline{D_{12}}) \gtrsim \|\delta_1\|_{H^1}^2 + \|\delta_2\|_{H^1}^2.
\end{aligned} \tag{5.99}$$

We can easily exclude the case $\delta_1, \delta_2 = 0$ for then it is clear $M^2(\phi_1 \wedge \phi_2) \gtrsim D(|\phi_1|^2, |\phi_2|^2)$ thanks to $\langle \phi_1 \,,\, \phi_2 \rangle = 0$. Say then that $\|\delta_1\|_{H^1} \ge \|\delta_2\|_{H^1}$: $\delta_1 \neq 0$. The case $\delta_2 = 0$ and $\delta_1 \neq 0$ is an easy adaptation of what follows, we treat it later. As there holds

$$|\phi_2|^2 * \tfrac{1}{|\cdot|}(x) \le \tfrac{1}{|x-z_2|}$$

where z_2 is the center of ϕ_2, Estimate (5.99) is true only if there lies a mass of δ_1 near z_2 : the quantity $\|\delta_1^*\phi_2\|_{\mathcal{C}}^2$ must compensate $D(|\delta_1|^2, |\phi_2|^2)$. Eventually the same phenomena occurs for δ_2 around z_1 the center of ϕ_1. Up to extraction :

$$\frac{\delta_k(\cdot - z_k)}{\|\delta_k\|_{H^1}} \rightharpoonup_{H^1} \ell_k,$$

and $(\ell_1, \ell_2) \neq (0,0)$. Indeed up to contraction there is convergence in L^2_{loc} and if $\ell_k = 0$ then for all $r > 0$ and $(i_1, i_2) \in \big\{(1,2),(2,1)\big\}$

$$\limsup_{j\to+\infty} \int \frac{|\delta_{i_1}(x)|^2}{\|\delta_{i_1}\|_{H^1}^2}|\phi_{i_2}|^2 * \frac{1}{|\cdot|}(x)dx \le \frac{1}{r} + \limsup_{j\to+\infty} \int_{|x-z_{i_2}|\le r} \frac{|\delta_{i_1}(x)|^2}{\|\delta_{i_1}\|_{H^1}^2}|\phi_2|^2 * \frac{1}{|\cdot|}(x)dx = \frac{1}{r},$$

this would contradict (5.99). Then as we have :

$$\lim_{j\to+\infty} M^2\big(\frac{\delta_1}{\|\delta_1\|_{H^1}}\wedge\phi_2\big) = \lim_{j\to+\infty}\frac{1}{\underline{D_{12}}}M^2\big(\delta_1\wedge\phi_2\big)=0,$$

then necessarily $\ell_1 = \varepsilon_1\phi_{2,\infty}$ with $|\varepsilon_1|\leq 1$. Furthermore, either $\|\delta_2\|_{H^1} = \underset{j\to+\infty}{o}(\|\delta_1\|_{H^1})$ or $\|\delta_2\|_{H^1} = \underset{j\to+\infty}{\Theta}(\|\delta_1\|_{H^1})$.

– In the first case then $\|\delta_2\|^2_{H^1} = \underset{j\to+\infty}{o}(\underline{D_{12}})$ and $\ell_1\neq 0$. We get a contradiction by computing :

$$\begin{aligned} 0=\int \underline{h_1}^*\underline{h_2} &= \int\phi_1^*\phi_2+\int\delta_1^*\phi_2+\int\phi_1^*\delta_2+\int\delta_1^*\delta_2\\ &= \underset{j\to+\infty}{\mathcal{O}}(e^{-\overline{\varepsilon}\mathrm{R}_g})+\int\delta_1^*\phi_2+\underset{j\to+\infty}{\mathcal{O}}(\|\delta_2\|_{L^2}(1+\|\delta_1\|_{L^2}))\\ &= \int\delta_1^*\phi_2+\underset{j\to+\infty}{o}(\|\delta_1\|_{H^1}).\end{aligned}$$

– In the second case we also get $\underset{j\to+\infty}{\lim}\|\delta_2\|^{-2}_{H^1}M^2(\delta_2\wedge\phi_1)$ and $\ell_2=\varepsilon_2\phi_{1,\infty}$, $|\varepsilon_2|\leq 1$. Writing for $k\neq k'$: $\underline{h_k} = \phi_k+\varepsilon_k\|\delta_k\|_{H^1}\phi_{k'}+h_k^{(r)}$, up to extraction the following holds :

$$\begin{aligned} 0=\int\underline{h_1}^*\underline{h_2} &= \underset{j\to+\infty}{\mathcal{O}}(e^{-\overline{\varepsilon}\mathrm{R}_g})+\varepsilon_1^*\|\delta_1\|_{H^1}+\varepsilon_2\|\delta_2\|_{H^1}+\int(h_1^{(r)})^*\underline{h_2}+\int\underline{h_1}^*h_2^{(r)}\\ \int(h_1^{(r)})^*\underline{h_2} &= \int(h_1^{(r)})^*\phi_2+\int(h_1^{(r)})^*(\varepsilon_1\|\delta_1\|_{H^1}\phi_1)+\int(h_1^{(r)})^*h_2^{(r)}\\ &= \underset{j\to+\infty}{o}(\|\delta_1\|_{H^1})+\underset{j\to+\infty}{\mathcal{O}}(\|\delta_1\|^2_{H^1})+\underset{j\to+\infty}{\mathcal{O}}(\|\delta_1\|_{H^1}\|\delta_2\|_{H^1}).\end{aligned}$$

The $\underset{j\to+\infty}{o}(\|\delta_1\|_{H^1})$ comes from the L^2_{loc}-convergence to 0 of $\frac{h_1^{(r)}(\cdot-z_2)}{\|\delta_1\|_{H^1}}$ and the uniform shape of the $\phi_2(\cdot-z_2)$'s. In particular :

$$\varepsilon_1^*\|\delta_2\|_{H^1} = -\varepsilon_2\|\delta_1\|_{H^1}+\underset{j\to+\infty}{o}(\|\delta\|_{H^1}).$$

Writing $\varepsilon_1\|\delta_1\|_{H^1}=a$ and $\varepsilon_2\|\delta_2\|_{H^2}=b=-a^*+(\delta a)$:

$$\left\{\begin{aligned}\underline{h_1} &= \phi_1+a\phi_2+h_1^{(r)}\\ \underline{h_2} &= \phi_2-a^*\phi_1+(\delta a)\phi_1+h_2^{(r)}\end{aligned}\right. \quad\left|\quad\begin{aligned} h_1^{(r)} &= \delta_1-a\phi_2\\ h_2^{(r)} &= \delta_2-b\phi_2.\end{aligned}\right.$$

We apply $\begin{pmatrix}\sqrt{1-|a|^2} & a^*\\ -a & \sqrt{1-|a|^2}\end{pmatrix}$ with $\sqrt{1-|a|^2}=:s$

$$\begin{pmatrix}\underline{g_1}\\ \underline{g_2}\end{pmatrix}=\begin{pmatrix}\phi_1(s+|a|^2-a(\delta a))+\phi_2(a(s-1))+sh_1^{(r)}-ah_2^{(r)}\\ \phi_2(s+|a|^2)+\phi_1(a^*(1-s)+(\delta a)s)+sh_2^{(r)}+a^*h_1^{(r)}\end{pmatrix},$$

replacing $s=1-\frac{|a|^2}{2}+\underset{j\to+\infty}{\mathcal{O}}(|a|^4)$ and neglecting the term $\mathcal{O}_{H^1}(|a|^3)$:

$$\begin{pmatrix}\underline{g_1}\\ \underline{g_2}\end{pmatrix}=\begin{pmatrix}\phi_1(1+\frac{|a|^2}{2}-a(\delta a))+h_1^{(r)}-ah_2^{(r)}+\mathcal{O}_{H^1}(|a|^3)\\ (1+\frac{|a|^2}{2})\phi_2+\phi_1((\delta a)(1-\frac{|a|^2}{2}))+h_2^{(r)}+a^*h_1^{(r)}+\mathcal{O}_{H^1}(|a|^3)\end{pmatrix}.$$

By L^2_{loc}-convergence, it is clear that $D(|\phi_k|^2,|h_{k'}^{(r)}|^2)=\underset{j\to+\infty}{o}(\|\delta_{k'}\|^2_{H^1})$ for (k,k') equal to $(1,2)$ or $(2,1)$. Using $\delta a=\underset{j\to+\infty}{o}(\|\delta\|_{H^1})$, at last we have :

$$D(|\underline{g_1}|^2,|\underline{g}_2|^2)\lesssim D(|\phi_1|^2,|\phi_2|^2)+\underset{j\to+\infty}{o}(\|\delta\|^2_{H^1})=\underset{j\to+\infty}{o}(\|\delta\|^2_{H^1})=\underset{j\to+\infty}{o}(\underline{D_{12}}=d_\Psi),$$

which gives the desired contradiction.
– Let us treat at last the case $\delta_1 \neq 0$ and $\delta_2 = 0$. Then as before :

$$D(|\underline{h_1}|^2, |\phi_2|^2) \quad = D(|\delta_1|^2, |\phi_2|^2) + \mathcal{O}\big(\tfrac{1+\|\delta_1\|_{L^2}}{\mathrm{R}_g}\big) = D(|\delta_1|^2, |\phi_2|^2) + \underset{j\to+\infty}{o}(\underline{D_{12}}).$$

Then necessarily there lies some mass of δ_1 near z_2 and :

$$\frac{\delta_1(\cdot - z_2)}{\|\delta_1\|_{H^1}} \rightharpoonup_{H^1} \ell_1 \neq 0.$$

As before necessarily : $\ell_1 = \varepsilon_1 \phi_{2,\infty}$ with $0 < |\varepsilon_1| \leq 1$. But this contradicts :

$$0 = \int \underline{h_1}^* \phi_2 = \int \delta_1^* \phi_2 + \int \phi_1^* \phi_2 = \int \delta_1^* \phi_2 + \underset{j\to+\infty}{\mathcal{O}}(e^{-\overline{\varepsilon}\mathrm{R}_g}).$$

5.B.2 Proof of Proposition 5.4

The proof is similar to that of Proposition 5.3 : by contradiction we assume the existence of $(a_j)_j$ decreasing to 0 together with $(\Psi_j = h_1 \wedge h_2)$ with $\mathcal{E}_{\mathrm{PT}}^U(\Psi_j) < a_j$ and $M^2(\Psi_j) < a_j R_{\mathrm{g};j}$. We re-use the same notations of the previous Subsection.

Thanks to Proposition 5.5 we know that d_{Ψ_j} is bounded from below by

$$(1 - \kappa\sqrt{a_0'})\big\{D(|\phi_1|^2, |\phi_2|^2) + D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2)\big\} + D(|\delta_1|^2, |\delta_2|^2)$$

As $(h_{k;j}(\cdot - z_{k;j}))_j$ tends to $\phi_{k,\infty} \in \mathscr{P}$ in H^1 for $k = 1, 2$, then for any $A > 0$:

$$\lim_{j\to+\infty} \int_{B(z_{k,j},A)} |h_{k,j}(x)|^2 dx = \int_{B(z_{k,j},A)} |\phi_{k,\infty}(x)|^2 dx.$$

For any $2^{-1/2} < \lambda < 1$ let $A_\lambda > 0$ be the number such that the last integral with $A = A_\lambda$ is equal to λ. We have :

$$\iint_{|x-y|<\mathrm{R}_g+2A_\lambda} \frac{|h_1 \wedge h_2(x,y)|^2}{|x-y|} dxdy \geq \frac{2}{\mathrm{R}_g + 2A_\lambda} \iint_{|x-y|<\mathrm{R}_g+2A_\lambda} |h_1(x)|^2 |h_2(y)|^2 dxdy$$
$$- \frac{2}{\mathrm{R}_g + 2A_\lambda} \int dx h_1^* h_2(x) \int_{y \in B(x,\mathrm{R}_g+2A_\lambda)} h_2^* h_1(y) dy$$
$$\liminf_{j\to+\infty} \iint_{|x-y|<\mathrm{R}_g+2A_\lambda} \frac{|h_1 \wedge h_2(x,y)|^2}{|x-y|} dxdy \geq \tfrac{2}{\mathrm{R}_g+2A_\lambda}(\lambda^2 - 2^{-1}).$$

We used the following trick : if $\displaystyle\int h_1^* h_2 = 0$ where $\|h_k\|_{L^2} = 1$, then for any Borelian set B :

$$\Big|\int_B h_1^* h_2\Big| \leq \frac{1}{2}.$$

The more precise result has the same proof : in the limit there holds similar inequality : for sufficiently small $a > 0$, $\lambda \mathrm{R}_g > A_\varepsilon$ where

$$\int_{|x|\leq A_\varepsilon} |\phi(x)|^2 dx = \varepsilon,\ \varepsilon > 2^{-1/2},\ \phi \in \mathscr{P}_0.$$

We conclude with the same argument.

5.C Localisation in Direct space : the $\underline{\psi_j}$'s

5.C.1 Proof of Lemma 5.7

Notation 5.11. For convenience here we write $V \cdot \underline{\varphi_k} := v'_{\underline{\gamma}}\varphi_k - R_{\underline{N}}\underline{\varphi_k}$ (and a similar expression for $\underline{\chi_k}$). The function $r_k := R_{\underline{\gamma}}\underline{\psi_k}$ is split into its upper part $r_{k,\uparrow} := (R_{\underline{\gamma}}\underline{\psi_k})_\uparrow$ and its lower part $r_{k,\downarrow}$ both in $L^2(\mathbb{R}^3, \mathbb{C}^2)$.

Moreover we write :

$$P_k(-\Delta) := c^2(1-\mu_k^2\mathcal{L}_{c\Lambda}^{-2}) - \Delta \text{ and } y_c := \mathcal{L}_{c\Lambda}^{-1} = \frac{c^2\Lambda^2}{c^2\Lambda^2 - \Delta}.$$

The operator $P_k(-\Delta)$ can be rewritten as follows : with $a_k := c^2(1-\mu_k)$ and $b := c\Lambda$ then

$$\begin{aligned} c^2(1-\mu_k y_c^2) - \Delta &= a_k(1+\mu_k) - \Delta\Big[1 + \tfrac{\mu_k c^2 - a_k}{c^2\Lambda^2}\tfrac{b^2}{b^2-\Delta} + \tfrac{\mu_k^2}{\Lambda^2}\Big(\tfrac{b^2}{b^2-\Delta^2}\Big)^2\Big] \\ &= (a_k(1+\mu_k) - \Delta)\Big\{1 + \big(1 - \tfrac{a_k(1+\mu_k)}{a_k(1+\mu_k)-\Delta}\big)\Big[\tfrac{\mu_k c^2 - a_k}{c^2\Lambda^2}\tfrac{b^2}{b^2-\Delta} + \tfrac{\mu_k^2}{\Lambda^2}\Big(\tfrac{b^2}{b^2-\Delta^2}\Big)^2\Big]\Big\} \end{aligned} \tag{5.100}$$

Proof We remark that $\underline{n}(x) = |h_1(x)|^2 + |h_2(x)|^2 = |\underline{\psi_1}(x)|^2 + |\underline{\psi_2}(y)|^2$.

Thanks to (5.46)-(5.47), there holds :

$$(\mathbf{D} + \alpha B)\psi_k = (1 + \tfrac{3E_{\rm PT(1)}}{2c^2} + \mathcal{O}(\alpha^{1/4}c^{-2}))\psi_k. \tag{5.101}$$

Up to applying some $\mathbf{m} \in \mathbf{SU}(2)$ to $\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}$, we consider $\underline{\psi_k} = h_k$ with the following :

$$(c^2\beta - ic\boldsymbol{\alpha}\cdot\nabla h_k) + \alpha c y_c(V\cdot h_k - R_{\underline{\gamma}}h_k) = (c^2 - \tfrac{3E_{\rm PT}(1)}{2})y_c h_k + \mathcal{O}(\alpha^{1/4}y_c h)$$

We write $a = -\frac{3E_{\rm PT}(1)}{2}$ and the additional term $\mathcal{O}(\alpha^{1/4}y_c h) = \delta_k h$.

– We now rewrite (5.72) once again : by substitution, we get :

$$\begin{cases} \underline{\varphi_k} &= \alpha c y_c \dfrac{1+\mu_k y_c}{P_k(-\Delta)}(V\cdot\underline{\varphi_k} - r_{k,\uparrow}) + \dfrac{\alpha y_c}{P_k(-\Delta)} i\sigma\cdot\nabla\big[V\cdot\underline{\chi_k} - r_{k,\downarrow}\big] \\ \underline{\chi_k} &= \alpha\dfrac{y_c}{P_k(-\Delta)} i\sigma\cdot\nabla(V\cdot\underline{\varphi_k} - r_{k,\uparrow}) + \alpha y_c\dfrac{c^2(1-\mu_k y_c)}{cP_k(-\Delta)}\big[V\cdot\underline{\chi_k} - r_{k,\downarrow}\big] \end{cases} \tag{5.102}$$

There holds similar equation for h_k but with additional terms $\frac{1}{\alpha c}(\delta_k h)_\uparrow$ with $-r_{k,\uparrow}$ and $\frac{1}{\alpha c}(\delta_k h)_\downarrow$ with $-r_{k,\downarrow}$.

There holds :

$$\alpha c(1-\mu_k y_c) = \alpha c(1-\mu_k) + \alpha c\mu_k(1-y_c).$$

For any $A \geq \Gamma(\mathrm{R_g})\mathrm{R}_g$, we multiply each term by $|D_0|^{1/2}$ and then by $d_{A,\lambda}(\cdot)$ defined by $d(\cdot)\xi_A(\cdot)\boldsymbol{\eta}^\lambda_{\mathrm{R}_g}$.

We take the L^2-norm, let us show estimates *independent* of A (but depending on ξ_1) :

$$\|d_{A,\lambda}|D_0|^{1/2}\underline{\psi_k}\|_{L^2} \leq K_\lambda + \varepsilon_{(\lambda)}\|E^{1/2}_{A,\lambda}|D_0|^{1/2}\underline{\psi_k}\|_{L^2},\ \text{with } \varepsilon_{(\lambda)} < 1.$$

This will end the proof, the family $(K_\lambda)_\lambda$ depending on $(\varepsilon_{(\lambda)})_\lambda$ and the latter being nonincreasing in $\lambda \in (\lambda_0, 2^{-1})$.

We prove the estimation of $\|d^{(2)}_{A,\lambda}|D_0|^{1/2}\underline{\psi_j}\|_{L^2}$ with $j = 1, 2$ by the same method : we need finiteness of $\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g}|D_0|^{1/2}\underline{\psi_k}\|_{L^2}$ with $k = 1, 2$ and of $\||x-y|\gamma\|_{\mathfrak{S}_2}$. We refer to Appendix 5.C for more details.

– In Appendix 5.C, we show :

$$|d_{A,\lambda}(x) - d_{A,\lambda}(y)| \lesssim |x-y|. \tag{5.103}$$

Let us first multiply (5.102) by $|D_0|^{1/2}$: let $\mathcal{F}_{j,k} := \frac{|D_0|^{1/2}\partial_j}{P_k(-\Delta)}$ and $\mathcal{F}_{0,k} := \frac{|D_0|^{1/2}}{P_k(-\Delta)}$. It is clear that they are bounded (convolution) operators, we show in Appendix 5.C that

$$\||\cdot|\mathcal{F}_{j,k}\|_{L^1} \lesssim 1,\ j \in \{1,2,3\},\ k \in \{1,2\}. \tag{5.104}$$

The function associated to y_c is a Yukawa potential Y_c [LL97, Section 6.23] :

$$Y_c(x-y) = \sqrt{\frac{\pi}{2}}\frac{(c\Lambda)^2 e^{-c\Lambda|x-y|}}{|x-y|},$$

in particular $\| |\cdot| Y_c\|_{L^1} \lesssim \frac{1}{c\Lambda}$. The idea is to take first the commutator $[d_{A,\lambda}, \mathcal{F}_{j,k}]$ and $[d_{A,\lambda}, y_c]$. Then we study $d_{A,\lambda} v \underline{\varpi_k}$ ($\varpi_k \in \{\varphi_k, \chi_k\}$) and $d_{A,\lambda} r_{\uparrow/\downarrow}$.

Estimate of $\alpha c\|V\cdot \underline{\varphi_k}\|_{L^2}, \alpha c\|V\cdot\underline{\chi_k}\|_{L^2}$ We use the same method for both cases. We recall the following :

$$v_{\underline{\gamma}} = \big(-\underline{\check{F_\Lambda}} * \underline{n} + (\delta_0 - \underline{\check{F_\Lambda}}) * (\mathfrak{t}_{\underline{N}} - \alpha^2 \underline{\widetilde{\tau}_2})\big) * \frac{1}{|\cdot|} = -\underline{\check{F_\Lambda}} * \underline{n} * \frac{1}{|\cdot|} + \underline{\rho_{rem}} * \frac{1}{|\cdot|}.$$

By (5.57) :

$$\begin{aligned} \big|\alpha c \underline{\check{F_\Lambda}} * \underline{n} * \tfrac{1}{|\cdot|}\big|(x) &\leq \underline{n} * \tfrac{1}{|\cdot|}(x) + \alpha c\big|(\underline{\check{F_\Lambda}} - F_\Lambda(0)\delta_0) * v_{\underline{n}}(x)\big| \\ &\leq \underline{n} * \tfrac{1}{|\cdot|}(x) + \mathcal{O}\big(\tfrac{1}{\sqrt{c}}\big). \end{aligned}$$

We used $\|f\|_{L^\infty} \lesssim \|\widehat{f}\|_{L^1}$, split the integral in Fourier space at level $2c$ and used Cauchy-Schwarz inequality. By Appendix 5.A.2 and Proposition 5.5 :

$$\begin{aligned} \big|\alpha c \underline{\rho_{rem}} * \tfrac{1}{|\cdot|}\big|(x) &\lesssim \alpha c (c^{1/2}\|\rho_{rem}\|_{\mathcal{C}} + c^{3/2}\|\rho_{rem}\|_{L^2}) \\ &\lesssim \alpha c^{3/2}(\alpha c^{-1} + \alpha^2 c^{-1}) + \alpha c^{5/2}(c^{-2} + c^{-1}(\alpha(a_{12}+a_{21}))^{1/2}) \\ &\lesssim \tfrac{\alpha}{\sqrt{\log(\Lambda)}} + \tfrac{1}{\sqrt{\log(\Lambda)}} + \tfrac{\alpha^{5/4}}{\sqrt{\log(\Lambda)}} \lesssim \tfrac{1}{\sqrt{\log(\Lambda)}}. \end{aligned}$$

We recall $a_{jk} = \|v_k\psi_k - v_{kj}\psi_k\|_{L^2}$ and by Proposition 5.5 we know it is $\mathcal{O}(c^{-1}\alpha^{3/2})$. We decompose each $\underline{\psi_j}$ in sum of h_1, h_2 : $\underline{\psi_k} = c_{k1}h_1 + c_{k2}h_2$. Then :

$$\begin{aligned} v_{\underline{\gamma}}\underline{\psi_k} &= v_{\underline{\gamma}}(c_{k1}h_1 + c_{k2}h_2) \\ (v_{\underline{n}} - R_{\underline{N}})\underline{\psi_k} &= c_{k1}(v_{|h_2|^2}h_1 - v_{h_2^*h_1}h_2) + c_{k2}(v_{|h_1|^2}h_2 - v_{h_1^*h_2}h_1). \end{aligned}$$

We write $h_k = \delta_k + \phi_k$ where $\phi_k \in \mathscr{P}$: as in Section 5.B $\|\delta_k\|_{H^1}^2 \lesssim \alpha$. By fast decay of the ϕ_k's : $(|\phi_k|^2 * \frac{1}{|\cdot|}(x))^2 = \Theta(|\phi_k|^2 * \frac{1}{|\cdot|^2}(x))$ and for $|x| \gtrsim 1$ this is $\mathcal{O}(\frac{1}{|x-z_k|^2})$.

In particular for $|x| > \lambda \mathrm{R}_g$

$$v\big[|h_k|^2\big](x) \lesssim \frac{1+\|\delta_k\|_{L^2}}{|x-z_k|} + \langle |\nabla|\delta_k\,,\,\delta_k\rangle \lesssim \frac{1}{\lambda\mathrm{R}_g} + \alpha,$$

we choose $C_0 > 1$ such that $\frac{\alpha c}{\lambda \mathrm{R}_g} < 1 - \varepsilon_0$ where $0 < \varepsilon_0 < 1$ is fixed (for instance 2^{-1}).

By Cauchy-Schwarz inequality we have $v\big[h_1^*h_2\big](x), v\big[h_2^*h_1\big](x) = \mathcal{O}(\|\delta\|_{L^2})$. It follows that

$$\alpha c\|d_{A,\lambda}V\cdot\underline{\varphi_k}\|_{L^2} \lesssim \varepsilon'_{(\lambda)}\|d_{A,\lambda}\underline{\varphi_k}\|_{L^2},\ \text{with } 0 < \varepsilon'_{(\lambda)} < 1.$$

Estimate of $\alpha c d_{A,\lambda} R_{\underline{\gamma}\underline{\psi_k}}$

$$\begin{aligned} |[d_{A,\lambda}, R_{\underline{\gamma}}](x,y)| &\lesssim |\underline{\gamma}(x,y)| \text{ so :} \\ \alpha c\|[d_{A,\lambda}, R_{\underline{\gamma}}]\underline{\psi_k}\|_{L^2} &\lesssim \alpha c\|\underline{\gamma}\|_{\mathfrak{S}_2}\|\underline{\psi_k}\|_{L^2} \lesssim \alpha^2 c^{1/2} = \mathcal{O}(\tfrac{\alpha}{\sqrt{\log(\Lambda)}}). \\ \|R_{\underline{\gamma}} d_{A,\lambda}\underline{\psi_k}\|_{L^2}^2 &\lesssim \mathrm{Tr}(\gamma R_{\underline{\gamma}})\langle |\nabla| d_{A,\lambda}\underline{\psi_k}\,,\, d_{A,\lambda}\underline{\psi_k}\rangle \\ &\lesssim c^{-1}\||D_0|^{1/2} d_{A,\lambda}\underline{\psi_k}\|_{L^2}^2. \end{aligned}$$

By Lemma (5.10), $[|D_0|^{1/2}, d_{A,\lambda}]|D_0|^{-1/2}$ is a bounded operator (with norm $\mathcal{O}(\|\nabla d_{A,\lambda}\|_{L^\infty})$) and at last we get :

$$\alpha c\|d_{A,\lambda}R_{\underline{\gamma}}\underline{\psi_k}\|_{L^2} \lesssim \alpha c^{1/2}(1 + \|d_{A,\lambda}|D_0|^{1/2}\underline{\psi_k}\|_{L^2}) \text{ and } \alpha c^{1/2} = \mathcal{O}\Big(\frac{1}{\sqrt{\log(\Lambda)}}\Big).$$

We know deal with the case of $d^{(2)}_{A,\lambda}R_{\underline{\gamma\psi_k}}$, using (5.107), proved below.

The aim is to prove :

$$\begin{aligned}\|d^{(2)}_{A,\lambda}R_{\underline{\gamma\psi_k}}\|_{L^2} \lesssim \||x-y|\underline{\gamma}\|_{\mathfrak{S}_2} + \|\underline{\gamma}\|_{\mathfrak{S}_2}\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}\underline{\psi_k}\|_{L^2}\\ +c^{1/2}\|\gamma\|_{\mathrm{Ex}}(\|\underline{\psi_k}\|_{L^2}+\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}\underline{\psi_k}\|_{L^2}).\end{aligned} \tag{5.105}$$

First of all we use Taylor's formula (5.107) to get :

$$\|[d^{(2)}_{1,\lambda}, R_{\underline{\gamma}]\underline{\psi_k}}\|_{L^2} \lesssim \||x-y|\underline{\gamma}\|_{\mathfrak{S}_2} + \|\underline{\gamma}\|_{\mathfrak{S}_2}\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}\underline{\psi_k}\|_{L^2}.$$

Let us prove at the end $\||x-y|\underline{\gamma}\|_{\mathfrak{S}_2} = c^{-1}\||x-y|\gamma\|_{\mathfrak{S}_2}\lesssim \alpha c^{-1}$.

There remains $\|R_{\underline{\gamma} d^{(2)}_{A,\lambda}\underline{\psi_k}}\|_{L^2}\lesssim \||D_0|^{1/2}d^{(2)}_{A,\lambda}\underline{\psi_k}\|_{L^2}$.

We commute : using (5.96), there holds

$$\begin{aligned}[|D_0|^{1/2}, d^{(2)}_{A,\lambda}] &= \frac{1}{2^{-1/2}\pi}\int_0^{+\infty}\frac{s^{1/4}ds}{1-\Delta+s}[-\Delta, d^{(2)}]\frac{1}{1-\Delta+s},\\ [-\Delta, d^{(2)}] &= (-\Delta d^{(2)}) - 2\sum_{j=1}^{3}(\partial_j d^{(2)})\partial_j.\end{aligned}$$

First $\|\Delta d^{(2)}\|_{L^\infty}\lesssim 1$. Then thanks to (5.107) :

$$\begin{aligned}\|(\partial_j d^{(2)})\tfrac{\partial_j}{1-\Delta+s}\underline{\psi_k}\|_{L^2} &\lesssim \|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}\tfrac{\partial_j}{1-\Delta+s}\underline{\psi_k}\|_{L^2}\\ &\lesssim \||x-y|\mathscr{F}^{-1}(\tfrac{p_j}{1+s+|p|^2})\|_{L^1}\|\underline{\psi_k}\|_{L^2} + \tfrac{\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}\underline{\psi_k}\|_{L^2}}{1+s}\\ &\lesssim \frac{1}{1+s}(\|\underline{\psi_k}\|_{L^2}+\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}\underline{\psi_k}\|_{L^2}).\end{aligned}$$

To end this section we prove $\||x-y|\gamma\|_{\mathfrak{S}_2}, \||x-y||\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}\lesssim\alpha$. This is almost trivial : for each $j\in\{1,2,3\}$ we consider $(x_j-y_j)\gamma(x,y)$ and use the Cauchy expansion of γ. For each $Q_{0,k}$, $k\in[|1,5|]$, we replace at least one $P^0_\varepsilon v'_\gamma P^0_{-\varepsilon}$ as in (5.93) ([GLS09]) and write :

$$x_j - y_j = x_j - \ell^{(1)}_j + \ell^{(1)}_j - \ell^{(2)}_j + \cdots + \ell^{(n)}_j - y_j.$$

For each convolution operator $\frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}(x-y)$, $\frac{P^0_\varepsilon}{\mathbf{D}+i\eta}(x-y)$, $\frac{1}{D_0+i\omega}(x-y)$, multiplying by (x_j-y_j) corresponds to take the derivative ∂_j in Fourier space enabling us to take KSS inequalities (5.13) under the integral sign. Indeed we have :

$$\begin{aligned}&|\partial_j \overline{E}^{1/2}_p|\lesssim \overline{E}^{1/6}_p, && |\partial_j\tfrac{1}{\overline{E}(p)+i\eta}|\lesssim\tfrac{1}{|\overline{E}_p+i\eta|^{1+3^{-1}}},\\ &|\partial_j\tfrac{1}{E(p)+i\omega}|\lesssim\tfrac{1}{E(\omega_2)+|p|^2}, && |\partial_j P^0_\varepsilon(p)|\lesssim\tfrac{1}{E(p)}.\end{aligned}$$

Then operators of type $\rho*\frac{1}{|\cdot|}$ or $\alpha_k\partial_k(\rho*\frac{1}{|\cdot|})$ remains unchanged while operators of type $(x_j-y_j)R_Q(x,y)$ are trivially Hilbert-Schmidt. This end the proof ; the biggest term comes from $Q_{1,0}((x_j-y_j)\gamma'(x,y))$.

5.C.2 Proof of (5.103) and variation for $d^{(2)}_{A,\lambda}$

1. We recall that ξ_1 is a *radial* smooth function with $\xi_1(x)=1$ for $|x|\le 1$ and $\xi_1(x)=0$ for $|x|\ge 2$. We study $d_{A,\lambda} := d(\cdot)\xi_A(\cdot)\boldsymbol{\eta}^\lambda_{\mathrm{R}_g}(\cdot)$.

First remark to be done : $H=\{x : |x-z_1|=|x-z_2|\}$ splits the space into two half-spaces E_1 (set of points closest to z_1) and E_2. Let s_H be the orthogonal symmetry with respect to H : $s_H(z_1)=z_2$. If $x\in E_1$ and $y\in E_2$, then

$$|d(x)-d(y)| = \big||x-z_1|-|s_H(y)-z_1|\big|\le |x-s_H(y)|\le|x-y|.$$

Moreover $d_{A,\lambda}(y)=d_{A,\lambda}(s_H(y))$ and

$$\big|d_{A,\lambda}(x)-d_{A,\lambda}(y)\big| = \big|d_{A,\lambda}(x)-d_{A,\lambda}(s_H(y))\big|.$$

So we may assume that $d(x)=|x-z_1|$ and $d(y)=|y-z_1|$, and in this case we can write :

$$d_{A,\lambda}(x)=F_\lambda(d(x))\xi_A(x):=d(x)\sqrt{1-\xi_{\lambda \mathrm{R}_g^2(d(x))}}G_A(|x-z_m|)$$

the same holds for y. We will write $F_\lambda(\cdot)$ for $x\mapsto F_\lambda(d(x))$ for convenience. There holds

$$\nabla d_{A,\lambda}(x)=\big(\nabla F_\lambda(x)\big)\xi_A(x)+F_\lambda(x)(\frac{\nabla\xi_1(x/A)}{A}),$$

and as we have chosen $A\gg \mathrm{R}_g$ we may assume that if $\nabla\xi_A(x)\neq 0$, then $|x-z_m|=\Theta(d(x))$. By simple computation :

$$|\nabla d_{A,\lambda}(x)| \quad\lesssim \big(1+\||\cdot|\nabla\xi_1\|_{L^\infty}+\||\cdot|\nabla\boldsymbol{\eta}_1^\lambda\|_{L^\infty}\big). \tag{5.106}$$

2. For $x,y\in E_\varepsilon$, $\varepsilon=1,2$ (say E_1) and $A\gg\mathrm{R}_g$, there holds :

$$\begin{aligned}d_{A,\lambda}^{(2)}(x)-d_{A,\lambda}^{(2)}(y)&=|x-z_1|^2\xi_A(x)\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}(x)-|y-z_1|^2\xi_A(y)\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}(y)\\ &=|y-z_1|^2\big(\tfrac{\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}(y)}{A}\nabla\xi_1(\tfrac{y}{A})+\tfrac{\xi_A(y)}{c\lambda\mathrm{R}_g}\nabla(\boldsymbol{\eta}_1^1)(\tfrac{y}{c\lambda\mathrm{R}_g})\big)\cdot(x-y)\\ &\quad+\xi_A(y)\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}(y)\langle y-z_1\,,\,x-y\rangle+|y-z_1|^2+\mathcal{O}\big(|x-y|^2\big)\\ &=\mathcal{O}\big(d(y)\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}(y)|x-y|+|x-y|^2\big).\end{aligned}\tag{5.107}$$

Above we used $\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}=\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$ and the $\mathcal{O}(\cdot)$ depends on $\xi_1,\boldsymbol{\eta}_1^1$. This estimate enables us to consider commutators with $\frac{|D_0|^{1/2}\sigma\cdot\nabla}{P_k(-\Delta)}$ and $y_c:=\frac{(c\Lambda)^2}{(c\Lambda)^2-\Delta}$, as shown in the next section.

5.C.3 Proof of (5.104) and variation for $d_{A,\lambda}^{(2)}$

1. For any borelian function $\mathcal{F}$:

$$\int_{\mathbb{R}^3}|x||\mathcal{F}(x)|dx\le\Big\{\int|x|^4E(x)^2|\mathcal{F}(x)|^2dx\int\frac{dx}{|x|^2E(x)^2}\Big\}^{1/2}.$$

To prove $|\cdot|\mathcal{F}\in L^1$ it suffices to check all integrals on the right side converge : in Fourier space, we have to prove :

$$\|\Delta\widehat{\mathcal{F}}\|_{L^2}^2+\|\nabla\Delta\widehat{\mathcal{F}}\|_{L^2}^2<+\infty.$$

Applying this method for $\mathcal{F}_{j,k}(x-y):=\frac{|D_0|^{1/2}\partial_j}{P_k(-\Delta)}(x-y)$:

$$\widehat{\mathcal{F}_{j,k}}(p)=\frac{E(p)^{1/2}p_j}{a_k+|p|^2}\Big\{1+\frac{\mu_k^2|p|^2}{\Lambda^2(a_k+|p|^2)}\frac{2b^4+b^2|p|^2}{(b^2+|p|^2)^2}\Big\}^{-1}$$

where we recall $b=c\Lambda$, $a_k=c^2(1-\mu_k)$. From this expression, it is easy to see that for $\ell=1,2,3$ and $m=1,2$ we have

$$\|\partial_\ell^m\mathcal{F}_{j,k}\|_{L^2}^2\lesssim 1.$$

The constant depends on a_k but for sufficiently small α,L,Λ^{-1} then $a_k>\varepsilon_0>0$.

2. By the same method we can show that :

$$\int_{\mathbb{R}^3}|x|^2|\mathcal{F}(x)|dx\le\Big\{\int|x|^6E(x)^2|\mathcal{F}(x)|^2dx\int\frac{dx}{|x|^2E(x)^2}\Big\}^{1/2},$$

enabling us to treat $d_{A,\lambda}^{(2)}$.

5.D Localisation in Direct space : γ

We recall we explain in Remark 5.15 how we use the technical results proved here : Propositions 5.7, 5.8 and 5.9.

5.D.1 Estimates on the localised density

Let $Q \in \mathcal{K}$ and $0 \leq \zeta \leq 1$ a smooth function (*e.g.* $\xi_{\lambda \mathrm{R}_g}$ or $\boldsymbol{\eta}_{\mathrm{R}_g}^{\lambda}$). Our aim is to give a semi-quantitative estimate of the localisation of the function $\zeta^2 \rho_Q = \rho_{\zeta Q \zeta}$ around the support of ζ.

Proposition 5.7. *Let Q and ζ be as above, then we have :*

$$\|\zeta^2 \rho_Q - \rho[\zeta^{++} Q \zeta^{++} + \zeta^{--} Q \zeta^{--}]\|_{\mathcal{C}} \leq F_{est}[\Lambda, \zeta, Q], \tag{5.108}$$

with

$$\begin{aligned} F_{est}[\Lambda, \zeta, Q] &= (\sqrt{\log(\Lambda)}\|\nabla\zeta\|_{L^3} + \|\nabla \zeta\|_{L^\infty})(\|\zeta P^0_{\pm} |D_0|^{a[\Lambda]} Q\|_{\mathfrak{S}_2} + \|\nabla\zeta\|_{L^\infty}\|Q\|_{\mathfrak{S}_2}) \\ &+ \|\nabla\zeta\|_{L^6}^2 \||D_0|^{a[\Lambda]} Q\|_{\mathfrak{S}_2} + \sqrt{\log(\Lambda)}(\|\zeta Q^{\pm\mp}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_2} + \|\zeta Q^{\pm\mp}\|_{\mathfrak{S}_2}\|\nabla\zeta\|_{L^\infty}) \\ &+ \sqrt{\log(\Lambda)}\|\nabla\zeta\|_{L^\infty}(\|\nabla\zeta\|_{L^\infty}\|Q^{\pm\pm}\|_{\mathfrak{S}_1} + \|\zeta|D_0|^{a[\Lambda]}Q^{\pm\pm}\|_{\mathfrak{S}_1}) \\ &+ (\log(\Lambda))^{1/6}\|\nabla\zeta\|_{L^\infty}^2 \||D_0|^{a[\Lambda]}Q^{\pm\pm}\|_{\mathfrak{S}_1}. \end{aligned} \tag{5.109}$$

Moreover there holds for $\varepsilon = \pm$:

$$\begin{aligned} \|\rho[\zeta^{\varepsilon\varepsilon} Q \zeta^{\varepsilon\varepsilon}]\|_{\mathcal{C}} &\leq \|[\zeta^{\varepsilon\varepsilon}, |D_0|^{a[\Lambda]}]\|_{\mathcal{B}}\|Q^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1} + \|\zeta^{\varepsilon\varepsilon}Q^{\varepsilon\varepsilon}|D_0|^{a[\Lambda]}\zeta^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1} \\ &\lesssim \|\nabla\zeta\|_{L^\infty}\|Q^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1} + \|\zeta^{\varepsilon\varepsilon}Q^{\varepsilon\varepsilon}|D_0|^{a[\Lambda]}\zeta^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1}. \end{aligned} \tag{5.110}$$

Remark 5.17. 1. In the case $Q = \Pi - P^0_-$ with $\Pi^* = \Pi^2 = \Pi$ then (*cf* [HLS05a]) :
$Q^2 = Q^{++} - Q^{--} \geq Q^{++}$. As shown in [Sok13] we can consider an orthonormal family of eigenvectors of Q^2 that split into those in $\mathrm{Ran}(P^0_+)$ and those in $\mathrm{Ran}(P^0_-)$. It is then clear that :

$$\begin{aligned} \|\zeta^{++}Q^{++}|D_0|^{a[\Lambda]}\zeta^{++}\|_{\mathfrak{S}_1} &\leq \|\zeta Q^{++}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_1} \\ &\leq \|\zeta|D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2}\|\zeta Q\|_{\mathfrak{S}_2} \end{aligned}$$

2. There is also an analogous estimate if we choose two different functions ζ_1, ζ_2, that is with $\zeta_1\zeta_2\rho(Q) = \rho(\zeta_1 Q \zeta_2)$. The same proof shows also localisation estimates, but we have to "polarize" the inequalities just like for a quadratic form and its associated bilinear form.

Proof : We prove it by duality. Let V be some Schwartz function : we study $\mathrm{Tr}_0(\zeta Q \zeta V)$. By symmetry we just treat $(\zeta Q \zeta V)^{++}$. There holds :

$$\begin{aligned} P^0_+ \zeta Q \zeta V P^0_+ &= P^0_+ \zeta (P^0_+ + P^0_-) Q (P^0_+ + P^0_-) \zeta (P^0_+ + P^0_-) V P^0_+ \\ &= \zeta^{++}Q^{++}\zeta^{++}V^{++} + \zeta^{++}Q^{++}\zeta^{+-}V^{-+} + \zeta^{++}Q^{+-}\zeta^{-+}V^{++} + \zeta^{++}Q^{+-}\zeta^{--}V^{-+} \\ &+ \zeta^{+-}Q^{-+}\zeta^{++}V^{++} + \zeta^{+-}Q^{-+}\zeta^{+-}V^{-+} + \zeta^{+-}Q^{--}\zeta^{-+}V^{++} + \zeta^{+-}Q^{--}\zeta^{--}V^{-+}. \end{aligned}$$

We first show those operators are trace-class and then prove (5.108).

Remark 5.18. We recall that by Sobolev inequality : $\|V\|_{L^6} \lesssim \|\nabla V\|_{L^2}$.
Moreover $\||D_0|^{-a[\Lambda]}V\|_{\mathfrak{S}_2} \lesssim \sqrt{\log(\Lambda)}\|V\|_{L^2}$.
As shown in Appendix 5.A :

$$\zeta^{-+} = \frac{i}{2\pi}\int_{-\infty}^{+\infty} \frac{1}{D_0 + i\eta}\boldsymbol{\alpha}\cdot\nabla\zeta \frac{P^0_+ d\eta}{D_0 + i\eta}. \tag{5.111}$$

It can be rewritten as :

$$\zeta^{-+} = \frac{i}{2}\int_0^{+\infty} e^{-s|D_0|}P^0_- \boldsymbol{\alpha}\cdot\nabla\zeta P^0_+ e^{-s|D_0|}ds, \tag{5.112}$$

by writing $\frac{1}{E(p)+E(q)} = \int_0^{+\infty} e^{-s(E(p)+E(q))}$ in the kernel of its Fourier transform *cf* Appendix 5.A.

$\zeta^{++}Q\zeta^{++}V^{++}$ **:**

$$\zeta^{++}Q\zeta^{++}V^{++}=\zeta^{++}(Q^{++}\zeta^{++}|D_0|^{a[\Lambda]})\frac{1}{|D_0|^{a[\Lambda]}}V^{++}$$

and $(Q^{++}\zeta^{++}|D_0|^{a[\Lambda]})\in\mathfrak{S}_1$, $\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\in\mathfrak{S}_6$ with norm $\mathcal{O}((\log(\Lambda))^{1/6}\|\nabla V\|_{L^2})$ by the KSS inequality (5.13). We write

$$\begin{aligned}\|\zeta Q^{++}\zeta^{++}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1} &\le \|\zeta Q^{++}\|_{\mathfrak{S}_1}\|[\zeta^{++},|D_0|^{a[\Lambda]}]\|_{\mathcal{B}}+\|\zeta Q^{++}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_1}\\ &\lesssim \|\zeta Q^{++}\|_{\mathfrak{S}_1}\|\nabla\zeta\|_{L^\infty}+\|\zeta Q^{++}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_1}.\end{aligned}$$

In general whenever there is Q^{++} or Q^{--} we can easily estimate.

$$\begin{aligned}|\mathrm{Tr}(\zeta^{++}Q^{++}\zeta^{+-}V^{-+})| &= |\mathrm{Tr}(V^{-+}\tfrac{1}{|D_0|^{a[\Lambda]}}|D_0|^{a[\Lambda]}\zeta^{++}Q^{++}\zeta^{+-})|\\ &\lesssim \sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}\|\nabla\zeta\|_{L^\infty}(\|\nabla\zeta\|_{L^\infty}\|Q^{++}\|_{\mathfrak{S}_1}+\|\zeta|D_0|^{a[\Lambda]}Q^{++}\|_{\mathfrak{S}_1}),\\ |\mathrm{Tr}(\zeta^{+-}Q^{--}\zeta^{-+}V^{++})| &\le \|\tfrac{1}{|D_0|^{a[\Lambda]}}V\|_{\mathfrak{S}_6}\|\zeta^{+-}\|_{\mathcal{B}}\|Q^{--}\zeta^{-+}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1}\\ &\lesssim (\log(\Lambda))^{1/6}\|\nabla V\|_{L^2}\|\nabla\zeta\|_{L^\infty}^2\|Q^{--}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1},\\ |\mathrm{Tr}(\zeta^{+-}Q^{--}\zeta^{--}V^{-+})| &\lesssim \sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}\|\nabla\zeta\|_{L^\infty}(\|\nabla\zeta\|_{L^\infty}\|Q^{--}\|_{\mathfrak{S}_1}+\|\zeta|D_0|^{a[\Lambda]}Q^{--}\|_{\mathfrak{S}_1}).\end{aligned}$$

The term $\zeta^{+-}Q^{-+}\zeta^{+-}V^{-+}$ **:**

$$\begin{aligned}\|\zeta^{+-}Q^{-+}\zeta^{+-}V^{-+}\|_{\mathfrak{S}_1} &\le \|\zeta^{-+}\|_{\mathfrak{S}_6}\|Q^{+-}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_2}\|\tfrac{1}{|D_0|^{a[\Lambda]}}\zeta^{-+}V^{++}\|_{\mathfrak{S}_3}\\ \|\tfrac{1}{|D_0|^{a[\Lambda]}}\zeta^{-+}V^{++}\|_{\mathfrak{S}_3} &\lesssim \sum_{j=1}^3\frac{1}{2\pi}\int_{-\infty}^{+\infty}\|\tfrac{1}{|D_0|^{a[\Lambda]}(D_0+i\eta)}\partial_j\zeta\tfrac{P_+^0}{D_0+i\eta}V\|_{\mathfrak{S}_3}d\eta\\ &\lesssim \sum_{j=1}^3\|\partial_j\zeta\|_{L^6}\|V\|_{L^6}\|\tfrac{1}{E(\cdot)^{5/8}}\|_{L^6}^2\int_{-\infty}^{+\infty}\frac{d\eta}{E(\eta)^{5/4}},\\ \|\zeta^{-+}\|_{\mathfrak{S}_6} &\lesssim \|\nabla\zeta\|_{L^6}.\end{aligned}$$

The term $\zeta^{++}Q^{+-}\zeta^{--}V^{-+}$:

$$|\mathrm{Tr}(\zeta^{++}Q^{+-}\zeta^{--}V^{-+})| \quad\lesssim \sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}(\|\zeta Q^{+-}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_2}+\|\zeta Q^{+-}\|_{\mathfrak{S}_2}\|\nabla\zeta\|_{L^\infty}).$$

The terms $\zeta^{+-}Q^{-+}\zeta^{++}V^{++}$ **and** $\zeta^{++}Q^{+-}\zeta^{-+}V^{++}$ These operators are difficult to handle. We use Lemma 5.10 (Appendix 5.A). First :

$$\zeta^{+-}Q^{-+}\zeta^{++}V^{++}=\big(\zeta^{+-}\frac{1}{|D_0|^{\frac{\varepsilon_\Lambda}{4}}}\big)\big(|D_0|^{\frac{\varepsilon_\Lambda}{4}}Q^{-+}\zeta^{++}|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}\big)\big(\frac{1}{|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}}V^{++}\big)\in\mathfrak{S}_1,$$

with norm $\mathcal{O}((\log(\Lambda))^{3/2}\|\nabla\zeta\|_{L^3}\|V\|_{L^6}\||D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2})$. We used the KSS inequality and Hölder-type inequality for $\mathfrak{S}_p$. Similarly we can show that $\zeta^{++}Q^{+-}\zeta^{-+}V^{++}\in\mathfrak{S}_1$. Then by density of $\mathfrak{S}_1$ in $\mathfrak{S}_2$, we approximate $\big(|D_0|^{\frac{\varepsilon_\Lambda}{4}}Q^{-+}\zeta^{++}|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}\big)$ by trace-class operators enabling us to say that :

$$\mathrm{Tr}(\zeta^{+-}Q^{-+}\zeta^{++}V^{++})=\mathrm{Tr}\Big(\big(|D_0|^{\frac{\varepsilon_\Lambda}{4}}Q^{-+}\zeta^{++}|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}\big)\big(\frac{1}{|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}}V^{++}\big)\big(\zeta^{+-}\frac{1}{|D_0|^{\frac{\varepsilon_\Lambda}{4}}}\big)\Big).$$

Let us show that $Q^{-+}\zeta^{++}V^{++}\zeta^{+-}\in\mathfrak{S}_1$. It suffices to show $\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\eta^{+-}\in\mathfrak{S}_2$. We go in Fourier space and used formula (5.112) to show $[V,P_+^0e^{-sE|D_0|}]\in\mathfrak{S}_2$.

$$\mathscr{F}([V,P_+^0e^{-sE|D_0|}];p,q)=\frac{1}{(2\pi)^{3/2}}\widehat{V}(p-q)\big(P_+^0(q)e^{-sE(q)}-P_-^0(p)e^{-sE(p)}\big);$$

then (*cf* Appendix 5.A)

$$\begin{aligned}
P^0_+(q)e^{-sE(q)} - P^0_-(p)e^{-sE(p)} &= (P^0_+(q) - P^0_+(p))e^{-sE(q)} + P^0_+(p)(e^{-sE(q)} - e^{-sE(p)}) \\
\left|P^0_+(q) - P^0_+(p)\right| &\lesssim \frac{|p-q|}{\max(E(p),E(q))} \\
\left|e^{-sE(q)} - e^{-sE(p)}\right| &= s|E(p)-E(q)|\frac{|e^{-sE(q)} - e^{-sE(p)}|}{s|E(p)-E(q)|} \\
&\leq s|p-q|\min(e^{-sE(p)}, e^{-sE(q)}) \\
&\leq s|p-q|(e^{-sE(p)} + e^{-sE(q)}).
\end{aligned}$$

By easy computation : $\|[V, P^0_+ e^{-sE|D_0|}]\|_{\mathfrak{S}_2} \lesssim s^{-1/2}e^{-s/\sqrt{2}}\|\nabla V\|_{L^2}$:

$$\int_{s=0}^{+\infty} \|[V, P^0_+ e^{-s|D_0|}]\boldsymbol{\alpha}\cdot\nabla\zeta e^{-s|D_0|}\|_{\mathfrak{S}_2} ds \lesssim \|\nabla\zeta\|_{L^\infty}\|\nabla V\|_{L^2}\int_0^{+\infty}\frac{e^{-s}ds}{s^{1/2}}.$$

At last there remains to show :

$$\mathcal{A}[V,\zeta] = \int_0^{+\infty}\frac{e^{-s|D_0|}}{|D_0|^{a[\Lambda]}}P^0_+\big(V\boldsymbol{\alpha}\cdot\nabla\zeta\big)P^0_- e^{-s|D_0|}ds \in \mathfrak{S}_2,$$

as in Appendix 5.A it suffices to go in Fourier space and remark $\|V\partial_j\zeta\|_{L^2} \leq \|V\|_{L^6}\|\partial_j\zeta\|_{L^3}$:

$$\|\mathcal{A}[V,\zeta]\|_{\mathfrak{S}_2} \lesssim \sqrt{\log(\Lambda)}\|V\nabla\zeta\|_{L^2} \lesssim \sqrt{\log(\Lambda)}\|V\|_{L^6}\|\partial_j\zeta\|_{L^3}.$$

The case of $\zeta^{++}Q^{+-}\zeta^{-+}V^{++}$ is similar : first we prove by density that

$$\mathrm{Tr}(\zeta^{++}Q^{+-}\zeta^{-+}V^{++}) = \mathrm{Tr}(\zeta^{-+}V^{++}\zeta^{++}Q^{+-}),$$

and we get *in fine*

$$\begin{aligned}
&\|\rho[\zeta^{++}Q^{+-}\zeta^{-+}V^{++}]\|_{\mathcal{C}} + \|\rho[\zeta^{-+}Q^{+-}\zeta^{-+}V^{++}]\|_{\mathcal{C}} \\
&\quad\lesssim (\sqrt{\log(\Lambda)}\|\nabla\zeta\|_{L^3} + \|\nabla\zeta\|_{L^\infty})(\|\zeta P^0_+|D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2} + \|\nabla\zeta\|_{L^\infty}\|Q\|_{\mathfrak{S}_2}).
\end{aligned} \tag{5.113}$$

□

5.D.2 Estimates on the localised operator γ

Here γ is the vacuum part of a (hypothetical) minimizer of $E^0_{\mathrm{BDF}}(2)$ or a minimizer of $E^0_{\mathrm{BDF}}(1)$. Our aim is to prove :

Proposition 5.8. *Let ζ be a smooth function with :*

$$\begin{cases} \|\nabla\zeta\|_{L^\infty}, \|\partial_j\partial_k\zeta\|_{L^\infty} < +\infty,\ j,k \in \{1,2,3\} \\ \|\zeta v'\|_{L^6}, \|\zeta\nabla v'\|_{L^2}, \|\zeta\gamma\|_{Ex}, \|\zeta R_N\|_{\mathfrak{S}_2} < +\infty. \end{cases}$$

Then there holds :

$$\begin{aligned}
\|\zeta|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2} \lesssim\; & c^{-1/2}\|\zeta\nabla v'\|_{L^2} + \alpha(\|\zeta\gamma\|_{Ex} + \|\zeta R_N\|_{\mathfrak{S}_2}) \\
&+\alpha^2(\|\zeta\nabla v'\|_{L^2} + \|\zeta v'\|_{L^6} + \|\zeta\gamma\|_{Ex} + \|\zeta R_N\|_{\mathfrak{S}_2})^2 \\
&+\big\{\|\nabla\zeta\|_{L^\infty} + \textstyle\sum_{1\leq j,k\leq 3}\|\partial_j\partial_k\zeta\|_{L^\infty}\big\}\big\{\alpha(\|\rho'_\gamma\|_{\mathcal{C}} + \||\nabla|^{1/2}\gamma'\|_{\mathfrak{S}_2})\big\}.
\end{aligned} \tag{5.114}$$

The same holds for $\|\zeta|D_0|^{\widetilde{a}}\gamma\|_{\mathfrak{S}_2}$ with $\widetilde{a} \in \{\frac{1}{2}, a[\Lambda]\}$.
We can replace $\|\zeta\gamma\|_{Ex} + \|\zeta R_N\|_{\mathfrak{S}_2}$ by $\|\gamma'\|_{Ex}$ and put $P^0_\pm\gamma$ instead of γ.

Idea of the proof

We will focus on the Cauchy expansion of $\gamma : \gamma = \sum_{j=1}^{+\infty} \alpha^j Q_j(\gamma', \rho'_\gamma)$.

As shown in [GLS09, Sok13, Sok14c], we substitute $P^0_\pm(\rho'_\gamma * \frac{1}{|\cdot|})P^0_\mp$ by its expression (5.93) whenever it is necessary (in $Q_{0,1}, Q_{0,3}, Q_{0,5}$)

We multiply γ by $|D_0|^{\widetilde{a}}$ (or $|\mathbf{D}|^{1/2}$) and then by ζ. We consider $\frac{|D_0|^{\widetilde{a}}}{\mathbf{D}+i\eta}$ (or $\frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}$) as a whole operator and we then commute ζ with this operator and maybe some P^0_ε and $\frac{1}{D_0+i\omega}$ (if it was necessary to use (5.93)) in order to stick ζ with a $v\rho'_\gamma * \frac{1}{|\cdot|}$, a R'_γ or a $\partial_j \rho'_\gamma * \frac{1}{|\cdot|}$ (if (5.93) was used). For instance in the case of $Q_{0,1}$:

$$\begin{aligned} Q_{0,1}^{+-} &= \int_{-\infty}^{+\infty} \frac{|\mathbf{D}|^{1/2} P^0_+}{\mathbf{D}+i\eta} v' \frac{P^0_-}{\mathbf{D}+i\eta} \\ &= \frac{i}{2\pi} \iint_{\mathbb{R}\times\mathbb{R}} \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \frac{1}{D_0+i\omega} \boldsymbol{\alpha}\cdot\nabla v' \frac{P^0_-}{D_0+i\omega} \frac{d\eta d\omega}{\mathbf{D}+i\eta}. \end{aligned} \tag{5.115}$$

We multiply by ζ and under the integral sign :

$$\begin{aligned} \zeta \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \frac{1}{D_0+i\omega} \boldsymbol{\alpha}\cdot\nabla v' &= \Big[\zeta, \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}\Big] \frac{1}{D_0+i\omega} \boldsymbol{\alpha}\cdot\nabla v' + \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \Big[\zeta, \frac{1}{D_0+i\omega}\Big] \boldsymbol{\alpha}\cdot\nabla v' \\ &\quad + \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \frac{1}{D_0+i\omega} \zeta \boldsymbol{\alpha}\cdot\nabla v'. \end{aligned} \tag{5.116}$$

We treat the first two terms in Section 5.D.2. For the latter we go in Fourier space and up to a constant the kernel of its Fourier transform is :

$$\frac{\overline{E}_p^{1/2}}{\overline{E}_p + \overline{E}_q} \frac{P^0_+(p)}{E(p)+E(q)} \big(\mathscr{F}(\zeta\boldsymbol{\alpha}\cdot\nabla v'; p-q)\big) P^0_-(q).$$

In particular its Hilbert-Schmidt norm is $\mathcal{O}(\sqrt{\log(\Lambda)} \|\zeta\nabla v'_{\rho_\gamma}\|_{L^2})$.

Doing the same for the other $Q_{k,\ell}$, we get terms with commutators treated in 5.D.2 and other terms with $\zeta v'_{\rho_\gamma}$, $\zeta\boldsymbol{\alpha}\cdot\nabla v'$ and $\zeta R_{\gamma'} = R_{\zeta\gamma'}$. In particular taking the $\|\cdot\|_{\mathfrak{S}_2}$ under the integral sign, we get the following estimates on those terms.

$$\mathcal{O}\Big(c^{-1/2}\|\zeta\nabla v'\|_{L^2} + \alpha\|\zeta\gamma'\|_{\mathrm{Ex}} + \alpha^2(\|\zeta\nabla v'\|_{L^2} + \|\zeta v'\|_{L^6} + \|\zeta\gamma'\|_{\mathrm{Ex}})^2\Big). \tag{5.117}$$

Remark 5.19. The term $\|\zeta\gamma'\|_{\mathrm{Ex}}$ is due to Ineq. (5.50) (l.h.s). Moreover we can deal with γ and N in γ' differently. Indeed as $R_N \in \mathfrak{S}_2$, $\|\zeta\gamma'\|_{\mathrm{Ex}}$ can be replaced by $K(\|\zeta\gamma\|_{\mathrm{Ex}} + \|\zeta R_N\|_{\mathfrak{S}_2})$.

Remark 5.20. The term $\mathcal{T}[\zeta, v'] := \zeta\boldsymbol{\alpha}\cdot\nabla v'$ appears in $P^0_{-\varepsilon} v' P^0_\varepsilon$, that equals up to a multiplicative constant to

$$\int_{\omega=-\infty}^{+\infty} \frac{d\omega}{D_0+i\omega} \mathcal{T}[\zeta, v'] \frac{P^0_\varepsilon}{D_0+i\omega}.$$

Up to a constant its Fourier transform is

$$\frac{P^0_{-\varepsilon}(p)\widehat{\mathcal{T}}(p-q)P^0_\varepsilon(q)}{E(p)+E(q)},$$

and we deal with this term as $\widehat{P^0_{-\varepsilon}}(p)\widehat{v'}(p-q)\widehat{P^0_\varepsilon}(q)$ in [HLS05a, Sok13, Sok14c].

Commutating ζ

We recall here that $[\zeta, P^0_\varepsilon]$ is treated in (5.93), Appendix 5.A.

In the same spirit of Lemma 5.10, we have the following Lemma.

Lemma 5.11. *Let $\eta \in \mathbb{R}$ and ζ smooth with*

$$\|\nabla\zeta\|_{L^\infty}, \|\partial_j\partial_k\zeta\|_{L^\infty} < +\infty, k, j \in \{1,2,3\}.$$

Then there holds :

$$\Big|\Big|\Big[\zeta, \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}\Big]|\mathbf{D}+i\eta|^{7/12}\Big|\Big|_{\mathcal{B}} \lesssim \|\nabla\zeta\|_{L^\infty} + \sum_{1\le j,k\le 3}\|\partial_j\partial_k\zeta\|_{L^\infty}.$$

Remark 5.21. We can do the same with $|D_0|^{a[\Lambda]}$ or $|D_0|^{1/2}$ instead of $|\mathbf{D}|^{1/2}$ by using the following formula [LS10, p. 87] :

$$|D_0|^a = \frac{\sin(a\pi)}{\pi}\int_{s=0}^{+\infty}\frac{ds}{s^{1-a}}\frac{|D_0|}{|D_0|+s},\ a = a[\Lambda], 1/2.$$

Here we show the proof for $|\mathbf{D}|^{1/2}$ because it enables us to localise the kinetic energy. But we can replace every $|D_0|^{a[\Lambda]}$ by $|\mathbf{D}|^{1/2}$ and vice-versa.

There is also :

Lemma 5.12. *There exists $K > 0$ such that for any $\eta \in \mathbb{R}$ and any smooth function ζ with $\|\nabla\zeta\|_{L^\infty} < +\infty$:*

$$\Big|\Big[\zeta, \frac{1}{D_0+i\omega}\Big](x-y)\Big| \le K\|\nabla\zeta\|_{L^\infty}\frac{e^{-E(\eta)/2(x-y)}}{|x-y|}. \tag{5.118}$$

Remark 5.22. We recall that up to some constant $\frac{1}{a^2-\Delta}(x-y) = \sqrt{\frac{\pi}{2}}\frac{e^{-a|x-y|}}{|x-y|}$ [LL97].

– The interesting fact here is that by taking the commutator of ζ and some function of $-i\nabla$ we gain some exponent for η or ω. Thus by using KSS inequalities under the integral sign we get the following estimates for the term with commutators :

$$\mathcal{O}\Big(\big(\|\nabla\zeta\|_{L^\infty} + \sum_{1\le j,k\le 3}\|\partial_j\partial_k\zeta\|_{L^\infty}\big)\big(\alpha(\|\rho'_\gamma\|_{\mathcal{C}} + \||\nabla|^{1/2}\gamma\|_{\mathfrak{S}_2} + \|\nabla N\|_{\mathfrak{S}_2})\big)\Big) \tag{5.119}$$

Proof of Lemma 5.11 : We decompose $\zeta = \zeta^{++}+\zeta^{+-}+\zeta^{-+}+\zeta^{--}$. We write for each term $\zeta^{\varepsilon\varepsilon'}, \varepsilon, \varepsilon' \in \{+,-\}$:

$$\Big[\zeta^{\varepsilon\varepsilon'}, \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}\Big] = [\zeta^{\varepsilon\varepsilon'}, |\mathbf{D}|^{1/2}]\frac{1}{\mathbf{D}+i\eta} + |\mathbf{D}|^{1/2}\Big[\zeta^{\varepsilon\varepsilon'}, \frac{1}{\mathbf{D}+i\eta}\Big].$$

It follows that :

$$|\mathbf{D}|^{1/2}\Big[\zeta^{\varepsilon\varepsilon'}, \frac{1}{\mathbf{D}+i\eta}\Big] = \frac{|\mathbf{D}|^{1/2}P^0_\varepsilon}{\mathbf{D}+i\eta}[\mathbf{D},\zeta]\frac{P^0_{\varepsilon'}}{\mathbf{D}+i\eta}. \tag{5.120}$$

The term $|\mathbf{D}|^{1/2}\Big[\zeta^{\varepsilon\varepsilon'}, \frac{1}{\mathbf{D}+i\eta}\Big]$ By simple computation we have :

$$\begin{aligned}
[\mathbf{D},\zeta] &= \Big(1-\frac{\Delta}{\Lambda^2}\Big)(-i\boldsymbol{\alpha}\cdot\nabla\zeta) + \frac{(-\Delta\zeta)}{\Lambda^2}D_0 + 2\nabla\zeta\cdot\frac{\nabla D_0}{\Lambda^2}\\
&= (-i\boldsymbol{\alpha}\cdot\nabla\zeta) - \sum_{j=1}^3\Big(\frac{\partial_j}{\Lambda^2}(-i\boldsymbol{\alpha}\cdot\nabla\partial_j\zeta) - 2(\partial_j^2\zeta)\frac{D_0}{\Lambda^2}\Big)\\
&\quad +(-\Delta\zeta)\frac{D_0}{\Lambda^2} - \sum_{j=1}^3\frac{\partial_j}{\Lambda}\Big((-i\boldsymbol{\alpha}\cdot\nabla\zeta)\frac{\partial_j}{\Lambda} - (\partial_j\zeta)\frac{D_0}{\Lambda}\Big).
\end{aligned} \tag{5.121}$$

Then there holds :

$$\|\frac{|D_0|}{\Lambda|\mathbf{D}|^{1/3}}\|_{\mathcal{B}} \lesssim 1. \tag{5.122}$$

Thus substituting in (5.120), on the right of derivatives of ζ, there is still an operator $\frac{1}{|\mathbf{D}+i\eta|^{2/3}}$ available for some KSS inequality. The $\|\cdot\|_{\mathcal{B}}-$norm of the operator on their left is $\mathcal{O}(\overline{E}_\eta^{-1/6})$. The $\|\cdot\|_{\mathcal{B}}-$norm of derivatives of ζ are $\mathcal{O}(\|\nabla\zeta\|_{L^\infty} + \|\Delta\zeta\|_{L^\infty})$.

The term $[\zeta^{\varepsilon\varepsilon'}, |\mathbf{D}|^{1/2}]\frac{1}{\mathbf{D}+i\eta}$ By symmetry it suffices to study ζ^{++} and ζ^{+-}. First :

$$[\zeta^{++}, |\mathbf{D}|^{1/2}]\frac{1}{\mathbf{D}+i\eta} \quad = \tfrac{1}{\pi}\int_0^{+\infty}\sqrt{s}ds\frac{P_+^0}{\mathbf{D}+s}[\mathbf{D},\zeta]\frac{P_+^0}{\mathbf{D}+s}\frac{1}{\mathbf{D}+i\eta}.$$

Once again, if we replace $[\mathbf{D},\zeta]$ by its expression in (5.121), we see that taking $|\mathbf{D}+i\eta|^{-1/4}$ from $\frac{1}{\mathbf{D}+i\eta}$, there remains $\frac{|\mathbf{D}+i\eta|^{1/4}}{\mathbf{D}+i\eta}$ for some KSS inequality.

This enables us to get a finite integral over the s variable :

$$\int_0^{+\infty}\frac{\sqrt{s}ds}{(1+s)^{2/3}}\frac{1}{(1+s)^{11/12}} < +\infty.$$

At last :

$$\begin{aligned}[\zeta^{+-}, |\mathbf{D}|^{1/2}]\frac{1}{\mathbf{D}+i\eta} &= -\frac{1}{\pi}\int_0^{+\infty}\sqrt{s}ds\frac{P_+^0}{|\mathbf{D}|+s}(\zeta\mathbf{D}+\mathbf{D}\zeta)\frac{P_-^0}{|\mathbf{D}|+s}\frac{1}{\mathbf{D}+i\eta}\\ &= -\frac{1}{\pi}\int_0^{+\infty}\sqrt{s}ds\frac{P_+^0}{|\mathbf{D}|+s}(2\zeta\mathbf{D}+[\mathbf{D},\zeta])\frac{P_-^0}{|\mathbf{D}|+s}\frac{1}{\mathbf{D}+i\eta}.\end{aligned}$$

The term with $[\mathbf{D},\zeta]$ is dealt with as before. There remains :

$$\int_0^{+\infty}\frac{\sqrt{s}ds}{|\mathbf{D}|+s}\zeta^{+-}\frac{\mathbf{D}}{|\mathbf{D}|+s}\frac{1}{\mathbf{D}+i\eta}. \tag{5.123}$$

We write (*cf* (5.93)) :

$$\zeta^{+-} = P_+^0[\zeta, P_-^0] = \frac{P_+^0}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\mathbf{D}+i\omega}[\mathbf{D},\zeta]\frac{1}{\mathbf{D}+i\omega}, \tag{5.124}$$

and substitute ζ^{+-} by this expression in (5.123). We must compensate $\frac{|D_0|}{\Lambda}$ on the left side of ζ and $\frac{|D_0|\mathbf{D}}{\Lambda}$ on its right side : we use $\frac{1}{|\mathbf{D}+i\omega|^{1/3}}$ on the left side and $\{|\mathbf{D}+i\omega|^{1/2}|\mathbf{D}+i\eta|^{5/12}(|\mathbf{D}|+s)^{5/12}\}^{-1}$ on the right side : there remains $\frac{1}{|\mathbf{D}+i\eta|^{7/12}}$ for some KSS inequality and :

$$\int_{s=0}^{+\infty}\int_{\omega=-\infty}^{+\infty}\frac{\sqrt{s}dsd\omega}{(1+s)^{19/12}E(\omega)^{7/6}} < +\infty.$$

Proof of lemma 5.12 : This is straightforward because everything is computable :

$$\frac{1}{D_0+i\eta} = \frac{D_0-i\eta}{E(\eta)^2-\Delta}.$$

However $\frac{1}{E(\eta)^2-\Delta}(x-y) = \frac{e^{-E(\eta)|x-y|}}{4\pi|x-y|}$ so it is clear that :

$$\Big|\frac{1}{D_0+i\eta}(x-y)\Big| \lesssim \frac{e^{-E(\eta)|x-y|/2}}{|x-y|^2}.$$

In Direct space we use $|\zeta(x)-\zeta(y)| \le \|\nabla\zeta\|_{L^\infty}|x-y|$ and

$$\Big|\Big[\zeta, \frac{1}{D_0+i\omega}\Big](x-y)\Big| \lesssim \|\nabla\zeta\|_{L^\infty}\frac{e^{-E(\eta)/2(x-y)}}{|x-y|}$$

Localisation of $\nabla v_{\rho'_\gamma}$ and R_N

We recall that $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$ is the following function :

$$\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}(x) := \big\{1-\xi_{c\lambda\mathrm{R}_g}^2(x-cz_1)-\xi_{c\lambda\mathrm{R}_g}^2(x-cz_2)\big\}^{-1/2},\ \lambda_0<\lambda<2^{-1}.$$

We will take $\lambda_0 \le \lambda \le 3^{-1}$ ($\lambda_0(L,\mathrm{R}_g)$ is defined in (5.81)). More generally except for $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\partial v\|_{L^2}, \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}v\|_{L^6}$, the estimates are true with ζ instead of $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$ in the case where ζ is $\zeta(x)=\zeta_0(x/A)$ with $0\le\zeta_0\le 1$ fixed . This part gives estimates with respect to ζ_0 and A.

Notation 5.12. We write $\theta_1^1(x) := \sqrt{1-\xi_1^2(x)}$, it is clear that

$$\|\nabla \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\|_{L^\infty} \le \frac{\|\nabla\theta_1^1\|_{L^\infty}}{c\lambda \mathrm{R}_g} \text{ and so on.}$$

Proposition 5.9. *Let $\gamma+N$ be a minimizer for $E^0(2)$ (or $E^0(1)$), $\rho\in L^1\cap L^2$ (e.g. $\rho=\rho_\gamma,\rho_N$) and $\lambda_0\le\lambda< 2^{-1}$. With the previous notations, there holds :*

$$\begin{cases} \|\boldsymbol{\eta}_{cR_g}^{(\lambda)} R[N_j]\|_{\mathfrak{S}_2}^2 & \lesssim \|\nabla\psi_j\|_{L^2}^2 \int_x (\boldsymbol{\eta}_{cR_g}^{(\lambda)})^2(x)|\psi_j(x)|^2dx \lesssim \big\{(\lambda R_g)^2c^2\big\}^{-1},\\ \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\gamma\|_{Ex} & \lesssim \|\nabla\theta_1^1\|_{L^\infty}(c\lambda R_g)^{-1}\||D_0|^{1/2}\gamma\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2},\\ \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}v_\rho\|_{L^6} & \lesssim \|(\nabla\boldsymbol{\eta}_{cR_g}^{(\lambda)})v_\rho\|_{L^2} + \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\nabla v_\rho\|_{L^2},\\ \|(\nabla\boldsymbol{\eta}_{cR_g}^{(\lambda)})v_\rho\|_{L^2} & \lesssim \|\rho\|_{L^1}\|\nabla|\nabla|\boldsymbol{\theta}_1^1\|_{L^2}(c\lambda R_g)^{-1/2},\\ \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\partial_j v_\rho\|_{L^2} & \lesssim \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\rho\,\boldsymbol{\eta}_{cR_g}^{(\lambda/2)}\|_{\mathcal{C}} + \|\rho\|_{L^1}\Big(\frac{\|\nabla\theta_1^1\|_{L^\infty}^{1/4}}{(c\lambda R_g)^{1/2}} + \frac{\|\nabla\theta_1^1\|_{L^\infty}}{(c\lambda R_g)^{3/4}}\Big)\\ & \quad +\|\rho\|_{L^2}^{1/6}\|\rho\|_{L^1}^{5/6}\frac{\|\nabla\theta_1^1\|_{L^\infty}^{3/4}}{(c\lambda R_g)^{1/2}} + \|\rho\|_{L^1}\Big(\frac{1+\|\nabla\theta_1^1\|_{L^\infty}}{(c\lambda R_g)^{1/2}}\Big). \end{cases} \tag{5.125}$$

Moreover if we write $\gamma=\alpha Q_{0,1}+\alpha Q_{1,0}+\alpha^2\widetilde{Q}_2$, $\rho_N=n$ we also have :

$$\begin{cases} \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\rho_\gamma\|_{\mathcal{C}} & \lesssim \frac{\alpha}{c\lambda R_g}\|\nabla\theta_1^1\|_{L^\infty}(\|n\|_{\mathcal{C}} + \|\alpha\rho_{1,0}+\alpha^2\widetilde{\rho}_2\|_{L^{6/5}})\\ & \quad +L\|\boldsymbol{\eta}_{cR_g}^{(\lambda)}n\|_{\mathcal{C}} + \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}(\alpha\rho_{1,0}+\alpha^2\widetilde{\rho}_2)\|_{\mathcal{C}}. \end{cases} \tag{5.126}$$

We recall that $\|\rho\|_{L^{6/5}}\lesssim \|\rho\|_{L^2}^{1/3}\|\rho\|_{L^1}^{2/3}$.

Proof : We will write $v_\rho = v$ for convenience.

The term $\|\boldsymbol{\eta}_{c\mathbf{R}_g}^{(\lambda)}R_N\|_{\mathfrak{S}_2}$

$$\begin{aligned} \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}N_j\|_{\mathfrak{S}_2}^2 & = \iint \frac{(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2(x)|\psi_j(x)|^2|\psi_j(y)|^2}{|x-y|^2}dxdy\\ & = \int_x dx(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2(x)|\psi_j(x)|^2\int_y\frac{|\psi_j(y)|^2}{|x-y|^2}dy\\ & \le 4\|\nabla\psi_j\|_{L^2}^2\int_x(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2(x)|\psi_j(x)|^2dx \lesssim \frac{1}{(\lambda\mathrm{R}_g)^2}\frac{1}{c^2} \end{aligned}$$

where we have used Lemma 5.7.

The term $\|\boldsymbol{\eta}_{c\mathbf{R}_g}^{(\lambda)}\gamma\|_{\mathbf{Ex}}$

$$\begin{aligned} \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\|_{\mathrm{Ex}} & \le \sqrt{\tfrac{\pi}{2}}\||D_0|^{1/2}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\|_{\mathfrak{S}_2}\\ & \le \sqrt{\tfrac{\pi}{2}}\big(\|[|D_0|^{1/2},\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}]\gamma\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}\big)\\ & \lesssim \|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\|_{L^\infty}\||D_0|^{1/2}\gamma\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}, \end{aligned}$$

and we can treat $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}$ as $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{a[\Lambda]}\gamma\|_{\mathfrak{S}_2}$.

The term $\|\boldsymbol{\eta}_{c\mathbf{R}_g}^{(\lambda)}v\|_{L^6}$ We use the Sobolev inequality :

$$\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}v\|_{L^6} \lesssim \|(\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})v\|_{L^2} + \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\nabla v\|_{L^2}.$$

We get a term $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\nabla v\|_{L^2}$ we will treat later.

– For the term $\|(\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g})v\|_{L^2}$, we use the fact that $\rho * \frac{1}{|\cdot|}$ is L^3_w with weak norm of order $\|\rho\|_{L^1}$ [Ste70] and we use rearrangement inequalities [LL97] : $\displaystyle\int |fg| \le \int |f|_* |g|_*$ and $\|\nabla|f|_*\|_{L^2} \le \|\nabla|f|\|_{L^2}$.

$$\begin{aligned}\|(\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g})v\|^2_{L^2} &= \int |\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2|v|^2 \le \int (|\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2)_*(|v|^2)_* \\ &\lesssim \int (|\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2)_*(x)\frac{\|\rho\|^2_{L^1}}{|x|^2}dx \\ &\lesssim \|\rho\|^2_{L^1}\|\nabla\sqrt{(|\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2)_*}\|^2_{L^2} = \|\rho\|^2_{L^1}\|\nabla(\sqrt{|\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2})_*\|^2_{L^2} \\ &\lesssim \|\rho\|^2_{L^1}\|\nabla|\nabla\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|\|^2_{L^2} \lesssim \|\rho\|^2_{L^1}\frac{\|\nabla|\nabla|\theta^1_1\|^2_{L^2}}{c\lambda\mathrm{R}_g}.\end{aligned}$$

– For the term $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\partial_j v\|_{L^2}$, we write :

$$\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\partial_j v(x) = \int \frac{(y_j - x_j)}{|x-y|^3}(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(x) - \boldsymbol{\eta}^{(y)}_{c\mathrm{R}_g})\rho(y)dy + (\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\rho) * \Big(\partial_j\frac{1}{|\cdot|}\Big). \tag{5.127}$$

The last term will give $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\rho\|_{\mathcal{C}}$. From this point, due to the particular form of $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}$ there holds :

$$\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} = \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g} \text{ so } \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\rho\|_{\mathcal{C}} = \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\rho\,\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g}\|_{\mathcal{C}}. \tag{5.128}$$

Let us treat the first term of (5.127). More generally we take $\zeta(x) = \zeta_0(x/A)$ and we use the properties of $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}$ at the very end.

Taking the squared norm we have :

$$\iint \rho(x)\rho(x)dxdy\int \frac{(\zeta(t)-\zeta(x))(\zeta(t)-\zeta(y))(t_j-x_j)(t_j-y_j)}{|t-x|^3|t-y|^3}dt.$$

We split at level $|x-y| \ge \sqrt{A}$:

$$\begin{aligned}&\iint_{|x-y|\ge\sqrt{A}} \frac{|\rho(x)||\rho(y)|}{|x-y|^{1/2}}\int \frac{\|\nabla\zeta\|^{1/2}_{L^\infty}dt}{|t|^{7/4}|t-\mathbf{e}|^{7/4}} \\ &\qquad \le \frac{\|\nabla\zeta\|^{1/2}_{L^\infty}}{\sqrt{A}}\|\rho\|^2_{L^1} \lesssim \frac{L^2\|\nabla\zeta_0\|^{1/2}_{L^\infty}}{A}.\end{aligned}$$

If $|x-y| \le \sqrt{A}$: $|x-y|\|\nabla\zeta\|_{L^\infty} \le \|\nabla\zeta_0\|_{L^\infty}\frac{1}{\sqrt{A}}$, thus $\zeta(x) = \zeta(y) + \zeta(x) - \zeta(y)$ and we substitute in the integral over t. We split $\mathbb{R}^3$ in $|t-x| < |x-y|/2$, $|t-y| < |x-y|/2$ and the remainder domain. For the first ball $B(x, |x-y|/2) = B_x$:

$$\int_{B_x}\frac{|\zeta(x)-\zeta(t)||\zeta(y)-\zeta(t)|}{|t-x|^2|t-y|^2}dt \le \frac{\|\nabla\zeta_0\|^2_{L^\infty}}{A^{3/2}}\int_{B_x}\frac{dt}{|t-x|^2|t-y|} \quad \lesssim \frac{\|\nabla\zeta_0\|^2_{L^\infty}}{A^{3/2}}.$$

The same holds for the ball B_y. For the remainder domain C_{xy} :

$$\begin{aligned}\int_{t\in C_{xy}} dt\frac{|(\zeta(x)-\zeta(y))(\zeta(t)-\zeta(y))|}{|x-t|^2|y-t|^2} &\le \frac{(\|\nabla\zeta_0\|_{L^\infty})^{3/2}}{A}\int\frac{dt}{|x-t|^2|y-t|^{3/2}} \\ &\lesssim \frac{(\|\nabla\zeta_0\|_{L^\infty})^{3/2}}{A}\frac{1}{|x-y|^{1/2}} \text{ and :}\end{aligned}$$

$$\iint\frac{|\rho(x)||\rho(y)|}{|x-y|^{1/2}}dxdy \lesssim \|\rho\|^{1/3}_{L^2}\|\rho\|^{5/3}_{L^1} \lesssim L^2c^{-1/2}.$$

We used here the Hardy-Littlewood-Sobolev inequality [LL97, Theorem 4.3].

At last we must handle :

$$\iint_{|x-y|\le\sqrt{A}} \rho(x)\rho(y)dxdy \int_{t\in C_{xy}} \frac{(\zeta(t)-\zeta(y))^2(t_j-y_j)(t_j-x_j)}{|x-t|^3|y-t|^3}dt.$$

As $t\in C_{xy}$ we can replace $|x-t|^{-2}$ by $K|y-t|^{-2}$.

$$\int_{t\in C_{xy}} \frac{(\zeta(t)-\zeta(y))^2}{|t-y|^4}dt \quad \le \int_t \frac{(\zeta(t)-\zeta(y))^2}{|t-y|^4}dt.$$

We use now the properties of the function $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}$. It is easy to see that no matter where $y\in\mathbb{R}^3$ is, this last integral is $\mathcal{O}((c\lambda\mathrm{R}_g)^{-1}K(\theta_1^1))$. Indeed let Ext be the domain defined by $\mathrm{Ext}=\{y\in\mathbb{R}^3 : f(y):=\mathrm{dist}(y,\{\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\neq 1\})> 2c\lambda\mathrm{R}_g\}$. If $y\in\mathrm{Ext}$, then it is clear that the previous integral is an

$$\mathcal{O}\Big(\frac{(c\lambda\mathrm{R}_g)^3}{f(y)^4}\Big)=\mathcal{O}\big(\frac{1}{c\lambda\mathrm{R}_g}\big).$$

Else we split $\mathbb{R}^3$ at level $|t-y|=2c\lambda\mathrm{R}_g$:

$$\int_{|t-y|\le 2c\lambda\mathrm{R}_g} dt\frac{(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(t)-\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(y))^2}{|t-y|^4}\lesssim \frac{\|\nabla\theta_1^1\|^2_{L^\infty}}{(c\lambda\mathrm{R}_g)^2}(c\lambda\mathrm{R}_g)=\mathcal{O}\big(\frac{\|\nabla\theta_1^1\|^2_{L^\infty}}{c\lambda\mathrm{R}_g}\big).$$

$$\int_{|t-y|>2c\lambda\mathrm{R}_g} dt\frac{(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(t)-\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(y))^2}{|t-y|^4}\le \int_{|t-y|>2c\lambda\mathrm{R}_g}\frac{dt}{|t-y|^4}=\mathcal{O}\Big(\frac{1}{c\lambda\mathrm{R}_g}\Big).$$

Proof of (5.126) To begin with we remark that by the Hardy-Littlewood-Sobolev inequality [LL97] : $\|\rho\|_{\mathcal{C}}\lesssim\|\rho\|_{L^{6/5}}$. Then we use formula (5.55) of ρ_γ. We write

$$\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(x)\check{F}_\Lambda*\rho(x)=\int_y(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(x)-\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(y))\check{F}_\Lambda(x-y)\rho(y)dy+\check{F}_\Lambda*(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\rho)(x).$$

So it suffices to show $\||\cdot|\check{F}_\Lambda\|_{L^1}\lesssim\alpha$ to end the proof : this is precisely (5.53)-(5.54), applied with $\ell=1$ to $\check{F}_\Lambda$ (true if α is less than some $K(\ell=1)$). □

Proof of Lemma 5.9

We write ξ instead of $\xi_j^{(\frac{1}{3})}$ and Q instead of γ' for convenience.

First remark : for any $\varepsilon,\varepsilon'\in\{+,-\}$:

$$P^0_\varepsilon\xi P^0_\varepsilon QP^0_{\varepsilon'}\xi P^0_{\varepsilon'}=[P^0_\varepsilon,\xi]Q^{\varepsilon\,\varepsilon'}[\xi,P^0_{\varepsilon'}]+[P^0_\varepsilon,\xi]Q^{\varepsilon\,\varepsilon'}\xi+\xi Q^{\varepsilon\,\varepsilon'}[\xi,P^0_{\varepsilon'}]+\xi Q^{\varepsilon\,\varepsilon'}\xi. \tag{5.129}$$

This gives the error term between $\xi Q\xi$ and $\xi[Q]$. We estimate their density as in Section 5.D.1, that is by duality.

Second remark : $\partial_j\xi^{(\lambda)}=(\partial_j\xi)\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g}$.

As in this section, by using (5.93), it is clear that

$$\|[P^0_\varepsilon,\xi]Q^{\varepsilon\,\varepsilon'}[\xi,P^0_{\varepsilon'}]\|_{\mathcal{C}}\lesssim\||D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2}\|\xi\|^2_{L^6}\lesssim\frac{\||D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2}}{(c\mathrm{R}_g)^2}.$$

We can drop terms involving the density of these operators.

We write :

$$\xi^{+-}=\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{D_0+i\omega}(\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g})^2(\boldsymbol{\alpha}\cdot\nabla\xi)\frac{d\omega}{D_0+i\omega}.$$

We commute $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}$ with $(D_0+i\omega)^{-1}$ on the right and on the left. As shown before there holds :

$$\Big|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}(x)-\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}(y))\frac{1}{D_0+i\omega}(x-y)\Big|\lesssim \frac{e^{-E(\omega)|x-y|/2}}{|x-y|}\|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{L^\infty}.$$

So taking KSS inequalities under the integral sign we obtain for instance :

$$\begin{aligned}&\mathrm{Tr}\big(P_-^0\xi Q\xi^{+-}VP_-^0\big)=\mathrm{Tr}\Big(P_-^0\xi Q\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\xi^{+-}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}VP_-^0\Big)\\&+\mathcal{O}\Big(\|V\|_{L^6}\|Q|D_0|^{1/2}\|_{\mathfrak{S}_2}\|\nabla\xi\|_{L^3}\|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{L^\infty}\int_{\mathbb{R}}\frac{d\omega}{E(\omega/2)^{5/4}}\Big)\\&+\mathcal{O}\Big(\|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{L^\infty}^2\|V\|_{L^6}\|\nabla\xi\|_{L^3}\|Q\|_{\mathfrak{S}_2}\int_{\mathbb{R}}\frac{d\omega}{E(\omega/2)^2}\Big).\end{aligned}$$

There remains the first trace. First of all, for any V Schwartz, we can show as in Section 5.D.1 that the operator is trace-class with norm controlled by

$$\sqrt{\log(\Lambda)}\|\nabla(\xi\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}V)\|_{L^2}\||D_0|^{1/2}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}Q^{+-}\|_{\mathfrak{S}_2}+\|\nabla\xi\|_{L^\infty}\|\nabla(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}V)\|_{L^2}\|QP_+^0\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{\mathfrak{S}_2}.$$

We have *a priori* $\|\nabla(\xi\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}V)\|_{L^2}\lesssim\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\nabla V\|_{L^2}+\|\nabla(\xi\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)})\|_{L^3}\|V\|_{L^6}$.
In particular :

$$\|[P_\varepsilon^0,\xi]Q^{\varepsilon\,\varepsilon'}\xi\|_{\mathcal{C}}\lesssim\sqrt{\log(\Lambda)}\||D_0|^{1/2}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}Q^{\varepsilon'\,\varepsilon}\|_{\mathfrak{S}_2}\lesssim\frac{L}{\sqrt{c\lambda\mathrm{R}_g}}.$$

We use now the fact that we want the trace *for a particular* V, namely $\rho[\xi Q\xi]*\frac{1}{|\cdot|}$. So as in Proposition 5.9, the function $(\xi^2\rho'_\gamma)*\frac{1}{|\cdot|}$ is in L^3_w and

$$\|(\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)})\big[(\xi^2\rho'_\gamma)*\tfrac{1}{|\cdot|}\big]\|_{L^2}\lesssim\frac{\sqrt{2}}{\sqrt{\lambda c\mathrm{R}_g}}\|\rho'_\gamma\|_{L^1}\lesssim\frac{\sqrt{2}}{\sqrt{\lambda c\mathrm{R}_g}}.$$

Then we write $(\xi^2\rho'_\gamma)*\frac{1}{|\cdot|}=\rho'_\gamma*\frac{1}{|\cdot|}-((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2\rho'_\gamma)*\frac{1}{|\cdot|}$ and

$$\begin{aligned}\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\nabla\big[(\xi^2\rho'_\gamma)*\tfrac{1}{|\cdot|}\big]\|_{L^2}&\lesssim\|\nabla((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2\rho'_\gamma)*\tfrac{1}{|\cdot|}\|_{L^2}+\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\nabla(\rho'_\gamma)*\tfrac{1}{|\cdot|}\|_{L^2}\\&\lesssim\|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2\rho'_\gamma\|_{\mathcal{C}}+\sum_{j=1}^3\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\partial_j v'_{\rho_\gamma}\|_{L^2},\end{aligned}$$

and those terms are dealt with Propositions 5.9 and 5.8.

Putting everything together, we get an error term of order :

$$\sqrt{\log(\Lambda)}\times\frac{1}{c\sqrt{\mathrm{R}_g}}\times\frac{1}{\sqrt{c\mathrm{R}_g}}=\mathcal{O}\Big(\frac{L}{c\mathrm{R}_g}\Big).$$

Troisième partie

Existence d'états excités du vide : le positronium et le dipositronium

Chapitre 6

Sur l'ortho-positronium

The positronium in a mean-field approximation of quantum electrodynamics

Abstract

The Bogoliubov-Dirac-Fock (BDF) model is a no-photon, mean-field approximation of quantum electrodynamics. It describes relativistic electrons in the Dirac sea. In this model, a state is fully characterized by its one-body density matrix, an infinite rank nonnegative operator. We prove the existence of the positronium, the bound state of an electron and a positron, represented by a critical point of the energy functional in the absence of external field. This state is interpreted as the ortho-positronium, where the two particles have parallel spins.

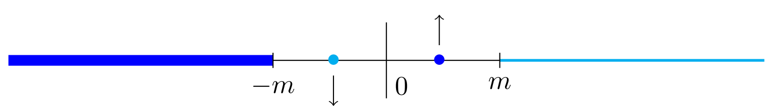

FIGURE 6.1 – Spectre de l'ortho-positronium

Contents

6.1 Introduction and main results

THE DIRAC OPERATOR

In relativistic quantum mechanics, the kinetic energy of an electron is described by the so-called *Dirac operator* D_0. Its expression is [Tha92] :

$$D_0 := m_e c^2 \beta - i\hbar c \sum_{j=1}^{3} \alpha_j \partial_{x_j} \tag{6.1}$$

where m_e is the (bare) mass of the electron, c the speed of light and $\hbar$ the reduced Planck constant, β and the α_j's are 4×4 matrices defined as follows :

$$\beta := \begin{pmatrix} \mathrm{Id}_{\mathbb{C}^2} & 0 \\ 0 & -\mathrm{Id}_{\mathbb{C}^2} \end{pmatrix},\ \alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix},\ j \in \{1,2,3\}$$

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}.$$

The Dirac operator acts on spinors *i.e.* square-integrable $\mathbb{C}^4$-valued functions :

$$\mathfrak{H} := L^2(\mathbb{R}^3, \mathbb{C}^4). \tag{6.2}$$

It corresponds to the Hilbert space associated to one electron. The operator D_0 is self-adjoint on $\mathfrak{H}$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$, but contrary to $-\Delta/2$ in quantum mechanics, it is unbounded from below.

Indeed its spectrum is $\sigma(D_0) = (-\infty, m_e c^2] \cup [m_e c^2, +\infty)$. Dirac postulated that all the negative energy states are already occupied by "virtual electrons", with one electron in each state, and that the uniform filling is unobservable to us. Then, by Pauli's principle real electrons can only have a positive energy.

It follows that the relativistic vacuum, composed by those negatively charged virtual electrons, is a polarizable medium that reacts to the presence of an external field. This phenomenon is called the *vacuum polarization.*

If one turns on an external field that gets strong enough, it leads to a transition of an electron of the Dirac sea from a negative energy state to a positive one. The resulting system – an electron with positive energy plus a hole in the Dirac sea – is interpreted as an electron-positron pair. Indeed the absence of an electron in the Dirac sea is equivalent to the addition of a particle with same mass and opposite charge : the positron.

Its existence was predicted by Dirac in 1931. Although firstly observed in 1929 independently by Skobeltsyn and Chung-Yao Chao, it was recognized in an experiment lead by Anderson in 1932.

CHARGE CONJUGATION

Following Dirac's ideas, the free vacuum is described by the negative part of the spectrum $\sigma(D_0)$:

$$P_-^0 = \chi_{(-\infty,0)}(D_0).$$

The correspondence between negative energy states and positron states is given by the *charge conjugation* C [Tha92]. This is an antiunitary operator that maps $\mathrm{Ran}\, P_-^0$ onto $\mathrm{Ran}(1 - P_-^0)$. In our convention [Tha92] it is defined by the formula :

$$\forall\, \psi \in L^2(\mathbb{R}^3),\ \mathrm{C}\psi(x) = i\beta\alpha_2 \overline{\psi}(x), \tag{6.3}$$

where $\overline{\psi}$ denotes the usual complex conjugation. More precisely :

$$\mathrm{C} \cdot \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_2 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \overline{\psi}_4 \\ -\overline{\psi}_3 \\ -\overline{\psi}_2 \\ \overline{\psi}_1 \end{pmatrix}. \tag{6.4}$$

In our convention it is also an *involution* : $\mathrm{C}^2 = \mathrm{id}$. An important property is the following :

$$\forall\, \psi \in L^2, \forall\, x \in \mathbb{R}^3,\ |\mathrm{C}\psi(x)|^2 = |\psi(x)|^2. \tag{6.5}$$

Positronium

The positronium is the bound state of an electron and a positron. This system was independently predicted by Anderson and Mohorovičić in 1932 and 1934 and was experimentally observed for the first time in 1951 by Martin Deutsch.

It is unstable : depending on the relative spin states of the positron and the electron, its average lifetime in vacuum is 125 ps (para-positronium) or 142 ns (ortho-positronium) (see [Kar04]).

In this paper, we are looking for a positronium state within the Bogoliubov-Dirac-Fock (BDF) model : the state we found can be interpreted as the ortho-positronium where the electron and positron have parallel spins. Our main results are Theorem 6.1 and 6.3. In our state, the wave function of the real electron and that of the virtual electron defining the positronium are charge conjugate of each other.

BDF model

The BDF model is a no-photon approximation of quantum electrodynamics (QED) which was introduced by Chaix and Iracane in 1989 [CI89], and studied in many papers [BBHS98a, HLS05a, HLS05b, HLS07, HLS09, GLS09, Sok14b].

It allows to take into account real electrons together with the Dirac vacuum in the presence of an external field.

This is a Hartree-Fock type approximation in which a state of the system "vacuum + real electrons" is given by an infinite Slater determinant $\psi_1 \wedge \psi_2 \wedge \cdots$. Equivalently, such a state is represented by the projector onto the space spanned by the ψ_j's : its so-called one-body density matrix. For instance P^0_- represents the free Dirac vacuum.

Here we just give main ideas of the derivation of the BDF model from QED, we refer the reader to [CI89, HLS05a, HLS07] for full details.

Remark 6.1. To simplify the notations, we choose relativistic units in which, the mass of the electron m_e, the speed of light c and $\hbar$ are set to 1.

Let us say that there is an external density ν, *e.g.* that of some nucleus and let us write $\alpha > 0$ the so-called *fine structure constant* (physically $e^2/(4\pi\varepsilon_0\hbar c)$), where e is the elementary charge and ε_0 the permittivity of free space).

The starting point is the (complicated) Hamiltonian of QED $\mathbb{H}_{\text{QED}}$ that acts on the Fock space of the electron $\mathcal{F}_{\text{elec}}$ [Tha92]. The (formal) difference between the infinite energy of a Hartree-Fock state Ω_P and that of $\Omega_{P^0_-}$, state of the free vacuum taken as a reference state, gives a function of the reduced one-body density matrix $Q := P - P^0_-$.

It can be shown that a projector P is the one-body density matrix of a Hartree-Fock state in $\mathcal{F}_{\text{elec}}$ *iff* $P - P^0_-$ is Hilbert-Schmidt, that is compact such that its singular values form a sequence in ℓ^2.

To get a well-defined energy, one has to impose an ultraviolet cut-off $\Lambda > 0$: we replace $\mathfrak{H}$ by its subspace

$$\mathfrak{H}_\Lambda := \big\{ f \in \mathfrak{H},\ \operatorname{supp} \widehat{f} \subset B(0,\Lambda) \big\}.$$

This procedure gives the BDF energy introduced in [CI89] and studied for instance in [HLS05a, HLS05b].

Notation 6.1. Our convention for the Fourier transform $\mathscr{F}$ is the following

$$\forall\, f \in L^1(\mathbb{R}^3),\ \widehat{f}(p) := \frac{1}{(2\pi)^{3/2}} \int f(x) e^{-ixp} dx.$$

Let us notice that $\mathfrak{H}_\Lambda$ is invariant under D_0 and so under P^0_-.

For the sake of clarity, we will emphasize the ultraviolet cut-off and write Π_Λ for the orthogonal projection onto $\mathfrak{H}_\Lambda$: Π_Λ is the following Fourier multiplier

$$\Pi_\Lambda := \mathscr{F}^{-1} \chi_{B(0,\Lambda)} \mathscr{F}. \tag{6.6}$$

By means of a thermodynamical limit, Hainzl *et al.* showed in [HLS07] that the formal minimizer and hence the reference state should not be given by $\Pi_\Lambda P^0_-$ but by another projector $\mathcal{P}^0_-$ in $\mathfrak{H}_\Lambda$ that satisfies the self-consistent equation <u>*in* $\mathfrak{H}_\Lambda$</u> :

$$\begin{cases} \mathcal{P}^0_- - \frac{1}{2} & = & -\operatorname{sign}\big(\mathcal{D}^0\big), \\ \mathcal{D}^0 & = & D_0 - \dfrac{\alpha}{2}\dfrac{(\mathcal{P}^0_- - \frac{1}{2})(x-y)}{|x-y|} \end{cases} \tag{6.7}$$

We have $\mathcal{P}^0_- = \chi_{(-\infty,0)}(\mathcal{D}^0)$.

In $\mathfrak{H}$, the operator $\mathcal{D}^0$ coincides with a bounded, matrix-valued Fourier multiplier whose kernel is $\mathfrak{H}_\Lambda^\perp \subset \mathfrak{H}$.

The resulting BDF energy $\mathcal{E}^\nu_{\mathrm{BDF}}$ is defined on Hartree-Fock states represented by their one-body density matrix P :

$$\mathscr{N} := \big\{P \in \mathcal{B}(\mathfrak{H}_\Lambda),\ P^* = P^2 = P,\ P - \mathcal{P}^0_- \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\big\}.$$

This energy depends on three parameters : the fine structure constant $\alpha > 0$, the cut-off $\Lambda > 0$ and the external density ν. We assume that ν has finite *Coulomb energy*, that is

$$D(\nu,\nu) := 4\pi \int_{\mathbb{R}^3} \frac{|\widehat{\nu}(k)|^2}{|k|^2} dk. \tag{6.8}$$

Remark 6.2. The Coulomb energy coincides with $\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\nu(x)^*\nu(y)}{|x-y|} dxdy$ whenever this integral is well-defined.

Remark 6.3. The operator $\mathcal{D}^0$ was previously introduced by Lieb *et al.* in [LS00] in another context in the case $\alpha\log(\Lambda)$ small.

Notation 6.2. We recall that $\mathcal{B}(\mathfrak{H}_\Lambda)$ is the set of bounded operators and $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ the set of compact operators whose singular values form a sequence in ℓ^p [RS75, Appendix IX.4 Vol II], [Sim79] ($p \geq 1$). In particular $\mathfrak{S}_\infty(\mathfrak{H}_\Lambda)$ is the set $\mathrm{Comp}(\mathfrak{H}_\Lambda)$ of compact operators.

Notation 6.3. Throughout this paper we write

$$m = \inf \sigma\big(|\mathcal{D}^0|\big) \geq 1, \tag{6.9}$$

and

$$\mathcal{P}^0_+ := \Pi_\Lambda - \mathcal{P}^0_- = \chi_{(0,+\infty)}(\mathcal{D}^0). \tag{6.10}$$

The same symmetry holds for $\mathcal{P}^0_-$ and $\mathcal{P}^0_+$: the charge conjugation C maps $\operatorname{Ran}\mathcal{P}^0_-$ onto $\operatorname{Ran}\mathcal{P}^0_+$.

Minimizers and critical points

The charge of a state $P \in \mathscr{N}$ is given by the so-called $\mathcal{P}^0_-$-trace of $P - \mathcal{P}^0_-$

$$\mathrm{Tr}_{\mathcal{P}^0_-}\big(P - \mathcal{P}^0_-\big) := \mathrm{Tr}\big(\mathcal{P}^0_-(P-\mathcal{P}^0_-)\mathcal{P}^0_- + \mathcal{P}^0_+(P-\mathcal{P}^0_-)\mathcal{P}^0_+\big).$$

This trace is well defined as we can check from the formula [HLS05a]

$$(P - \mathcal{P}^0_-)^2 = \mathcal{P}^0_+(P-\mathcal{P}^0_-)\mathcal{P}^0_+ - \mathcal{P}^0_-(P-\mathcal{P}^0_-)\mathcal{P}^0_-. \tag{6.11}$$

Minimizers of the BDF energy with charge constraint $N \in \mathbb{N}$ corresponds to ground states of a system of N electrons in the presence of an external density ν.

The problem of their existence was studied in several papers [HLS09, Sok14b, Sok13]. In [HLS09], Hainzl *et al.* proved that it was sufficient to check binding inequalities and showed existence of ground states in the presence of an external density ν, provided that $N - 1 < \int \nu$, under technical assumptions on α, Λ.

In [Sok14b], we proved that, due to the vacuum polarization, there exists a minimizer for $\mathcal{E}^0_{\mathrm{BDF}}$ with charge constraint 1 : in other words an electron can bind alone in the vacuum without any external charge (still under technical assumptions on α, Λ).

In [Sok13], the effect of charge screening is studied : due to vacuum polarization, the observed charge of a minimizer $P \neq \mathcal{P}^0_-$ is different from its real charge $\mathrm{Tr}_{\mathcal{P}^0_-}(P - \mathcal{P}^0_-)$.

Here we are looking for a positronium state, that is an electron and a positron in the vacuum without any external density. So we have to study $\mathcal{E}^0_{\mathrm{BDF}}$ on

$$\mathscr{M} := \Big\{ P \in \mathscr{N},\ \mathrm{Tr}_{\mathcal{P}^0_-}\big(P - \mathcal{P}^0_-\big) = 0 \Big\}. \tag{6.12}$$

From a geometrical point of view $\mathscr{M}$ is a Hilbert manifold and $\mathcal{E}^0_{\mathrm{BDF}}$ is a differentiable map on $\mathscr{M}$ (Propositions 6.1 and 6.2).

We thus seek a critical point on $\mathscr{M}$, that is some $P \in \mathscr{M},\ P \neq \mathcal{P}^0_-$ such that $\nabla \mathcal{E}^0_{\mathrm{BDF}}(P) = 0$. We also must ensure that this is a positronium state. A good candidate is a projector P that is obtained from $\mathcal{P}^0_-$ by substracting a state $\psi_- \in \mathrm{Ran}\,\mathcal{P}^0_-$ and adding a state $\psi_+ \in \mathrm{Ran}\,\mathcal{P}^0_+$, that is

$$P = \mathcal{P}^0_- + |\psi_+\rangle\langle\psi_+| - |\psi_-\rangle\langle\psi_-|. \tag{6.13}$$

But there is no reason why such a projector would be a critical point. If it were that would mean that there exists a positronium state in which, apart from the excitation of the virtual electron giving the electron-positron pair, the vacuum is not polarized.

Keeping (6.13) in mind, we identify a subset $\mathscr{M}_{\mathscr{C}} \subset \mathscr{M}$, made of C-symmetric states.

Definition 6.1. The set $\mathscr{M}_{\mathscr{C}}$ of C-symmetric states is defined as :

$$\mathscr{M}_{\mathscr{C}} = \{P \in \mathscr{M},\ -\mathrm{C}(P - \mathcal{P}^0_-)\mathrm{C} = P - \mathcal{P}^0_-\}. \tag{6.14}$$

Remark 6.4. Let $P \in \mathscr{M}_{\mathscr{C}}$. As $-\mathrm{C}(\mathcal{P}^0_- - \mathcal{P}^0_+)\mathrm{C} = \mathcal{P}^0_- - \mathcal{P}^0_+$, writing

$$P - \mathcal{P}^0_- = \tfrac{1}{2}\big(P - (\Pi_\Lambda - P) - \mathcal{P}^0_- + \mathcal{P}^0_+\big),$$

there holds :

$$P \in \mathscr{M}_{\mathscr{C}} \Rightarrow P + \mathrm{C}P\mathrm{C} = \Pi_\Lambda, \tag{6.15}$$

that is

$$\forall\, P \in \mathscr{M}_{\mathscr{C}},\ \mathrm{C} : \mathrm{Ran}\,P \to \mathrm{Ran}(\Pi_\Lambda - P) \text{ is an isometry.}$$

The set $\mathscr{M}_{\mathscr{C}}$ has fine properties : this is a submanifold, invariant under the gradient flow of $\mathcal{E}^0_{\mathrm{BDF}}$ (Proposition 6.3). Moreover it has two connected components $\mathscr{E}_1$ and $\mathscr{E}_{-1}$ (Proposition 6.4). In particular, any extremum of the BDF energy restricted to $\mathscr{M}_{\mathscr{C}}$ is a critical point on $\mathscr{M}$.

So we are lead to seek a minimizer over each of these connected components : the first ($\mathscr{E}_1$) gives $\mathcal{P}^0_-$, which is the global minimizer over $\mathscr{N}$, but the second gives a non-trivial critical point. It corresponds to the positronium and is a perturbation of a state which can be written as in (6.13).

Our main Theorems are the following :

Theorem 6.1. *There exist $\alpha_0, \Lambda_0, L_0 > 0$ such that if $\alpha \leq \alpha_0, \Lambda^{-1} \leq \Lambda_0^{-1}$, and $\alpha \log(\Lambda) \leq L_0$, then there exists a minimizer of $\mathcal{E}^0_{\mathrm{BDF}}$ over $\mathscr{E}_{-1}$ (see Proposition 6.4 for its definition). Moreover we have*

$$E_{1,1} := \inf\{\mathcal{E}^0_{\mathrm{BDF}}(P),\ P \in \mathscr{E}_{-1}\} \leq 2m + \frac{\alpha^2 m}{g_1'(0)^2} E_{\mathrm{CP}} + \mathcal{O}(\alpha^3),$$

where $E_{\mathrm{CP}} < 0$ is the Choquard-Pekar energy defined as follows [Lie77] :

$$E_{\mathrm{CP}} = \inf\Big\{ \|\nabla\phi\|^2_{L^2} - D\big(|\phi|^2, |\phi|^2\big),\ \phi \in L^2(\mathbb{R}^3),\ \|\phi\|_{L^2} = 1 \Big\}. \tag{6.16}$$

Theorem 6.2. *Under the same assumptions as in Theorem 6.1, let $\overline{P}$ be a minimizer for $E_{1,1}$. Then there exists an anti-unitary map $A \in \mathbf{A}(\mathfrak{H}_\Lambda)$, and $P^0_{1,1}$ of form (6.13) such that*

$$\left|\begin{array}{l} \overline{P} = e^A P^0_{1,1} e^A, \\ e^A \psi_\varepsilon = \psi_\varepsilon,\ \varepsilon \in \{+,-\} \text{ and } \psi_- = \mathrm{C}\psi_+, \\ A = \big[[A, \mathcal{P}^0_-], \mathcal{P}^0_-\big] \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ \|A\|_{\mathfrak{S}_2} \lesssim \alpha, \\ \text{and } \mathrm{CAC} = A. \end{array}\right. \tag{6.17}$$

Moreover, the following holds :

$$E_{1,1} = 2m + \frac{\alpha^2 m}{g_1'(0)^2} E_{\mathrm{CP}} + \mathcal{O}(\alpha^3). \tag{6.18}$$

We emphasize that ψ_+ *does not* represent the electron state.

Theorem 6.3. *Under the same assumptions as in Theorem 6.1, let $\overline{P}$ be a minimizer for $E_{1,1}$ and $Q_0 = \overline{P} - \mathcal{P}^0_-$. Let $\overline{\boldsymbol{\pi}}$ be*

$$\overline{\boldsymbol{\pi}} := \chi_{(-\infty,0)}\big(\Pi_\Lambda D_{Q_0}\Pi_\Lambda\big). \tag{6.19}$$

Then there holds $\mathrm{Ran}\,(\Pi_\Lambda - \overline{\boldsymbol{\pi}}) \cap \mathrm{Ran}\,\overline{P} = \mathbb{C}\psi_e$. The unitary wave function ψ_e satisfies the equation

$$D_{Q_0}\psi_e = \mu_e\psi_e, \tag{6.20}$$

where μ_e is some constant

$$K_0\alpha^2 \leq m - \mu_e \leq K_1\alpha^2,\ \ K_0, K_1 > 0.$$

By C*-symmetry $\psi_v := \mathrm{C}\psi_e$ satisfies $D_{Q_0}\psi_v = -\mu_e\psi_v$, and we have*

$$\overline{P} = \overline{\boldsymbol{\pi}} + |\psi_e\rangle\langle\psi_e| - |\psi_v\rangle\langle\psi_v|. \tag{6.21}$$

Moreover the following holds. We split ψ_e into upper spinor $\varphi_e \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ and lower spinor $\chi_e \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ and scale φ_e by $\lambda := \frac{g_1'(0)^2}{\alpha m}$:

$$\widetilde{\varphi}_e(x) := \lambda^{3/2}\varphi_e\big(\lambda x\big).$$

Then in the non-relativistic limit $\alpha \to 0$ (with $\alpha\log(\Lambda)$ kept small), the lower spinor χ_e tends to 0 and, up to translation, $\widetilde{\varphi}_e$ tends to a Pekar minimizer.

Remark 6.5. As ψ_e and $\psi_v = \mathrm{C}\psi_e$ have antiparallel spins, the state $\overline{P}$ represents one electron in state ψ_e and the absence of one electron in state ψ_v in the Dirac sea, that is an electron and a positron with *parallel spins.*

Remark 6.6. To prove that $\widetilde{\varphi}_e$ tends to a Pekar minimizer up to translation, it suffices to prove that its Pekar energy tends to E_{CP} [Lie77].

Notation 6.4. Throughout this paper we write K to mean a constant independent of α, Λ. Its value may differ from one line to the other. We also use the symbol $\lesssim$: $0 \leq a \lesssim b$ means there exists $K > 0$ such that $a \leq Kb$.

Remarks and notations about $\mathcal{D}^0$

$\mathcal{D}^0$ has the following form [HLS07] :

$$\mathcal{D}^0 = g_0(-i\nabla)\beta - i\boldsymbol{\alpha}\cdot\frac{\nabla}{|\nabla|}g_1(-i\nabla) \tag{6.22}$$

where g_0 and g_1 are smooth radial functions on $B(0,\Lambda)$ and $\boldsymbol{\alpha} = (\alpha_j)_{j=1}^3$. Moreover we have :

$$\forall\, p \in B(0,\Lambda),\ 1 \leq g_0(p),\ \text{and } |p| \leq g_1(p) \leq |p|g_0(p). \tag{6.23}$$

Notation 6.5. For $\alpha\log(\Lambda)$ sufficiently small, we have $m = g_0(0)$ [LL97, Sok14b].

Remark 6.7. In general the smallness of α is needed to ensure technical estimates hold. The smallness of $\alpha\log(\Lambda)$ is needed to get estimates of $\mathcal{D}^0$: in this case $\mathcal{D}^0$ can be obtained by a fixed point scheme [HLS07, LL97], and we have [Sok14b, Appendix A] :

$$\begin{gathered} g_0'(0) = 0,\ \text{and } \|g_0'\|_{L^\infty}, \|g_0''\|_{L^\infty} \leq K\alpha \\ \|g_1' - 1\|_{L^\infty} \leq K\alpha\log(\Lambda) \leq \tfrac{1}{2} \text{ and } \|g_1''\|_{L^\infty} \lesssim 1. \end{gathered} \tag{6.24}$$

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6.2 Description of the model

6.2.1 The BDF energy

Definition 6.2. Let $\alpha > 0, \Lambda > 0$ and $\nu \in \mathcal{S}'(\mathbb{R}^3)$ a generalized function with $D(\nu,\nu) < +\infty$. The BDF energy $\mathcal{E}^0_{\mathrm{BDF}}$ is defined on $\mathscr{N}$ as follows : for $P \in \mathscr{N}$ we write $Q := P - \mathcal{P}^0_-$ and

$$\begin{cases} \mathcal{E}^0_{\mathrm{BDF}}(Q) = \mathrm{Tr}_{\mathcal{P}^0_-}\big(\mathcal{D}^0 Q\big) - \alpha D(\rho_Q,\nu) + \dfrac{\alpha}{2}\Big(D(\rho_Q,\rho_Q) - \|Q\|^2_{\mathrm{Ex}}\Big), \\ \forall\, x,y \in \mathbb{R}^3,\ \rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big),\ \|Q\|^2_{\mathrm{Ex}} := \displaystyle\iint \frac{|Q(x,y)|^2}{|x-y|}dxdy, \end{cases} \tag{6.25}$$

where $Q(x,y)$ is the integral kernel of Q.

Remark 6.8. The term $\mathrm{Tr}_{\mathcal{P}^0_-}\big(\mathcal{D}^0 Q\big)$ is the kinetic energy, $-\alpha D(\rho_Q,\nu)$ is the interaction energy with ν. The term $\dfrac{\alpha}{2}D(\rho_Q,\rho_Q)$ is the so-called *diract term* and $-\dfrac{\alpha}{2}\|Q\|^2_{\mathrm{Ex}}$ is the *exchange term.*

1. Let us see that this function is well-defined and more generally that formula (6.25) is well-defined whenever Q is $\mathcal{P}^0_-$-trace-class [HLS05a, HLS09].

– We start by defining this notion. For any $\varepsilon,\varepsilon' \in \{+,-\}$ and $A \in \mathcal{B}(\mathfrak{H}_\Lambda)$, we write

$$A^{\varepsilon,\varepsilon'} := \mathcal{P}^0_\varepsilon A \mathcal{P}^0_{\varepsilon'}.$$

The set $\mathfrak{S}_1^{\mathcal{P}^0_-}$ of $\mathcal{P}^0_-$-trace class operator is the following Banach space :

$$\mathfrak{S}_1^{\mathcal{P}^0_-} = \big\{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ Q^{++}, Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\big\}, \tag{6.26}$$

with the norm

$$\|Q\|_{\mathfrak{S}_1^{\mathcal{P}^0_-}} := \|Q^{+-}\|_{\mathfrak{S}_2} + \|Q^{-+}\|_{\mathfrak{S}_2} + \|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1}. \tag{6.27}$$

We have $\mathscr{N} \subset \mathcal{P}^0_- + \mathfrak{S}_1^{\mathcal{P}^0_-}$ thanks to Eq. (6.11). The closed convex hull of $\mathscr{N} - \mathcal{P}^0_-$ in the $\mathfrak{S}_1^{\mathcal{P}^0_-}$-topology gives

$$\mathcal{K} := \big\{Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ Q^* = Q,\ -\mathcal{P}^0_- \le Q \le \mathcal{P}^0_+\big\}$$

and we have [HLS05a, HLS05b] : $\forall\, Q \in \mathcal{K},\ Q^2 \le Q^{++} - Q^{--}$.

– For Q in $\mathfrak{S}_1^{\mathcal{P}^0_-}$, we show $\mathcal{E}^\nu_{\mathrm{BDF}}(Q)$ is well defined. We have

$$\mathcal{P}^0_-(\mathcal{D}^0 Q)\mathcal{P}^0_- = -|\mathcal{D}^0|Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda),\ \text{because}\,|\mathcal{D}^0| \in \mathcal{B}(\mathfrak{H}_\Lambda),$$

this proves that the kinetic energy is defined.

– Thanks to the Kato-Seiler-Simon inequality [Sim79, Chapter 4], the operator Q is locally trace-class :

$$\forall\, \phi \in \mathbf{C}_0^\infty(\mathbb{R}^3),\ \phi\Pi_\Lambda \in \mathfrak{S}_2 \text{ so } \phi Q\phi = \phi\Pi_\Lambda Q\phi \in \mathfrak{S}_1(L^2(\mathbb{R}^3)).$$

We recall this inequality states that for all $2 \le p \le \infty$ and $d \in \mathbb{N}$, we have

$$\forall\, f,g \in L^p(\mathbb{R}^d),\ f(x)g(-i\nabla) \in \mathfrak{S}_p(\mathfrak{H}_\Lambda) \text{ and } \|f(x)g(-i\nabla)\|_{\mathfrak{S}_p} \le (2\pi)^{-d/p}\|f\|_{L^p}\|g\|_{L^p}. \tag{6.28}$$

In particular the *density* ρ_Q of Q, given by the formula

$$\forall\, x \in \mathbb{R}^3,\ \rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big)$$

is well defined. In [HLS05a] Hainzl *et al.* prove that its Coulomb energy is finite $D(\rho_Q,\rho_Q) < +\infty$. By Cauchy-Schwartz inequality, $D(\nu,\rho_Q)$ is defined.

– By Kato's inequality

$$\frac{1}{|\cdot|} \le \frac{\pi}{2}|\nabla|, \tag{6.29}$$

the exchange term is well-defined : this implies that $\|Q\|^2_{\mathrm{Ex}} \le \frac{\pi}{2}\mathrm{Tr}\big(|\nabla|Q^*Q\big)$.
– Furthermore the following holds : if $\alpha < \frac{4}{\pi}$, then the BDF energy is bounded from below on $\mathcal{K}$ [BBHS98a, HLS05b, HLS09]. Here we assume it is the case.

2. For $Q \in \mathcal{K}$, its charge is its $\mathcal{P}^0_-$-trace : $q = \mathrm{Tr}_{\mathcal{P}^0_-}(Q)$. So we define charge sectors sets :

$$\forall\, q \in \mathbb{R}^3,\ \mathcal{K}^q := \big\{Q \in \mathcal{K},\ \mathrm{Tr}(Q) = q\big\}.$$

A minimizer of $\mathcal{E}^\nu_{\mathrm{BDF}}$ over $\mathcal{K}$ is interpreted as the polarized vacuum in the presence of ν while minimizer over charge sector $N \in \mathbb{N}$ is interpretreted as the ground state of N electrons in the presence of ν. We define the energy functional E^ν_{BDF} :

$$\forall\, q \in \mathbb{R}^3,\ E^\nu_{\mathrm{BDF}}(q) := \inf\big\{\mathcal{E}^\nu_{\mathrm{BDF}}(Q),\ Q \in \mathcal{K}^q\big\}. \tag{6.30}$$

We also write :

$$\mathcal{K}^0_{\mathscr{C}} := \{Q \in \mathcal{K},\ \mathrm{Tr}_{\mathcal{P}^0_-}(Q) = 0,\ -\mathrm{C}Q\mathrm{C} = Q\}. \tag{6.31}$$

Lemma 6.1 states that this set is sequentially weakly-$*$ closed in $\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$.

Notation 6.6. For an operator $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, we write R_Q the operator given by the integral kernel :

$$R_Q(x,y) := \frac{Q(x,y)}{|x-y|}.$$

6.2.2 Structure of manifold

We define

$$\mathscr{V} = \big\{P - \mathcal{P}^0_-,\ P^* = P^2 = P \in \mathcal{B}(\mathfrak{H}_\Lambda),\ \mathrm{Tr}_{\mathcal{P}^0_-}\big(P - \mathcal{P}^0_-\big) = 0\big\} \subset \mathfrak{S}_2(\mathfrak{H}_\Lambda).$$

Up to adding $\mathcal{P}^0_-$, we deal with

$$\mathscr{M} := \mathcal{P}^0_- + \mathscr{V} = \big\{P,\ P^* = P^2 = P,\ \mathrm{Tr}_{\mathcal{P}^0_-}\big(P - \mathcal{P}^0_-\big) = 0\big\}.$$

From a geometrical point of view, we recall that these sets are Hilbert manifolds : $\mathscr{V}$ lives in the Hilbert space $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ and $\mathscr{M}$ lives in the affine space $\mathcal{P}^0_- + \mathfrak{S}_2(\mathfrak{H}_\Lambda)$.

Proposition 6.1. *The set $\mathscr{M}$ is a Hilbert manifold and for all $P \in \mathscr{M}$,*

$$\mathrm{T}_P\mathscr{M} = \{[A,P],\ A \in \mathcal{B}(\mathfrak{H}_\Lambda),\ A^* = -A \text{ and } PA(1-P) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}. \tag{6.32}$$

Writing

$$\mathfrak{m}_P := \{A \in \mathcal{B}(\mathfrak{H}_\Lambda),\ A^* = -A,\ PAP = (1-P)A(1-P) = 0 \text{ and } PA(1-P) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}, \tag{6.33}$$

any $P_1 \in \mathscr{M}$ can be written as $P_1 = e^A P e^{-A}$ where $A \in \mathfrak{m}_P$.

The BDF energy $\mathcal{E}^\nu_{\mathrm{BDF}}$ is a differentiable function in $\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$ with :

$$\begin{cases} \forall\, Q, \delta Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ \mathrm{d}\mathcal{E}^\nu_{\mathrm{BDF}}(Q)\cdot\delta Q = \mathrm{Tr}_{\mathcal{P}^0_-}\big(D_{Q,\nu}\delta Q\big). \\ D_{Q,\nu} := \mathcal{D}^0 + \alpha\big((\rho_Q - \nu) * \frac{1}{|\cdot|} - R_Q\big). \end{cases} \tag{6.34}$$

We may rewrite (6.34) as follows :

$$\forall\, Q, \delta Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ \mathrm{d}\mathcal{E}^\nu_{\mathrm{BDF}}(Q)\cdot\delta Q = \mathrm{Tr}_{\mathcal{P}^0_-}\big(\Pi_\Lambda D_{Q,\nu}\Pi_\Lambda\delta Q\big) \tag{6.35}$$

Notation 6.7. In the case $\nu = 0$ we write $D_Q := D_{Q,0}$.

Proposition 6.2. *Let (P,v) be in the tangent bundle $\mathrm{T}\mathscr{M}$ and $Q = P - \mathcal{P}^0_-$. Then $[[\Pi_\Lambda D_Q \Pi_\Lambda, P], P]$ is a Hilbert-Schmidt operator in $\mathrm{T}_P\mathscr{M}$ and :*

$$\mathrm{d}\mathcal{E}^0_{BDF}(P)\cdot v = \mathrm{Tr}\Big(\big[\big[\Pi_\Lambda D_Q\Pi_\Lambda, P\big], P\big]v\Big). \tag{6.36}$$

Remark 6.9. The operator $[[\Pi_\Lambda D_Q \Pi_\Lambda, P], P]$ is the "projection" of $\Pi_\Lambda D_Q \Pi_\Lambda$ onto $\mathrm{T}_P\mathscr{M}$. It properly defines a vector in the tangent plane which is exactly the *gradient* of $\mathcal{E}^0_{\mathrm{BDF}}$ at the point P.

$$\forall\, P \in \mathscr{M},\ \nabla\mathcal{E}^0_{\mathrm{BDF}}(P) = \big[\big[\Pi_\Lambda D_Q \Pi_\Lambda, P\big], P\big]. \tag{6.37}$$

We recall $\mathscr{M}_{\mathscr{C}}$ is the set of C-symmetric states (6.14).

Proposition 6.3. *The set $\mathscr{M}_{\mathscr{C}}$ is a* submanifold *of $\mathscr{M}$, which is* invariant *under the flow of $\mathcal{E}^0_{BDF}$. For any $P \in \mathscr{M}_{\mathscr{C}}$, writing*

$$\mathfrak{m}_P^{\mathscr{C}} = \{a \in \mathfrak{m}_P,\ \mathrm{C}a\mathrm{C} = a\}, \tag{6.38}$$

we have

$$\mathrm{T}_P\mathscr{M}_{\mathscr{C}} = \{[a, P],\ a \in \mathfrak{m}_P^{\mathscr{C}}\} = \{v \in \mathrm{T}_P\mathscr{M},\ -\mathrm{C}v\mathrm{C} = v\}. \tag{6.39}$$

Furthermore, for any $P \in \mathscr{M}_{\mathscr{C}}$ we have

$$\rho_{P-\mathcal{P}^0_-} = 0. \tag{6.40}$$

Proposition 6.4. *The set $\mathscr{M}_{\mathscr{C}}$ has two connected components $\mathscr{E}_1$ and $\mathscr{E}_{-1}$:*

$$\forall\, P \in \mathscr{M}_{\mathscr{C}},\ P \in \mathscr{E}_1 \iff \mathrm{Dim}\,\mathrm{Ran}\,P \cap \mathrm{Ran}\,\mathcal{P}^0_+ \equiv 0[2]. \tag{6.41}$$

In particular, $\mathscr{E}_1$ contains $\mathcal{P}^0_-$ and $\mathscr{E}_{-1}$ contains any $\mathcal{P}^0_- + |\psi\rangle\langle\psi| - |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|$ where $\psi \in \mathrm{Ran}\,\mathcal{P}^0_+$.

We end this section by stating technical results needed to prove Propositions 6.1,6.3 and 6.4.

6.2.3 Form of trial states

Theorem 6.4 (Form of trial states)**.** *Let P_1, P_0 be in $\mathscr{N}$ and $Q = P_1 - P_0$. Then there exist $M_+, M_- \in \mathbb{Z}_+$ such that there exist two orthonormal families*

$$\begin{aligned} &(a_1, \dots, a_{M_+}) \cup (e_i)_{i\in\mathbb{N}} && \text{in } \mathrm{Ran}\,\mathcal{P}^0_+,\\ &(a_{-1}, \dots, a_{-M_+}) \cup (e_{-i})_{i\in\mathbb{N}} && \text{in } \mathrm{Ran}\,\mathcal{P}^0_-, \end{aligned}$$

and a nonincreasing sequence $(\lambda_i)_{i\in\mathbb{N}} \in \ell^2$ satisfying the following properties.

1. *The a_i's are eigenvectors for Q with eigenvalue 1 (resp. -1) if $i > 0$ (resp. $i < 0$).*
2. *For each $i \in \mathbb{N}$ the plane $\Pi_i := Span(e_i, e_{-i})$ is spanned by two eigenvectors f_i and f_{-i} for Q with eigenvalues λ_i and $-\lambda_i$.*
3. *The plane Π_i is also spanned by two orthogonal vectors v_i in $Ran(1-P)$ and v_{-i} in $Ran(P)$. Moreover $\lambda_i = \sin(\theta_i)$ where $\theta_i \in (0, \frac{\pi}{2})$ is the angle between the two lines $\mathbb{C}v_i$ and $\mathbb{C}e_i$.*
4. *There holds :*
$$Q = \sum_{i=1}^{M_+} |a_i\rangle\langle a_i| - \sum_{i=1}^{M_-} |a_{-i}\rangle\langle a_{-i}| + \sum_{j\in\mathbb{N}} \lambda_j(|f_j\rangle\langle f_j| - |f_{-j}\rangle\langle f_{-j}|).$$

Remark 6.10. We have

$$\begin{aligned} Q^{++} &= \sum_{i=1}^{M_+} |a_i\rangle\langle a_i| + \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 |e_j\rangle\langle e_j|,\\ Q^{--} &= -\sum_{i=1}^{M_-} |a_{-i}\rangle\langle a_{-i}| - \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 |e_{-j}\rangle\langle e_{-j}|. \end{aligned} \tag{6.42}$$

Thanks to Theorem 6.4, it is possible to characterize C-symmetric states.

Proposition 6.5. *Let $\gamma = P - \mathcal{P}^0_-$ be in $\mathscr{M}_{\mathscr{C}}$. For $-1 \le \mu \le 1$ and $A = \in \{\gamma, \gamma^2\}$, we write*

$$E^A_\mu = Ker(A - \mu).$$

Then for any $\mu \in \sigma(\gamma)$, we have $\mathrm{C}E_\mu^\gamma = E_{-\mu}^\gamma$. Moreover for $|\mu| < 1$: if we decompose $E_\mu^\gamma \oplus E_{-\mu}^\gamma$ into a sum of planes Π as in Theorem 6.4, then each Π is not C-*invariant and $\dim E_\mu^\gamma$ is even. Equivalently $\dim E_{\mu^2}^{\gamma^2}$ is divisible by 4.*

Moreover there exists a decomposition

$$E_{\mu^2}^{\gamma^2} = \overset{\perp}{\bigoplus_{1\le j\le \frac{N}{2}}} V_{\mu,j} \text{ and } V_{\mu,j} = \Pi_{\mu,j}^a \overset{\perp}{\oplus} \mathrm{C}\Pi_{\mu,j}^a$$

where the $\Pi_{\mu,j}^a$'s and $\mathrm{C}\Pi_{\mu,j}^a$'s are spectral planes described in Theorem 6.4.

6.3 Proof of Theorem 6.1

6.3.1 Strategy and tools of the proof

Topologies

The upper bound in (6.18) comes from minimization over C-symmetric state of form (6.13).

We prove the existence of the minimizer over $\mathscr{E}_{-1}$ by using a lemma of Borwein and Preiss [BP87, HLS09], a smooth generalization of Ekeland's Lemma [Eke74] : we study the behaviour of a specific minimizing sequence $(P_n)_n$ or equivalently $(P_n - \mathcal{P}_-^0 =: Q_n)_n$.

Each element of the sequence satisfies an equation close to the one satisfied by a real minimizer and we show this equation remains in some weak limit.

Remark 6.11. We recall different topologies over bounded operators, besides the norm topology $\|\cdot\|_{\mathcal{B}}$ [RS75].

1. The so-called *strong topology*, the weakest topology $\mathcal{T}_s$ such that for any $f \in \mathfrak{H}_\Lambda$, the map

$$\begin{array}{ccc} \mathcal{B}(\mathfrak{H}_\Lambda) & \longrightarrow & \mathfrak{H}_\Lambda \\ A & \mapsto & Af \end{array}$$

   is continuous.

2. The so-called *weak operator topology*, the weakest topology $\mathcal{T}_{w.o.}$ such that for any $f, g \in \mathfrak{H}_\Lambda$, the map

$$\begin{array}{ccc} \mathcal{B}(\mathfrak{H}_\Lambda) & \longrightarrow & \mathbb{C} \\ A & \mapsto & \langle Af\,,\,g\rangle \end{array}$$

   is continuous.

We can also endow $\mathfrak{S}_1^{\mathcal{P}_-^0}$ with its weak-$*$ topology, the weakest topology such that the following maps are continuous :

$$\left|\begin{array}{ccc} \mathfrak{S}_1^{\mathcal{P}_-^0} & \longrightarrow & \mathbb{C} \\ Q & \mapsto & \mathrm{Tr}\big(A_0(Q^{++}+Q^{--}) + A_2(Q^{+-}+Q^{-+})\big) \\ \multicolumn{3}{l}{\forall\,(A_0, A_2) \in \mathrm{Comp}(\mathfrak{H}_\Lambda)\times \mathfrak{S}_2(\mathfrak{H}_\Lambda).} \end{array}\right.$$

We emphasize that the weak-$*$ topology is different from the weak topology (where $\mathrm{Comp}(\mathfrak{H}_\Lambda)$ must be replaced by $\mathcal{B}(\mathfrak{H}_\Lambda)$).

The following Lemma is important in our proof.

Lemma 6.1. *The set $\mathcal{K}_{\mathscr{C}}^0$ (defined in (6.31)) is weakly-$*$ sequentially closed in $\mathfrak{S}_1^{\mathcal{P}_-^0}(\mathfrak{H}_\Lambda)$.*

We prove this Lemma at the end of this Subsection.

Borwein and Preiss Lemma

We recall this Theorem as stated in [HLS09] :

Theorem 6.5. *Let $\mathcal{M}$ be a closed subset of a Hilbert space $\mathcal{H}$, and $F : \mathcal{M} \to (-\infty, +\infty]$ be a lower semi-continuous function that is bounded from below and not identical to $+\infty$. For all $\varepsilon > 0$ and all $u \in \mathcal{M}$ such that $F(u) < \inf_{\mathcal{M}} + \varepsilon^2$, there exist $v \in \mathcal{M}$ and $w \in \overline{\mathrm{Conv}(\mathcal{M})}$ such that*

1. *$F(v) < \inf_{\mathcal{M}} + \varepsilon^2$,*
2. *$||u - v||_{\mathcal{H}} < \sqrt{\varepsilon}$ and $||v - w||_{\mathcal{H}} < \sqrt{\varepsilon}$,*
3. *$F(v) + \varepsilon||v - w||_{\mathcal{H}}^2 = \min\big\{F(z) + \varepsilon||z - w||_{\mathcal{H}}^2,\ z \in \mathcal{M}\big\}$.*

Here we apply this Theorem with $\mathcal{H} = \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, $\mathcal{M} = \mathscr{E}_{-1} - \mathcal{P}_-^0$ and $F = \mathcal{E}_{\mathrm{BDF}}^0$.

The BDF energy is continuous in the $\mathfrak{S}_1^{\mathcal{P}_-^0}$-norm topology, thus its restriction over $\mathscr{V}$ is continuous in the $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$-norm topology.

This subspace $\mathcal{H}$ is closed in the Hilbert-Schmidt norm topology because $\mathscr{V} = \mathscr{M}_{\mathscr{C}}$ is closed in $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ and $\mathscr{E}_{-1} - \mathcal{P}_-^0$ is closed in $\mathscr{V}$.

Moreover, we have

$$\overline{\mathrm{Conv}(\mathscr{E}_{-1} - \mathcal{P}_-^0)}^{\mathfrak{S}_2} \subset \mathcal{K}_{\mathscr{C}}^0.$$

For every $\eta > 0$, we get a projector $P_\eta \in \mathscr{E}_{-1}$ and $A_\eta \in \mathcal{K}_{\mathscr{C}}^0$ such that P_η that minimizes the functional

$$F_\eta : P \in \mathscr{E}_{-1} \mapsto \mathcal{E}_{\mathrm{BDF}}^0(P - \mathcal{P}_-^0) + \varepsilon\|P - \mathcal{P}_-^0 - A_\eta\|_{\mathfrak{S}_2}^2.$$

We write

$$Q_\eta := P_\eta - \mathcal{P}_-^0,\ \Gamma_\eta := Q_\eta - A_\eta,\ \widetilde{D}_{Q_\eta} := \Pi_\Lambda\big(\mathcal{D}^0 - \alpha R_{Q_\eta} + 2\eta\Gamma_\eta\big)\Pi_\Lambda. \tag{6.43}$$

Studying its differential on $\mathrm{T}_{P_\eta}\mathscr{M}_{\mathscr{C}}$, we get that

$$\big[\widetilde{D}_{Q_\eta}, P_\eta\big] = 0. \tag{6.44}$$

In particular, by functional calculus, we get that

$$\big[\boldsymbol{\pi}_-^\eta, P_\eta\big] = 0,\ \boldsymbol{\pi}_\eta^- := \chi_{(-\infty,0)}(\widetilde{D}_{Q_\eta}). \tag{6.45}$$

We also write

$$\boldsymbol{\pi}_\eta^+ := \chi_{(0,+\infty)}(\widetilde{D}_{Q_\eta}) = \Pi_\Lambda - \boldsymbol{\pi}_\eta^-. \tag{6.46}$$

We can decompose $\mathfrak{H}_\Lambda$ as follows (here R means Ran) :

$$\mathfrak{H}_\Lambda = \mathrm{R}(P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}_\eta^-) \overset{\perp}{\oplus} \mathrm{R}(P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}_\eta^+) \overset{\perp}{\oplus} \mathrm{R}(\Pi_\Lambda - P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}_\eta^-) \overset{\perp}{\oplus} \mathrm{R}(\Pi_\Lambda - P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}_\eta^+). \tag{6.47}$$

We will prove

1. $\mathrm{Ran}\, P \cap \mathrm{Ran}\, \boldsymbol{\pi}_\eta^+$ has dimension 1, spanned by a unitary $\psi_\eta \in \mathfrak{H}_\Lambda$.
2. As η tends to 0, up to translation and a subsequence, $\psi_\eta \rightharpoonup \psi_e \neq 0$, $Q_\eta \rightharpoonup \overline{Q}$. There holds $\overline{Q} + \mathcal{P}_-^0 \in \mathscr{E}_{-1}$, ψ_e is a unitary eigenvector of $\Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda$ and

$$\overline{Q} + \mathcal{P}_-^0 = \chi_{(-\infty,0)}\big(\Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda\big) + |\psi_e\rangle\langle\psi_e| - |\mathrm{C}\psi_e\rangle\langle\mathrm{C}\psi_e|.$$

In the following part we write the spectral decomposition of trial states and prove Lemma 6.1.

Spectral decomposition

Let $(Q_n)_n$ be any minimizing sequence for $E_{1,1}$. We consider the spectral decomposition of the trial states Q_n : thanks to the upper bound, $\mathrm{Dim}\,\mathrm{Ker}(Q_n - 1) = 1$, as shown in Subsection 6.3.2.

There exist a *non-increasing* sequence $(\lambda_{j;n})_{j\in\mathbb{N}} \in \ell^2$ of eigenvalues and an orthonormal basis $\mathbf{B}_n$ of $\mathrm{Ran}\, Q_n$:

$$\mathbf{B}_n := (\psi_n, \mathrm{C}\psi_n) \cup (e_{j;n}^a, e_{j;n}^b, \mathrm{C}e_{j;n}^a, \mathrm{C}e_{j;n}^b),\ \mathcal{P}_-^0\psi_n = \mathcal{P}_-^0 e_{j;n}^\star = 0,\ \star \in \{a, b\}, \tag{6.48}$$

such that the following holds. We omit the index n :

$$\forall j \in \mathbb{N},\ \ e^a_{-j} := -\mathrm{C}e^b_j,\ e^b_{-j} := \mathrm{C}e^a_j, \tag{6.49a}$$

$$\begin{array}{rcl} f^\star_j & := & \sqrt{\frac{1-\lambda_j}{2}}e^\star_{-j} + \sqrt{\frac{1+\lambda_j}{2}}e^\star_j, \\ f^\star_{-j} & := & -\sqrt{\frac{1+\lambda_j}{2}}e^\star_{-j} + \sqrt{\frac{1+\lambda_j}{2}}e^\star_j. \end{array} \tag{6.49b}$$

$$\left\{\begin{array}{rcl} Q_n & = & |\psi_n\rangle\langle\psi_n| - |\mathrm{C}\psi_n\rangle\langle \mathrm{C}\psi_n| + \sum_{j\geq 1}\lambda_j q_{j;n} \\ q_{j;n} & = & |f^a_j\rangle\langle f^a_j| - |f^a_{-j}\rangle\langle f^a_{-j}| + |f^b_j\rangle\langle f^b_j| - |f^b_{-j}\rangle\langle f^b_{-j}|. \end{array}\right. \tag{6.49c}$$

Remark 6.12. Thanks to the cut-off, the sequences $(\psi_n)_n$ and $(e_{j;n})_n$ are H^1-bounded.

Up to translation and extraction ($(n_k)_k \in \mathbb{N}^{\mathbb{N}}$ and $(x_{n_k})_k \in (\mathbb{R}^3)^{\mathbb{N}}$), we assume that the weak limit of $(\psi_n)_n$ is non-zero (if it were then there would hold $E_{1,1} = 2m$).

We consider the weak limit of each (e_n) : by means of a diagonal extraction, we assume that all the $(e_{j,n_k}(\cdot - x_{n_k}))_k$ and $(\psi_{j,n_k}(\cdot - x_{n_k}))_k$, converge along the same subsequence $(n_k)_k$. We also assume that

$$\forall j \in \mathbb{N},\ \lambda_{j,n_k} \to \mu_j,\ (\mu_j)_j \in \ell^2,\ (\mu_j)_j \text{ non-increasing}, \tag{6.50}$$

and that the above convergences also hold in L^2_{loc} and almost everywhere.

Proof of Lemma 6.1

Let $(Q_n)_n$ be a sequence in $\mathcal{K}^0_{\mathscr{C}}$ that converges to $Q \in \mathcal{K}$ in the weak-$*$ topology of $\mathfrak{S}_1{}^{\mathcal{P}^0_-}$, that is :

$$\forall (G_0, G_2) \in \mathrm{Comp}(\mathfrak{H}_\Lambda) \times \mathfrak{S}_2(\mathfrak{H}_\Lambda) :$$

$$\left\{\begin{array}{l} \mathrm{Tr}(Q^{+-}_n G_2) \underset{n\to+\infty}{\to} \mathrm{Tr}(Q^{+-}G_2) \quad\text{and}\quad \mathrm{Tr}(Q^{-+}_n G_2) \underset{n\to+\infty}{\to} \mathrm{Tr}(Q^{-+}G_2), \\ \mathrm{Tr}(Q^{++}_n G_0) \underset{n\to+\infty}{\to} \mathrm{Tr}(Q^{++}G_0) \quad\text{and}\quad \mathrm{Tr}(Q^{--}_n G_0) \underset{n\to+\infty}{\to} \mathrm{Tr}(Q^{--}G_0). \end{array}\right.$$

In particular we have $S := \sup_n \|Q_n\|_{\mathfrak{S}_2} < +\infty$ by the uniform boundedness principle. The C-symmetry is a weak-$*$ condition : for all $\phi_1, \phi_2 \in \mathfrak{H}_\Lambda$:

$$\mathrm{Tr}\big(-\mathrm{C}Q_n\mathrm{C}|\phi_1\rangle\langle\phi_2|\big) = -\langle Q_n\mathrm{C}\phi_1\,,\,\mathrm{C}\phi_2\rangle$$

thus $-\mathrm{C}Q\mathrm{C} = Q$. There remains to prove that $\mathrm{Tr}_{\mathcal{P}^0_-}(Q) = 0$.

We consider the spectral decomposition of $P_n := \mathcal{P}^0_- + Q_n$. We know that this is compact perturbation of $\mathcal{P}^0_-$, thus its essential spectrum is $\{0, 1\}$ and there exist an ONB of $\mathfrak{H}_\Lambda$:

$$(e_{k;n})_{k=1}^{K_1} \cup (f_{j;n})_{j\in\mathbb{N}} \cup (g_{j;n})_{j\in\mathbb{N}},\ K_1 \in \mathbb{Z}_+$$

and two sequences $(r_{j;n})_j, (s_{j;n})_j$ in $[0, \frac{1}{2})$ that tend to 0, such that

$$P_n = \frac{1}{2}\sum_{k=1}^{K_1}|e_{k;n}\rangle\langle e_{k;n}| + \sum_{j\in\mathbb{N}}\Big\{r_{j;n}|f_{j;n}\rangle\langle f_{j;n}| + (1 - s_{j;n})|g_{j;n}\rangle\langle g_{j;n}|\Big\}.$$

Our aim is to prove we can rewrite P_n as follows :

$$\left|\begin{array}{l} P_n = \overline{P}_n + \overline{\gamma}_n, \\ \overline{\gamma}_n = \sum_j t_{j;n}\big(|\phi_{j;n}\rangle\langle\phi_{j;n}| - |\mathrm{C}\phi_{j;n}\rangle\langle\mathrm{C}\phi_{j;n}|\big), \\ \overline{P}_n \in \mathscr{M}_{\mathscr{C}},\ 2\sum_j t_{j;n} \leq \mathrm{Tr}\big(Q^{++}_n - Q^{--}_n\big), \\ (\phi_{j;n})_j \cup (\mathrm{C}\phi_{j;n})_j \text{ orthonormal family.} \end{array}\right. \tag{6.52}$$

Let us assume this point for the moment. Up to extraction, it is clear that the weak limit $\overline{\gamma}_\infty$ of $(\overline{\gamma}_n)$ has trace 0 : the eventual loss of mass of $(\phi_{j;n})_n$ is compensated by that of $(\mathrm{C}\phi_{j;n})_n$: $|\phi_{j;n}(x)|^2 = |\mathrm{C}\phi_{j;n}(x)|^2$ for all $x \in \mathbb{R}^3$. So the weak limit of

$$t_{j;n}\big(|\phi_{j;n}\rangle\langle\phi_{j;n}| - |\mathrm{C}\phi_{j;n}\rangle\langle\mathrm{C}\phi_{j;n}|\big)$$

has trace 0.

The same goes for $\overline{Q}_n := \overline{P}_n - \mathcal{P}^0_-$. We write $S := \limsup_n \mathrm{Tr}_{\mathcal{P}^0_-}(\overline{Q}_n) < +\infty$. We decompose each $\overline{Q}_n$ as in (6.49) and take the same notations. We may have $D_n := \mathrm{Dim}(\overline{Q}_n^2 - 1) > 2$ but the sequence $(D_n)_n$ is bounded by S. There is at most $\frac{S}{2}$ different $\psi_{j;n}$ in the spectral decomposition of $\overline{Q}_n$ $(j = 1, \dots, \lfloor \frac{S}{2} \rfloor)$.

We study the weak-limit of the $\psi_{j;n}$'s and the $e^\star_{j;n}$'s : there may be a loss of mass. However from (6.42), we see that the loss of mass in $\psi_{j;n}$ is compensated by that of $\mathrm{C}\psi_{j;n}$, and that of $e^\star_{j;n}$ is compensated by that of $\mathrm{C}e^\star_{j;n}$.

The subscript ∞ means we take the weak limit. If the sequences of eigenvalues $(\lambda_j)_j \in \ell^2$ weakly converges to $(\mu_j)_j \in \ell^2$, then we get that

$$\begin{cases} Q^{++} = \displaystyle\sum_{1\le j\le \lfloor S/2\rfloor} |\psi_{j;\infty}\rangle\langle\psi_{j;\infty}| + \sum_{j\in\mathbb{N}} \mu_j^2 \Big\{ |e^a_{j,\infty}\rangle\langle e^a_{j,\infty}| + |e^b_{j,\infty}\rangle\langle e^b_{j,\infty}| \Big\} \\ Q^{--} = -\displaystyle\sum_{1\le j\le \lfloor S/2\rfloor} |\psi_{-j;\infty}\rangle\langle\psi_{-j;\infty}| - \sum_{j\in\mathbb{N}} \mu_j^2 \Big\{ |e^a_{-j,\infty}\rangle\langle e^a_{-j,\infty}| + |e^b_{-j,\infty}\rangle\langle e^b_{-j,\infty}| \Big\} \end{cases}$$

where $|\psi_{j,\infty}|^2 = |\psi_{-j,\infty}|^2$ resp. $|e^\star_{j,\infty}|^2 = |e^\star_{-j,\infty}|^2$. Thus

$$\mathrm{Tr}\big(Q^{++} + Q^{--}\big) = 0.$$

Proof of (6.52) The condition $-\mathrm{C}Q_n\mathrm{C} = Q_n$ is equivalent to $\mathrm{C}P_n\mathrm{C} = \Pi_\Lambda - P_n$, so for any $\mu \in \mathbb{R}$ we have

$$\mathrm{CKer}\,\big(P_n - \mu\big) = \mathrm{Ker}\,\big(P_n - (1-\mu)\big).$$

Up to reindexing the sequences, we can assume that $r_{j;n} = s_{j;n}$ and up to changing the ONB, we can assume that $g_{j;n} = \mathrm{C}f_{j;n}$. Let us remark that

$$\mathrm{C}B_n\mathrm{C} = B_n \text{ where } B_n := \frac{1}{2}\sum_{k=1}^{K_0} |e_{k;n}\rangle\langle e_{k;n}|.$$

As shown in [HLS09, Lemma 15, Appendix B], the condition $Q_n \in \mathfrak{S}_1^{\mathcal{P}^0_-}$ gives

$$\begin{aligned} \mathrm{Tr}\big(Q_n^{++} - Q_n^{--}\big) &= \frac{K_1}{2} + \sum_{j\ge1} \Big\{ r_{j;n}\|\mathcal{P}^0_+ f_{j;n}\|^2_{L^2} + (1-r_{j;n})\|\mathcal{P}^0_- f_{j;n}\|^2_{L^2} \Big\} \\ &\quad + \sum_{j\ge1} \Big\{ (1-s_{j;n})\|\mathcal{P}^0_+ g_{j;n}\|^2_{L^2} + s_{j;n}\|\mathcal{P}^0_- g_{j;n}\|^2_{L^2} \Big\}, \end{aligned}$$

which implies

$$\Big| \; \frac{K_1}{2} + \sum_{j\ge1}(r_{j;n} + s_{j;n}) \le \mathrm{Tr}_{\mathcal{P}^0_-}(Q_n).$$

In particular we can write

$$\left|\begin{aligned} &P_n = \overline{P}_n + \gamma_n + B_n, \\ &\gamma_n = \sum_{j\ge1} r_{j:n}\big(|f_{j;n}\rangle\langle f_{j;n}| - |\mathrm{C}f_{j;n}\rangle\langle\mathrm{C}f_{j;n}|\big), \\ &P'_n = \sum_{j\ge1} |\mathrm{C}f_{j;n}\rangle\langle\mathrm{C}f_{j;n}|. \end{aligned}\right.$$

Both γ_n and B_n are trace-class, thus $P'_n - \mathcal{P}^0_- \in \mathfrak{S}_1^{\mathcal{P}^0_-}$. We know that $\mathrm{Tr}_{\mathcal{P}^0_-}(P'_n - \mathcal{P}^0_-)$ is an integer [HLS05a], this gives

$$\frac{K_1}{2} = K_0 \in \mathbb{N}.$$

Let us prove that we can decompose $\operatorname{Ran} B_n$ as follows :

$$\operatorname{Ran} B_n = F_n \overset{\perp}{\oplus} \mathrm{C}F_n,\ \operatorname{Dim} F_n = K_0. \tag{6.53}$$

This ends the proof : we have

$$B_n = \operatorname{Proj}(\mathrm{C}F_n) + \frac{1}{2}\big(\operatorname{Proj}(F_n) - \operatorname{Proj}(\mathrm{C}F_n)\big)$$

where $\operatorname{Proj}(E)$ is the orthogonal projection onto E. We choose then

$$\left|\begin{array}{l} \overline{P}_n := P'_n + \operatorname{Proj}(\mathrm{C}F_n), \\ \overline{\gamma}_n := \gamma_n + \frac{1}{2}\big(\operatorname{Proj}(F_n) - \operatorname{Proj}(\mathrm{C}F_n)\big). \end{array}\right.$$

Let $\phi \in \operatorname{Ran} B_n$ with $\mathrm{C}\phi \notin \mathbb{C}\phi$. Else, we take $\phi \perp \phi'$ with

$$\mathrm{C}\phi = e^{i\theta}\phi,\ \mathrm{C}\phi' = e^{i\theta'}\phi',\ \theta, \theta' \in \mathbb{R}.$$

Up to considering $e^{i\theta/2}\phi$ and $e^{i\theta'/2}\phi'$ we may assume that $\mathrm{C}\phi = \phi$, $\mathrm{C}\phi' = \phi'$. Then writing

$$\phi_\pm := \frac{1}{\sqrt{2}}\big(\phi \pm i\phi'\big)$$

we have $\langle \mathrm{C}\phi_+\,,\,\phi_+\rangle = 0$, which is absurd.

Let us consider $\operatorname{Span}(\phi, \mathrm{C}\phi)$ and assume $\|\phi\|_{L^2} = 1$. Thus $z = \langle \mathrm{C}\phi\,,\,\phi\rangle = -re^{i\theta}$ with $0 \le r \le 1$. There exist $a, b \in \mathbb{C}$ such that

$$\langle \mathrm{C}(a\phi + b\mathrm{C}\phi)\,,\,a\phi + b\mathrm{C}\phi\rangle = 0.$$

If $r = 0$ we take $a = 1$ and $b = 0$, else it suffices to take $a = r_0 e^{-i\theta/2}$ and $b = r_1 e^{i\theta/2}$ where $r_0, r_1 > 0$ are any number that satisfies

$$\frac{r_0}{r_1} + \frac{r_1}{r_0} = \frac{2}{r}.$$

This is possible because as $0 < r \le 1$ we have $\frac{2}{r} \ge 2$. By an easy induction, we can write $\operatorname{Ran} B_n$ as in (6.53).

□

6.3.2 Upper and lower bounds of $E_{1,1}$

Upper bound

We consider trial states of the following form :

$$Q = |\psi\rangle\langle\psi| - |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|,\ \|\psi\|_{L^2} = 1 \text{ and } \mathcal{P}^0_-\psi = 0.$$

The set of these states is written $\mathscr{E}^0_{-1}$. We will prove that the energy of a particular Q gives the upper bound. For such a Q, the BDF energy is simply :

$$2\langle|\mathcal{D}^0|\psi\,,\,\psi\rangle - \frac{\alpha}{2}\iint \frac{|\psi \wedge \mathrm{C}\psi(x,y)|^2}{|x-y|}dxdy. \tag{6.54}$$

Following [Sok14b], we take $\phi_{\mathrm{CP}} \in L^2(\mathbb{R}^3, \mathbb{C})$ the unique positive radial minimizer of the Choquard-Pekar energy. *We know that this minimizer is in the Schwartz class* (here we just need it to be in H^2). We form the spinor :

$$\phi := \big(\,\phi_{\mathrm{CP}}\ \ 0\ \ 0\ \ 0\,\big)^{\mathrm{T}},$$

and scale ϕ by a constant $\lambda^{-1} \sim \alpha$ to be chosen later :

$$\phi_\lambda(x) := \lambda^{-3/2}\phi(x/\lambda).$$

We define $\psi_\lambda := \Pi_\Lambda \phi_\lambda$ and write :

$$\psi_+ := \frac{\mathcal{P}^0_+ \psi_\lambda}{\|\mathcal{P}^0_+ \psi_\lambda\|_{L^2}} \text{ and } \psi_- := \frac{\mathcal{P}^0_- \mathrm{C}\psi_\lambda}{\|\mathcal{P}^0_- \mathrm{C}\psi_\lambda\|_{L^2}} = \mathrm{C}\psi_+. \tag{6.55}$$

Let us compute the energy of

$$Q_0 := |\psi_+\rangle\langle\psi_+| - |\psi_-\rangle\langle\psi_-|. \tag{6.56}$$

We have :

$$\begin{aligned}
\|\mathcal{P}^0_+ \psi_\lambda\|^2_{L^2} &= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2 \frac{g_0(p)}{2}\big(1 + \tfrac{1}{\widetilde{E}(p)}\big)dp,\\
&= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2 g_0(p)\big(1 - \tfrac{g_1(p)^2}{4g_0(p)^2}\big)dp + \mathcal{O}(\lambda^{-4}),\\
&= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2 \big(m - \tfrac{g_1'(0)^2}{4m}\big)dp + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}),\\
&= 1 - \frac{g_1'(0)^2}{4\lambda^2 m}\|\phi_{\mathrm{CP}}\|^2_{L^2} + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}).
\end{aligned}$$

Similarly the following holds :

$$\begin{aligned}
\langle |\mathcal{D}^0| \mathcal{P}^0_+ \psi_\lambda\, ,\, \psi_\lambda\rangle &= \int\limits_{B(0,\Lambda)} \widetilde{E}\,(p)\, \langle \widehat{\mathcal{P}^0_+}(p)\widehat{\psi}_\lambda(p)\, ,\, \widehat{\psi}_\lambda(p)\rangle_{\mathbb{R}^3} dp\\
&= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2 \frac{1}{2}\big(g_0(p) + \widetilde{E}\,(p)\,\big)dp\\
&= m + \frac{g_1'(0)^2}{4\lambda^2 m}\|\phi_{\mathrm{CP}}\|^2_{L^2} + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}).
\end{aligned}$$

Then we estimate :

$$\begin{aligned}
\iint \frac{|\psi_+ \wedge \psi_-(x,y)|^2}{|x-y|} dxdy &= 2\Big\{ D\big(|\psi_+|^2, |\psi_-|^2\big) - D\big(\psi_+^*\psi_-, \psi_+^*\psi_-\big)\Big\}\\
&= 2\Big\{ \tfrac{1}{\lambda} D\big(|\phi_{\mathrm{CP}}|^2, |\phi_{\mathrm{CP}}|^2\big) + \mathcal{O}(\lambda^{-2}) - D\big(\psi_+^*\psi_-, \psi_+^*\psi_-\big)\Big\}\\
&= 2\Big\{ \tfrac{1}{\lambda} D\big(|\phi_{\mathrm{CP}}|^2, |\phi_{\mathrm{CP}}|^2\big) + \mathcal{O}(\lambda^{-2})\Big\}.
\end{aligned}$$

Indeed we have :

$$\begin{aligned}
\|\psi_+^*\psi_-\|_{L^1} &\lesssim \|\nabla\psi_\lambda\|_{L^2}\|\psi_\lambda\|_{L^2} = \mathcal{O}(\lambda^{-1}).\\
|\psi_+^*\psi_-| * \tfrac{1}{|\cdot|} &\leq |\psi_+|^2 * \tfrac{1}{|\cdot|} \leq \tfrac{\pi}{2}\langle |\nabla|\psi_+\, ,\, \psi_+\rangle\\
&= \mathcal{O}(\lambda^{-1}).
\end{aligned}$$

Thus we get that :

$$\mathcal{E}^0_{\mathrm{BDF}}(Q_0) = 2m + \frac{g_1'(0)^2}{\lambda^2 m}\|\nabla\phi_{\mathrm{CP}}\|^2_{L^2} - \frac{\alpha}{\lambda} D\big(|\phi_{\mathrm{CP}}|^2, |\phi_{\mathrm{CP}}|^2\big) + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}). \tag{6.57}$$

If we *choose*

$$\frac{1}{\lambda} := \frac{\alpha m}{g_1'(0)^2} \tag{6.58}$$

we get the following upper bound :

$$E_{1,1} \leq \mathcal{E}^0_{\mathrm{BDF}}(Q_0) = 2m + \alpha^2 \frac{m}{g_1'(0)^2} E_{\mathrm{CP}} + \mathcal{O}(\alpha^3). \tag{6.59}$$

Let $Q\in\mathscr{M}-\mathcal{P}^0_-$ be an approximate minimizer such that

$$\mathcal{E}^0_{\rm BDF}(Q)<E_{1,1}+\alpha^2\frac{m}{2g_1'(0)^2}|E_{\rm CP}|<2m.$$

Our aim is to prove the following

$$\left\{\begin{array}{rcl} E_{1,1}-2m & \geq & -K\alpha^2,\\ \mathrm{Tr}\big(|\nabla|Q^2\big) & \leq & K\alpha.\end{array}\right. \tag{6.60}$$

We have

$$\Big(1-\alpha\frac{\pi}{4}\Big)\mathrm{Tr}(|\mathcal{D}^0|Q^2)\leq\mathcal{E}^0_{\rm BDF}<2m \text{ so } \|Q\|^2_{\mathfrak{S}_2}<\frac{2m}{1-\alpha\frac{\pi}{4}}<3.$$

However $\|Q\|^2_{\mathfrak{S}_2}\geq\mathrm{Dim\,Ker}(Q^2-1)=2\mathrm{Dim\,Ker}(Q-1)$, thus Q has the form written in (6.49) ; in particular we have :

$$Q=|\psi\rangle\langle\psi|-|\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|+\gamma,\ \psi\in\mathrm{Ran}(\mathcal{P}^0_+),\ \psi_+:=\psi,\psi_-:=\mathrm{C}\psi\in\mathrm{Ker}\,\gamma.$$

Let us remark that $\gamma+\mathcal{P}^0_-\in\mathscr{M}$. The energy of Q is :

$$\mathcal{E}^0_{\rm BDF}(Q)=\mathcal{E}^0_{\rm BDF}(\gamma)+2\langle|\mathcal{D}^0|\psi\,,\,\psi\rangle-\frac{\alpha}{2}\iint\frac{|\psi\wedge\mathrm{C}\psi(x,y)|^2}{|x-y|}dxdy-\alpha\sum_{\varepsilon\in\{+,-\}}\big(\langle\psi_\varepsilon R_\gamma\,,\,\psi_\varepsilon\rangle\big). \tag{6.61}$$

We substract $2m$: as $g_0'(0)=0$ and $\|g_0''\|_{L^\infty}\leq K\alpha$ [Sok14b, Appendix A], we have

$$|g_0(p)-m|\leq p^2\int_0^1|g_0''(tp)|(1-t)dt\leq K\alpha p^2,$$

thus :

$$\begin{aligned}\widetilde{E}(p)-m&=\frac{g_1(p)^2+(g_0(p)-m)(g_0(p)+m)}{\widetilde{E}(p)+m}\\&\leq\frac{g_1(p)^2(1-K\alpha)}{2\widetilde{E}(p)}.\end{aligned}$$

Going back to the energy, we have by Cauchy-Schwartz inequality :

$$|\langle\psi_\varepsilon\,,\,R_\gamma\psi_\varepsilon\rangle|\leq\|N[\psi_\varepsilon]\|_{\rm Ex}\|\gamma\|_{\rm Ex},\ N[\psi_\varepsilon]:=|\psi_\varepsilon\rangle\langle\psi_\varepsilon|.$$

The quantity $\|N[\psi_\varepsilon]\|^2_{\rm Ex}$ is simply $D\big(|\psi_\varepsilon|^2,|\psi_\varepsilon|^2\big)$ and we get :

$$\begin{aligned}&(1-K\alpha)\langle\tfrac{g_1^2(-i\nabla)}{|\mathcal{D}^0|}\psi\,,\,\psi\rangle+\mathrm{Tr}(|\mathcal{D}^0|\gamma^2)\leq K_1\alpha^2+2\alpha D\big(|\psi|^2,|\psi|^2\big)+\tfrac{3\alpha}{2}\|\gamma\|^2_{\rm Ex},\\&(1-K\alpha)\langle\tfrac{g_1^2(-i\nabla)}{|\mathcal{D}^0|}\psi\,,\,\psi\rangle+\big(1-\tfrac{3\alpha\pi}{4}\big)\mathrm{Tr}(|\mathcal{D}^0|\gamma^2)\leq K_1\alpha^2+\alpha\pi\langle\,|\nabla|\psi\,,\,\psi\rangle.\end{aligned}$$

Now we have :

$$(1-K\alpha)\frac{p^2}{\widetilde{E}(p)}\geq2\alpha|p|\iff p^2\geq4\alpha^2(1-K\alpha)\widetilde{E}(p)^2\,. \tag{6.62}$$

We can take $K=\|g_0\|_{L^\infty}$: this inequality holds for

$$|p|\geq r_0:=\frac{2\alpha\|g_0\|_{L^\infty}\sqrt{1-\alpha\|g_0\|_{L^\infty}}}{\sqrt{1-4\alpha^2\|g_1'\|^2_{L^\infty}(1-\alpha\|g_0\|_{L^\infty})}}. \tag{6.63}$$

If we split $\langle|\nabla\psi|\,,\,\psi\rangle$ at level $|p|=r_0$, we have :

$$\frac{1-\|g_0\|_{L^\infty}\alpha}{2}\langle\tfrac{g_1^2(-i\nabla)}{|\mathcal{D}^0|}\psi\,,\,\psi\rangle+\big(1-\frac{3\alpha\pi}{4}\big)\mathrm{Tr}(|\mathcal{D}^0|\gamma^2)\leq K_1\alpha^2+\alpha r_0\lesssim\alpha^2. \tag{6.64}$$

and

$$\langle |\nabla|\psi\,,\,\psi\rangle \lesssim \alpha. \tag{6.65}$$

Substituting these estimates in (6.61), we get :

$$E_{1,1}-2m \geq \mathcal{E}^0_{\mathrm{BDF}}(Q)-2m+\alpha^2\frac{m}{2g_1'(0)^2}E_{\mathrm{CP}} \geq -K\alpha^2. \tag{6.66}$$

Form of a minimizer for $E_{1,1}$

If a minimizer $\overline{P}\in\mathscr{E}_{-1}$ exists, then it satisfies the following :

$$\left|\begin{array}{l}\overline{P}=\mathcal{P}^0_-+\overline{Q}=\mathcal{P}^0_-+|\psi_+\rangle\langle\psi_+|-|\mathrm{C}\psi_+\rangle\langle\mathrm{C}\psi_+|+\gamma\\ \psi_+,\mathrm{C}\psi_+\in\mathrm{Ker}\,\gamma,\ \mathcal{P}^0_-\psi_+=0.\end{array}\right.$$

Moreover the proof of the lower bound ensures that $\|\gamma\|_{\mathfrak{S}_2}\lesssim\alpha$. So let $\mathrm{P}^0_{1,1}$ be :

$$\mathrm{P}^0_{1,1}:=\mathcal{P}^0_-+|\psi_+\rangle\langle\psi_+|-|\mathrm{C}\psi_+\rangle\langle\mathrm{C}\psi_+|.$$

Then we have $\|\mathrm{P}^0_{1,1}-\overline{P}\|_{\mathfrak{S}_2}=\|\gamma\|_{\mathfrak{S}_2}\lesssim\alpha$. Using Propositions 6.1 and 6.3, we write

$$\overline{P}=e^{A}\mathrm{P}^0_{1,1}e^{-A},\ A\in\mathfrak{m}^{\mathscr{C}}_{\mathrm{P}^0_{1,1}}$$

where there exist $(\theta_j)_j\in\ell^2$ decreasing and $K_0>0$ such that

$$\begin{aligned}\|\gamma\|_{\mathfrak{S}_2}&=4\sum_{j=1}^{+\infty}\sin(\theta_j)^2\leq K_0\alpha^2,\ \text{thus}\\ \|A\|^2_{\mathfrak{S}_2}&=4\sum_{j=1}^{\infty}\theta_j^2\leq\frac{\pi^2}{4}K_0\alpha^2.\end{aligned}$$

Assuming Theorem 6.1, this proves the description of Theorem 6.2.

6.3.3 Existence of a minimizer for $E_{1,1}$

We consider a family of almost minimizers $(P_{\eta_n})_n$ of type (6.43) where $(\eta_n)_n$ is any decreasing sequence. We assume that $\Lambda^2\alpha^{-2}\eta_n$ is small. We also consider the spectral decomposition (6.49) of any $Q_n:=P_{\eta_n}-\mathcal{P}^0_-$.

For short we write $P_n:=P_{\eta_n}$ and in general replace the subscript η_n by n.

– We study weak limits of $(Q_n)_n$. We recall that $\mathbb{C}\psi_n=\mathrm{Ker}(Q_n-1)$, and

$$Q_n=|\psi_n\rangle\langle\psi_n|-|\mathrm{C}\psi_n\rangle\langle\mathrm{C}\psi_n|+\gamma_n,\ \psi_n,\mathrm{C}\psi_n\in\mathrm{Ker}\,\gamma_n. \tag{6.67}$$

– We first prove that there is no vanishing :

$$\exists A>0,\ \limsup_n\sup_{z\in\mathbb{R}^3}\int_{B(z,A)}|\psi_n(x)|^2dx>0.$$

Indeed, let us assume this is false. Then for any $A>0$ the following holds :

$$D\big(|\psi_n|^2,|\psi_n|^2\big)\leq\frac{1}{A}+2\Lambda\Big\{\sup_{z\in\mathbb{R}^3}\int_{B(z,A)}|\psi_n(x)|^2dx\Big\}^{1/2},$$

where we have used Cauchy-Schwarz inequality and Hardy inequality. In the limit $n\to+\infty$ and then $A\to+\infty$, we have : $\limsup_n D\big(|\psi_n|^2,|\psi_n|^2\big)=0$.

There holds *a priori* estimates (6.60) : using Kato's inequality we would get

$$\liminf_n \mathcal{E}^0_{\rm BDF}(Q_n) \geq 2 \liminf_n \langle |\mathcal{D}^0| \psi_n \, , \, \psi_n \rangle + \liminf_n \mathcal{E}^0_{\rm BDF}(\gamma_n) \geq 2m.$$

Thus, up to translation, we assume that $Q_n \rightharpoonup Q_\infty \neq 0$.

– As the BDF energy is sequential weakly lower continuous [HLS05b], we have

$$E_{1,1} \geq \mathcal{E}^0_{\rm BDF}(Q_\infty).$$

Our aim is to prove that $Q_\infty + \mathcal{P}^0_- \in \mathscr{M}_{\mathscr{C}}$: in other words that Q_∞ is a minimizer for $E_{1,1}$.

– The spectral decomposition (6.67) is not the relevant one : let us prove we can describe P_n in function of the spectral spaces of the "mean-field operator" $\widetilde{D}_{Q_n}$: the first step is to prove (6.69) below.

We recall that Q_n satisfies Eq. (6.44), that we have the decomposition (6.47).

The following holds :

$$\begin{aligned}\langle \widetilde{D}_{Q_n} \psi_n \, , \, \psi_n \rangle &= \langle |\mathcal{D}^0| \psi_n \, , \, \psi_n \rangle + \mathcal{O}\big(\alpha \| \, |\nabla|^{1/2} \psi_n \|_{L^2} \| \, |\nabla|^{1/2} Q \|_{\mathfrak{S}_2} + \eta_n \|\Gamma_n\|_{\mathfrak{S}_2}\big) \\ &= \langle |\mathcal{D}^0| \psi_n \, , \, \psi_n \rangle + \mathcal{O}(\alpha^2) \geq m - K\alpha^2.\end{aligned}$$

Thus $\mathrm{Ran}\, P_n \cap \mathrm{Ran}\, \boldsymbol{\pi}^n_+ \neq \{0\}$. Let us prove this subspace has dimension 1 : we use the minimizing property of Q_n. The condition on the first derivative gives (6.44), what is the condition on the second derivative ? For any $A \in \mathfrak{m}^{\mathscr{C}}_{P_n}$, expanding $e^A P_n e^{-A} - P_n$ in power of A, we get that the Hessian $\mathrm{Hess}_{P_n}(F_n)$ of $F_n := F_{\eta_n}$ at point P_n is

$$\begin{aligned}&\forall\, V \in \mathrm{T}_{P_n} \mathscr{M}_{\mathscr{C}}, \; A = \big[V, P_n\big], \\ &\mathrm{Hess}_{F_n}(P_n; V, V) = \mathrm{Tr}\big(\widetilde{D}_{Q_n}(A^2 P_n - A P_n A)\big) + \eta_n \|V\|^2_{\mathfrak{S}_2} - \frac{\alpha}{2}\|V\|^2_{\rm Ex}.\end{aligned}$$

This Hessian is non-negative. For any unitary $f \perp g$ in $\mathrm{Ran}(\Pi_\Lambda - P_n)$ we choose

$$A := |f\rangle\langle -\mathrm{C} g| - | - \mathrm{C} g\rangle\langle f| + |g\rangle\langle \mathrm{C} f| - |\mathrm{C} f\rangle\langle g| \in \mathfrak{m}^{\mathscr{C}}_{P_n}.$$

As $-\mathrm{C}\widetilde{D}_{Q_n}\mathrm{C} = \widetilde{D}_{Q_n}$, the condition on the Hessian gives

$$2\big(\langle \widetilde{D}_{Q_n} f \, , \, f \rangle + \langle \widetilde{D}_{Q_n} g \, , \, g \rangle\big) + 4\eta_n \geq \frac{\alpha}{2} \big|\big| \, \big[A, P_n\big] \big|\big|^2_{\rm Ex} \geq 0. \tag{6.68}$$

We have $\mathrm{C}\psi_n \in \mathrm{Ran}(\Pi_\Lambda - P_n)$ and

$$\langle \widetilde{D}_{Q_n} \mathrm{C}\psi_n \, , \, \mathrm{C}\psi_n \rangle = -\langle \widetilde{D}_{Q_n} \psi_n \, , \, \psi_n \rangle \leq -m + K\alpha^2,$$

thus necessarily for n large, there is no plane in $\mathrm{Ran}(\Pi_\Lambda - P_n) \cap \mathrm{Ran}(\boldsymbol{\pi}^n_-)$, equivalently there is no plane in $\mathrm{Ran}\, P_n \cap \mathrm{Ran}\, \boldsymbol{\pi}^n_+$.

There exists a unitary $\psi_{e;n} \in \mathfrak{H}_\Lambda$ that spans $\mathrm{Ran}\, P_n \cap \mathrm{Ran}\, \boldsymbol{\pi}^n_+$. Equivalently $\psi_{v;n} := \mathrm{C}\psi_{e;n}$ spans the other one.

Thus :

$$P_n = |\psi_{e;n}\rangle\langle \psi_{e;n}| + \boldsymbol{\pi}^n_-. \tag{6.69}$$

- We thus write

$$Q_n = |\psi_{e;n}\rangle\langle \psi_{e;n}| - |\psi_{v;n}\rangle\langle \psi_{v;n}| + \overline{\gamma}_n = \overline{N}_n + \overline{\gamma}_n. \tag{6.70}$$

As $\mathrm{Ran}\, P_n$ is $\widetilde{D}_{Q_n}$-invariant and that $\widetilde{D}_{Q_n}$ is bounded (with a bound that depends on Λ), necessarily

$$\widetilde{D}_{Q_n} \psi_{e;n} = \mu_n \psi_{e;n}, \; \mu_n \in \mathbb{R}_+.$$

The condition on the Hessian enables us to say that

$$m - \mu_n + 2\eta_n \geq 0.$$

– As for ψ_n, there is no vanishing for $(\psi_{e,n})_n$ for α sufficiently small : decomposing $\psi_+ \in \mathrm{Ran}\, P_n$:

$$\psi_+ = a\psi_{e;n} + \phi, \; \phi \in \mathrm{Ran}\, P_n \cap \mathrm{Ran}\, \boldsymbol{\pi}^n_-,$$

we have

$$|a|^2 \geq \frac{1}{\mu}\big(m + \langle|\widetilde{D}_{Q_n}|\phi\,,\,\phi\rangle - K(\alpha^2 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2})\big).$$

Provided that μ_n is close to 1, the absence of vanishing for ψ_n implies that of $\psi_{e;n}$.

By Kato's inequality (6.29) :

$$\begin{aligned}\widetilde{D}^2_{Q_n} &\geq |\mathcal{D}^0|\big(1 - 2\alpha\|R_{Q_n}|\mathcal{D}^0|^{-1}\|_{\mathcal{B}} - 4\eta_n\|\Gamma_n\|_{\mathcal{B}}\big)|\mathcal{D}^0| \\ &\geq |\mathcal{D}^0|^2\big(1 - \alpha\|Q_n\|_{\mathrm{Ex}} - 4\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big)\end{aligned}$$

Thus

$$\big|\widetilde{D}_{Q_n}\big| \geq |\mathcal{D}^0|\big(1 - \alpha\|Q_n\|_{\mathrm{Ex}} - 2\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big) \text{ and } \mu_n \geq 1 - K(\alpha^2 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2}).$$

In the same way we can prove that

$$|\mu_n - m| \lesssim \alpha^2 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2}$$

So

$$\psi_{e,n} \rightharpoonup \psi_e \neq 0.$$

– We decompose $\overline{\gamma_n} = \boldsymbol{\pi}^n_- - \mathcal{P}^0_- \in \mathscr{E}_1 - \mathcal{P}^0_-$ as in (6.49) : using Cauchy's expansion [HLS05a], we have

$$\boldsymbol{\pi}^n_- - \mathcal{P}^0_- = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\omega}{\mathcal{D}^0 + i\omega}\big(2\eta_n\Gamma_n - \alpha\Pi_\Lambda R_{Q_n}\Pi_\Lambda + 2\eta_n\Gamma_n\big)\frac{1}{\widetilde{D}_{Q_n} + i\omega}\Pi_\Lambda. \tag{6.71}$$

To justify this equality, we remark that $|\widetilde{D}_{Q_n}|$ is uniformly bounded from below : the r.h.s. of (6.71) is well-defined. Integrating the norm of bounded operator in (6.71), we get that

$$\|\boldsymbol{\pi}^n_- - \mathcal{P}^0_-\|_{\mathcal{B}} \lesssim \alpha\|Q_n\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2} < 1.$$

In fact, we can also expand in power of $Y_n := -\alpha\Pi_\Lambda R_{Q_n}\Pi_\Lambda + 2\eta_n\Gamma_n$:

$$\begin{cases} \boldsymbol{\pi}^n_- - \mathcal{P}^0_- &= \displaystyle\sum_{j\geq 1}\alpha^j M_j[B_n], \\ M_j[Y_n] &= \displaystyle -\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\mathcal{D}^0 + i\omega}\Big(Y_n\frac{1}{\mathcal{D}^0 + i\omega}\Big)^j. \end{cases} \tag{6.72}$$

We take the Hilbert-Schmidt norm [HLS05a, Sok14b] : as $\|R_{Q_n}\frac{1}{|\nabla|^{1/2}}\|_{\mathfrak{S}_2} \lesssim \|Q\|_{\mathrm{Ex}}$, we have

$$\|\overline{\gamma}_n\|_{\mathfrak{S}_2} \lesssim \alpha\|Q_n\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2} \lesssim \alpha^2. \tag{6.73}$$

We thus write

$$\overline{\gamma}_n = \sum_{j\geq 1}\lambda_{j;n}q_{j;n},$$

where $q_{j;n}$ has the same form as the one in (6.49).

– Up to a subsequence, we assume all weak convergences as in Remark (6.12) : the sequence of eigenvalues $(\lambda_{j;n})_n$ tends to $(\mu_j)_j \in \ell^2$ and each $(e^\star_{j;n})_n$ (with $\star \in \{a, b\}$) tends to $e^\star_{j;\infty}$, $(\psi_{e;n})_n$ tends to ψ_e. We also assume that the sequence $(\mu_n)_n$ tends to μ with $0 \leq \mu \leq m$. For shot we write $\psi_v := \mathrm{C}\psi_e$.

– We write $\overline{P} := Q_\infty + \mathcal{P}^0_-$ and $\overline{\boldsymbol{\pi}} := \chi_{(-\infty,0)}(D_{Q_\infty})$. We will prove that

1. $\big[D^{(\Lambda)}_{Q_\infty}, \overline{P}\big] = 0$,
2. $D_{Q_\infty}\psi_e = \mu\psi_e$ and so $\overline{\boldsymbol{\pi}}\psi_e = 0$.
   Moreover $D_{Q_\infty}\mathrm{C}\psi_e = -\mu\mathrm{C}\psi_e$ and $\langle\mathrm{C}\psi_e\,,\,\psi_e\rangle = 0$.
3. $\overline{\boldsymbol{\pi}} = \overline{P} - |\psi_e\rangle\langle\psi_e| + |\mathrm{C}\psi_e\rangle\langle\mathrm{C}\psi_e|$.

Notation 6.8. We write $D^{(\Lambda)}_{Q_\infty} := \Pi_\Lambda D_{Q_\infty}\Pi_\Lambda$ for short.

This all comes from the fact that

$$\mathrm{s}-\lim_n R_{Q_n} = R_{Q_\infty}. \tag{6.74}$$

This fact enables us to show

$$\left|\begin{array}{l} R_{Q_n}\psi_{e;n} \rightharpoonup_n R_{Q_\infty}\psi_e \text{ in } L^2,\\ \mathrm{s.\,op.}-\lim_n \left(\boldsymbol{\pi}_-^n - \mathcal{P}_-^0\right) = \overline{\boldsymbol{\pi}} - \mathcal{P}_-^0 \text{ in } \mathcal{B}(\mathfrak{H}_\Lambda),\\ \mathrm{w.\,op.}-\lim_n P_n = \overline{\boldsymbol{\pi}} - \mathcal{P}_-^0 + |\psi_e\rangle\langle\psi_e| - |\psi_v\rangle\langle\psi_v| \text{ in } \mathcal{B}(\mathfrak{H}_\Lambda). \end{array}\right. \tag{6.75}$$

Indeed for any $f \in \mathfrak{H}_\Lambda$ we have

$$\begin{aligned} \|R_{Q_n}f - R_{Q_\infty}f\|_{L^2}^2 &= \int \Big| \int \frac{(Q_n - Q_\infty)(x,y)}{|x-y|} f(y)dy\Big|^2 dx\\ &\le \|f\|_{L^2}^2 \Big(\frac{1}{A^2}\|Q_n - Q_\infty\|_{\mathfrak{S}_2}^2 + 4\Lambda^2 \iint_{B(0,2A)^2} |(Q_n - Q_\infty)(x,y)|^2 dxdy\Big)\\ &\quad + 4\Lambda^2 \|Q_n - Q_\infty\|_{\mathfrak{S}_2}^2 \int_{B(0,A)^c} |f(y)|^2 dy. \end{aligned}$$

We have just split as follows : for $x \in \mathbb{R}^3$ we consider

$$\mathbb{R}^3 = B(x,A)^c \sqcup B(x,A)\cap B(0,A) \sqcup B(x,A)\cap B(0,A)^c.$$

Taking the limsup $n \to +\infty$ we get that

$$\forall\, A>0,\ \limsup_n \|R_{Q_n}f - R_{Q_\infty f}\|_{L^2}^2 \le 4 \limsup_n \|Q_n\|_{\mathfrak{S}_2}^2 \Big(\frac{\|f\|_{L^2}^2}{A^2} + 4\Lambda^2 \int_{B(0,A)^c} |f(y)|^2 dy\Big),$$

taking the limit $A \to +\infty$ we get that

$$\limsup_n \|R_{Q_n}f - R_{Q_\infty f}\|_{L^2}^2 = 0.$$

In particular for any $f \in \mathfrak{H}_\Lambda$

$$\langle R_{Q_n}\psi_{e;n}\,,\, f\rangle = \langle \psi_{e;n}\,,\, R_{Q_n}f\rangle \underset{n\to+\infty}{\longrightarrow} \langle \psi_e\,,\, R_{Q_\infty}f\rangle = \langle R_{Q_\infty}\psi_e\,,\, f\rangle.$$

Thus $\widetilde{D}_{Q_n}\psi_{e;n} \underset{n\to+\infty}{\rightharpoonup} D_{Q_\infty}\psi_e$, and $D_{Q_\infty}\psi_e = \mu\psi_e$.
– Let us prove that

$$\mathrm{s.\,op.}-\lim_n \boldsymbol{\pi}_-^n = \overline{\boldsymbol{\pi}}. \tag{6.76}$$

We have

$$R_{Q_n}\frac{1}{\mathcal{D}^0 + i\omega}f = R[Q_n - Q_\infty]\frac{1}{\mathcal{D}^0 + i\omega}f + R_{Q_\infty}\frac{1}{\mathcal{D}^0 + i\omega}f$$

and at fixed ω and f

$$R[Q_n - Q_\infty]\frac{1}{\mathcal{D}^0 + i\omega}f \underset{n\to+\infty}{\longrightarrow} 0 \text{ in } L^2.$$

Generally for $J \ge 1$, we expand $\Big(R_{Q_n}\frac{1}{\mathcal{D}^0+i\omega}\Big)^J$ in power of $R[Q_n - Q_\infty]$ and Q_∞. We get :

$$\forall\,\omega, f,\ \Big(R_{Q_n}\frac{1}{\mathcal{D}^0 + i\omega}\Big)^J \underset{n\to+\infty}{\longrightarrow} 0 \text{ in } L^2.$$

Moreover

$$\Big|\Big|\Big(R_{Q_n}\frac{1}{\mathcal{D}^0+i\omega}\Big)^J\Big|\Big|_{L^2}\le \widetilde{E}\,(\omega)^{-J/2}\,\|Q_n\frac{1}{|\mathcal{D}^0|^{1/2}}\|_{\mathcal{B}}^J\|f\|_{L^2},$$
$$\le \big(\limsup_n\|Q_n\|_{\rm Ex}\widetilde{E}\,(\omega)^{-1/2}\big)^J\|f\|_{L^2}.$$

By dominated convergence as

$$u_j\|f\|_{L^2}:=\int\frac{d\omega}{\widetilde{E}\,(\omega)^{1+J/2}}\big(\alpha\|Q_n\|_{\rm Ex}+\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big)^J\|f\|_{L^2}<+\infty,\tag{6.77}$$

we get

$$M_j[Y_n]f\underset{n\to+\infty}{\longrightarrow}M_j[\alpha R_{Q_\infty}]f\text{ in }L^2.$$

To end this argument we remark that the series $\sum_{j\ge1}u_j$ is convergent for α and η_n sufficiently small : thus we have

$$\sum_{j\ge1}M_j[Y_n]f\underset{n\to+\infty}{\longrightarrow}\sum_{j\ge1}M_j[\alpha R_{Q_\infty}]f\text{ in }L^2,$$

that is (6.76) holds.

– Thanks to (6.76), there holds (in the weak operator topology for instance)

$$Q_\infty=\lim_n Q_n=|\psi_e\rangle\langle\psi_e|-|\psi_v\rangle\langle\psi_v|+\overline{\boldsymbol{\pi}}-\mathcal{P}_-^0,$$

that is

$$\overline{P}=|\psi_e\rangle\langle\psi_e|-|\psi_v\rangle\langle\psi_v|+\overline{\boldsymbol{\pi}}.\tag{6.78}$$

In the weak operator topology we also have

$$\text{w. op.}-\lim_n\big[\widetilde{D}_{Q_n},Q_n+\mathcal{P}_-^0\big]=\big[D_{Q_\infty}^{(\Lambda)},Q_\infty+\mathcal{P}_-^0\big],$$

by strong convergence of R_{Q_n} to R_{Q_∞} and norm convergence of $\eta_n\Gamma_n$ to 0.

– There remains to prove that $\|\psi_e\|_{L^2}=1$. We assume for the moment that we can uniformly separate the μ_n's from the remainder of the positive spectrum $\sigma\big(|\widetilde{D}_{Q_n}|\big)\backslash\{\mu_n\}$. Let us write a_n the bottom of this last set : there exists $\varepsilon>0$ (of order α^2 in fact) such that for n_0 sufficiently large :

$$\forall n\ge n_0,\ a_n-\mu_n\ge5\varepsilon.\tag{6.79}$$

In particular, we can draw a small circle in $\mathbb{C}$ that intersects $\mathbb{R}$ only at points $\mu\pm2\varepsilon$. We write $\mathcal{C}_\varepsilon$ this circle : it has been chosen such that if $|\mu_n-\mu|\le\varepsilon$ (true for $n\ge n_1$ where $n_1\ge n_0$ is sufficiently large),

$$\forall n\ge n_0,\ \text{dist}\big(\mu_n;\mathcal{C}_\varepsilon\big)\ge\varepsilon.$$

By functional calculus we have

$$|\psi_{e;n}\rangle\langle\psi_{e;n}|=\frac{1}{2i\pi}\int_{\mathcal{C}_\varepsilon}\frac{dz}{z-\widetilde{D}_{Q_n}}.$$

We want to substract $\chi_{(\mu-2\varepsilon,\mu+2\varepsilon)}\big(D_{Q_\infty}^{(\Lambda)}\big)$. If (6.79) is true, then the same holds for the limit $D_{Q_\infty}^{(\Lambda)}$ by strong convergence. Indeed, for any $f\in\text{Ran}\big(\overline{\boldsymbol{\pi}}_+\big)$ (where $\overline{\boldsymbol{\pi}}_+:=\Pi_\Lambda-\overline{\boldsymbol{\pi}}$) we have

$$\|\boldsymbol{\pi}_+^n f-f\|_{L^2}\to0.$$

For $f_1\perp f_2$ in $\text{Ran}\big(\overline{\boldsymbol{\pi}}_+\big)$, there holds

$$\min_j\big(\frac{1}{\|\overline{\boldsymbol{\pi}}_+^n f_j\|_{L^2}^2}\big)\langle\widetilde{D}_{Q_n}\overline{\boldsymbol{\pi}}_+^n f_1\,,\,f_1\rangle+\langle\widetilde{D}_{Q_n}\overline{\boldsymbol{\pi}}_+^n f_2\,,\,f_2\rangle\ge a_n+\mu_n$$

– We prove the gap (6.79) for $D^{(\Lambda)}_{Q_\infty}$ by taking the liminf. Thus, we can isolate the bottom of $\sigma\big(|A|\big)$ for $A=\widetilde{D}_{Q_n}$ or $A=D^{(\Lambda)}_{Q_\infty}$ by the same circle and get

$$|\psi_{e;n}\rangle\langle\psi_{e;n}|-\frac{1}{\|\psi_e\|^2_{L^2}}|\psi_e\rangle\langle\psi_e|=\frac{1}{2i\pi}\int_{\mathcal{C}_\varepsilon}\frac{dz}{z-\widetilde{D}_{Q_n}}\big(\alpha R[Q_\infty-Q_n]+2\eta_n\Gamma_n\big)\frac{1}{z-D^{(\Lambda)}_{Q_\infty}}.$$

By dominated convergence, this operator strongly converges to 0 : this proves

$$\|\psi_e\|_{L^2}=1.$$

Proof of (6.79) **and estimate on** $E_{1,1}$ This proof is based on the method of [Sok14b] : we know that

$$|m-\mu_n|\le K\alpha^2$$

and that

$$\widetilde{D}_{Q_n}\psi_{e;n}=\mu_n\psi_{e;n}. \tag{6.80}$$

In the following, we will get estimates on the Sobolev norms of $\psi_{e;n}$, this will enable us to estimate $\langle\widetilde{D}_{Q_n}\psi_{e;n}\,,\,\psi_{e;n}\rangle$. We will use estimates on g_0,g_1 written in (6.24).

Estimate on $\nabla\psi_{e;n}$ From (6.80) we have

$$\begin{aligned}\|\mathcal{D}^0\psi_{e;n}\|^2_{L^2}-m^2\le K\alpha^2+4\alpha\|Q_n\|_{\mathfrak{S}_2}\|\nabla\psi_{e;n}\|_{L^2}+4\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\\ +2\|\nabla\psi_{e;n}\|^2_{L^2}\big(\alpha\|Q_n\|^2_{\mathfrak{S}_2}+4\eta_n^2\|\Gamma_n\|^2_{\mathfrak{S}_2}\big)\end{aligned}$$

and $\|\nabla\psi_{e;n}\|^2_{L^2}\lesssim\alpha^2$. In the same way, for n sufficiently large, we can prove that

$$\langle\,|\nabla|^3\psi_{e;n}\,,\,\psi_{e;n}\rangle\lesssim\alpha^3.$$

We multiply (6.80) by $|\nabla|^{1/2}$ and take the L^2-norm. We can drop all terms with $2\eta_n\Gamma_n$ because all the operators that we consider are bounded in $\mathfrak{H}_\Lambda$ and $\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}$ tends to 0 as n tends to $+\infty$. We just have to deal with $|\nabla|^{1/2}R_{Q_n}\psi_{e;n}$. We recall that in Fourier space, the following holds [HLS05a]

$$\forall\,Q\in\mathfrak{S}_2(\mathfrak{H}_\Lambda),p,q\in\mathbb{R}^3,\ \mathscr{F}\big(R_Q;p,q\big)=\frac{1}{2\pi}\int_{\mathbb{R}^3}\frac{d\ell}{|\ell|^2}\widehat{Q}(p-\ell,q-\ell).$$

So, writing $\mathfrak{A}_n$ the operator whose Fourier transform is given by the integral kernel

$$\mathscr{F}\big(\mathfrak{A}_n;p,q\big):=|p-q|^{1/2}|\widehat{Q}(p,q)|,$$

we have

$$\Big|\mathscr{F}\big([|\nabla|^{1/2},R_{Q_n}]\big)\Big|\le\mathscr{F}\big(R_{\mathfrak{A}_n};p,q\big).$$

By Hardy's inequality, we have

$$\big|\big|[|\nabla|^{1/2},R_{Q_n}]\psi_{e;n}\big|\big|_{L^2}\le 4\|\,|\nabla|^{1/2}Q_n\|_{\mathfrak{S}_2}\|\nabla\psi_{e;n}\|_{L^2}\lesssim\alpha^{3/2}.$$

As

$$\|R_{Q_n}|\nabla|^{1/2}\psi_{e;n}\|_{L^2}\le\frac{\pi}{2}\|\,|\nabla|^{1/2}Q_n\|_{\mathfrak{S}_2}\|\nabla\psi_{e;n}\|_{L^2}\lesssim\alpha^{3/2},$$

we have $\|\,|\nabla|^{1/2}R_{Q_n}\psi_{e;n}\|_{L^2}\lesssim\alpha^{3/2}$ and

$$\langle\,|\nabla||\mathcal{D}^0|^2\psi_{e;n}\,,\,\psi_{e;n}\rangle-m^{\langle}|\nabla|\psi_{e;n}\,,\,\psi_{e;n}\rangle\lesssim\alpha^3. \tag{6.81}$$

Estimates on $\chi_{e;n}$ We scale (6.80) by α^{-1}, that is we consider

$$\underline{\psi_{e;n}}(x) := \alpha^{-3/2}\psi_{e;n}(\tfrac{x}{\alpha}),\ x \in \mathbb{R}^3.$$

This enables us to get an estimate of the lower spinor of $\psi_{e;n}$. We write

$$\psi_{e;n} =: \begin{pmatrix} \varphi_{e;n} \\ \chi_{e;n} \end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^2)^2$$

For short we also write

$$\mathbf{g}_1(p) := g_1(p)\tfrac{p}{|p|},\ p \in \mathbb{R}^3.$$

We write

$$\underline{Q_n}(x,y) := \alpha^{-3}\underline{Q_n}(\frac{x}{\alpha}, \frac{y}{\alpha}) \text{ and } \underline{\Gamma_n}(x,y) := \alpha^{-3}\underline{\Gamma_n}(\frac{x}{\alpha}, \frac{y}{\alpha}$$

The upper and lower spinors $\underline{\varphi_{e;n}}$ and $\underline{\chi_{e;n}}$ of $\underline{\psi_{e;n}}$ satisifies

$$\underline{\chi_{e;n}} = \frac{\mathbf{g}_1\big(\frac{-i\nabla}{\alpha}\big)\cdot\boldsymbol{\sigma}}{\alpha^2(\mu_n + g_0\big(\frac{)i\nabla}{\alpha}\big))}\underline{\varphi_{e;n}} + \big(-\alpha^2 R_{\underline{Q_n}}\underline{\psi_{e;n}} + 2\alpha\eta_n\underline{\Gamma_n}\underline{\psi_{e;n}}\big)_{\downarrow}. \tag{6.82}$$

By Hardy's inequality, we get that

$$\|\chi_{e;n}\|_{L^2} = \|\underline{\chi_{e;n}}\|_{L^2} \lesssim \alpha.$$

As there holds :

$$\langle -\Delta\chi_{e;n}\,,\,\chi_{e;n}\rangle \le \|\,|\nabla|^{3/2}\chi_{e;n}\|_{L^2}\sqrt{\|\chi_{e;n}\|_{L^2}\|\nabla\chi_{e;n}\|_{L^2}}$$

we also get the following (rough) estimate

$$\|\chi_{e;n}\|_{L^2} \lesssim \alpha^{4/3}.$$

Estimate on $E_{1,1}$ Using (6.24), we have (here $g_\star$ means $g_\star(-i\nabla)$)

$$\begin{aligned}
\langle \mathcal{D}^0\psi_{e;n}\,,\,\psi_{e;n}\rangle &= \langle g_0\psi_{e;n}\,,\,\psi_{e;n}\rangle + 2\mu_n\langle \tfrac{g_1^2}{(g_0+\mu_n)^2}\phi_{e;n}\,,\,\phi_{e;n}\rangle + \mathcal{O}\big(\alpha(\alpha^2 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2})\big)\\
&= \langle g_0\psi_{e;n}\,,\,\psi_{e;n}\rangle + 2m\langle \tfrac{g_1^2}{(g_0+m)^2}\phi_{e;n}\,,\,\phi_{e;n}\rangle + \mathcal{O}\big(\alpha^3\big),\\
&= m + \frac{g_1'(0)^2}{2m}\|\nabla\phi_{e;n}\|_{L^2}^2 + \mathcal{O}\big(\alpha^3\big).
\end{aligned}$$

As $\psi_{v;n} = \mathrm{C}\psi_{e;n}$, we have

$$\frac{1}{2}\iint \frac{|\psi_{e;n}\wedge\psi_{v;n}(x,y)|^2}{|x-y|}dxdy = D\big(|\varphi_{e;n}|^2, |\varphi_{e;n}|^2\big) + \mathcal{O}(\alpha^3).$$

Using (6.73), we finally get for n sufficiently large

$$\langle \widetilde{D}_{Q_n}\psi_{e;n}\,,\,\psi_{e;n}\rangle = m + \frac{g_1'(0)^2}{2m}\|\nabla\phi_{e;p}\|_{L^2}^2 - \alpha D\big(|\varphi_{e;n}|^2, |\varphi_{e;n}|^2\big) + \mathcal{O}(\alpha^3). \tag{6.83}$$

As $\|\varphi_{e;n}\|_{L^2}^2 = 1 - K\alpha^2$, we get

$$E_{1,1} \ge \mathcal{E}^0_{\mathrm{BDF}}(Q_\infty) = 2m + \frac{\alpha^2 m}{g_1'(0)^2}\mathcal{E}_{\mathrm{CP}}\big(\widetilde{\varphi_{e;n}}\big) + \mathcal{O}(\alpha^3),$$

where $\mathcal{E}_{\mathrm{CP}}$ denotes the Pekar energy [LL97] and $\widetilde{\varphi_{e;n}}$ is the scaling of $\varphi_{e;n}$ by $\frac{g_1'(0)^2}{\alpha m}$.

We already have an upper bound of $E_{1,1}$: it has the same expansion with $\mathcal{E}_{\mathrm{CP}}\big(\varphi_{e;n}\big)$ replaced by the smallest possible value E_{CP}. As there holds

$$\mathcal{E}_{\mathrm{CP}}\big(\underline{\varphi_{e;n}}\big) \ge (1 - \|\chi_{e;n}\|_{L^2}^2)^3 E_{\mathrm{CP}}$$

we thus have

$$\mathcal{E}_{\rm CP}\big(\underline{\varphi_{e;n}}\big) = E_{\rm CP} + \mathcal{O}(\alpha), \tag{6.84}$$

and

$$\mu_n = m + 2m\frac{\alpha^2}{g_1'(0)^2}E_{\rm CP} + \mathcal{O}(\alpha^3). \tag{6.85}$$

Thus $\mu_n < m$ for α sufficiently small. Are there other eigenvalues in $(0, m)$? As the Hessians are non-negative (see (6.68)), we have

$$\sigma\,|\widetilde{D}_{Q_n}| \subset [\mu_n - 2\eta_n, +\infty)$$

Let $\xi_n \perp \psi_n$ in Ran $\in (\boldsymbol{\pi}_+^n)$ and $s_n \in (\mu_n - 2\eta_n, m)$ such that

$$\widetilde{D}_{Q_n}\xi_n = s_n\xi_n.$$

By the same method as before used for $\psi_{e;n}$, we can prove the following :

$$\begin{array}{r|l} \|\nabla\xi_n\|_{L^2} \lesssim \alpha, & \|\,|\nabla|^{3/2}\xi_n\|_{L^2} \lesssim \alpha^{3/2}, \\ \|(\xi_n)_\downarrow\|_{L^2} \lesssim \alpha, & \|\nabla(\xi_n)_\downarrow\|_{L^2} \lesssim \alpha^{4/3}. \end{array}$$

The arrow $\downarrow$ means we take the lower spinor (which is in $L^2(\mathbb{R}^3, \mathbb{C}^2)$). In particular we have

$$s_n = \langle \widetilde{D}_{Q_n}\xi_n\,,\,\xi_n\rangle = m + \frac{g_1'(0)^2}{2m}\|\nabla\xi_n\|_{L^2}^2 - \alpha D(\xi_n^*\psi_{e;n};\xi_n^*\psi_{e;n}) + \mathcal{O}(\alpha^{8/3}).$$

Remark 6.13. We have lost $\alpha^{1/3}$ due to the rough estimate $\|\nabla(\xi_n)_\downarrow\|_{L^2} \lesssim \alpha^{4/3}$. We can prove that this quantity is of order α^2, but the proof is technical.

Estimate on $\underline{\psi_{e;n}}$ We know that $\underline{\psi_{e;n}}$ is close to a Pekar minimizer : its Pekar energy is

$$E_{CP} + \mathcal{O}(\alpha^{2/3}).$$

For α sufficiently small, we know that this gives information about the distance between $\underline{\psi_{e;n}}$ and the manifold $\mathscr{P}$ of Pekar minimizer [Len09] :

$$\mathrm{dist}_{H^1}(\underline{\psi_{e;n}}, \mathscr{P})^2 \le K\mathcal{E}_{\rm CP}(\underline{\psi_{e;n}}) - E_{\rm CP}.$$

The notation dist_{H^1} means the distance in the H^1-norm.

This result is stated in $L^2(\mathbb{R}^3, \mathbb{C})$, but it is not hard to prove it is also true in $L^2(\mathbb{R}^3, \mathbb{C}^4)$: in this case $\mathscr{P}$ is isomorphic to $\mathbb{R}^3 \times \mathbb{S}^3$ (and not simply to $\mathbb{R}^3 \times \mathbb{S}^1$).

If $\underline{\xi_n}$ denotes the scaling of ξ_n by $\frac{g_1'(0)^2}{2\alpha m}$, there holds

$$\frac{g_1'(0)^2}{2\alpha^2 m}(s_n - m) = \|\nabla\underline{\xi_n}\|_{L^2}^2 - D\big(\underline{\xi_n}^*\underline{\psi_{e;n}}, \underline{\xi_n}^*\underline{\psi_{e;n}}\big) + \mathcal{O}(\alpha^{2/3}). \tag{6.86}$$

Eventually by replacing $\underline{\psi_{e;n}}$ by its projection $\phi_{\rm CP}^n$ onto $\mathscr{P}$, we also have

$$\frac{g_1'(0)^2}{2\alpha^2 m}(s_n - m) = \|\nabla\underline{\xi_n}\|_{L^2}^2 - D\big(\underline{\xi_n}^*\phi_{\rm CP}^n, \underline{\xi_n}^*\phi_{\rm CP}^n\big) + \mathcal{O}(\alpha^{1/3}). \tag{6.87}$$

Proof of (6.79) We just have to study the spectrum of $\sigma(-\Delta - R\big(|\phi_{\rm CP}^n\rangle\langle\phi_{\rm CP}^n|\big))$, and precisely its negative eigenvalues. Its smallest eigenvalue is $E_{\rm CP}$ with eigenvector $\phi_{\rm CP}^n$. Now we seek the second smallest eigenvalue, that is

$$F_{\rm CP} := \inf\Big\{\langle\big(-\Delta - R\big(|\phi_{\rm CP}^n\rangle\langle\phi_{\rm CP}^n|\big)\big)f\,,\,f\rangle,\ f \perp \phi_{\rm CP}^n \in H^1,\ \|f\|_{L^2} = 1\Big\}. \tag{6.88}$$

By studying a minimizing sequence, we get

$$F_{\rm CP} > E_{\rm CP}. \tag{6.89}$$

By continuity the same holds for the spectrum of $-\Delta - R\big(|\underline{\psi_{e;n}}\rangle\langle\underline{\psi_{e;n}}|\big)$: for α sufficiently small (and n sufficiently big) its smallest eigenvalue t_n has multiplicity one and its second smallest eigenvalue $\widetilde{t_n}$ is away from t_n, uniformly in α (and n) :

$$\widetilde{t_n} - t_n > \frac{F_{\mathrm{CP}} - E_{\mathrm{CP}}}{2} > 0.$$

As a consequence, we get from (6.86) the following :

$$s_n - \mu_n \geq \frac{\alpha^2 m}{g_1'(0)^2}\big(F_{\mathrm{CP}} - E_{\mathrm{CP}}\big) + \mathcal{O}(\alpha^{7/3}), \tag{6.90}$$

and (6.79) holds.

6.3.4 Proof of Theorems 6.2 and 6.3

In fact, it suffices to follow the proof of Theorem 6.1 : instead of having an almost minimizer, we deal with a real minimizer $\overline{P} = \overline{Q} + \mathcal{P}^0_-$. Technically speaking, we just have to drop the term $\eta_n\Gamma_n$ in the equations and by the same method we prove the following.

1. There exist $0 < \mu < m$ and a wave function $\psi_e \in \mathfrak{H}_\Lambda$ such that

$$\begin{cases} \overline{P} = |\psi_e\rangle\langle\psi_e| - |\mathrm{C}\psi_e\rangle\langle\mathrm{C}\psi_e| + \chi_{(-\infty,0)}\big(\Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda\big), \\ \Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda\psi_e = \mu\psi_e. \end{cases} \tag{6.91}$$

2. We have $\|\,|\nabla|^3\psi_e\|_{L^2} \lesssim \alpha^{3/2}$. Splitting ψ_e into upper and lower spinors φ_e and χ_e, we have $\|\chi_e\|_{L^2} \lesssim \alpha$. We write $\widetilde{\varphi_e}(x) := \lambda^{3/2}\varphi_e(\lambda x)$ with $\lambda = \frac{g_1'(0)^2}{\alpha m}$. The following holds :

$$\begin{cases} E_{1,1} &= 2m + \frac{\alpha^2 m}{g_1'(0)^2}\mathcal{E}_{\mathrm{CP}}\big(\widetilde{\varphi_e}\big) + \mathcal{O}(\alpha^3) \\ &= 2m + \frac{\alpha^2 m}{g_1'(0)^2}\mathrm{E}_{\mathrm{CP}} + \mathcal{O}(\alpha^3), \\ \mu &= m + 2m\frac{\alpha^2}{g_1'(0)^2}E_{\mathrm{CP}} + \mathcal{O}(\alpha^3). \end{cases} \tag{6.92}$$

3. In the limit $\alpha \to 0$ we have

$$\lim_{\alpha\to 0}\|\chi_e\|_{L^2} = 0 \text{ and } \lim_{\alpha\to 0}\mathcal{E}_{\mathrm{CP}}\big(\widetilde{\varphi_e}\big) = \mathrm{E}_{\mathrm{CP}}.$$

The *geometrical* description of a minimizer of Theorem 6.2 has already been proved at the end of Subsection 6.3.2 under the assumption of existence.

6.4 Proofs on results on the variational set

6.4.1 On the manifold $\mathscr{M}$: Theorem 6.4, Propositions 6.1, 6.2

Proof of Theorem 6.4

– As Q is a compact self-adjoint operator, we apply the spectral theorem and write

$$Q = \sum_{i\in\mathbb{Z}^*}\mu_i|b_i\rangle\langle b_i|,$$

where $(\mu_i)_{i\in\mathbb{N}}$ (resp. $(\mu_i)_{i\in\mathbb{Z}^*_-}$) is the non-increasing sequence of positive eigenvalues of Q (resp. increasing sequence of negative eigenvalues).

It is clear that $-1 \leq Q \leq 1$. If $Q\psi = \psi$, then necessarily $P_1\psi = \psi$ and $P_0\psi = 0$, analogously if $Q\psi = -\psi$, then $P_1\psi = 0$ and $P_0\psi = \psi$.

Up to index translation we have :

$$A := Q - \Big\{\sum_{i=1}^{M_+}|a_i\rangle\langle a_i| - \sum_{i=1}^{M_-}|a_{-i}\rangle\langle a_{-i}|\Big\} = \sum_{i\in\mathbb{Z}^*}\mu_i|b_i\rangle\langle b_i| = A_p - A_n, \tag{6.93}$$

where A_p is the sum over positive i and $-A_n$ over negative i.

Notation 6.9. For short, for any $\mu \in \mathbb{R}$ and any self-adjoint operator S, we write $E^S_\mu = \mathrm{Ker}(S-\mu)$ the spectral subspace of S.

Furthermore, for an operator B we write

$$B^{\varepsilon_1\ \varepsilon_2} = P_0(\varepsilon_1) B P_0(\varepsilon_2),\ \varepsilon_i = \pm,\ P_0(-) = P_0,\ P_0(+) = 1 - P_0.$$

– We know that

$$Q^{++} - Q^{--} = Q^2 = \sum_{i=1}^{M_+} |a_i\rangle\langle a_i| + \sum_{i=1}^{M_-} |a_{-i}\rangle\langle a_{-i}| + \sum_{i\in\mathbb{Z}^*} \mu_i^2 |b_i\rangle\langle b_i|.$$

In particular $[Q^2, P_0] = 0$ and all the spectral subspaces of Q^2 are P_0-invariant. For any $\mu > 0$,

$$E^{Q^2}_{\mu^2} = E^Q_\mu \overset{\perp}{\oplus} E^Q_{-\mu} = E^{Q^{++}}_{\mu^2} \overset{\perp}{\oplus} E^{Q^{--}}_{-\mu^2}.$$

For $i \in \mathbb{N}$, let c_i be a unitary eigenvector for Q^{++} with eigenvalue $0 < \mu_i^2 < 1$. We write

$$c_i = c_p + c_n,\ c_p \in \mathrm{Ran}(A_p),\ c_n \in \mathrm{Ran}(A_n).$$

We have $A_p c_p = \mu_i c_p$ and $A_n c_n = -\mu_i c_n$. Moreover $c_n \neq 0$, otherwise $(1-P_0)c_p = c_p$ and

$$A c_p = \mu_i c_p = ((1-P_0) - (1-P_1))c_p \ i.e.\ (1-P_1)c_p = (1-\mu_i)c_p.$$

This would give $\mu_i = 1$ or $\mu_i = 0$. By the same argument $c_p \neq 0$. We have $P_0 c_p = -P_0 c_n$ and this vector is non-zero, otherwise $(1-P_0)c_p = c_p$. Thus the two-dimensional plane $\Pi = \mathrm{Span}(c_p, c_n)$ is in $E^{Q^2}_{\mu_i^2}$ and there exists an orthonormal basis $(e_+ = c_i, e_-)$ of Π such that $P_0 e_- = e_-$ (and $(1-P_0)c_i = c_i$).

We write $c_p = ||c_p|| d_p$ and $c_n = ||c_n|| d_n$ and up to a phase, we have :

$$c_i = \cos(\phi) d_p + \sin(\phi) d_n.$$

There holds :

$$Q^2 c_i = \mu_i^2 c_i = A_p c_i = \mu_i (1-P_0)(\cos(\phi) d_p + \sin(\phi) d_n) = \mu_i(\cos(\phi)^2 - \sin(\phi)^2) c_i,$$

and $\mu_i = \cos(2\phi)$. We have

$$E^{Q^2}_{\mu_i^2} = \Pi \overset{\perp}{\oplus} R.$$

– By induction over the dimension of the remainder $\mathrm{Dim}(R \cap E^{Q^{++}}_{\mu_i^2})$, we can decompose $E^{Q^2}_{\mu_i^2}$ as a sum of orthogonal planes : by symmetry there holds $\mathrm{Dim}\, E^{Q^{++}}_{\mu_i^2} = \mathrm{Dim}\, E^{Q^{--}}_{\mu_i^2}$. Each plane Π is invariant under the action of Q and $\mathcal{P}^0_-$ and so also under that $P = Q + \mathcal{P}^0_-$. Therefore, there also exists an orthonormal basis (v_+, v_-) of Π such that $P_1 v_- = v_-$ and $(1-P_1)v_+ = v_+$. Up to a phase we suppose that

$$v_- = \cos(\theta) e_- + \sin(\theta) e_+ \text{ and } v_+ = -\sin(\theta) e_- + \cos(\theta) e_+,\ \theta \in (0, \tfrac{\pi}{2}). \tag{6.94}$$

In the plane Π we thus have :

$$Q|_\Pi = |v_-\rangle\langle v_-| - |e_-\rangle\langle e_-|.$$

Such an operator has eigenvalues $\pm\sin(\theta)$ with eigenvectors

$$\begin{cases} f_+ = \sqrt{\frac{1-\sin(\theta)}{2}} e_- + \sqrt{\frac{1+\sin(\theta)}{2}} e_+ & \text{associated to } \sin(\theta), \\ f_- = -\sqrt{\frac{1+\sin(\theta)}{2}} e_- + \sqrt{\frac{1-\sin(\theta)}{2}} e_+ & \text{associated to } -\sin(\theta) \end{cases} \tag{6.95}$$

□

Proof of Proposition 6.1 In general, let P_1 and P_2 be two orthogonal projectors in $\mathfrak{H}_\Lambda$. If $P_2 = U P_1 U^{-1}$ where U is a unitary operator, we have :

$$P_2 - P_1 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \iff [U, P_1]U^{-1} \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\ i.e.\ [U, P_1] \in \mathfrak{S}_2(\mathfrak{H}_\Lambda). \tag{6.96}$$

– For any $P_1 \in \mathscr{M}$ and any $P_2 \in \mathscr{M}$ with $\|P_1 - P_2\|_{\mathcal{B}} < 1$, we can decompose $P_2 - P_1$ as in Theorem 6.4 but with P_1 as new reference (the decomposition is the same but with $e_j \in \mathrm{Ran}\,(1-P_1)$ and $e_{-j} \in \mathrm{Ran}\,P_1$) :

$$\begin{cases} P_2 - P_1 = \sum_{j\in\mathbb{N}} (|v_{-j}\rangle\langle v_{-j}| - |e_{-j}\rangle\langle e_{-j}|),\ v_{-j} = \cos(\theta_j)e_{-j} + \sin(\theta_j)e_j \\ P_2 v_{-j} = v_{-j},\ P_1 e_{-j} = e_{-j}, P_1 e_j = 0 \text{ and } \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 < +\infty. \end{cases}$$

Above we have $\theta_j \in (0, \frac{\pi}{2})$ for all $j \in \mathbb{N}$. Let A be defined as follows :

$$A = \sum_{j\in\mathbb{N}} \theta_j (|e_j\rangle\langle e_{-j}| - |e_{-j}\rangle\langle e_j|),\ \theta_j \in (0, \tfrac{\pi}{2}),$$

then we have $P_2 = e^A P_1 e^{-A}$, $A^* = -A$ and

$$[A, P_1] = \sum_{j\in\mathbb{N}} \theta_j (|e_j\rangle\langle e_{-j}| + |e_{-j}\rangle\langle e_j|) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda). \tag{6.97}$$

Furthermore $[\exp(A), P_1] \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$: for all $k \in \mathbb{N}$, there holds :

$$[A^k, P_1] = \sum_{j=0}^{k-1} A^j [A, P_1] A^{k-1-j},$$

and

$$\|[\exp(A), P_1]\|_{\mathfrak{S}_2} \le \sum_{k=1}^{+\infty} \frac{1}{k!} \big\{ k \|[A, P_1]\|_{\mathfrak{S}_2} \|A\|_{\mathcal{B}}^{k-1} \big\} = \|[A, P_1]\|_{\mathfrak{S}_2} \exp \|A\|_{\mathcal{B}}. \tag{6.98}$$

Let us call this A the *canonical* antiunitary operator $L_{P_1}(P_2)$ associated to P_2 : we will see it does not depend on the choice of eigenvectors e_j.

Remark 6.14. In the case $\|P_2 - P_1\|_{\mathcal{B}} = 1$, we have $1, -1 \in \sigma(P_2 - P_1)$: indeed $P_2 - P_1$ may be decomposed as in (6.93) with $M_+ = M_-$ because $\mathrm{Tr}(P_2 - P_1) = 0$.

We still have $P_2 = e^A P_1 e^{-A}$ with

$$A = \sum_{i=1}^{M_+} \frac{\pi}{2} \Big(|a_i\rangle\langle a_{-i}| - |a_{-i}\rangle\langle a_i| \Big) + \sum_{j\ge1} \theta_j \Big(|e_j\rangle\langle e_{-j}| - |e_{-j}\rangle\langle e_j| \Big), \tag{6.99}$$

where $a_i, e_j \in \mathrm{Ran}(1 - P_1)$ and $a_{-i}, e_{-j} \in \mathrm{Ran}\,P_1$ form an orthonormal family as in the decomposition of Theorem 6.4 (in particular the non-zero eigenvalues in $(-1,1)$ are the $\pm\sin(\theta_i)$).

– Let $(\mathfrak{m}_{P_1}, \|\cdot\|_{\mathfrak{S}_2})$ be the set of compact operators :

$$\mathfrak{m}_{P_1} := \{ a \in \mathcal{B}(\mathfrak{H}_\Lambda),\ ((1-P_1)aP_1)^* = -P_1 a(1-P_1) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ (1-P_1)a(1-P_1) = P_1 P_1 = 0\}.$$

Remark 6.15. As we consider operators in $\mathcal{B}(\mathfrak{H}_\Lambda)$ we can replace 1 by Π_Λ in the definition.

The map Φ_{P_1}

$$\Phi_{P_1} : \begin{array}{ccc} (\mathfrak{m}_{P_1}, 0) & \longrightarrow & (\mathscr{M}, P_1) \\ a & \mapsto & e^a P_1 e^{-a} \end{array} \tag{6.100}$$

is differentiable and we have :

$$\forall A \in \mathfrak{m}_{P_1},\ \mathrm{d}\Phi_{P_1}(P_1) \cdot A = [A, P_1].$$

This map

$$\mathrm{d}\Phi_{P_1} : \mathfrak{m}_{P_1} \to \{[A, P_1],\ A \in \mathfrak{m}_{P_1}\} =: \mathrm{Ran}(\mathrm{d}\Phi_{P_1})$$

is invertible with inverse

$$\mathrm{d}\Phi_{P_1}^{-1} : v \in \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \mapsto [v, P_1] \in \mathfrak{m}_{P_1}.$$

This proves that in a neighbourhood of P_1, the corresponding part of $\mathscr{M}$ is the graph of some function $\mathcal{F}_{P_1}$.

Indeed, if we see the set

$$\mathcal{P}^0_- + \mathfrak{S}_2(\mathfrak{H}_\Lambda) = P_1 + \mathfrak{S}_2(\mathfrak{H}_\Lambda)$$

as an affine space with associated vector space $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$, then we have

$$\mathfrak{S}_2(\mathfrak{H}_\Lambda) = \mathfrak{m}_{P_1} \overset{\perp}{\oplus} \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \overset{\perp}{\oplus} \{u \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ P_1 u(1-P_1) = (1-P_1)uP_1 = 0\}.$$

We decompose any $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ with respect to $\mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \oplus (\mathrm{Ran}(\mathrm{d}\Phi_{P_1}))^\perp$:

$$Q = v[P_1;Q] + w[P_1;Q] \in \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \oplus (\mathrm{Ran}(\mathrm{d}\Phi_{P_1}))^\perp.$$

In a neighbourhood $\mathcal{V}_{P_1}$ of P_1, the set $\mathcal{V}_{P_1} \cap \mathscr{M}$ is a portion of the graph of

$$\mathcal{F}_{P_1} : v \in \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \mapsto P_1 + w\big[P_1; e^{[v,P_1]} P_1 e^{-[v,P_1]} - P_1\big] \in P_1 + (\mathrm{Ran}\,\mathrm{d}\Phi_{P_1})^\perp.$$

– Thus for any $P_1 \in \mathscr{M}$, there exists a neighbourhood $\mathcal{V}_{P_1} \ni P_1$ such that $\mathscr{M} \cap \mathcal{V}_{P_1}$ is a manifold with $\mathrm{T}_{P_1}\mathscr{M} = \mathrm{Ran}(\mathrm{d}\Phi_{P_1})$. To conclude $\mathscr{M}$ is a proper manifold, it suffices to compare the neighbourhood of $\mathscr{M}$ (or prove that $\mathscr{M}$ is connected) : for $P_1, P_3 \in \mathscr{M}$, we use Remark 6.14 and write $P_3 = e^A P_1 e^{-A}$ with $A \in \mathfrak{m}_{P_1}$. Then it is clear that the map

$$\mathfrak{T}(P_1,P_3) : \begin{array}{ccc} (\mathscr{M}, P_1) & \longrightarrow & (\mathscr{M}, P_3) \\ P & \mapsto & e^A P e^{-A} \end{array}$$

is an isometry and that its differential $\mathfrak{t}(P_1,P_3)$ is an isometry that maps $\mathrm{T}_{P_1}\mathscr{M}$ onto $\mathrm{T}_{P_3}\mathscr{M}$. The map $t \in [0,1] \mapsto e^{tA} P_1 e^{-tA} \in \mathscr{M}$ links P_1 and P_3.

Moreover the map

$$L_{P_1} : \begin{array}{ccc} \{P \in \mathscr{M},\ \|P - P_1\|_{\mathcal{B}} < 1\} & \longrightarrow & \mathfrak{m}_{P_1} \\ P & \mapsto & A \end{array}$$

is locally invertible around P_1 with (local) inverse Φ_{P_1}.

More generally, we can prove that the restriction of Φ_{P_1} to the $a \in \mathfrak{m}_{P_1}$ with $\|a\|_{\mathcal{B}} < \frac{\pi}{2}$ is one-to-one : it suffices to consider the spectral decomposition of a and link spectral subspaces with rotations.

□

Proof of proposition 6.2

Remark 6.16. 1. We recall that if P_1 and P_2 are two projectors such that $P_1 - P_2$ is Hilbert-Schmidt, then

$$A \in \mathfrak{S}_1^{P_1} \iff A \in \mathfrak{S}_1^{P_2} \text{ and } \mathrm{Tr}_{P_1}(A) = \mathrm{Tr}_{P_2}(A). \tag{6.101}$$

2. For any $A \in \mathcal{B}$ and any projector P we have :

$$[[A,P],P] = (1-P)AP + PA(1-P). \tag{6.102}$$

If we restrict $\mathcal{E}_{\mathrm{BDF}}$ to $\mathscr{M}$, using (6.101) and (6.102) we get that for $(P,v) \in \mathrm{T}\mathscr{M}$:

$$\mathrm{d}\mathcal{E}^0_{\mathrm{BDF}}(P) \cdot v = \mathrm{Tr}_P(\Pi_\Lambda D_{P-\mathcal{P}^0_-} \Pi_\Lambda v) = \mathrm{Tr}_P\big([[\Pi_\Lambda D_{P-\mathcal{P}^0_-}\Pi_\Lambda, P], P] v\big). \tag{6.103}$$

We write $Q = P - \mathcal{P}^0_-$, $\boldsymbol{\pi} = \chi_{(-\infty,0)}(\Pi_\Lambda D_Q \Pi_\Lambda)$ and $\Gamma = P - \boldsymbol{\pi}$. We have :

$$\begin{aligned} P\Pi_\Lambda D_Q \Pi_\Lambda (1-P) &= (\boldsymbol{\pi} + \Gamma)\Pi_\Lambda D_Q \Pi_\Lambda (1 - \boldsymbol{\pi} - \Gamma), \\ &= \boldsymbol{\pi} - \Pi_\Lambda D_Q \Pi_\Lambda \Gamma + \Gamma \Pi_\Lambda D_Q \Pi_\Lambda (1-\boldsymbol{\pi}) - \Gamma \Pi_\Lambda D_Q \Pi_\Lambda \Gamma. \end{aligned}$$

Thus

$$[[\Pi_\Lambda D_Q \Pi_\Lambda, P], P] = |\Pi_\Lambda D_Q \Pi_\Lambda|\Gamma + \Gamma|\Pi_\Lambda D_Q \Pi_\Lambda| - 2\Gamma \Pi_\Lambda D_Q \Pi_\Lambda \Gamma. \tag{6.104}$$

We have :

$$\begin{aligned} |\Pi_\Lambda D_Q \Pi_\Lambda|^2 &= \Pi_\Lambda (\mathcal{D}^0)^2 + \alpha\big(\Pi_\Lambda B_Q \Pi_\Lambda \mathcal{D}^0 + \mathcal{D}^0 \Pi_\Lambda B_Q \Pi_\Lambda\big) + \alpha^2 (\Pi_\Lambda B_Q \Pi_\Lambda)^2 \\ &\le \Pi_\Lambda (\mathcal{D}^0)^2 \Big(1 + \alpha \|\Pi_\Lambda B_Q \Pi_\Lambda \mathrm{inv}(\mathcal{D}^0)\|_{\mathcal{B}}\Big)^2, \\ &\le \Pi_\Lambda (\mathcal{D}^0)^2 \Big(1 + \alpha K \|V_Q \tfrac{\Pi_\Lambda}{\sqrt{1-\Delta}}\|_{\mathcal{B}} + \|R_Q \tfrac{\Pi_\Lambda}{\sqrt{1-\Delta}}\|_{\mathcal{B}}\Big)^2. \end{aligned}$$

We have $\Gamma = (P - \mathcal{P}^0_-) + (\mathcal{P}^0_- - \boldsymbol{\pi}) \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$. So the following holds :

$$\big|\big|\,|\Pi_\Lambda D_Q \Pi_\Lambda|\Gamma\big|\big|_{\mathfrak{S}_2} \lesssim E(\Lambda)^{1/2} \|\,|\mathcal{D}^0|^{1/2}\Gamma\|_{\mathfrak{S}_2}(1+\alpha(\sqrt{D(\rho_Q,\rho_Q)} + \||\mathcal{D}^0|^{1/2}Q\|_{\mathfrak{S}_2}))^2,$$

and

$$\|\Gamma\Pi_\Lambda D_Q \Pi_\Lambda \Gamma\|_{\mathfrak{S}_2} \leq 2\big|\big|\,|\Pi_\Lambda D_Q \Pi_\Lambda|^{1/2}\Gamma\big|\big|^2_{\mathfrak{S}_2} < +\infty.$$

□

6.4.2 On the manifold $\mathscr{M}_{\mathscr{C}}$: Propositions 6.3, 6.4 and 6.5

Proof of Proposition 6.3

Let $P_1, P_2 \in \mathscr{M}_{\mathscr{C}}$ such that $\|P_2 - P_1\|_{\mathcal{B}} < 1$. Thanks to Theorem 6.4, we know that P_2 can be written as $P_2 = e^A P_1 e^{-A}$ where $A \in \mathcal{B}(\mathfrak{H}_\Lambda)$ is antiunitary and

$$P_1 A P_1 = (1-P_1)A(1-P_1).$$

– Taking into account the C-symmetry we can say more : thanks to (6.15) we can follow the proof of Proposition 6.5 with $\mathcal{P}^0_-$ replaced by P_1. This gives

$$\mathrm{C}A\mathrm{C} = A. \tag{6.105}$$

Indeed there exist $\mathcal{J} \subset \mathbb{Z}^*$ with $-\mathcal{J} = \mathcal{J}$ and $(e_j)_{j\in J}$ in $\mathfrak{H}_\Lambda^{\mathcal{J}}$ such that

1. $(e_j)_j \cup (Ce_j)_j$ is an orthonormal basis for $\mathrm{Ran}(P_2 - P_1)$,
2. for all $j \in \mathcal{J}$, $j > 0$: $P_1 e_j = 0$ and $P_1 e_{-j} = e_{-j}$,
3. each 4-dimensional space $\mathrm{Span}(e_j, e_{-j}, \mathrm{C}e_j, \mathrm{C}e_{-j})$ is spanned by four eigenvectors $f_j \perp \mathrm{C}f_{-j}$ with eigenvalue $\sin(\theta_i) > 0$ and $f_{-j} \perp \mathrm{C}f_j$ with eigenvalue $-\sin(\theta_i)$.

Then A is defined as follows :

$$A = \sum_{j\in\mathcal{J}} \theta_j \Big(|e_j\rangle\langle e_{-j}| - |e_{-j}\rangle\langle e_j| - |\mathrm{C}e_{-j}\rangle\langle \mathrm{C}e_j| + |\mathrm{C}e_j\rangle\langle \mathrm{C}e_{-j}|\Big)$$

It is easy to check (6.105) from this formula. Reciprocally, let $A \in \mathfrak{m}_P$ be an antiunitary map satisfying (6.105). Then we know that $e^A P e^{-A} \in \mathscr{M}$. Moreover we have $-\mathrm{C}e^A\mathrm{C} = -e^A$. It follows that

$$\begin{aligned} -\mathrm{C}(e^A P e^{-A} - P)\mathrm{C} &= \mathrm{C}e^A\mathrm{C}(-\mathrm{C}P\mathrm{C})\mathrm{C}e^{-A}\mathrm{C} + \mathrm{C}P\mathrm{C}, \\ &= e^A(-(\Pi_\Lambda - P))e^{-A} + (\Pi_\Lambda - P), \\ &= -\Pi_\Lambda + e^A P e^{-A} + \Pi_\Lambda - P = e^A P e^{-A} - P. \end{aligned}$$

In other words $e^A P e^{-A} \in \mathscr{M}_{\mathscr{C}}$. Thus Φ_{P_1} (*cf* (6.100)) is a local isomorphism from $(\mathfrak{m}_{P_1}, 0)$ to $(\mathscr{M}, P_1)$, and its restriction

$$\Phi^{\mathscr{C}}_{P_1} : \begin{array}{ccc} \mathfrak{m}^{\mathscr{C}}_{P_1} & \longrightarrow & \mathscr{M}_{\mathscr{C}} \\ a & \mapsto & e^a P_1 e^{-a} \end{array}$$

is well-defined and is a local isomorphism from $(\mathfrak{m}^{\mathscr{C}}_{P_1}, 0)$ to $(\mathscr{M}_{\mathscr{C}}, P)$. There remains to prove that for any $P_1, P_2 \in \mathscr{M}_{\mathscr{C}}$, there exists an isometry of $\mathfrak{S}_2$, that maps $\mathfrak{m}^{\mathscr{C}}_{P_1}$ onto $\mathfrak{m}^{\mathscr{C}}_{P_2}$. If $\|P_1 - P_2\|_{\mathcal{B}} < 1$, this isometry is given by

$$\phi^0_{\mathscr{C}}(P_1, P_2) : X \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \mapsto \exp(L_{P_1}(P_2))\, X \exp(-L_{P_1}(P_2)) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda).$$

The restriction is :

$$\phi_{\mathscr{C}}(P_1, P_2) : X \in \mathfrak{m}^{\mathscr{C}}_{P_1} \mapsto \exp(L_{P_1}(P_2))\, a \exp(-L_{P_1}(P_2)),$$

indeed, as $\mathrm{C}L_{P_1}(P_2)\mathrm{C} = L_{P_1}(P_2)$ we have $\mathrm{C}\phi_{\mathscr{C}}(P_1, P_2; a)\mathrm{C} = \phi_{\mathscr{C}}(P_1, P_2; a)$. If $\|P_1 - P_2\|_{\mathcal{B}} = 1$ then we can write

$$P_2 - P_1 = \sum_{k=1}^K \big(|a_k\rangle\langle a_k| - |\mathrm{C}a_k\rangle\langle \mathrm{C}a_k|\big) + \gamma(P_1, P_2),$$

where $(a_k)_k \cup (\mathrm{C}a_k)_k$ is an orthonormal family which is orthogonal to $\mathrm{Ran}\,\gamma(P_1,P_2)$ and $\|\gamma(P_1,P_2)\|_{\mathcal{B}} < 1$. We also have $P_1\mathrm{C}a_k = \mathrm{C}a_k$ and $P_1 a_k = 0$. We define

$$\begin{cases} P_{12} & := & P_1 + \displaystyle\sum_{k=1}^{K} \big(|a_k\rangle\langle a_k| - |\mathrm{C}a_k\rangle\langle \mathrm{C}a_k|\big) \in \mathscr{M}_{\mathscr{C}}, \\ U_{12} & := & \displaystyle\sum_{k=1}^{K} \big(|\mathrm{C}a_k\rangle |a_k\rangle - |a_k\rangle\langle \mathrm{C}a_k|\big) \in \mathbf{U}(\mathfrak{H}_\Lambda). \end{cases}$$

Then $\|P_2 - P_{12}\|_{\mathcal{B}} < 1$ and $U_{12}P_1U_{12}^* = -U_{12}P_1U_{12} = P_{12}$. Moreover

$$\phi_{\mathscr{C},P_1,P_{12}} : \begin{array}{ccc} \mathfrak{m}^{\mathscr{C}}_{P_1} & \longrightarrow & \mathfrak{m}^{\mathscr{C}}_{P_{12}} \\ a & \mapsto & U_{12}aU_{12}^{-1} \end{array}$$

is well-defined and is an isometry. Indeed, as $\mathrm{C}U_{12}\mathrm{C} = -U_{12}$, we get that

$$\mathrm{C}U_{12}aU_{12}^{-1}\mathrm{C} = U_{12}aU_{12}^{-1}.$$

This proves the isometric isomorphisms

$$\left| \begin{array}{ccccc} \mathfrak{S}_2(\mathfrak{H}_\Lambda) & \xrightarrow[\phi^0_{\mathscr{C}}(P_1,P_{12})]{\simeq} & \mathfrak{S}_2(\mathfrak{H}_\Lambda) & \xrightarrow[\phi^0_{\mathscr{C}}(P_{12},P_2)]{\simeq} & \mathfrak{S}_2(\mathfrak{H}_\Lambda), \\ \mathfrak{m}^{\mathscr{C}}_{P_1} & \xrightarrow[\phi_{\mathscr{C}}(P_1,P_{12})]{\simeq} & \mathfrak{m}^{\mathscr{C}}_{P_{12}} & \xrightarrow[\phi_{\mathscr{C}}(P_{12},P_2)]{\simeq} & \mathfrak{m}^{\mathscr{C}}_{P_2}. \end{array} \right.$$

So $\mathscr{M}_{\mathscr{C}}$ is a submanifold and the characterization of the tangent planes (6.39) follows from that of $\mathscr{M}$.

– Let us show that $\mathscr{M}_{\mathscr{C}}$ is invariant under the flow of $\mathcal{E}^0_{\mathrm{BDF}}$: it suffices to show that for any $P \in \mathscr{M}_{\mathscr{C}}$, the gradient $\nabla\mathcal{E}^0_{\mathrm{BDF}}(P)$ (*cf* (6.37)) is in $\mathrm{T}_P\mathscr{M}_{\mathscr{C}}$. For a C-symmetric state P, we write $Q := P - \mathcal{P}^0_-$.

That the density ρ_Q vanishes is clear from (6.107) and the fact that for any $\psi \in \mathfrak{H}_\Lambda$ and $x \in \mathbb{R}^3$ we have $|\mathrm{C}\psi(x)|^2 = |\psi(x)|^2$. From (6.4), we get that for $-\mathrm{C}Q\mathrm{C} = Q$ there holds :

$$-\mathrm{C}Q\mathrm{C}(x,y) = Q(x,y) \text{ so } -\mathrm{C}R_Q\mathrm{C}(x,y) = R_Q(x,y) = \frac{Q(x,y)}{|x-y|}.$$

As $-\mathrm{C}\mathcal{D}^0\mathrm{C} = \mathcal{D}^0$, it follows that :

$$-\mathrm{C}\big(\mathcal{D}^0 + \alpha(\rho_Q * \tfrac{1}{|\cdot|} - R_Q)\big)\mathrm{C} = -\mathrm{C}(\mathcal{D}^0 - \alpha R_Q)\mathrm{C} = \mathcal{D}^0 - \alpha R_Q. \tag{6.106}$$

We remark that $[\Pi_\Lambda, \mathrm{C}] = 0$, and $\mathrm{C}P\mathrm{C} = 1 - P$ and $\mathrm{C}(1-P)\mathrm{C} = P$. Thus

$$\begin{aligned} -\mathrm{C}\big[[\Pi_\Lambda D_Q \Pi_\Lambda; P]; P\big]\mathrm{C} &= -\mathrm{C}\big(P\Pi_\Lambda D_Q\Pi_\Lambda(1-P) + (1-P)\Pi_\Lambda D_Q \Pi_\Lambda P\big)\mathrm{C} \\ &= (1-P)\big(-\Pi_\Lambda \mathrm{C}D_Q\mathrm{C}\Pi_\Lambda\big)P + P\big(-\Pi_\Lambda\mathrm{C}D_Q\mathrm{C}\Pi_\Lambda\big)(1-P) \\ &= (1-P)\Pi_\Lambda D_Q\Pi_\Lambda P + P\Pi_\Lambda D_Q \Pi_\Lambda(1-P) \\ &= \big[[\Pi_\Lambda D_Q\Pi_\Lambda; P]; P\big]. \end{aligned}$$

Proof of Proposition 6.4 Let $c : t \in [0,1] \mapsto c(t) \in \mathscr{M}_{\mathscr{C}}$ be a continuous map such that $c(0) = 0$ and $\|c(1)\|_{\mathcal{B}} = 1$. By Theorem 6.4 and Proposition 6.5, any $c(t)$ has the following form :

$$\begin{aligned} c(t) = &\sum_{j\in\mathbb{N}} \lambda_j(|f_j(t)\rangle\langle f_j(t)| - |f_{-j}(t)\rangle\langle f_{-j}(t)| + |\mathrm{C}f_{-j}(t)\rangle\langle\mathrm{C}f_{-j}(t)| - |\mathrm{C}f_j(t)\rangle\langle f_j(t)|) \\ &+ \sum_{j=1}^{N(t)} (|a_j(t)\rangle\langle a_j(t)| - |\mathrm{C}a_j(t)\rangle\langle\mathrm{C}a_j(t)|), \end{aligned}$$

where $(a_j)_j \cup (\mathrm{C}a_j)_j \cup (f_j)_j \cup (\mathrm{C}f_j)$ is an orthonormal family and $(\lambda_j)_j$ is the sequence of positive eigenvalues lesser than 1. Each plane $\mathrm{Span}(f_j, f_{-j})$ (resp. $\mathrm{Span}(\mathrm{C}f_j, \mathrm{C}f_{-j})$) is spanned by $e_j \in \mathrm{Ran}(\mathcal{P}^0_+)$ and $e_{-j} \in \mathrm{Ran}(\mathcal{P}^0_-)$ (resp. $\mathrm{C}e_{-j} \in \mathrm{Ran}(\mathcal{P}^0_+)$ and $\mathrm{C}e_j \in \mathrm{Ran}(\mathcal{P}^0_-)$).

Let t_0 be $\inf\{t \in [0,1],\ \|c(t)\|_{\mathcal{B}} = 1\}$. For any $t \in [0,1]$ and any $\mu \in \sigma(c(t))\backslash\{1,0\},\ 4\,|\ \mathrm{Dim}\, E_{\mu^2}^{c(t)^2}$. In particular, for $t < t_0$ the number

$$J(c(t)) = \mathrm{Dim} \bigoplus_{\frac{1}{2}<\mu\leq 1} E_{\mu^2}^{c(t)^2} \text{ is divisible by 4.}$$

By continuity, $J(c(t))$ is divisible by 4 for any t : the variations of J follow the variations of the λ_i's (λ_i equals $\sin(\widehat{\mathbb{C}v_j, \mathbb{C}e_j})$ in the notations of Theorem 6.4). Such an eigenvalue is associated to 4-dimensional spaces of type $\mathrm{Span}(f_j, f_{-j}, \mathrm{C}f_j, \mathrm{C}f_{-j})$ and each of them has a basis made of four eigenvectors in $E_{\lambda_i^2}^{c(t)^2}$.

Thus $4\,|\ J(c(1))$ and for any unitary $\psi \in \mathrm{Ran}\,\mathcal{P}_+^0$, there is no continuous path in $\mathscr{M}_{\mathscr{C}}$ that links 0 and $Q_\psi = |\psi\rangle\langle\psi| - |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|$. It is then straightforward to prove that for any $\gamma \in \mathscr{M}_{\mathscr{C}}$, if $4\,|\ J(\gamma)$ then there exists a path that links 0 and γ else there exists a path that links Q_ψ and γ. □

Proof of Proposition 6.5

A direct computation shows that for any $\psi \in L^2$:

$$\mathrm{C}|\psi\rangle\langle\psi|\mathrm{C} = |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|. \tag{6.107}$$

By Theorem 6.4, for $\mu \in \sigma(\gamma) \cap (0,1)$, there exist $N \in \mathbb{N}$ and N orthogonal planes $\Pi_\mu^1, \ldots \Pi_\mu^N$ such that

$$E_{\mu^2}^{\gamma^2} = E_\mu^\gamma \overset{\perp}{\oplus} E_{-\mu}^\gamma = \bigoplus_{1\leq j\leq N} \Pi_\mu^j,$$

where each plane is γ-invariant with $\gamma|_{\Pi_\mu} = |v_-\rangle\langle v_-| - |e_-\rangle\langle e_-|$ with $Pv_= v_-$ and $\mathcal{P}_-^0 e_- = e_-$. The expression of its eigenvectors f_+ and f_- are written in (6.95), where $e_+ \in \mathrm{Ran}\,\mathcal{P}_+^0$ is chosen such that $v_- = \cos(\theta)e_- + \sin(\theta)e_+$.

As C is *isometric*, then necessarily $E_{\mu^2}^{\gamma^2}$ is C-invariant, and $\mathrm{C}\Pi_\mu^j$ is some plane $\widetilde{\Pi}_\mu^j$ in $E_{\mu^2}^{\gamma^2}$, γ-*invariant* (there holds $\mu = \sin(\widehat{\mathbb{C}v_-, \mathbb{C}e_-})$). Let us show that $\Pi_\mu^j \neq \widetilde{\Pi}_\mu^j$. Indeed, using (6.95) this would imply that $\mathrm{C}e_- = e^{i\phi_1}e_+$ and $\mathrm{C}e_+ = e^{i\phi_2}e_-$ for some $\phi_1, \phi_2 \in \mathbb{R}$ and

$$-(|\mathrm{C}e_-\rangle\langle\mathrm{C}e_+| + |\mathrm{C}e_+\rangle\langle\mathrm{C}e_-|) = |e_-\rangle\langle e_+| + |e_+\rangle\langle e_-|.$$

In particular there would hold $-e^{i(\phi_1-\phi_2)} = 1$ that is $\phi_1 - \phi_2 \equiv \pi[2\pi]$. However C is an involution so $\mathrm{C}^2 e_+ = e_+$ and $e^{i(\phi_1-\phi_2)}e_+ = e_+$: this gives $\phi_1 - \phi_2 \equiv 0[2\pi]$ and contradicts the previous result.

Thus the two planes are different and the 4-dimensional space V_μ they span is C and γ-invariant : $E_{\mu^2}^{\gamma^2} = V_\mu \overset{\perp}{\oplus} W_\mu$. By induction over $\mathrm{Dim}\, W_\mu$, we get that $2N$ is divisible by 4, that is N is even. We obtain $\frac{N}{2}$ such V_μ, written V_μ^j.

In each V_μ^j, let $u_j^a \perp u_j^b$ be two unitary eigenvectors associated to μ. Thus $\mathrm{C}u_j^a \perp \mathrm{C}u_j^b$ are two eigenvectors associated to $-\mu$. We use Theorem 6.4 to decompose $V_\mu^j = \Pi^a \overset{\perp}{\oplus} \Pi^b$ with

$$\left|\begin{array}{l} \forall \star \in \{a,b\},\ \Pi_\star = \mathrm{Span}(u_j^\star, u_{-j}^\star) = \mathrm{Span}(e_j^\star, e_{-j}^\star) \\ \gamma u_{\pm j}^\star = \pm\mu u_\pm^\star,\ \mathcal{P}_\mp^0 e_{\pm j}^\star = 0. \end{array}\right.$$

We may assume (6.95) holds for both planes. Our aim is to prove that up to a phase, $\mathrm{C}u_{\pm j}^a = u_\mp^b$. *A priori* there exist $\phi_0, \phi_1, \phi_2, \theta \in [-\pi, \pi)$ such that

$$\left|\begin{array}{l} \mathrm{C}u_j^a = e^{i\phi_1}\cos(\theta)u_{-j}^a + e^{i\phi_2}\sin(\theta)u_{-j}^b, \\ \mathrm{C}u_j^b = -e^{i(\phi_1+\phi_0)}\sin(\theta)u_{-j}^a + e^{i(\phi_2+\phi_0)}\cos(\theta)u_{-j}^b. \end{array}\right.$$

We may assume $\cos(\theta), \sin(\theta) > 0$. Using (6.95), and writing $\overline{\phi}_k = \phi_k + \phi_0$, $k \in \{1,2\}$, we get

$$\begin{array}{r|l} \mathrm{C}e_j^a = -e^{i\phi_1}\cos(\theta)e_{-j}^a - e^{i\phi_2}\sin(\theta)e_{-j}^b, & \mathrm{C}e_j^b = e^{i\overline{\phi}_1}\sin(\theta)e_{-j}^a - e^{i\overline{\phi}_2}\cos(\theta)e_{-j}^b, \\ \mathrm{C}e_{-j}^a = e^{i\phi_1}\cos(\theta)e_j^a + e^{i\phi_2}\sin(\theta)e_j^b, & \mathrm{C}e_{-j}^b = -e^{i\overline{\phi}_1}\sin(\theta)e_j^a + e^{i\overline{\phi}_2}\cos(\theta)e_j^b. \end{array}$$

Applying C to Ce_j^a we get

$$e_j^a = e^{i(\overline{\phi}_1 - \phi_2)}\big(\sin(\theta)^2 - e^{i(\phi_2 - \overline{\phi}_1)}\cos(\theta)^2\big)e_j^a - e^{i\phi_0}\frac{\sin(2\theta)}{2}\big(e^{i(\phi_2-\overline{\phi}_1)} + 1\big)e_j^b.$$

Thus $\sin(\theta) = 1$ and $\overline{\phi}_1 - \phi_2 \equiv 0[2\pi]$. This gives :

$$E_{\mu^2}^{\gamma^2} = \overset{\perp}{\bigoplus_{1\leq j\leq \frac{N}{2}}} V_\mu^j \text{ and } V_\mu^j = \Pi_{\mu,j}^a \overset{\perp}{\oplus} \mathrm{C}\Pi_{\mu,j}^a, \tag{6.108}$$

where each $\Pi_{\mu,j}^a$ and $\mathrm{C}\Pi_{\mu,j}^a$ is a spectral plane described in Theorem 6.4. □

Chapitre 7

Sur le para-positronium et le dipositronium

The positronium and the dipositronium in a mean-field model of quantum electrodynamics

Abstract

The Bogoliubov-Dirac-Fock (BDF) model is a no-photon, mean-field approximation of quantum electrodynamics. It describes relativistic electrons in the Dirac sea. In this model, a state is fully characterized by its one-body density matrix, an infinite rank nonnegative operator. We prove the existence of the positronium, the bound state of an electron and a positron, represented by a critical point of the energy functional in the absence of external field. This state is interpreted as the ortho-positronium, where the two particles have parallel spins.

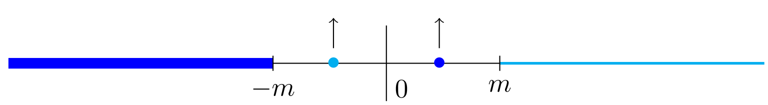

FIGURE 7.1 – Spectre du para-positronium

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7.1 Introduction and main results

7.1.1 The Dirac operator

Relativistic quantum mechanics is based on the *Dirac operator* D_0, which is the Hamiltonian of the free electron. Its expression is [Tha92] :

$$D_0 := m_e c^2 \beta - i\hbar c \sum_{j=1}^{3} \alpha_j \partial_{x_j} \tag{7.1}$$

where m_e is the (bare) mass of the electron, c the speed of light and $\hbar$ the reduced Planck constant and β and the α_j's are 4×4 matrices defined as follows :

$$\beta := \begin{pmatrix} \mathrm{Id}_{\mathbb{C}^2} & 0 \\ 0 & -\mathrm{Id}_{\mathbb{C}^2} \end{pmatrix},\ \alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix},\ j\in\{1,2,3\}$$

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ \sigma_3 \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}.$$

The operator D_0 acts on the Hilbert space $\mathfrak{H}$:

$$\mathfrak{H} := L^2(\mathbb{R}^3, \mathbb{C}^4); \tag{7.2}$$

it is self-adjoint on $\mathfrak{H}$ with domain $H^1(\mathbb{R}^3,\mathbb{C}^4)$. Its spectrum is $\sigma(D_0) = (-\infty, m_e c^2] \cup [m_e c^2, +\infty)$, which leads to the existence of states with arbitrary small energy.

Dirac postulated that all the negative energy states are already occupied by "virtual electrons", with one electron in each state : by Pauli's principle real electrons can only have a positive energy.

In this interpretation the Dirac sea, composed by those negatively charged virtual electrons, constitutes a polarizable medium that reacts to the presence of an external field. This phenomenon is called the *vacuum polarization*.

After the transition of an electron of the Dirac sea from a negative energy state to a positive, there is a real electron with positive energy plus the absence of an electron in the Dirac sea. This hole can be interpreted as the addition of a particle with same mass, but opposite charge : the so-called positron. The existence of this particle was predicted by Dirac in 1931. Although firstly observed in 1929 independently by Skobeltsyn and Chung-Yao Chao, it was recognized in an experiment lead by Anderson in 1932.

7.1.2 Positronium and dipositronium

The positronium is the bound state of an electron and a positron. This system was independently predicted by Anderson and Mohorovičić in 1932 and 1934 and was experimentally observed for the first time in 1951 by Martin Deutsch.

It is unstable : depending on the relative spin states of the positron and electron, its average lifetime in vacuum is 125 ps (para-positronium) or 142 ns (ortho-positronium) [Kar04].

Here we are interested in positronium states in the Bogoliubov-Dirac-Fock (BDF) model.

In a previous paper we have proved the existence of a state that can be interpreted as the ortho-positronium. Our aim in this paper is to find another one that can be interpreted as the para-positronium and to find another state that can be interpreted as the dipositronium, the bound state of two electrons and two positrons. To find these states, we use symmetric properties of the Dirac operator.

7.1.3 Symmetries

– Following Dirac's ideas, the free vacuum is described by the negative part of the spectrum $\sigma(D_0)$:

$$P^0_- = \chi_{(-\infty,0)}(D_0).$$

A correspondence between negative energy states and positron states is given by the *charge conjugation* C [Tha92]. This is an antiunitary operator that maps $\mathrm{Ran}\, P^0_-$ onto $\mathrm{Ran}(1-P^0_-)$. In our convention [Tha92] it is defined by the formula :

$$\forall\, \psi \in L^2(\mathbb{R}^3),\ \mathrm{C}\psi(x) = i\beta\alpha_2 \overline{\psi}(x), \tag{7.3}$$

where $\overline{\psi}$ denotes the usual complex conjugation. More precisely :

$$\mathrm{C}\cdot\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_2\\ \psi_4\end{pmatrix}=\begin{pmatrix}\overline{\psi}_4\\ -\overline{\psi}_3\\ -\overline{\psi}_2\\ \overline{\psi}_1\end{pmatrix}. \tag{7.4}$$

In our convention it is also an *involution* : $\mathrm{C}^2=\mathrm{id}$. An important property is the following :

$$\forall\,\psi\in L^2,\forall\,x\in\mathbb{R}^3,\ |\mathrm{C}\psi(x)|^2=|\psi(x)|^2. \tag{7.5}$$

The Dirac operator anti-commutes with D_0, or equivalently there holds

$$-\mathrm{C}D_0\mathrm{C}^{-1}=-\mathrm{C}D_0\mathrm{C}=D_0.$$

– There exists another simple symmetry. We define

$$\mathrm{I_s}:=\begin{pmatrix}0 & -\mathrm{Id}_{\mathbb{C}^2}\\ \mathrm{Id}_{\mathbb{C}^2} & 0\end{pmatrix}\in\mathbb{C}^{4\times 4}. \tag{7.6}$$

This operator is $-i$ the *time reversal operator* L_T [Tha92, 2.5.7] in $\mathfrak{H}$, interpreted as a unitary reprsentation of the Poincaré group.

It acts on the spinor by simple multiplication, furthermore we have $\mathrm{I_s^2}=-\mathrm{Id}$ and

$$\mathrm{I_s}:\begin{array}{ccc}\mathrm{Ran}\,P^0_- & \xrightarrow{\simeq} & \mathrm{Ran}\,(1-P^0_-)\\ \psi(x) & \mapsto & \mathrm{I_s}\psi(x)\end{array}$$

Similarly we have $-\mathrm{I_s}D_0\mathrm{I_s^{-1}}=\mathrm{I_s}D_0\mathrm{I_s}=D_0$.
– To end this part we recall that $\mathbf{SU}(2)$ acts on $\mathfrak{H}$ [Tha92]. Writing $\boldsymbol{\alpha}=(\alpha_j)_{j=1}^3$ and

$$\mathbf{p}:=-i\hbar\nabla,\ L:=\mathbf{x}\wedge\mathbf{p},\ \mathbf{S}:=-\frac{i}{4}\boldsymbol{\alpha}\wedge\boldsymbol{\alpha}=\frac{1}{2}\begin{pmatrix}\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma}\end{pmatrix}, \tag{7.7}$$

we define

$$\mathbf{J}:=\mathbf{L}+\mathbf{S}. \tag{7.8}$$

The operator $\mathbf{L}$ is the angular momentum operator and $\mathbf{J}$ is the total angular momentum. From a geometrical point of view, $-i\mathbf{J}$ gives rise to a unitary representation of $\mathbf{SU}(2)$ in $\mathfrak{H}$ by the following formula :

$$\begin{cases} e^{-i\theta\mathbf{J}\cdot\omega}\psi(x)=e^{-i\mathbf{S}\cdot\omega}\psi\big(\mathbf{R}^{-1}_{\omega,\theta}\big),\\ \forall\theta\in[0,4\pi),\forall\psi\in\mathfrak{H},\forall\omega\in\mathbb{S}^2,\end{cases}$$

where $\mathbf{R}_{\omega,\theta}\in\mathrm{SO}(3)$ is the rotation with axis ω and angle θ.

As each S_j is diagonal by block, it is clear that this group representation can be decomposed in two representations, the first acting on the upper spinors $\phi\in L^2(\mathbb{R}^3,\mathbb{C}^2)$ and the second on the lower spinors $\chi\in L^2(\mathbb{R}^3,\mathbb{C}^2)$:

$$\psi=:\begin{pmatrix}\phi\\ \chi\end{pmatrix}.$$

In [Tha92, pp. 122-129] it is proved that D_0 commutes with the action of $\mathbf{SU}(2)$, thus the representation can also be decomposed with respect to $\mathrm{Ran}\,P^0_-$ and $\mathrm{Ran}\,(1-P^0_-)$.

From an algebraic point of view, there exists a group morphism $\Phi_{\mathrm{SU}}:\mathbf{SU}(2)\to\mathbf{U}(\mathfrak{H}_\Lambda)$ where $\mathbf{U}(\mathfrak{H})$ is the set of unitary operator of $\mathfrak{H}$. We write

$$\mathbf{S}:=\Phi_{\mathrm{SU}}\big(\mathbf{SU}(2)\big). \tag{7.9}$$

The irreducible representations of Φ_{SU} are known and are expressed in terms of eigenspaces of $\mathbf{J}^2,\mathbf{S}$. The proofs of the following can be found in [Tha92, pp. 122-129].

The operators $\mathbf{J}^2, \mathrm{J}_3, \mathbf{K}$ all commute with each other, and $\mathbf{J}^2, \mathbf{K}$ with D_0. Moreover $\mathbf{K}$ commutes with the action Φ_{SU}.

We have $\mathfrak{H}_\Lambda \subset L^2(\mathbb{R}^3) \simeq L^2((0,\infty),dr) \otimes L^2(\mathbb{S}^2)^4$, and $\mathbf{J}$, $\mathbf{L}$ only act on the part $L^2(\mathbb{S}^2)^4$.

Restricted to $L^2(\mathbb{S}^2)^4$, we have

$$\sigma\left(\mathbf{J}^2\right) = \big\{j(j+1),\ j \in \frac{1}{2} + \mathbb{Z}_+\big\}, \tag{7.10}$$

and for each eigenvalue $j(j+1) \in \sigma\,\mathbf{J}^2$, the eigenspace $\mathrm{Ker}\big(\mathbf{J}^2 - j(j+1)\big)$ may be decomposed with respect to the eigenspaces of J_3 and $\mathbf{S}$. The corresponding eigenvalues are

1. $m_j = -j, -j+1, \cdots, j-1, j$ for J_3,
2. $\kappa_j = \pm\big(j + \frac{1}{2}\big)$ for $\mathbf{S}$.

The eigenspace $\mathfrak{k}_{m_j,\kappa_j}$ of a triplet (j, m_j, κ_j) has dimension 2 and is spanned by $\Phi^+_{m_j,\kappa_j} \perp \Phi^-_{m_j,\kappa_j}$, which have respectively a zero lower spinor and zero upper spinor.

Lemma 7.1. *For each irreducible subrepresentation Φ'_{SU} of Φ_{SU}, there exists*

$$(j, \varepsilon, \mathbf{z} = [z_1 : z_2], a_1(r), a_2(r)) \in \big(\frac{1}{2} + \mathbb{Z}_+\big) \times \{+,-\} \times \mathbb{C}P^1 \times \big(\mathbb{S}L^2((0,\infty),dr)\big)^2,$$

such that the representation Φ'_{SU} is spanned by $\psi(x)$ defined as follows :

$$\forall x = r\omega \in \mathbb{R}^3, \psi(x) := z_1 r a_1(r) \Phi^+_{j,\varepsilon(j+\frac{1}{2})}(\omega) + z_2 r a_2(r) \Phi^-_{j,\varepsilon(j+\frac{1}{2})}.$$

Remark 7.1. We recall that for any Hilbert space $\mathfrak{h}$ and any subspace $V \subset \mathfrak{h}$, we define $\mathbb{S}V$ as the unitary vector in V :

$$\mathbb{S}V := \{x \in V,\ \|x\|_{\mathfrak{h}} = 1\}.$$

We will use this notation throughout this paper.

We prove this Lemma in Section 7.4.

Remark 7.2. An irreducible subrepresentation of Φ_{SU} is characterized by the two numbers (j, κ_j). Indeed, the irreducible representations of $\mathbf{SU}(2)$ are known : they can be described by homogeneous polynomials, and for any $n \in \mathbb{Z}_+$, there is but one irreducible representation of dimension $n+1$, up to isomorphism.

In the case of Φ_{SU}, the two cases $\kappa_j = \pm(j + \frac{1}{2})$ are different but *isomorphic*.

Notation 7.1. An irreducible subrepresentation of Φ_{SU} spanned by an eigenvector of $\mathbf{J}^2$ and $\mathbf{K}$ with respective eigenvalues $j(j+1)$ and $\varepsilon(j+\frac{1}{2})$ will be refered as beeing of type (j,ε) (where $\varepsilon \in \{+,-\}$).

Notation 7.2. Throughout this paper we write $\mathrm{Proj}\,E$ to mean the orthonormal projection onto the vector space E.

7.1.4 The BDF model

This model is a no-photon approximation of quantum electrodynamics (QED) which was introduced by Chaix and Iracane in 1989 [CI89], and studied in many papers [BBHS98a, HLS05a, HLS05b, HLS07, HLS09, GLS09, Sok14b].

It allows to take into account the Dirac vacuum together an electronic system in the presence of an external field.

This is a Hartree-Fock type approximation in which a state of the system "vacuum plus real electrons" is given by an infinite Slater determinant $\psi_1 \wedge \psi_2 \wedge \cdots$. Such a state is represented by the projector onto the space spanned by the ψ_j's : its so-called one-body density matrix. For instance P^0_- represents the free Dirac vacuum.

We do not recall the derivation of the BDF model from QED : we refer the reader to [CI89, HLS05a, HLS07] for full details.

Remark 7.3. To simplify the notations, we choose relativistic units in which, the mass of the electron m_e, the speed of light c and $\hbar$ are set to 1.

Let us say that there is an external density ν, *e.g.* that of some nucleus. We write $\alpha > 0$ the so-called *fine structure constant* (physically $e^2/(4\pi\varepsilon_0\hbar c)$), where e is the elementary charge and ε_0 the permittivity of free space).

The relative energy of a Hartree-Fock state represented by its 1pdm P with respect to a state of reference (P_-^0 in [CI89, HLS05a]) turns out to be a function of $Q = P - P_-^0$, the so-called reduced one-body density matrix. We emphasize that this procedure is mathematically ill-defined : we substract an infinite energy to an infinite energy.

A projector P is the one-body density matrix of a Hartree-Fock state in $\mathcal{F}_{\text{elec}}$ *iff* $P - P_-^0$ is Hilbert-Schmidt, that is compact such that its singular values form a sequence in ℓ^2 [HLS05a, Appendix].

An ultraviolet cut-off $\Lambda > 0$ is needed : we only consider electronic states in

$$\mathfrak{H}_\Lambda := \left\{ f \in \mathfrak{H},\ \operatorname{supp} \widehat{f} \subset B(0,\Lambda) \right\},$$

where $\widehat{f}$ is the Fourier transform of f.

This procedure gives the BDF energy introduced in [CI89] and studied in [HLS05a, HLS05b].

Notation 7.3. Our convention for the Fourier transform $\mathscr{F}$ is the following

$$\forall\, f \in L^1(\mathbb{R}^3),\ \widehat{f}(p) := \frac{1}{(2\pi)^{3/2}} \int f(x) e^{-ixp} dx.$$

Let us notice that $\mathfrak{H}_\Lambda$ is invariant under D_0 and so under P_-^0.

We write Π_Λ for the orthogonal projection onto $\mathfrak{H}_\Lambda$: Π_Λ is the Fourier multiplier $\mathscr{F}^{-1}\chi_{B(0,\Lambda)}\mathscr{F}$.

By means of a thermodynamical limit, Hainzl *et al.* showed that the formal minimizer and hence the reference state should not be given by $\Pi_\Lambda P_-^0$ but by another projector $\mathcal{P}_-^0$ in $\mathfrak{H}_\Lambda$ that satisfies the self-consistent equation <u>*in* $\mathfrak{H}_\Lambda$</u> [HLS07] :

$$\begin{cases} \mathcal{P}_-^0 - \frac{1}{2} &= -\operatorname{sign}\big(\mathcal{D}^0\big), \\ \mathcal{D}^0 &= D_0\Pi_\Lambda - \dfrac{\alpha}{2}\dfrac{(\mathcal{P}_-^0 - \frac{1}{2})(x-y)}{|x-y|} \end{cases} \tag{7.11}$$

We have $\mathcal{P}_-^0 = \chi_{(-\infty,0)}(\mathcal{D}^0)$. This operator $\mathcal{D}^0$ was previously introduced by Lieb *et al.* in [LS00]. In $\mathfrak{H}$, the operator $\mathcal{D}^0$ coincides with a bounded, matrix-valued Fourier multiplier whose kernel is $\mathfrak{H}_\Lambda^\perp \subset \mathfrak{H}$.

Notation 7.4. Throughout this paper we write

$$m = \inf \sigma\big(|\mathcal{D}^0|\big) \geq 1, \tag{7.12}$$

and

$$\mathcal{P}_+^0 := \Pi_\Lambda - \mathcal{P}_-^0 = \chi_{(0,+\infty)}(\mathcal{D}^0). \tag{7.13}$$

The resulting BDF energy $\mathcal{E}_{\text{BDF}}^\nu$ is defined on Hartree-Fock states represented by their one-body density matrix P :

$$\mathscr{N} := \left\{ P \in \mathcal{B}(\mathfrak{H}_\Lambda),\ P^* = P^2 = P,\ P - \mathcal{P}_-^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \right\}.$$

We recall that $\mathcal{B}(\mathfrak{H}_\Lambda)$ is the set of bounded operators and that for $p \geq 1$, $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ is the set of compact operators A such that $\operatorname{Tr}\big(|A|^p\big) < +\infty$ [RS75, Sim79]. In particular $\mathfrak{S}_\infty(\mathfrak{H}_\Lambda)$ is the set $\operatorname{Comp}(\mathfrak{H}_\Lambda)$ of compact operators.

This energy depends on three parameters : the fine structure constant $\alpha > 0$, the cut-off $\Lambda > 0$ and the external density ν. We assume that ν has finite *Coulomb energy*, that is

$$D(\nu,\nu) := 4\pi \int_{\mathbb{R}^3} \frac{|\widehat{\nu}(k)|^2}{|k|^2} dk. \tag{7.14}$$

The above integral coincides with $\iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\nu(x)^*\nu(y)}{|x-y|} dxdy$ whenever this last one is well-defined.

Remark 7.4. The same symmetries holds for $\mathcal{P}_-^0$ and $\mathcal{P}_+^0$: the charge conjugation C and the operator $\mathrm{I_s}$ maps $\operatorname{Ran}\mathcal{P}_-^0$ onto $\operatorname{Ran}\mathcal{P}_+^0$. Moreover thanks to [Tha92, pp. 122-129] we can easily check that $\mathcal{D}^0$ also commutes with the action of $\mathbf{SU}(2)$ and with the operators $\mathbf{J}^2$ and $\mathbf{K}$.

This results is proved in the Appendix.

7.1.5 Minimizers and critical points

For $P \in \mathscr{N}$, we have the identity

$$(P-\mathcal{P}_-^0)^2 = \mathcal{P}_+^0(P-\mathcal{P}_-^0)\mathcal{P}_+^0 - \mathcal{P}_-^0(P-\mathcal{P}_-^0)\mathcal{P}_-^0 \in \mathfrak{S}_1. \tag{7.15}$$

The charge of a state P is given by the $\mathcal{P}_-^0$-trace of $P-\mathcal{P}_-^0$, defined by the formula :

$$\mathrm{Tr}_{\mathcal{P}_-^0}\big(P-\mathcal{P}_-^0\big) := \mathrm{Tr}\big(\mathcal{P}_-^0(P-\mathcal{P}_-^0)\mathcal{P}_-^0 + \mathcal{P}_+^0(P-\mathcal{P}_-^0)\mathcal{P}_+^0\big), \tag{7.16}$$

$$= \mathrm{DimRan}(\mathcal{P}_+^0)\cap \mathrm{Ran}(P) - \mathrm{DimRan}(\mathcal{P}_-^0)\cap\mathrm{Ran}(1-P). \tag{7.17}$$

A minimizer over states with charge $N\in\mathbb{N}$ is interpreted as a ground state of a system with N electrons, in the presence of an external density ν

The existence problem was studied in several papers [HLS09, Sok14b, Sok13] : by [HLS09, Theorem 1], it is sufficient to check binding inequalities.

The following results hold under technical assumptions on α and Λ (different for each result).

In [HLS09], Hainzl *et al.* proved existence of minimizers for the system of N electrons with $\nu \geq 0$, provided that $N-1<\int \nu$.

In [Sok14b], we proved the existence of a ground state for $N=1$ and $\nu=0$: an electron can bind alone in the vacuum. This surprising result holds due to the vacuum polarization.

In [Sok13], we studied the charge screening effect : due to vacuum polarization, the observed charge of a minimizer $P\neq\mathcal{P}_-^0$ is different from its real charge $\mathrm{Tr}_{\mathcal{P}_-^0}(P-\mathcal{P}_-^0)$. We also proved it is possible to keep track of this effect in the non-relativistic limit $\alpha\to 0$: the resulting limit is an altered Hartree-Fock energy.

Here we are looking for states with an equal number of electrons and positrons, that is we study $\mathcal{E}_{\mathrm{BDF}}^0$ on

$$\mathscr{M} := \Big\{P\in\mathscr{N},\ \mathrm{Tr}_{\mathcal{P}_-^0}\big(P-\mathcal{P}_-^0\big)=0\Big\}. \tag{7.18}$$

From a geometrical point of view $\mathscr{M}$ is a Hilbert manifold and $\mathcal{E}_{\mathrm{BDF}}^0$ is a differentiable map on $\mathscr{M}$ (Propositions 7.3 and 7.4).

We thus seek a critical point on $\mathscr{M}$, that is some $P\in\mathscr{M},\ P\neq\mathcal{P}_-^0$ such that $\nabla\mathcal{E}_{\mathrm{BDF}}^0(P)=0$.

In [Sok14d], we have found the ortho-positronium by studying the BDF energy restricted to states with the C-symmetry :

$$P\in\mathscr{M} \text{ s.t. } P+\mathrm{C}P\mathrm{C} = \mathrm{Id}_{\mathfrak{H}_\Lambda}. \tag{7.19}$$

We write $\mathscr{M}_{\mathscr{C}}$ the set of such states. We will seek the para-positronium in the set $\mathscr{M}_{\mathscr{I}}$ of states having the $\mathrm{I_s}$-symmetry.

Definition 7.1.

$$\mathscr{M}_{\mathscr{I}} := \{P\in\mathscr{M} \text{ s.t. } P+\mathrm{I_s}P\mathrm{I_s}^{-1} = P-\mathrm{I_s}P\mathrm{I_s} = \mathrm{Id}_{\mathfrak{H}_\Lambda}\}. \tag{7.20}$$

Equivalently $P\in\mathscr{M}_{\mathscr{I}}$ if and only if $Q:=P-\mathcal{P}_-^0$ is Hilbert-Schmidt and satisfies

$$-\mathrm{I_s}Q\mathrm{I_s}^{-1} = \mathrm{I_s}Q\mathrm{I_s} = Q.$$

We seek a projector P "close" to a state P_0 that can be written as :

$$P_0 = \mathcal{P}_-^0 + |\mathrm{I_s}\psi_-\rangle\langle\mathrm{I_s}\psi_-| - |\psi_-\rangle\langle\psi_-|,\ \mathcal{P}_+^0\psi_-=0. \tag{7.21}$$

To deal with the dipositronium, we impose an additional symmetry : we define $\mathscr{W}\subset\mathscr{M}_{\mathscr{C}}$ as follows.

Definition 7.2.

$$\mathscr{W} := \big\{P\in\mathscr{M}_{\mathscr{C}},\ \forall U\in\mathbf{S},\ UPU^{-1}=P\big\}. \tag{7.22}$$

Equivalently

$$P\in\mathscr{W} \iff Q:=P-\mathcal{P}_-^0 \text{ satisfies } -\mathrm{C}Q\mathrm{C}=Q \text{ and } UQU^{-1}=Q,\ \forall U\in\mathbf{S}.$$

Those sets $\mathscr{M}_{\mathscr{C}}, \mathscr{M}_{\mathscr{I}}, \mathscr{W}$ have fine properties : they are all submanifolds of $\mathscr{M}$, invariant under the gradient flow of $\mathcal{E}^0_{\rm BDF}$ (Proposition 7.5).

However while $\mathscr{M}_{\mathscr{C}}$ has two connected components, $\mathscr{M}_{\mathscr{I}}$ has only one connected component and $\mathscr{W}$ has countable connected components. So we may find critical points by searching a minimizer of the BDF energy over the different connected components of $\mathscr{W}$. For the para-positronium, a critical point is found by an argument of mountain pass.

Proposition 7.1. *There is a one-to-one correspondence between the connected components of $\mathscr{W}$ and the set $\mathbb{Z}_2^2[X]$ of polynomials with coefficients in the ring $\mathbb{Z}_2\times\mathbb{Z}_2$.*

Let P be in $\mathscr{W}$. The vector space $E_1 := \operatorname{Ran} P \cap \operatorname{Ran}\mathcal{P}^0_+$ has finite dimension and is invariant under $\Phi_{\rm SU}$. We decompose it into irreducible representations.

The projector is associated to $\sum_{\ell=1}^{\ell_0} t_\ell X^\ell$ with $t_\ell = (t_{\ell,1};t_{\ell,-1})$ if and only if for any $j\in \frac12+\mathbb{Z}_+$:

1. *The number $b_{j-\frac12,1}$ of irreducible representations of E_1 of type $(j,+)$ satisfies $b_{j-\frac12,1}\equiv t_{j-\frac12,1}[2]$.*
2. *The number $b_{j-\frac12,-1}$ of irreducible representations of E_1 of type $(j,-)$ satisfies $b_{j-\frac12,-1}\equiv t_{j-\frac12,-1}[2]$.*

Notation 7.5. The symbols $\mathscr{Y}$ and Y denotes respectively $\mathscr{C}$ and C or $\mathscr{I}$ and $\mathrm{I_s}$.

Furthermore the different connected components of $\mathscr{W}$ are written $\mathscr{W}_{p(X)}$ with $p(X)\in\mathbb{Z}_2^2[X]$.

To state our main Theorems, we need to introduce the mean-field operator.

Notation 7.6 (mean-field operator). An operator $Q\in\mathscr{V}$ is Hilbert-Schmidt and we write $Q(x,y)$ its integral kernel. Its density ρ_Q is defined by the formula

$$\forall x\in\mathbb{R}^3,\ \rho_Q(x) := \operatorname{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big), \tag{7.23}$$

we prove in the next Section that it is well-defined. The mean-field operator $D_Q^{(\Lambda)}$ associated to Q *in the vacuum* is :

$$D_Q^{(\Lambda)} := \Pi_\Lambda\Big(\mathcal{D}^0 + \alpha\big(\rho_Q * \frac{1}{|\cdot|} - \frac{Q(x,y)}{|x-y|}\big)\Big). \tag{7.24}$$

Theorem 7.1. *There exist $\alpha_0, L_0, \Lambda_0>0$ such that if*

$$\alpha\le\alpha_0;\ \alpha\log(\Lambda) := L\le L_0 \text{ and } \Lambda^{-1}\le\Lambda_0^{-1},$$

then there exists a critical point $\overline{P}=\overline{Q}+\mathcal{P}^0_-$ of $\mathcal{E}^0_{BDF}$ in $\mathscr{M}_{\mathscr{I}}$ that satisfies the following equation.

$$\exists 0<\mu<m,\ \exists\psi_a\in\operatorname{Ker}\big(D_Q^{(\Lambda)}-\mu\big),\ \overline{P} = \chi_{(-\infty,0)}\big(D_Q^{(\Lambda)}\big) + |\psi_a\rangle\langle\psi_a| - |\mathrm{I_s}\psi_a\rangle\langle\mathrm{I_s}\psi_a|. \tag{7.25}$$

As α tends to 0, the upper spinor of $U_\lambda\psi_a := \lambda^{3/2}\psi_a(\lambda(\cdot))$ with $\lambda := \frac{g_1'(0)^2}{\alpha m}$ tends to a Pekar minimizer.
– We recall that the Pekar energy is defined as follows

$$\forall\,\psi\in H^1,\ \mathcal{E}_{PT}(\psi) := \|\nabla\psi\|^2_{L^2} - D\big(|\psi|^2,|\psi|^2\big).$$

The infimum over $\mathbb{S}L^2\cap H^1$ is written $E_{\rm PT}(1)$.

Theorem 7.2. *There exist $L_0,\Lambda_0>0$, and for any $j\in\frac12+\mathbb{Z}_+$, there exists α_j such that if*

$$\alpha\le\alpha_j;\ \alpha\log(\Lambda) := L\le L_0 \text{ and } \Lambda^{-1}\le\Lambda_0^{-1},$$

then there exists a minimizer $P_{\mathbf{t}X^{\ell_0}} = Q+\mathcal{P}^0_-$ of $\mathcal{E}^0_{BDF}$ over the connected component of $\mathscr{W}_{\mathbf{t}X^{\ell_0}}$ with $\mathbf{t}\in\{(1,0),(0,1)\}$.

Moreover there exists $0<\mu_{\ell_0,\mathbf{t}}<1$ and $\psi\in\operatorname{Ker}\big(D_Q^{(\Lambda)}-\mu_{\ell_0,\mathbf{t}}\big)$ such that

$$P_{\mathbf{t}X^{\ell_0}} = \chi_{(-\infty,0)}(D_Q^{(\Lambda)}) + \operatorname{Proj}\Phi_{\rm SU}(\psi) - \operatorname{Proj}\Phi_{\rm SU}(\mathrm{C}\psi).$$

Any upper spinor $\widetilde{\varphi}$ of $\widetilde{\psi}\in\Phi_{\rm SU}(\psi)$ can be written as

$$\forall\,x=r\omega_x\in\mathbb{R}^3,\ \widetilde{\varphi} =: ra(r)\sum_{m=-j}^{j} c_m(\widetilde{\varphi})\Phi^+_{m,\varepsilon(j_0+\frac12)},\ c_m(\widetilde{\varphi})\in\mathbb{C}.$$

Furthermore, as α tends to 0, the function $U_\lambda a(r) = \lambda^{3/2}a(\lambda r)$ tends to a minimizer of the energy $\mathcal{E}_{\mathbf{t}X^{\ell_0}}$ over $\mathbb{S}L^2(\mathbb{R}_+, r^2dr) \cap H^1(\mathbb{R}_+, r^2dr)$:

$$\mathcal{E}_{\mathbf{t}X^{\ell_0}}\big(f(r)\big) := \mathrm{Tr}\big(-\Delta\,\mathrm{Proj}\,\Phi_{\mathrm{SU}}(rf(r)\Phi^+_{j_0,\varepsilon(\mathbf{t})})\big) - \|\mathrm{Proj}\,\Phi_{\mathrm{SU}}\,(rf(r)\Phi^+_{j_0,\varepsilon(\mathbf{t})})\|^2_{Ex}. \tag{7.26}$$

In particular, the dipositronium corresponds to the case $\ell_0 = j_0 - \frac{1}{2} = 0$.

Notation 7.7. The minimum is written $E^{nr}_{\mathbf{t}X^{\ell_0}}$ for the non-relativistic energy and $E_{j_0,\varepsilon(\mathbf{t})}$ for the BDF energy over $\mathscr{W}_{\mathbf{t}X^{j_0-1/2}}$.

Notation 7.8. For $\mathbf{t}X^{\ell_0} \in \mathbb{Z}_2^2[X]$ as in Theorem 7.2, $\varepsilon(\mathbf{t}) \in \{+,-\}$ denotes $+$ if $\mathbf{t} = (1,0)$ or $-$ if $\mathbf{t} = (0,1)$.

Remark 7.5. We expect the existence of minimizers over any connected components of $\mathscr{W}$ (associated to $p(X) \in \mathbb{Z}_2^2[X]$), provided that α is smaller than some $\alpha_{p(X)}$.

Remark 7.6. The non-relativistic energy can be computed :

$$\begin{cases} \mathcal{E}_{\mathbf{t}X^{\ell_0}}\big(f(r)\big) &:= (2j_0+1)\displaystyle\int_0^{+\infty}\Big[r^2|f'(r)|^2 + (j_0+\varepsilon\tfrac{1}{2})(j_0+1+\varepsilon\tfrac{1}{2})|f(r)|^2\Big]dr \\ & \quad -\displaystyle\iint_{\mathbb{R}_+^2} r_1^2r_2^2|f(r_1)|^2|f(r_2)|^2 w_{j_0,\varepsilon(\mathbf{t})}(r_1,r_2), \\ w_{j_0,\varepsilon(\mathbf{t})}(r_1,r_2) &:= \displaystyle\iint_{(\mathbb{S}^2)^2} \tfrac{dn_1dn_2}{|r_1n_1-r_2n_2|}\Big(\sum_{m_1,m_2}((\Phi^+_{m_1,\varepsilon(j_0+\frac{1}{2})})^*\Phi^+_{m_1,\varepsilon(j_0+\frac{1}{2})})(n_1)\Big) \\ & \quad \times\Big(\displaystyle\sum_{m_1,m_2}((\Phi^+_{m_1,\varepsilon(j_0+\frac{1}{2})})^*\Phi^+_{m_1,\varepsilon(j_0+\frac{1}{2})})(n_2)\Big). \end{cases} \tag{7.27}$$

It corresponds to the energy

$$\mathcal{E}_{nr}\big(\Gamma\big) := \mathrm{Tr}\big(-\Delta\Gamma\big) - \|\Gamma\|^2_{\mathrm{Ex}},\ 0 \le \Gamma \le 1,\ \Gamma \in \mathfrak{S}_1(H^1(\mathbb{R}^3,\mathbb{C}^2))$$

restricted to the subspace

$$\mathscr{S}_{(j_0,\varepsilon(\mathbf{t}))} := \big\{\Gamma,\ \Gamma^* = \Gamma^2 = \Gamma,\ \mathrm{Ran}\,(\Phi_{\mathrm{SU}})\big|_{\Gamma} \text{ irreducible of type } (j_0,\varepsilon(\mathbf{t}))\big\}.$$

This subspace is invariant under the action of Φ_{SU} and it is easy to see that it is a submanifold of $\big\{\Gamma,\ \Gamma^* = \Gamma^2 = \Gamma,\ \mathrm{Tr}\,\Gamma = 2j_0+1\big\}$.

The subspace $\mathscr{S}_{(j_0,\varepsilon(\mathbf{t}))}$ is invariant under the flow of $\mathcal{E}_{nr}$.

The energies can be estimated.

Proposition 7.2. *In the same regime as in Theorem 7.1, the following holds. The critical point $\overline{P}$ of the BDF functional over $\mathscr{M}_{\mathscr{G}}$ satisfies*

$$\mathcal{E}^0_{BDF}(\overline{P}) = 2m + \frac{\alpha^2 m}{g_1'(0)^2}E_{PT}(1) + \mathcal{O}(\alpha^3). \tag{7.28}$$

Furthermore the minimizer $\overline{P}_{\ell_0}$ over $\mathscr{W}_{\mathbf{t}X^{\ell_0}}$ satisfies :

$$\mathcal{E}^0_{BDF}(\overline{P}_{\ell_0}) = 2(2j_0+1) + \frac{\alpha^2 m}{g_1'(0)^2}E^{nr}_{\mathbf{t}X^{\ell_0}} + \mathcal{O}(\alpha^3 K(j_0)). \tag{7.29}$$

Remark 7.7. The Pekar model describes an electron trapped in its own hole in a polarizable medium. Thus it is not surprising to find it here. We recall that there is a unique minimizer of the Pekar energy up to translation and a phase in $\mathbb{S}^7$ (in $\mathbb{C}^4$).

The asymptotic expansion (7.28) coincides with that of the ortho-positronium [Sok14d]. In fact, it can be proved that the first difference between the energies occurs at order α^4.

Notation 7.9. Throughout this paper we write K to mean a constant independent of α, Λ. Its value may differ from one line to the other. When we write $K(a)$, we mean a constant that depends solely on a. We also use the symbol $\lesssim$: $0 \le a \lesssim b$ means there exists $K > 0$ such that $a \le Kb$.

We also recall the reader our use of the notation $\mathbb{S}V$ for any subspace V of some Hilbert space that denotes the set of unitary vector in V.

7.1.6 Remarks and notations about $\mathcal{D}^0$

$\mathcal{D}^0$ has the following form [HLS07] :

$$\mathcal{D}^0 = g_0(-i\nabla)\beta - i\boldsymbol{\alpha}\cdot\frac{\nabla}{|\nabla|}g_1(-i\nabla) \tag{7.30}$$

where g_0 and g_1 are smooth radial functions on $B(0,\Lambda)$. Moreover we have :

$$\forall\, p\in B(0,\Lambda),\ 1\le g_0(p),\ \text{and } |p|\le g_1(p)\le |p|g_0(p). \tag{7.31}$$

Notation 7.10. For $\alpha\log(\Lambda)$ sufficiently small, we have $m = g_0(0)$ [LL97, Sok14b].

Remark 7.8. The smallness of α is needed to get estimates that hold close to the non-relativistic limit.

The smallness of $\alpha\log(\Lambda)$ is needed to get estimates of $\mathcal{D}^0$: in this case $\mathcal{D}^0$ can be obtained by a fixed point scheme [HLS07, LL97], and we have [Sok14b, Appendix A] :

$$\begin{aligned} g_0'(0)=0,\ \text{and } \|g_0'\|_{L^\infty}, \|g_0''\|_{L^\infty} \le K\alpha\\ \|g_1'-1\|_{L^\infty}\le K\alpha\log(\Lambda)\le \tfrac12 \text{ and } \|g_1''\|_{L^\infty}\lesssim 1.\end{aligned} \tag{7.32}$$

7.2 Description of the model

7.2.1 The BDF energy

Notation 7.11. For any $\varepsilon,\varepsilon'\in\{+,-\}$ and $A\in\mathcal{B}(\mathfrak{H}_\Lambda)$, we write

$$A^{\varepsilon,\varepsilon'} := \mathcal{P}^0_\varepsilon A \mathcal{P}^0_{\varepsilon'}. \tag{7.33}$$

Notation 7.12. For an operator $Q\in\mathfrak{S}_2(\mathfrak{H}_\Lambda)$, we write R_Q the operator given by the integral kernel :

$$R_Q(x,y) := \frac{Q(x,y)}{|x-y|}.$$

Definition 7.3 (BDF energy)**.** Let $\alpha>0,\Lambda>0$ and $\nu\in\mathcal{S}'(\mathbb{R}^3)$ a generalized function with $D(\nu,\nu)<+\infty$. For $P\in\mathscr{N}$ we write $Q:=P-\mathcal{P}^0_-$ and

$$\begin{cases} \mathcal{E}^0_{\text{BDF}}(Q) = \mathrm{Tr}_{\mathcal{P}^0_-}\big(\mathcal{D}^0 Q\big) - \alpha D(\rho_Q,\nu) + \dfrac{\alpha}{2}\Big(D(\rho_Q,\rho_Q) - \|Q\|^2_{\text{Ex}}\Big),\\ \forall\, x,y\in\mathbb{R}^3,\ \rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big),\ \|Q\|^2_{\text{Ex}} := \displaystyle\iint \frac{|Q(x,y)|^2}{|x-y|}dxdy,\end{cases} \tag{7.34}$$

where $Q(x,y)$ is the integral kernel of Q.

Remark 7.9. The term $\mathrm{Tr}_{\mathcal{P}^0_-}\big(\mathcal{D}^0 Q\big)$ is the kinetic energy, $-\alpha D(\rho_Q,\nu)$ is the interaction energy with ν. The term $\dfrac{\alpha}{2}D(\rho_Q,\rho_Q)$ is the so-called *diract term* and $-\dfrac{\alpha}{2}\|Q\|^2_{\text{Ex}}$ is the *exchange term.*

Let us see that formula (7.34) is well-defined whenever Q is $\mathcal{P}^0_-$-trace-class [HLS05a, HLS09].

$\mathfrak{S}_1^{\mathcal{P}^0_-}$ and the variational set $\mathcal{K}$ The set $\mathfrak{S}_1^{\mathcal{P}^0_-}$ of $\mathcal{P}^0_-$-trace class operator is the following Banach space :

$$\mathfrak{S}_1^{\mathcal{P}^0_-} = \big\{Q\in\mathfrak{S}_2(\mathfrak{H}_\Lambda),\ Q^{++},Q^{--}\in\mathfrak{S}_1(\mathfrak{H}_\Lambda)\big\}, \tag{7.35}$$

with the norm

$$\|Q\|_{\mathfrak{S}_1^{\mathcal{P}^0_-}} := \|Q^{+-}\|_{\mathfrak{S}_2} + \|Q^{-+}\|_{\mathfrak{S}_2} + \|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1}. \tag{7.36}$$

We have $\mathscr{N}\subset\mathcal{P}^0_- + \mathfrak{S}_1^{\mathcal{P}^0_-}$ thanks to (7.15). The closed convex hull of $\mathscr{N}-\mathcal{P}^0_-$ under $\mathfrak{S}_1^{\mathcal{P}^0_-}$ is

$$\mathcal{K} := \big\{Q\in\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ Q^*=Q,\ -\mathcal{P}^0_-\le Q\le\mathcal{P}^0_+\big\}$$

and we have [HLS05a, HLS05b]

$$\forall\, Q\in\mathcal{K},\ Q^2\le Q^{++}-Q^{--}.$$

The BDF energy for $Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}$ We have

$$\mathcal{P}^0_-(\mathcal{D}^0 Q)\mathcal{P}^0_- = -|\mathcal{D}^0|Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda),\ \text{because}\,|\mathcal{D}^0| \in \mathcal{B}(\mathfrak{H}_\Lambda),$$

this proves that the kinetic energy is defined.

By the Kato-Seiler-Simon (KSS) inequality [Sim79], Q is locally trace-class :

$$\forall\, \phi \in \mathbf{C}_0^\infty(\mathbb{R}^3),\ \phi\Pi_\Lambda \in \mathfrak{S}_2 \text{ so } \phi Q\phi = \phi\Pi_\Lambda Q\phi \in \mathfrak{S}_1(L^2(\mathbb{R}^3)).$$

We recall this inequality states that for all $2 \leq p \leq \infty$ and $d \in \mathbb{N}$, we have

$$\forall\, f, g \in L^p(\mathbb{R}^d),\ f(x)g(-i\nabla) \in \mathfrak{S}_p(\mathfrak{H}_\Lambda) \text{ and } \|f(x)g(-i\nabla)\|_{\mathfrak{S}_p} \leq (2\pi)^{-d/p}\|f\|_{L^p}\|g\|_{L^p}.$$

It follows that the *density* ρ_Q of Q, defined in (7.34) is well-defined. By the KSS inequality, we can also prove that $\|\rho_Q\|_{\mathcal{C}} \lesssim K(\Lambda)\|Q\|_{\mathfrak{S}_1^{\mathcal{P}^0_-}}$ [GLS09, Proposition 2].

By Kato's inequality :

$$\frac{1}{|\cdot|} \leq \frac{\pi}{2}|\nabla|, \tag{7.37}$$

the exchange term is well-defined.

Moreover the following holds : if $\alpha < \frac{4}{\pi}$, then the BDF energy is bounded from below on $\mathcal{K}$ [BBHS98a, HLS05b, HLS09]. We have

$$\forall\, Q_0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ \mathcal{E}^0_{\mathrm{BDF}}(Q_0) \geq \big(1 - \alpha\frac{\pi}{4}\big)\mathrm{Tr}\big(|\mathcal{D}^0||Q_0|^2\big). \tag{7.38}$$

Here we assume it is the case. This result will be often used throughout this paper.

Minimizers For $Q \in \mathcal{K}$, its charge is its $\mathcal{P}^0_-$-trace : $q = \mathrm{Tr}_{\mathcal{P}^0_-}(Q)$. We define the Charge sector sets :

$$\forall\, q \in \mathbb{R}^3,\ \mathcal{K}^q := \big\{Q \in \mathcal{K},\ \mathrm{Tr}(Q) = q\big\}.$$

A minimizer of $\mathcal{E}^\nu_{\mathrm{BDF}}$ over $\mathcal{K}$ is interpreted as the polarized vacuum in the presence of ν while a minimizer over charge sector $N \in \mathbb{N}$ is interpreted as the ground state of N electrons in the presence of ν, by Lieb's principle [HLS09, Proposition 3], such a minimizer is in $\mathscr{N} - \mathcal{P}^0_-$.

We define the energy functional E^ν_{BDF} :

$$\forall\, q \in \mathbb{R}^3,\ E^\nu_{\mathrm{BDF}}(q) := \inf\big\{\mathcal{E}^\nu_{\mathrm{BDF}}(Q),\ Q \in \mathcal{K}^q\big\}. \tag{7.39}$$

We also write :

$$\mathcal{K}^0_{\mathscr{Y}} := \{Q \in \mathcal{K},\ \mathrm{Tr}_{\mathcal{P}^0_-}(Q) = 0,\ -\mathrm{Y}Q\mathrm{Y}^{-1} = Q\}. \tag{7.40}$$

Proposition 7.2 states that this set is sequentially weakly-$*$ closed in $\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$.

7.2.2 Structure of manifold

We consider

$$\mathscr{V} = \big\{P - \mathcal{P}^0_-,\ P^* = P^2 = P \in \mathcal{B}(\mathfrak{H}_\Lambda),\ \mathrm{Tr}_{\mathcal{P}^0_-}\big(P - \mathcal{P}^0_-\big) = 0\big\} \subset \mathfrak{S}_2(\mathfrak{H}_\Lambda).$$

and write : $\mathscr{M} := \mathcal{P}^0_- + \mathscr{V} = \big\{P,\ P^* = P^2 = P,\ \mathrm{Tr}_{\mathcal{P}^0_-}\big(P - \mathcal{P}^0_-\big) = 0\big\}$.

We recall the following proposition, proved in [Sok14d].

Proposition 7.3. *The set $\mathscr{M}$ is a Hilbert manifold and for all $P \in \mathscr{M}$,*

$$\mathrm{T}_P\mathscr{M} = \{[A, P],\ A \in \mathcal{B}(\mathfrak{H}_\Lambda),\ A^* = -A \text{ and } PA(1-P) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}. \tag{7.41}$$

Writing

$$\mathfrak{m}_P := \{A \in \mathcal{B}(\mathfrak{H}_\Lambda),\ A^* = -A,\ PAP = (1-P)A(1-P) = 0 \text{ and } PA(1-P) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}, \tag{7.42}$$

any $P_1 \in \mathscr{M}$ can be written as $P_1 = e^A P e^{-A}$ where $A \in \mathfrak{m}_P$.

The BDF energy $\mathcal{E}^\nu_{\rm BDF}$ is a differentiable function in $\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$ with :

$$\begin{cases} \forall\, Q, \delta Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ \mathrm{d}\mathcal{E}^\nu_{\rm BDF}(Q)\cdot \delta Q = \mathrm{Tr}_{\mathcal{P}^0_-}\big(D_{Q,\nu}\delta Q\big). \\ D_{Q,\nu} := \mathcal{D}^0 + \alpha\big((\rho_Q-\nu)*\frac{1}{|\cdot|} - R_Q\big). \end{cases} \tag{7.43}$$

We may rewrite (7.43) as follows :

$$\forall\, Q, \delta Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ \mathrm{d}\mathcal{E}^\nu_{\rm BDF}(Q)\cdot \delta Q = \mathrm{Tr}_{\mathcal{P}^0_-}\big(\Pi_\Lambda D_{Q,\nu}\Pi_\Lambda\delta Q\big) \tag{7.44}$$

We recall the mean-field operator $D_Q^{(\Lambda)}$ is defined in Notation 7.24.

Proposition 7.4. *Let (P,v) be in the tangent bundle $\mathrm{T}\mathscr{M}$ and $Q = P-\mathcal{P}^0_-$. Then we have $[[\Pi_\Lambda D_Q\Pi_\Lambda, P],P]\in \mathrm{T}_P\mathscr{M}$ and :*

$$\mathrm{d}\mathcal{E}^0_{BDF}(P)\cdot v = Tr\Big(\big[\big[D_Q^{(\Lambda)},P\big],P\big]v\Big). \tag{7.45}$$

In other words :

$$\forall\, P\in\mathscr{M},\ \nabla\mathcal{E}^0_{BDF}(P) = \big[\big[\Pi_\Lambda D_Q\Pi_\Lambda, P\big],P\big]. \tag{7.46}$$

Remark 7.10. The operator $[[\Pi_\Lambda D_Q\Pi_\Lambda, P],P]$ is the "projection" of $\Pi_\Lambda D_Q\Pi_\Lambda$ onto $\mathrm{T}_P\mathscr{M}$.

In [Sok14d], we proved that $\mathscr{M}_{\mathscr{C}}$ is a submanifold of $\mathscr{M}$. We recall that the notations $\mathscr{Y}$, Y are specified in Notation 7.5.

Proposition 7.5. *The sets $\mathscr{M}_{\mathscr{I}}$ and $\mathscr{W}$ are* submanifolds *of $\mathscr{M}$, which are* invariant *under the flow of $\mathcal{E}^0_{BDF}$. The following holds : for any $P\in\mathscr{M}_{\mathscr{Y}}$, writing*

$$\mathfrak{m}_P^{\mathscr{Y}} = \{a\in\mathfrak{m}_P,\ \mathrm{Y}a\mathrm{Y}^{-1} = a\}, \tag{7.47}$$

we have

$$\mathrm{T}_P\mathscr{M}_{\mathscr{Y}} = \{[a,P],\ a\in\mathfrak{m}_P^{\mathscr{Y}}\} = \{v\in\mathrm{T}_P\mathscr{M},\ -\mathrm{Y}v\mathrm{Y}^{-1} = v\}. \tag{7.48}$$

Furthermore, for any $P\in\mathscr{M}_{\mathscr{Y}}$ we have $\rho_{P-\mathcal{P}^0_-} = 0$.

For $P\in\mathscr{W}$, the same holds with

$$\begin{cases} \mathfrak{m}_P^{\mathscr{W}} & := & \big\{a\in\mathfrak{m}_P^{\mathscr{C}},\ \forall\, U\in\mathbf{S},\ UaU^{-1} = a\big\}, \\ \mathrm{T}_P\mathscr{W} & := & \big\{[a,P],\ a\in\mathfrak{m}_P^{\mathscr{W}}\big\}. \end{cases}$$

Remark 7.11 (Lagrangians)*.* The operator $\mathrm{I_s}$ induced a symplectic structure on the *real* Hilbert space $(\mathfrak{H}_\Lambda, \mathfrak{Re}\langle\cdot\,,\,\cdot\rangle_{\mathfrak{H}})$:

$$\forall\, f,g\in\mathfrak{H}_\Lambda,\ \omega_{\rm I}(f,g) := \mathfrak{Re}\langle f\,,\,\mathrm{I_s}g\rangle.$$

The manifold $\mathscr{M}_{\mathscr{I}}$ is constituted by *Lagrangians* of $\omega_{\rm I}$ that are in $\mathscr{M}$.

We end this section by stating technical results.

7.2.3 Form of trial states

The following Theorem is stated in [HLS09, Appendix] and proved in [Sok14d].

Theorem 7.3 (Form of trial states)**.** *Let P_1,P_0 be in $\mathscr{N}$ and $Q = P_1 - P_0$. Then there exist $M_+, M_-\in\mathbb{Z}_+$ such that there exist two orthonormal families*

$$\begin{array}{ll} (a_1,\dots,a_{M_+})\cup(e_i)_{i\in\mathbb{N}} & \text{in } \mathrm{Ran}\,\mathcal{P}^0_+, \\ (a_{-1},\dots,a_{-M_+})\cup(e_{-i})_{i\in\mathbb{N}} & \text{in } \mathrm{Ran}\,\mathcal{P}^0_-, \end{array}$$

and a nonincreasing sequence $(\lambda_i)_{i\in\mathbb{N}}\in\ell^2$ satisfying the following properties :

1. *The a_i's are eigenvectors for Q with eigenvalue 1 (resp. -1) if $i>0$ (resp. $i<0$).*

2. *For each* $i \in \mathbb{N}$ *the plane* $\Pi_i := Span(e_i, e_{-i})$ *is spanned by two eigenvectors* f_i *and* f_{-i} *for* Q *with eigenvalues* λ_i *and* $-\lambda_i$.
3. *The plane* Π_i *is also spanned by two orthogonal vectors* v_i *in* $\mathrm{Ran}(1-P)$ *and* v_{-i} *in* $\mathrm{Ran}(P)$. *Moreover* $\lambda_i = \sin(\theta_i)$ *where* $\theta_i \in (0, \frac{\pi}{2})$ *is the angle between the two lines* $\mathbb{C}v_i$ *and* $\mathbb{C}e_i$.
4. *There holds :*

$$Q = \sum_i^{M_+} |a_i\rangle\langle a_i| - \sum_i^{M_-} |a_{-i}\rangle\langle a_{-i}| + \sum_{j\in\mathbb{N}} \lambda_j(|f_j\rangle\langle f_j| - |f_{-j}\rangle\langle f_{-j}|).$$

Remark 7.12. We have

$$\begin{aligned} Q^{++} &= \sum_i^{M_+} |a_i\rangle\langle a_i| + \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 |e_j\rangle\langle e_j|, \\ Q^{--} &= -\sum_i^{M_-} |a_{-i}\rangle\langle a_{-i}| - \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 |e_{-j}\rangle\langle e_{-j}|. \end{aligned} \tag{7.49}$$

Thanks to Theorem 7.3, it is possible to characterize states in $\mathscr{M}_{\mathscr{Y}}$ and $\mathscr{W}$. We restate a proposition of [Sok14d] and add the case of $\mathrm{I_s}$.

Proposition 7.6. *Let* $\gamma = P - \mathcal{P}^0_-$ *be in* $\mathscr{M}_{\mathscr{Y}}$. *For* $-1 \le \mu \le 1$ *and* $X \in \{\gamma, \gamma^2\}$, *we write*

$$E^X_\mu = \mathrm{Ker}(X - \mu).$$

Then for any $\mu \in \sigma(\gamma)$, $\mathrm{Y}E^\gamma_\mu = E^\gamma_{-\mu}$. *Moreover for* $|\mu| < 1$ *if we decompose* $E^\gamma_\mu \oplus E^\gamma_{-\mu}$ *into a sum of planes* Π *as in Theorem 7.3, then*

1. *If* $\mathrm{Y} = \mathrm{I_s}$, *then we can choose the* Π*'s to be* $\mathrm{I_s}$*-invariant.*
2. *If* $\mathrm{Y} = \mathrm{C}$, *then each* Π *is* not C*-invariant and* $\mathrm{Dim}\, E^\gamma_\mu$ *is even.*

   Equivalently Dim $E^{\gamma^2}_{\mu^2}$ *is divisible by* 4. *Moreover there exists a decomposition*

$$E^{\gamma^2}_{\mu^2} = \overset{\perp}{\bigoplus_{1\le j\le \frac{N}{2}}} V_{\mu,j} \text{ and } V_{\mu,j} = \Pi^a_{\mu,j} \overset{\perp}{\oplus} \mathrm{C}\Pi^a_{\mu,j}$$

   where the $\Pi^a_{\mu,j}$*'s and* $\mathrm{C}\Pi^a_{\mu,j}$*'s are spectral planes described in Theorem 7.3.*

7.2.4 The Cauchy expansion

In this part, we introduce a useful trick in the model. The Cauchy expansion (7.54) is an application of functional calculus : we refer the reader to [HLS05a, Sok14b] for further details.

We assume $Q_0 \in \mathfrak{S}_2$ with

$$\alpha \| |\mathcal{D}^0|^{1/2} Q_0 \|_{\mathfrak{S}_2} \ll 1. \tag{7.50}$$

We recall the following inequality, proved in [Sok14b]

$$\forall\, Q_0 \in \mathfrak{S}_2,\ \| R_{Q_0} \tfrac{1}{|\nabla|^{1/2}} \|^2_{\mathfrak{S}_2} \lesssim \|Q\|^2_{\mathrm{Ex}} \lesssim \iint |p+q| |\widehat{Q}(p,q)|^2 dpdq, \tag{7.51}$$

From now on, we only deal with Q_0 whose density vanishes : $\rho_{Q_0} = 0$. The mean-field operator $D^{(\Lambda)}_{Q_0}$ is away from 0 thanks to (7.50). Indeed, there holds

$$\begin{aligned} |\Pi_\Lambda R_{Q_0} \Pi_\Lambda|^2 &\le |\nabla|^{1/2} \frac{\Pi_\Lambda}{|\nabla|^{1/2}} R^*_{Q_0} R_{Q_0} \frac{\Pi_\Lambda}{|\nabla|^{1/2}} |\nabla|^{1/2} \\ &\le \Pi_\Lambda |\nabla| \| \tfrac{1}{|\nabla|^{1/2}} R_{Q_0} \|^2_{\mathcal{B}} \\ &\lesssim \Pi_\Lambda |\nabla| \|Q_0\|_{\mathrm{Ex}} \lesssim |\mathcal{D}^0|^2 \|Q_0\|^2_{\mathrm{Ex}}, \end{aligned}$$

thus

$$|D^{(\Lambda)}_{Q_0}| \gtrsim |\mathcal{D}^0|\big(1-\alpha K\|Q_0\|_{\rm Ex}\big). \tag{7.52}$$

The Cauchy expansion gives an expression of

$$\gamma_0 := \chi_{(-\infty,0)}\big(D^{(\Lambda)}_{Q_0}\big) - \mathcal{P}^0_- := \overline{\boldsymbol{\pi}}_0.$$

We have [HLS05a]

$$\chi_{(-\infty,0)}\big(D^{(\Lambda)}_{Q_0}\big) - \mathcal{P}^0_- = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\mathcal{D}^0+i\omega}\big(\alpha\Pi_\Lambda R_{Q_n}\Pi_\Lambda\big)\frac{1}{D_{Q_0}+i\omega}\Pi_\Lambda. \tag{7.53}$$

We also expand in power of $Y[Q_0] := -\alpha\Pi_\Lambda R_{Q_0}\Pi_\Lambda$:

$$\begin{cases} \boldsymbol{\pi}^n_- - \mathcal{P}^0_- &= \displaystyle\sum_{j\geq 1}\alpha^j M_j[Y[Q_0]],\\ M_j[Y_n] &= \displaystyle -\frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\mathcal{D}^0+i\omega}\Big(Y_n\frac{1}{\mathcal{D}^0+i\omega}\Big)^j. \end{cases} \tag{7.54}$$

Each $M_j[Y[Q_0]]$ is polynomial in $\Pi_\Lambda R_{Q_0}\Pi_\Lambda$ of degree j.

By using (7.51), the decomposition (7.54) is well-defined in several Banach space, provided that $\alpha\|Q_0\|_{\rm Ex}$ is small enough.

– First, integrating the norm of bounded operator in (7.53), we obtain

$$\|\overline{\boldsymbol{\pi}}_0 - \mathcal{P}^0_-\|_{\mathcal{B}} \lesssim \alpha\|Q_0\|_{\rm Ex} < 1.$$

– We take the Hilbert-Schmidt norm [HLS05a, Sok14b] : we get

$$\|\gamma_0\|_{\mathfrak{S}_2} \lesssim \alpha\|Q_0\|_{\rm Ex}. \tag{7.55}$$

– We take the norm $\||\mathcal{D}^0|^{1/2}(\cdot)\|_{\mathfrak{S}_2}$ we get the rough estimate

$$\||\mathcal{D}^0|^{1/2}\gamma_0\|_{\mathfrak{S}_2} \lesssim \min\big(\sqrt{L\alpha}\|Q_0\|_{\rm Ex}, \alpha\|R_{Q_0}\|_{\mathfrak{S}_2}\big) + \alpha^2\|Q_0\|^2_{\rm Ex}. \tag{7.56}$$

Remark 7.13. The same estimates holds for the differential of $Q_0 \mapsto \gamma_0$, for sufficiently small α. As shown in [Sok14b], the upper bound of each norm is a power series of kind

$$\|\gamma_0\| \leq \alpha\|M_1[Y[Q_0]]\| + \sum_{j=1}^{+\infty}\sqrt{j}\alpha^j\big(K\|Q_0\|_{\rm Ex}\big)^j.$$

In the case of the differential, we get an upper bound of kind

$$\|{\rm d}\gamma_0\| \leq \alpha\|M_1[Y[Q_0]]\| + \sum_{j=1}^{+\infty}j^{3/2}\alpha^j\big(K\|Q_0\|_{\rm Ex}\big)^j.$$

The power series converge for sufficiently small $\alpha\|Q_0\|_{\rm Ex}$.

– It is also possible to consider other norms, using from the fact that a (scalar) Fourier multiplier $F(\mathbf{p}-\mathbf{q}) = F(-i\nabla_x + i\nabla_y)$ commutes with the operator $R[\cdot] : Q(x,y) \mapsto \frac{Q(x,y)}{|x-y|}$. We can also consider the norm

$$\|Q_0\|^2_w := \iint w(p-q)(\widetilde{E}\,(p)+\widetilde{E}\,(q))|\widehat{Q}_0(p,q)|^2 dpdq,$$

where $w(\cdot)\geq 0$ is any weight satisfying a subadditive condition [Sok14b] :

$$\forall\, p,q\in\mathbb{R}^3,\ \sqrt{w(p+q)} \leq K(w)\big(\sqrt{w(p)}+\sqrt{w(q)}\big).$$

7.3 Proof of Theorems 7.1 and 7.2

7.3.1 Strategy and tools of the proof : the dipositronium

Topologies

The existence of a minimizer over $\mathscr{W}_{\mathbf{t}X^\ell}$ (with $\mathbf{t} \in \mathbb{Z}_2^2$) is proved with the same method used in [Sok14d].

We use a lemma of Borwein and Preiss [BP87, HLS09], a smooth generalization of Ekeland's Lemma [Eke74] : we study the behaviour of a specific minimizing sequence $(P_n)_n$ or equivalently $(P_n - \mathcal{P}_-^0 =: Q_n)_n$.

This sequence satisfies an equation close to the one satisfied by a real minimizer and we show this equation remains in some weak limit.

Remark 7.14. We recall different topologies over bounded operator, besides the norm topology $\|\cdot\|_{\mathcal{B}}$ [RS75].

1. The so-called *strong topology*, the weakest topology $\mathcal{T}_s$ such that for any $f \in \mathfrak{H}_\Lambda$, the map
$$\begin{array}{ccc} \mathcal{B}(\mathfrak{H}_\Lambda) & \longrightarrow & \mathfrak{H}_\Lambda \\ A & \mapsto & Af \end{array}$$
is continuous.
2. The so-called *weak operator topology*, the weakest topology $\mathcal{T}_{w.o.}$ such that for any $f, g \in \mathfrak{H}_\Lambda$, the map
$$\begin{array}{ccc} \mathcal{B}(\mathfrak{H}_\Lambda) & \longrightarrow & \mathbb{C} \\ A & \mapsto & \langle Af\,,\,g\rangle \end{array}$$
is continuous.

We can also endow $\mathfrak{S}_1^{\mathcal{P}_-^0}$ with its weak-$*$ topology, the weakest topology such that the following maps are continuous :
$$\left|\begin{array}{l} \begin{array}{ccc} \mathfrak{S}_1^{\mathcal{P}_-^0} & \longrightarrow & \mathbb{C} \\ Q & \mapsto & \mathrm{Tr}\big(A_0(Q^{++}+Q^{--}) + A_2(Q^{+-}+Q^{-+})\big) \end{array} \\ \forall\,(A_0, A_2) \in \mathrm{Comp}(\mathfrak{H}_\Lambda) \times \mathfrak{S}_2(\mathfrak{H}_\Lambda). \end{array}\right.$$

Lemma 7.2. *The set $\mathcal{K}_{\mathscr{Y}}^0$, defined in* (7.40)*, is weakly-$*$ sequentially closed in $\mathfrak{S}_1^{\mathcal{P}_-^0}(\mathfrak{H}_\Lambda)$.*

Remark 7.15. This Lemma was stated for $\mathscr{Y} = \mathscr{C}$ in [Sok14d]. For $\mathscr{Y} = \mathscr{I}$ the proof is the same and we refer the reader to this paper.

The Borwein and Preiss Lemma

We recall this Theorem as stated in [HLS09] :

Theorem 7.4. *Let $\mathcal{M}$ be a closed subset of a Hilbert space $\mathcal{H}$, and $F : \mathcal{M} \to (-\infty, +\infty]$ be a lower semi-continuous function that is bounded from below and not identical to $+\infty$. For all $\varepsilon > 0$ and all $u \in \mathcal{M}$ such that $F(u) < \inf_{\mathcal{M}} + \varepsilon^2$, there exist $v \in \mathcal{M}$ and $w \in \overline{\mathrm{Conv}(\mathcal{M})}$ such that*

1. *$F(v) < \inf_{\mathcal{M}} + \varepsilon^2$,*
2. *$\|u - v\|_{\mathcal{H}} < \sqrt{\varepsilon}$ and $\|v - w\|_{\mathcal{H}} < \sqrt{\varepsilon}$,*
3. *$F(v) + \varepsilon\|v - w\|_{\mathcal{H}}^2 = \min\big\{F(z) + \varepsilon\|z - w\|_{\mathcal{H}}^2,\ z \in \mathcal{M}\big\}$.*

– Here we apply this Theorem with $\mathcal{H} = \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, $\mathcal{M} = \mathscr{W}_{p(X)} - \mathcal{P}_-^0$ and $F = \mathcal{E}_{\mathrm{BDF}}^0$.

The BDF energy is continuous in the $\mathfrak{S}_1^{\mathcal{P}_-^0}$-norm topology, thus its restriction over $\mathscr{V}$ is continuous in the $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$-norm topology.

This subspace $\mathcal{H}$ is closed in the Hilbert-Schmidt norm topology because $\mathscr{V} = \mathscr{M}_{\mathscr{C}}$ is closed in $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ and $\mathscr{E}_{-1} - \mathcal{P}_-^0$ is closed in $\mathscr{V}$.

Moreover, we have
$$\overline{\mathrm{Conv}(\mathscr{W}_{p(X)} - \mathcal{P}_-^0)}^{\mathfrak{S}_2} \subset \mathcal{K}_{\mathscr{C}}^0.$$

– For every $\eta > 0$, we get a projector $P_\eta \in \mathscr{W}_{p(X)}$ and $A_\eta \in \mathcal{K}^0_{\mathscr{C}}$ such that P that minimizes the functional $F_\eta : P \in \mathscr{E}_{-1} \mapsto \mathcal{E}^0_{\mathrm{BDF}}(P - \mathcal{P}^0_-) + \varepsilon \| P - \mathcal{P}^0_- - A_\eta \|^2_{\mathfrak{S}_2}$.

We write

$$Q_\eta := P_\eta - \mathcal{P}^0_-,\ \Gamma_\eta := Q_\eta - A_\eta,\ \widetilde{D}_{Q_\eta} := \Pi_\Lambda\big(\mathcal{D}^0 - \alpha R_{Q_\eta} + 2\eta\Gamma_\eta\big)\Pi_\Lambda. \tag{7.57}$$

Studying its differential on $\mathrm{T}_{P_\eta}\mathscr{W}$, we get :

$$\big[\widetilde{D}_{Q_\eta}, P_\eta\big] = 0. \tag{7.58}$$

In particular, by functional calculus, we have :

$$\big[\boldsymbol{\pi}^\eta_-, P_\eta\big] = 0,\ \boldsymbol{\pi}^-_\eta := \chi_{(-\infty,0)}(\widetilde{D}_{Q_\eta}). \tag{7.59}$$

We also write

$$\boldsymbol{\pi}^+_\eta := \chi_{(0,+\infty)}(\widetilde{D}_{Q_\eta}) = \Pi_\Lambda - \boldsymbol{\pi}^-_\eta. \tag{7.60}$$

We decompose $\mathfrak{H}_\Lambda$ as follows (here R means Ran) :

$$\mathfrak{H}_\Lambda = \mathrm{R}(P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}^-_\eta) \overset{\perp}{\oplus} \mathrm{R}(P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}^+_\eta) \overset{\perp}{\oplus} \mathrm{R}(\Pi_\Lambda - P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}^-_\eta) \overset{\perp}{\oplus} \mathrm{R}(\Pi_\Lambda - P_\eta) \cap \mathrm{R}(\boldsymbol{\pi}^+_\eta). \tag{7.61}$$

We will prove

1. $\mathrm{Ran}\, P \cap \mathrm{Ran}\, \boldsymbol{\pi}^+_\eta$ has dimension $2j+1$ and is invariant under Φ_{SU}, spanned by a unitary $\psi_\eta \in \mathfrak{H}_\Lambda$.
2. As η tends to 0, up to translation and a subsequence, $\psi_\eta \rightharpoonup \psi_a \neq 0$, $Q_\eta \rightharpoonup \overline{Q}$. There holds $\overline{P}_{j_0} = \overline{Q} + \mathcal{P}^0_- \in \mathscr{W}_{p(X)}$, ψ_a is a unitary eigenvector of $D^{(\Lambda)}_{\overline{Q}}$ and

$$\overline{Q} + \mathcal{P}^0_- = \chi_{(-\infty,0)}\big(D^{(\Lambda)}_{\overline{Q}}\big) + \mathrm{Proj}\, \Phi_{\mathrm{SU}}(\psi_a) - \mathrm{Proj}\, \Phi_{\mathrm{SU}}(\mathrm{C}\psi_a), \tag{7.62}$$

   where $\mathrm{Proj}\, E$ means the orthonormal projection onto the vector space E.

In the following part we write the spectral decomposition of trial states and prove Lemma 7.2.

Spectral decomposition

Let $(Q_n)_n$ be any minimizing sequence for $E^{nr}_{\mathbf{t}X^{(j_0-1/2)}}$ for $j_0 \in \frac{1}{2} + \mathbb{Z}_+$.

Thanks to the upper bound, $\mathrm{Dim}\,\mathrm{Ker}(Q_n - 1) = 1$, as shown in Subsection 7.3.2.

There exist a *non-increasing* sequence $(\lambda_{j;n})_{j\in\mathbb{N}} \in \ell^2$ of eigenvalues and an orthonormal family $\mathbf{B}_n$ of $\mathrm{Ran}\, Q_n$:

$$\mathbf{B}_n := (\psi_n, \mathrm{C}\psi_n) \cup (e^a_{j;n}, e^b_{j;n}, \mathrm{C}e^a_{j;n}, \mathrm{C}e^b_{j;n}),\ \mathcal{P}^0_-\psi_n = \mathcal{P}^0_- e^\star_{j;n} = 0,\ \star \in \{a,b\}, \tag{7.63}$$

such that the following holds. We omit the index n.

1. For any j, the vector spaces $V^\star_{j;n} := \Phi_{\mathrm{SU}}(e^\star_{j;n})$ are irreducible, and so is $V_{0;n} := \Phi_{\mathrm{SU}}(\psi_n)$.
2. That last one is of type $(\ell_0, \varepsilon(\mathbf{t}))$ (see Notation 7.8).
3. Moreover for any $j \in \mathbb{N}$ we write :

$$\left|\begin{array}{l} e^a_{-j} := -\mathrm{C}e^b_j \text{ and } e^b_{-j} := \mathrm{C}e^a_j, \\ V^a_{-j} := \Phi_{\mathrm{SU}}\, e^a_{-j} \text{ and } V^b_{-j} := \Phi_{\mathrm{SU}}\, e^b_{-j}. \end{array}\right. \tag{7.64a}$$

$$\begin{array}{rcl} f^\star_j & := & \sqrt{\frac{1-\lambda_j}{2}} e^\star_{-j} + \sqrt{\frac{1+\lambda_j}{2}} e^\star_j, \\ f^\star_{-j} & := & -\sqrt{\frac{1+\lambda_j}{2}} e^\star_{-j} + \sqrt{\frac{1+\lambda_j}{2}} e^\star_j, \end{array} \tag{7.64b}$$

and

$$\forall\, j \in \mathbb{Z}^*,\ F^\star_j := \Phi_{\mathrm{SU}}(f^\star_j). \tag{7.64c}$$

The trial state Q_n has the following form.

$$\left\{\begin{array}{rcl} Q_n & = & \mathrm{Proj}\, V_{0,n} - \mathrm{Proj}\, \mathrm{C}V_{0,n} + \sum_{j\geq 1} \lambda_j q_{j;n} \\ q_{j;n} & = & \mathrm{Proj}\, F^a_j - \mathrm{Proj}\, F^a_{-j} + \mathrm{Proj}\, F^b_j - \mathrm{Proj}\, F^b_{-j}. \end{array}\right. \tag{7.64d}$$

Remark 7.16. Thanks to the cut-off the sequences $(\psi_n)_n$ and $(e_{j;n})_n$ are H^1-bounded. Up to translation and extraction ($(n_k)_k \in \mathbb{N}^{\mathbb{N}}$ and $(x_{n_k})_k \in (\mathbb{R}^3)^{\mathbb{N}}$), we can assume that the weak limit of $(\psi_n)_n$ is non-zero (if it were then there would hold $E_{j_0,\varepsilon(\mathbf{t})} = 2m(2j_0+1)$).

We can consider the weak limit of each (e_n) : by means of a diagonal extraction, we assume that all the $(e_{j,n_k}(\cdot - x_{n_k}))_k$ and $(\psi_{j,n_k}(\cdot - x_{n_k}))_k$, converge along the same subsequence $(n_k)_k$. We also assume that

$$\forall\, j \in \mathbb{N},\ \lambda_{j,n_k} \to \mu_j,\ (\mu_j)_j \in \ell^2,\ (\mu_j)_j \text{ non-increasing,} \tag{7.65}$$

and that the above convergences also hold in L^2_{loc} and almost everywhere.

7.3.2 Upper bound and rough lower bound of $E_{j_0,\pm}$

We aim to prove the upper bound of Proposition 7.2. The method will also give a rough lower bound of $E_{j_0,\pm}$.

Notation 7.13. We write :

$$C(j_0) := j_0^2 \sup_{-j_0\le m\le j_0} \|\Psi_{m,j_0\pm\frac12}\|^4_{L^\infty},$$

where the functions $\Psi_{m,j_0\pm\frac12}$ are defined in [Tha92, p. 125] : they are the upper or lower spinors of the $\Phi^{\pm}_{m,\kappa_{j_0}}$'s.

For $E_{j_0,\varepsilon(\mathbf{t})}$, we only consider $\mathbf{t} \in \{(1,0);(0,1)\}$ and $\varepsilon(\mathbf{t})$ is defined in Notation 7.8.

– We consider trial state of the following form :

$$Q = \operatorname{Proj}\Phi_{\text{SU}}(\psi) - \operatorname{Proj}\Phi_{\text{SU}}(\mathrm{C}\psi),$$

where $\Phi_{\text{SU}}(\psi)$ is of type $(\ell_0 + \frac12, \varepsilon(\mathbf{t}))$ and $\mathcal{P}^0_-\psi = 0$. For short, we write

$$N_\psi := \operatorname{Proj}\Phi_{\text{SU}}(\psi) \text{ and } N_{\mathrm{C}\psi} := \operatorname{Proj}\Phi_{\text{SU}}(\mathrm{C}\psi).$$

The set of these states is written $\mathscr{W}^0_{\mathbf{t}X^{\ell_0}}$. We will prove that the energy of a particular Q gives the upper bound. The BDF energy of $Q \in \mathscr{W}^0_{\mathbf{t}X^{\ell_0}}$ is :

$$2\mathrm{Tr}\big(|\mathcal{D}^0|N_\psi\big) - \alpha\|N_\psi\|^2_{\text{Ex}} - \alpha\,\mathfrak{Re}\,\mathrm{Tr}\big(N_\psi R[N_{\mathrm{C}\psi}]\big). \tag{7.66}$$

– We will study the non-relativistic limit $\alpha \to 0$.

– To get an upper bound, we choose a specific trial state in $\mathscr{W}_{\mathbf{t}X^{\ell_0}}$, the idea is the same as in [Sok14b, Sok14d] : the trial state is written in (7.69). Before that, we precise the structure of elements in $\mathscr{W}^0_{\mathbf{t}X^{\ell_0}}$.

Minimizer for $E^{nr}_{\mathbf{t}X^{\ell_0}}$ By an easy scaling argument, there exists a minimizer for the non-relativistic energy $E^{nr}_{\mathbf{t}X^{\ell_0}}$ (7.26). The scaling argument enables us to say that this energy is negative. Then it is clear that a minimizing sequence converges to a minimizer $\overline{\Gamma}$, up to extraction. Writing

$$H_{\overline{\Gamma}} := -\Delta - R_{\overline{\Gamma}},$$

this minimizer satisfies the self-consistent equation

$$\big[H_{\overline{\Gamma}}, \overline{\Gamma}\big] = 0.$$

This comes from Remark 7.6. In particular, $H_{\overline{\Gamma}}$ restricted to $\operatorname{Ran}\Gamma$ is a homothety by some $-e^2 < 0$, so

$$\forall\,\psi \in \operatorname{Ran}\overline{\Gamma},\ \|\psi\|_{L^2} = 1,\ \|\Delta\psi\|_{L^2} \le \|R_{\overline{\Gamma}}\psi\|_{L^2} \lesssim \|\overline{\Gamma}\|_{\text{Ex}}\|\,|\nabla|^{1/2}\psi\|_{L^2},$$

and we get

$$\|\Delta\psi\|^{3/4}_{L^2} \lesssim \|\overline{\Gamma}\|_{\text{Ex}}\ \textit{i.e.}\ \|\Delta\psi\|_{L^2} \lesssim \|\overline{\Gamma}\|^{4/3}_{\text{Ex}} \lesssim (2j_0+1)^{2/3}.$$

The last estimate comes from a simple study of a minimizer for $E^{nr}_{\mathbf{t}X^{\ell_0}}$: we have

$$\mathrm{Tr}\big(-\Delta\overline{\Gamma}\big) - \frac{\pi}{2}\mathrm{Tr}\big(|\nabla|\overline{\Gamma}\big) \le \mathcal{E}_{nr}(\overline{\Gamma}) < 0,$$

thus $\mathrm{Tr}\big(-\Delta\overline{\Gamma}\big) \lesssim j_0^2$ and $\mathrm{Tr}\big((-\Delta)^2\overline{\Gamma}\big) \lesssim j_0^{5/2}$.

We end this bootstrap argument at $\||\nabla|^3\psi\|_{L^2}$ for $\psi \in \mathrm{Ran}\,\psi$: we have

$$|\nabla|^3\psi = \frac{-\Delta}{e^2-\Delta}\Big([|\nabla|, R_{\overline{\Gamma}}]\psi + R_{\overline{\Gamma}}\psi\Big),$$
$$\|\,|\nabla|^3\psi\|_{L^2} \lesssim \|\Delta\overline{\Gamma}\|_{\mathfrak{S}_2} + \|\nabla\overline{\Gamma}\|_{\mathfrak{S}_2} \lesssim j_0^{5/2}.$$

Trial state We take the following trial state. First, let $\overline{\Gamma} = \mathrm{Proj}\, ra_0(r)\Psi_{j_0, j_0+\varepsilon(\mathbf{t})\frac{1}{2}}$ be a minimizer for $E^{nr}_{\mathbf{t}X^{\ell_0}}$. We form

$$\overline{N}_+ := \mathrm{Proj}\,\Phi_{\mathrm{SU}}\,\mathcal{P}^0_+ U_{\lambda^{-1}}(ra_0(r)\Phi^+_{j_0,\varepsilon(\mathbf{t})(j_0+\frac{1}{2})}) \tag{7.67}$$

where we recall that

$$\lambda := \frac{g_1'(0)^2}{\alpha m} \text{ and } U_a\phi(x) := a^{3/2}\phi(ax),\ a>0.$$

This corresponds to dilating $\overline{\Gamma}$ by λ^{-1} and projecting the range of the dilation onto $\mathrm{Ran}\,\mathcal{P}^0_+$. Of course $\Gamma \in \mathfrak{S}_1(L^2(\mathbb{R}^3,\mathbb{C}^2))$ is embedded in $\mathfrak{S}_1(L^2(\mathbb{R}^3,\mathbb{C}^2\times\mathbb{C}^2))$ as follows :

$$\overline{\Gamma} \mapsto \begin{pmatrix}\overline{\Gamma} & 0\\ 0 & 0\end{pmatrix} \in \mathfrak{S}_1(L^2(\mathbb{R}^3,\mathbb{C}^2\times\mathbb{C}^2)).$$

Then we define

$$\overline{N}_- := \mathrm{C}\overline{N}_-\mathrm{C}^{-1} = \mathrm{C}\overline{N}_-\mathrm{C}. \tag{7.68}$$

Our trial state is

$$\overline{N} := \overline{N}_+ - \overline{N}_-. \tag{7.69}$$

Upper bound for $E_{j_0,\pm}$ We compute $\mathcal{E}^0_{\mathrm{BDF}}(\overline{N})$.

Before that, we study a general projector $\mathrm{Proj}\,\Phi_{\mathrm{SU}}\,\psi$ where $\mathcal{P}^0_-\psi = 0$ and $\Phi_{\mathrm{SU}}\,\psi$ irreducible of type $(j_0,\varepsilon(\mathbf{t}))$.

As an element of $\mathrm{Ran}\,\mathcal{P}^0_+$, the wave function ψ can be written

$$\psi = \mathcal{P}^0_+\begin{pmatrix}\varphi\\ 0\end{pmatrix}.$$

As it spans an irreducible representation of type $(j_0,\varepsilon(\mathbf{t}))$, we can choose

$$\forall\, x = r\omega_x \in \mathbb{R}^3,\ \varphi(x) := ia(r)\Psi^{j_0}_{j_0+\varepsilon(\mathbf{t})\frac{1}{2}}(\omega_x),\ a(r) \in L^2\big((0,\infty), r^2dr\big),$$

where we used notations of [Tha92, p. 126]. This corresponds to taking

$$\psi := \mathcal{P}^0_+ ra(r)\Phi^+_{j_0,\varepsilon(j_0+\frac{1}{2})},\ \varepsilon = \varepsilon(\mathbf{t}).$$

We recall the following formulae of [Tha92, pp. 125-127] (with $\boldsymbol{\omega} : x \mapsto \frac{x}{|x|}$)

$$\begin{aligned}&-i\boldsymbol{\alpha}\cdot\nabla = -i(\boldsymbol{\alpha}\cdot\boldsymbol{\omega})\partial_r + \tfrac{i}{r}(\boldsymbol{\alpha}\cdot\boldsymbol{\omega})(2\mathbf{S}\cdot\mathbf{L}),\\ &\big\{\mathbf{S}\cdot\mathbf{L}, \boldsymbol{\alpha}\cdot\boldsymbol{\omega}\big\} = -\boldsymbol{\alpha}\cdot\boldsymbol{\omega} \text{ and } i\boldsymbol{\sigma}\cdot\boldsymbol{\omega}\Psi^{m_j}_{j\pm\frac{1}{2}} = \Psi^{m_j}_{j\mp\frac{1}{2}}.\end{aligned} \tag{7.70}$$

This gives

$$\begin{aligned}\mathcal{P}^0_+ a(r)\Phi^+_{m,\varepsilon(\mathbf{t})(j_0+\frac{1}{2})} &= \frac{1}{2}\begin{pmatrix} i\big(1+\frac{g_0(|\nabla|)}{|\mathcal{D}^0|}\big)a(r)\Psi^m_{j_0+\varepsilon\frac{1}{2}}\\ \frac{g_1(|\nabla|)}{|\mathcal{D}^0||\nabla|}\big(\partial_r(a(r)) + \varepsilon(j_0+\frac{1}{2})\frac{a(r)}{r}\big)\Psi^m_{j_0-\varepsilon\frac{1}{2}}\end{pmatrix},\\ &=: \begin{pmatrix} ia_\uparrow(r)\Psi^m_{j_0+\varepsilon\frac{1}{2}}\\ a_\downarrow(\varepsilon,j_0;r)\Psi^m_{j_0-\varepsilon\frac{1}{2}}\end{pmatrix}.\end{aligned} \tag{7.71}$$

We write $\mathrm{Op} := \frac{g_1(|\nabla|)}{|\mathcal{D}^0||\nabla|}$: the following holds.

$$\left|\mathrm{Tr}\big(N_\psi R[N_{\mathrm{C}\psi}]\big)\right| \begin{array}{ll} \lesssim & j_0^2 \sup_m \|\Psi^m_{j_0\pm\frac12}\|^2_{L^\infty} \| \, |a_\uparrow a_\downarrow(\varepsilon, j_0, \cdot)|\|^2_{\mathcal{C}} \\ \lesssim & C(j_0) D\Big(|a_\uparrow|^2; |\mathrm{Op}\cdot\partial_r(a(r))|^2 + j_0^2|\mathrm{Op}\cdot r^{-1}a(r)|^2\Big), \\ \lesssim & C(j_0)\langle|\nabla|\psi\,,\,\psi\rangle\|\nabla\psi\|^2_{L^2} =: \mathcal{R}em_0(j_0,\psi). \end{array} \tag{7.72}$$

In fact, we have $\mathrm{Tr}\big(N_\psi R[N_{\mathrm{C}\psi}]\big) \geq 0$ by direct computation.

Let us deal with $\|N_\psi\|^2_{\mathrm{Ex}}$.

Notation 7.14. We write $P_\uparrow$ the projection onto the upper part of $\mathbb{C}^2\times\mathbb{C}^2$ and $P_\downarrow$ the projection onto the lower part. That is : $P_\uparrow\psi$ has no lower spinor and the same upper spinor as ψ.

Similarly,

$$\begin{aligned} \|N_\psi\|^2_{\mathrm{Ex}} - \|P_\uparrow N_\psi P_\uparrow\|^2_{\mathrm{Ex}} &= \mathrm{Tr}\big(P_\uparrow N_\psi P_\downarrow R_{N_\psi}\big) + \mathrm{Tr}\big(P_\downarrow N_\psi P_\uparrow R_{N_\psi}\big) \\ &\quad + \|P_\downarrow N_\psi P_\downarrow\|_{\mathrm{Ex}}, \\ &\lesssim \mathcal{R}em(j_0,\psi) + C(j_0)\|\nabla\psi\|^2_{L^2}\|\tfrac{|\nabla|^{3/2}}{|D_0|}\psi\|^2_{L^2}, \\ &=: \mathcal{R}em_1(j_0,\psi). \end{aligned}$$

For the trial state (7.69), this gives :

$$\begin{aligned} \|\overline{N}_+\|^2_{\mathrm{Ex}} &= \|P_\uparrow N_\psi P_\uparrow\|^2_{\mathrm{Ex}} + \mathcal{O}\Big(C(j_0)\big(\alpha^3 j_0 + \alpha^5 j_0^{5/3}\big)\Big) \\ &= \frac{\alpha m}{g_1'(0)^2}\|\overline{\Gamma}\|^2_{\mathrm{Ex}}(1+\mathcal{O}(\|\nabla\psi\|^2_{L^2})) \\ &\quad + \mathcal{O}\big(\|\tfrac{\Delta}{1-\Delta}\psi\|^2_{L^2}(\|\tfrac{|\nabla|^{5/2}}{1-\Delta}\psi\|_{L^2} + \|\nabla\psi\|^2_{L^2})\big), \\ &= \frac{\alpha m}{g_1'(0)^2}\|\overline{\Gamma}\|^2_{\mathrm{Ex}} \\ &\quad + \mathcal{O}\Big[C(j_0)\Big(\alpha^3 j_0^{5/3} + \inf_{0\leq s\leq 1}(\alpha^{4s}j_0^{4s/3})\big(\alpha^2 j_0^{2/3} + \inf_{2^{-1}\leq s\leq 1}(\alpha^{4s}j_0^{4s/3})\big)\Big)\Big]. \end{aligned}$$

We compute the kinetic energy as in [Sok14b, Sok14d] : we get

$$\begin{aligned} \mathrm{Tr}\big(|\mathcal{D}^0|\overline{N}_+\big) &= \frac{\alpha^2 m}{g_1'(0)^2}\mathrm{Tr}\big(-\Delta\overline{\Gamma}\big)\big(1+K\alpha\big) + \mathcal{O}\big(\alpha^4\mathrm{Tr}\big((\Delta)^2\overline{\Gamma}\big)\big), \\ &= \frac{\alpha^2 m}{g_1'(0)^2}\mathrm{Tr}\big(-\Delta\overline{\Gamma}\big) + \mathcal{O}\big(\alpha^3 j_0 + \alpha^4 j_0^{5/2}\big). \end{aligned}$$

This proves

$$\left| \begin{array}{l} E_{j_0,\varepsilon(\mathbf{t})} \leq 2m(2j_0+1) + \frac{\alpha^2 m}{g_1'(0)^2}E^{nr}_{\mathbf{t}X^{\ell_0}} + \mathcal{O}\big(\varrho(\alpha,j_0)\big) \\ \varrho(\alpha,j_0) := \alpha^3 j_0 + \alpha^4 j_0^{5/2} + C(j_0)\Big(\alpha^3 j_0^{5/3} + \inf_{0\leq s\leq 1}(\alpha^{4s}j_0^{4s/3})\big(\alpha^2 j_0^{2/3} + \inf_{2^{-1}\leq s\leq 1}(\alpha^{4s}j_0^{4s/3})\big)\Big). \end{array}\right. \tag{7.73}$$

First, by Kato's inequality (7.37), we have

$$\|N_\psi - N_{\mathrm{C}\psi}\|^2_{\mathrm{Ex}} \leq \frac{\pi}{2}\mathrm{Tr}\big(|\nabla|(N_\psi + N_{\mathrm{C}\psi})\big) = \pi\mathrm{Tr}\big(|\nabla|N_\psi\big).$$

So

$$\mathcal{E}^0_{\mathrm{BDF}}(Q) \geq 2\Big(\mathrm{Tr}\big(|\mathcal{D}^0|N_\psi\big) - \alpha\frac{\pi}{2}\mathrm{Tr}\big(|\nabla|N_\psi\big)\Big) =: 2\big((2j_0+1)m + \mathcal{F}(N_\psi)\big).$$

As α tends to 0, a minimizer over $\mathscr{W}^0_{\mathbf{t}X^{\ell_0}}$ should be localized in Fourier space around 0. Indeed, for α, L sufficiently small, we have

$$\forall\, p\in B(0,\Lambda),\ \widetilde{E}\,(p) - m = \frac{g_0(p)^2 - m^2 + g_1(p)^2}{\widetilde{E}\,(p)+m} \geq \frac{p^2}{2\|g_0\|_{L^\infty}|D_0|},$$

and for any $0 < s \leq 2$:

$$\frac{p^2}{2\|g_0\|_{L^\infty}|D_0|} \geq s\frac{\alpha\pi}{2}|p| \iff |p| \geq \frac{\alpha s\pi\|g_0\|_{L^\infty}}{\sqrt{1-(\alpha s\pi\|g_0\|_{L^\infty})^2}} =: \vartheta_s.$$

We get

$$2\mathcal{F}\big(\Pi_{\vartheta_1}N_\psi\Pi_{\vartheta_1}\big) \leq \mathcal{E}^0_{\rm BDF}(Q) - 2(2j_0+1)m.$$

By Cauchy-Schwartz inequality, we get a rough lower bound

$$\mathrm{Tr}\big(-\Delta\Pi_{\vartheta_1}N_\psi\Pi_{\vartheta_1}\big) \lesssim \alpha^2(2j_0+1) \text{ and } \mathcal{E}^0_{\rm BDF}(Q) - 2(2j_0+1)m \gtrsim -\alpha^2(2j_0+1).$$

For an almost minimizer Q, the same argument shows that

$$\mathrm{Tr}\big(\frac{-\Delta}{|\mathcal{D}^0|}Q^2\big) \lesssim \alpha^2(2j_0+1). \tag{7.74}$$

A precise lower bound is obtained once we know that there exists a minimizer $\overline{P}_{j_0}$. This state satisfies the self-consistent equation (7.62) : see Subsection 7.3.5.

Remark 7.17. The same method can be used to get an upper bound of $E^{nr}_{p(X)}$ for any $p(X) = \sum_{\ell=0}^{\ell_0}\mathbf{t}_\ell X^\ell$. By scaling we have $E^{nr}_{p(X)} < 0$.

7.3.3 Strategy of the proof : the para-positronium

The method is more subtle because $\mathscr{M}_{\mathscr{I}}$ has only one connected component. We first consider the subset $\mathscr{M}^1_{\mathscr{I}}$ defined by :

$$\mathscr{M}^1_{\mathscr{I}} = \big\{P_\psi := \mathcal{P}^0_- + |\psi\rangle\langle\psi| - |\mathrm{I_s}\psi\rangle\langle\mathrm{I_s}\psi|,\ \psi \in \mathbb{S}\mathrm{Ran}\,\mathcal{P}^0_+\big\}. \tag{7.75}$$

Lemma 7.3. *Let $F_{\mathscr{I}}$ be the infimum of the BDF energy over $\mathscr{M}^1_{\mathscr{I}}$. Then we have*

$$F_{\mathscr{I}} \geq 2m - \alpha^2\frac{E_{\rm PT}(1)m}{g_1'(0)^2} + \mathcal{O}(\alpha^3). \tag{7.76}$$

We will prove the existence of a critical point in the neighbourhood of $\mathscr{M}^1_{\mathscr{I}}$ *via* a mountain pass argument. In this part, we aim to prove the following Proposition.

Proposition 7.7. *1. In the regime of Theorem 7.1, there exists a bounded sequence in $\mathscr{M}_{\mathscr{I}} - \mathcal{P}^0_-$ of almost critical points : $(Q_n = P_n - \mathcal{P}^0_-)_n$ such that*

$$\lim_{n\to+\infty}\|\nabla\mathcal{E}^0_{BDF}(P_n)\|_{\mathfrak{S}_2} = 0 \text{ with } \mathcal{E}^0_{BDF}(Q_n) = 2m - \frac{\alpha^2 m}{g_1'(0)^2}E_{PT}(1) + \mathcal{O}(\alpha^3).$$

Furthermore, for sufficiently big n, there exists $\psi_{a;n}$ such that

$$\mathbb{C}\psi_{a;n} = \mathrm{Ran}\,P_n \cap \mathrm{Ran}\,\chi_{(0,+\infty)}\big(D^{(\Lambda)}_{Q_n} - \nabla\mathcal{E}^0_{BDF}(P_n)\big)$$

and $P_n = \chi_{(-\infty,0)}\big(D^{(\Lambda)}_{Q_n} - \nabla\mathcal{E}^0_{BDF}(P_n)\big) + |\psi_{a;n}\rangle\langle\psi_{a;n}| - |\mathrm{I_s}\psi_{a;n}\rangle\langle\mathrm{I_s}\psi_{a;n}|$.
2. Up to a subsequence and up to translation the sequence tends to a critical point Q_∞ of $\mathcal{E}^0_{BDF}$ in $\mathscr{M}_{\mathscr{I}} - \mathcal{P}^0_-$. Moreover, writing $\overline{P} = Q_\infty + \mathcal{P}^0_-$, there exists $0 < \mu < m$ and $\psi_a \in \mathbb{S}\,\mathfrak{H}_\Lambda$ such that

$$\begin{cases} \overline{P} &= \chi_{(-\infty,0)}(D^{(\Lambda)}_{Q_\infty}) + |\psi_a\rangle\langle\psi_a| - |\mathrm{I_s}\psi_a\rangle\langle\mathrm{I_s}\psi_a|, \\ \mathbb{C}\psi_a &= \mathrm{Ker}\big(D^{(\Lambda)}_{Q_\infty} - \mu\big), \\ \inf\sigma(|D^{(\Lambda)}_{Q_\infty}|) &= \mu. \end{cases} \tag{7.77}$$

Proof of Proposition 7.7 : first part For any $\psi \in \mathbb{S}\mathrm{Ran}\,\mathcal{P}^0_+$, we define :

$$c_\psi : \begin{array}{ccl} [0,1] & \longrightarrow & \mathscr{M}_{\mathscr{I}} - \mathcal{P}^0_- \\ s & \mapsto & |\sin(\pi s)\psi + \cos(\pi s)\mathrm{I_s}\psi\rangle\langle \sin(\pi s)\psi + \cos(\pi s)\mathrm{I_s}\psi| - |\mathrm{I_s}\psi\rangle\langle\mathrm{I_s}\psi|. \end{array} \tag{7.78}$$

Remark 7.18. The loop $c_\psi + \mathcal{P}^0_-$ crosses $\mathscr{M}^1_{\mathscr{I}}$ at $t_0 = \frac{1}{2}$ where the BDF energy is maximal :

$$\sup_{s\in[0,1]} \mathcal{E}^0_{\mathrm{BDF}}(c(s)).$$

Indeed, there holds

$$\mathcal{E}^0_{\mathrm{BDF}}(c(s)) = 2\sin(\pi s)^2 \langle |\mathcal{D}^0|\psi\,,\,\psi\rangle - \alpha\sin(\pi s)^2\big[D\big(|\psi|^2,|\psi|^2\big) + \cos(2\pi s) D\big(\psi^*\mathrm{I_s}\psi,\psi^*\mathrm{I_s}\psi\big)\big],$$

and the derivative with respect to s is :

$$\begin{aligned}\tfrac{d}{ds}\mathcal{E}^0_{\mathrm{BDF}}(c(s_0)) = 2\pi\sin(2\pi s_0)\Big(&\langle|\mathcal{D}^0|\psi\,,\,\psi\rangle - \tfrac{\alpha}{2}\big[D\big(|\psi|^2,|\psi|^2\big)\\ &+(\sin(\pi s_0)^2 - \tfrac{1}{2}\cos(2\pi s_0))\alpha D\big(\psi^*\mathrm{I_s}\psi,\psi^*\mathrm{I_s}\psi\big)\big]\Big).\end{aligned}$$

For sufficiently small α, this quantity vanishes only at $2\pi s_0 \equiv 0[\pi]$.

What happens when we apply the gradient flow $\Phi_{\mathrm{BDF},t}$ of the BDF energy ? The loop c_ψ is transformed into $c_t := \Phi_{\mathrm{BDF},t}(c_\psi)$ and we still have

$$c_t(s=0) = c_t(s=1) = 0.$$

This follows from the fact that $\mathcal{P}^0_-$ is the global minimizer of $\mathcal{E}^0_{\mathrm{BDF}}$.

We recall that for all $s\in[0,1]$, the function $c_t(s)$ satisfies the equation

$$\forall\, t_0\in\mathbb{R}_+,\ \frac{d}{dt}(c_{t_0}(s)) = -\nabla\mathcal{E}^0_{\mathrm{BDF}}(c_{t_0}(s)) \in \mathrm{T}_{c_{t_0}(s)+\mathcal{P}^0_-}\mathscr{M}_{\mathscr{I}}.$$

The non-trivial result holds.

Lemma 7.4. *Let $P_\psi \in \mathscr{M}^1_{\mathscr{I}}$ be a state whose energy is close to the infimum $F_{\mathscr{I}}$:*

$$\mathcal{E}^0_{BDF}\big(P_\psi\big) < F_{\mathscr{I}} + \alpha^3.$$

Let c_ψ be the loop associated to ψ (see (7.78)) and $c_t := \Phi_{BDF,t}(c_\psi)$. Then for all $t\in\mathbb{R}_+$, the loop c_t crosses the set $\mathscr{M}^1_{\mathscr{I}}$ at some $\widetilde{s}(t)\in(0,1)$.

Lemma 7.5. *Let $(c_t)_{t\geq 0}$ be the family of loops defined in Lemma 7.4 and let $(s(t))_{t\geq 0}$ be a family of reals in $(0,1)$ such that*

$$\forall\, t\geq 0,\ \mathcal{E}^0_{BDF}\big(c_t(s(t))\big) = \sup_{s\in[0,1]}\mathcal{E}^0_{BDF}(c_t(s)).$$

Then there exists an increasing sequence $(t_n)_{n\in\mathbb{N}}$ the sequence $(c_{t_n}(s(t_n)))_{n\geq 0}$ satisfies the first point of Proposition 7.7

We prove Lemmas 7.3 and 7.4 in Subsection 7.3.6. We assume they are true to prove Lemma 7.5 and Proposition 7.7.

Remark 7.19. The proof of Lemma 7.4 uses an index argument. We kept it elementary but it is possible to rephrase it in terms of the Maslov index [Fur04] once we notice that $\mathrm{I_s}$ induces a symplectic structure and that the projectors in $\mathscr{M}_{\mathscr{I}}$ are Lagrangians (see Remark 7.11).

Spectral decomposition of P_n We define

$$F_1 := \liminf_{t\to+\infty} \mathcal{E}^0_{\rm BDF}(c_t(s(t))) = \liminf_{t\to+\infty} \sup_{s\in[0,1]} \mathcal{E}^0_{\rm BDF}(c_t(s)).$$

We assume $(t_n)_{n\geq 0}$ is a minimizing sequence for F_1.

We may assume that $\lim_{n\to+\infty} t_n = +\infty$.

– First we prove that along the path c_t the gradient $\nabla\mathcal{E}^0_{\rm BDF}$ (see (7.46)) is bounded in $\mathfrak{S}_2$. Indeed, for all $P = Q + \mathcal{P}^0_- \in \mathscr{M}$, we write

$$\widetilde{Q} := P - \chi_{(-\infty,0)}\big(\Pi_\Lambda D_Q \Pi_\Lambda\big),$$

We recall that $D_Q^{(\Lambda)} := \Pi_\Lambda D_Q \Pi_\Lambda$:

$$\begin{array}{rcl} \nabla\mathcal{E}^0_{\rm BDF}(P) & = & \big[\big[D_Q^\Lambda, P\big], P\big] = \big\{|D_Q^{(\Lambda)}|; \widetilde{Q}\big\} - 2\widetilde{Q}D_Q^{(\Lambda)}\widetilde{Q}, \\ \|\nabla\mathcal{E}^0_{\rm BDF}(P)\|_{\mathfrak{S}_2} & \lesssim & \|\widetilde{Q}\|_{\mathfrak{S}_2}\widetilde{E}\,(\Lambda)\Big[(1+\|Q\|_{\mathfrak{S}_2})(1+\|\widetilde{Q}\|_{\mathfrak{S}_2})\Big] \\ & \lesssim & K(\Lambda, F_1+\alpha^3). \end{array} \tag{7.79}$$

We have used the Cauchy expansion (7.54) to get an expression

$$\chi_{(-\infty,0)}\big(D_Q^{(\Lambda)}\big) - \mathcal{P}^0_- = \sum_{k=1}^{+\infty} \alpha^k M_k[Y[Q]]$$

where $M_k[Y[Q]]$ is a polynomial function of $\pi_\Lambda R_Q \Pi_\Lambda$ of degree k. We refer the reader to these papers or to (7.53)-(7.51) above for more details.

From formula (7.79) and Remark 7.13 we see that the gradient, as a function of Q is *locally Lipschitz*, at least in some ball $\{Q_0 :\ \||\mathcal{D}^0|^{1/2}Q_0\|_{\mathfrak{S}_2} \leq C_0\}$ in which there holds

$$\inf\sigma\big(|D_{Q_0}^{(\Lambda)}|\big) \geq K(C_0),$$

where C_0 is some constant. The Lipschitz constant depends on the constant C_0 and in the present case, we can take $C_0 \lesssim 1$.

Let us prove that

$$\lim_{n\to+\infty} \|\nabla\mathcal{E}^0_{\rm BDF}(c_{t_n}(s(t_n)))\|_{\mathfrak{S}_2} = 0. \tag{7.80}$$

If not, the $\limsup$ is bigger than some $\eta > 0$ and then we get a contradiction when we consider n_0 large enough such that

$$|F_1 - \mathcal{E}^0_{\rm BDF}(c_{t_{n_0}}(s(t_{n_0})))| \ll \eta \text{ and } \|\nabla\mathcal{E}^0_{\rm BDF}(c_{t_{n_0}}(s(t_{n_0})))\|_{\mathfrak{S}_2} \geq \frac{\eta}{2},$$

because

$$\forall\,\tau>0,\ \mathcal{E}^0_{\rm BDF}(c_{t_{n_0}+\tau}(s(t_{n_0}))) - \mathcal{E}^0_{\rm BDF}(c_{t_{n_0}}(s(t_{n_0}))) = -\int_0^\tau \|\nabla\mathcal{E}^0_{\rm BDF}(c_{t_{n_0}+u})(s_{t_{n_0}})\|^2_{\mathfrak{S}_2}du.$$

– We recall that the gradient at $P\in\mathscr{M}$ is the "projection" of the mean-field operator onto the tangent plane $\mathrm{T}_P\mathscr{M}$, in the sens that

$$\begin{array}{l} \forall\, v\in \mathrm{T}_P\mathscr{M}, PD_Q(1-P)\in\mathfrak{S}_1 \text{ and} \\ \qquad \mathrm{Tr}\big(PD_Q(1-P)v + (1-P)D_QPv\big) = \mathrm{Tr}\big(\nabla\mathcal{E}^0_{\rm BDF}\big) \end{array}$$

Notation 7.15. For short, we write

$$Q_n := c_{t_n}\big(s(t_n)\big) \text{ and } P_n := Q_n \text{ and } v_n := \nabla\mathcal{E}^0_{\rm BDF}(Q_n).$$

Moreover, we write

$$\widetilde{D}_{Q_n} := D_{Q_n} - v_n \text{ and } \widetilde{\boldsymbol{\pi}}_{-;n} := \chi_{(-\infty,0)}\big(D_{Q_n}^{(\Lambda)} - v_n\big).$$

We have shown that $\lim_{n\to+\infty}\|v_n\|_{\mathfrak{S}_2}=0$.

But as v_n is an element of the tangent plane $\mathrm{T}_{P_n}\mathscr{M}$, we have

$$\big[[v_n,P_n],P_n\big]=P_nv_n(1-P_n)+(1-P_n)v_nP_n=v_n$$

thus

$$\big[[D^{(\Lambda)}_{Q_n}-v_n,P_n],P_n\big]=0.$$

Equivalently, we have

$$\big[\widetilde{D}^{(\Lambda)}_{Q_n},P_n\big]=(1-P_n)\widetilde{D}^{(\Lambda)}_{Q_n}P_n-P_n\widetilde{D}^{(\Lambda)}_{Q_n}(1-P_n)=0. \tag{7.81}$$

Thus the projector P_n commutes with the distorted mean-field operator $\widetilde{D}_{Q_n}$. We recall that

$$\lim_n\|\widetilde{D}^{(\Lambda)}_{Q_n}-D^{(\Lambda)}_{Q_n}\|_{\mathfrak{S}_2}=0,$$

and thus up to taking n big enough, we can neglect the distortion v_n : all its Sobolev norms tend to zero as n tends to infinity *thanks to the cut-off*.

– Thanks to Lemma 7.3 we have the following energy condition :

$$2m+\mathcal{O}(\alpha^2)\le F_1\le\mathcal{E}^0_{\mathrm{BDF}}(Q_n)\le F_1+\alpha^3=2m+\mathcal{O}(\alpha^2).$$

Using the Cauchy expansion (7.53)-(7.51), we have

$$\|\,|\mathcal{D}^0|^{1/2}(\widetilde{\boldsymbol{\pi}}_{-;n}-\mathcal{P}^0_-)\|_{\mathfrak{S}_2}\lesssim\sqrt{L\alpha}\|Q_n\|_{\mathrm{Ex}}\lesssim\sqrt{L\alpha}.$$

Thus we get

$$\big|\|Q_n\|_{\mathfrak{S}_2}-\|P_n-\widetilde{\boldsymbol{\pi}}_{-;n}\|_{\mathfrak{S}_2}\big|\le\|\mathcal{P}^0_--\widetilde{\boldsymbol{\pi}}_{-;n}\|_{\mathfrak{S}_2}\lesssim\sqrt{L\alpha}.$$

As $\widetilde{D}_{Q_n}$ and P_n commutes, then necessarily $\|P_n-\widetilde{\boldsymbol{\pi}}_{-;n}\|^2_{\mathfrak{S}_2}$ is an integer equal to twice the dimension of $\mathrm{Ran}\,P_n\cap\mathrm{Ran}\,(1-\widetilde{\boldsymbol{\pi}}_{-;n})$.

But we know that

$$m\|Q_n\|^2_{\mathfrak{S}_2}\le\mathrm{Tr}\big(|\mathcal{D}^0|Q_n^2\big)\le\frac{1}{1-\alpha\frac{\pi}{4}}\mathcal{E}^0_{\mathrm{BDF}}(Q_n)\le\frac{2m}{1-\alpha\frac{\pi}{4}}=2m+\mathcal{O}(\alpha).$$

Then the above dimension is lesser than 1 and it cannot be 0 because of the energy condition

$$\mathcal{E}^0_{\mathrm{BDF}}(Q_n)\ge F_{\mathscr{I}}\ge 2m-K\alpha^2\gg\sqrt{L\alpha}.$$

This proves the first part of Proposition 7.7. We have $\mathrm{Ran}\,P_n\cap\mathrm{Ran}\,(1-\widetilde{\boldsymbol{\pi}}_{-;n})=\mathbb{C}\psi_{a;n}$ where $\psi_{a;n}$ is unitary. It is an eigenvector for $\widetilde{D}^{(\Lambda)}_{Q_n}$ with eigenvalue μ_n. From the equality :

$$\mathcal{E}^0_{\mathrm{BDF}}(Q_n)=\mathcal{E}^0_{\mathrm{BDF}}(\widetilde{\boldsymbol{\pi}}_{-;n}-\mathcal{P}^0_-)+2\mu_n-\frac{\alpha}{2}\iint\frac{|\psi_{a;n}\wedge\mathrm{I_s}\psi_{a;n}(x,y)|^2}{|x-y|}dxdy,$$

we get $0<\mu_n<m$. We end the proof as follows.

Proof of Proposition 7.7 : second part We follow the method of [Sok14d]. We recall the main steps and refer the reader to this paper for further details.

– The idea is simple : we must ensure that there exists a non-vanishing weak-limit and that this weak-limit is in fact a critical point.

Let us say that $\psi_{a;n}$ is associated to the eigenvalue μ_n.

– The condition of the energy ensures that the sequence $(\psi_{a;n})_n$ does not vanish in the sense that we *do not* have the following :

$$\forall\,A>0,\ \limsup_n\sup_{x\in\mathbb{R}^3}\int_{B(x,A)}|\psi_{a;n}|^2=0.$$

Up to translation and extraction of a subsequence, we may suppose that (Q_n) (resp. $(\psi_{a;n})$) converges in the weak topology of H^1 to $Q_\infty \neq 0$ (resp. $\psi_a \neq 0$). In particular these sequences also converge in L^2_{loc} and *a.e.* We recall that thanks to the cut-off and Kato's inequality (7.37) , we have $Q_n \in H^1(\mathbb{R}^3 \times \mathbb{R}^3)$ with

$$\||D_0|Q_n\|^2_{\mathfrak{S}_2} \leq \widetilde{E}\,(\Lambda)\,\||\mathcal{D}^0|^{1/2}Q_n\|^2_{\mathfrak{S}_2} \leq \frac{\widetilde{E}\,(\Lambda)}{1-\alpha\pi/4}\sup_n \mathcal{E}^0_{\mathrm{BDF}}(Q_n).$$

A similar estimate hold for $(\psi_{a;n})$. We also suppose that $\lim_n \mu_n = \mu_\infty$.
– As shown in [Sok14d], the operator R_{Q_n} converges in the strong operator topology to R_{Q_∞}. Thanks to the Cauchy expansion (7.54), we also have

$$\mathrm{s.}\lim_n \Big[\chi_{(-\infty,0)}\big(D^{(\Lambda)}_{Q_n} - \nabla\mathcal{E}^0_{\mathrm{BDF}}(P_n)\big) - \mathcal{P}^0_-\Big] = \chi_{(-\infty,0)}\big(D^{(\Lambda)}_{Q_\infty}\big) - \mathcal{P}^0_-.$$

By that strong convergence, we also have the weak-convergence of $\widetilde{D}^{(\Lambda)}_{Q_n}\psi_{a;n}$ to $D^{(\Lambda)}_{Q_\infty}\psi_a$ in L^2 and it follows that :

$$D^{(\Lambda)}_{Q_\infty}\psi_a = \mu_\infty\psi_a \neq 0.$$

– The condition of the energy ensures that for α sufficiently small, the $\psi_{a;n}$'s are close to a scaled Pekar minimizer : for any n, there exists a Pekar minimizer $\widetilde{\phi}_n$ such that

$$\|\psi_{a;n} - \lambda^{-3/2}\widetilde{\phi}_n(\lambda^{-1}(\cdot))\|^2_{H^1} \leq \alpha K \text{ where } \lambda := \frac{g_1'(0)^2}{\alpha m}.$$

The constant K depends on the energy estimate of Proposition 7.7.
– Thanks to that, for all n, μ_n is an isolated eigenvalue of $\widetilde{D}^{(\Lambda)}_{Q_n}$, uniformly in n : we have

$$\mathbb{C}\psi_{a;n} = \mathrm{Ker}\big(\widetilde{D}^{(\Lambda)}_{Q_n} - \mu_n\big),$$

and

$$\mathrm{dist}\Big(\mu_n; \sigma\big(\widetilde{D}^{(\Lambda)}_{Q_n}\big)\backslash\{\mu_n\}\Big) > K\alpha^2.$$

By functional calculus, we finally get the norm convergence of $(\psi_{a;n})_n$ to ψ_a in L^2.
– This proves that

$$\mathrm{s.}\lim_n P_n = \chi_{(-\infty,0)}\big(D^{(\Lambda)}_{Q_\infty}\big) + |\psi_a\rangle\langle\psi_a| - |\mathrm{I_s}\psi_a\rangle\langle\mathrm{I_s}\psi_a| \in \mathscr{M}_{\mathscr{I}},$$

and ends the proof.

7.3.4 Existence of a minimizer for $E_{j_0,\pm}$

We consider a family of almost minimizers $(P_{\eta_n})_n$ of type (7.57) where $(\eta_n)_n$ is any decreasing sequence. We also consider the spectral decomposition (7.64) of any
$Q_n := P_{\eta_n} - \mathcal{P}^0_-$.

For short we write $P_n := P_{\eta_n}$ and we replace the subscript η_n by n (for instance $\psi_n := \psi_{\eta_n}$). Moreover, we will often write ε instead of $\varepsilon(\mathbf{t})$.

We study weak limits of $(Q_n)_n$. We recall that Q_n can be written as follows :

$$\begin{cases} N_{+;n} = \mathcal{P}^0_+ N_{+;n} = \mathrm{Proj}\,\Phi_{\mathrm{SU}}\,\psi_{\eta_n} \text{ and } N_{-;n} = \mathrm{C}N_{+;n}\mathrm{C}, \\ Q_n = N_{+;n} - N_{-;n} + \gamma_n,\ \mathrm{Ran}\,N_{\pm;n} \cap \mathrm{Ker}\,\gamma_n = \{0\}. \end{cases} \tag{7.82}$$

We can suppose

$$\psi_n = \mathcal{P}^0_+ a_n(r)\Phi^+_{j_0,\varepsilon\mathbf{t}},\ a_n(r) \in \mathbb{S}L^2(\mathbb{R}_+, r^2dr).$$

Remark 7.20. The functions $\psi \in \mathrm{Ran}\,N_{\pm;n}$ are "almost" radial. We recall (7.71), giving

$$\left|\begin{array}{l} \forall\, x = r\omega_x \in \mathbb{R}^3,\ |\psi(x)| \leq \|\psi\|_{L^2}|s_n(r)|\|\Phi^\pm_{j_0,\pm(j_0+\frac12)}\|_{L^\infty}, \\ 4|s_n(r_0)|^2 := \big|(1+\frac{g_0(|\nabla|)}{|\mathcal{D}^0|})a_n\big|(r_0)^2 + \big|\frac{g_1(|\nabla|)}{|\nabla||\mathcal{D}^0|}(\partial_r a_n + \varepsilon\frac{a_n}{r})\big|(r_0)^2. \end{array}\right. \tag{7.83}$$

In particular by Newton's Theorem for radial function we have :

$$\forall\,\psi\in\mathrm{Ran}\,N_{\pm;n},\ |\psi|^2*\frac{1}{|\cdot|}(x_0)\le K(j_0)\frac{\|\psi\|_{L^2}^2}{|x_0|}. \tag{7.84}$$

– We first prove that there is no vanishing, that is

$$\exists A>0,\ \limsup_n \sup_{z\in\mathbb{R}^3}\int_{B(z,A)}|\psi_n(x)|^2dx>0.$$

Indeed, let assume this is false. Then using (7.84), it is clear that

$$\|N_{\pm;n}\|_{\mathrm{Ex}}^2\to 0,$$

and we get $\liminf\mathcal{E}^0_{\mathrm{BDF}}\ge 2(2j_0+1)m+\liminf\mathcal{E}^0_{\mathrm{BDF}}(\gamma_n)\ge 2(2j_0+1)m$, an inequality that is false as shown in the previous section.

Thus, we have : $Q_n\rightharpoonup Q_\infty\neq 0$.

– As the BDF energy is sequential weakly lower continuous [HLS05b], we have

$$E_{j_0,\varepsilon}\ge\mathcal{E}^0_{\mathrm{BDF}}(Q_\infty).$$

Our aim is to prove that $Q_\infty+\mathcal{P}^0_-\in\mathscr{W}_{\mathbf{t}X^{\ell_0}}$: in other words that Q_∞ is a minimizer for $E_{j_0,\varepsilon}$.

The spectral decomposition (7.82) is not the relevant one : let us prove we can describe P_n in function of the spectral spaces of the "mean-field operator" $\widetilde{D}_{Q_n}$: the first step is to prove (7.88) below.

We recall that Q_n satisfies Eq. (7.58), that we have the decomposition (7.61).

Using (7.74), we have for all ψ in $\mathbb{S}\mathrm{Ran}\,N_{+;n}$:

$$\begin{aligned}\langle\widetilde{D}_{Q_n}\psi\,,\,\psi\rangle-m&=\langle(|\mathcal{D}^0|-m)\psi\,,\,\psi\rangle-\langle(\alpha R_{Q_n}+2\eta_n\Gamma_n)\psi\,,\,\psi\rangle,\\&\gtrsim-\alpha\|Q_n\|_{\mathrm{Ex}}\|\,|\nabla|^{1/2}\psi\|_{L^2}-\end{aligned}$$
$$eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\gtrsim-\alpha^2(2j_0+1).$$

Thus $\mathrm{Ran}\,P_n\cap\mathrm{Ran}\,\boldsymbol{\pi}^n_+\neq\{0\}$.

– Let us prove this subspace has dimension $2j_0+1$: we use the minimizing property of Q_n. The condition on the first derivative gives (7.58). The estimation of the energy (from above and below) obtained in the previous section gives this result. Indeed, using the Cauchy expansion and the method of [Sok14b], we have

$$\left|\begin{array}{l}\sqrt{\mathrm{Tr}\big(|\mathcal{D}^0|\gamma_{vac;n}^2\big)}\lesssim\alpha(\|Q_n\|_{\mathrm{Ex}}+\eta_n\|\Gamma_n\|_{\mathfrak{S}_2})\lesssim\sqrt{L\alpha}\sqrt{\alpha j_0},\\ \gamma_{vac;n}:=\chi_{(-\infty,0)}\big(\widetilde{D}_{Q_n}\big)-\mathcal{P}^0_-.\end{array}\right. \tag{7.85}$$

The Cauchy expansion is explained in (7.53)-(7.54) below, we assume the above estimate for the moment (see (7.56)).

We write $Q_n=N_n+\overline{\gamma}_n$: there holds

$$\big|\|N_n\|_{\mathfrak{S}_2}^2-\|Q_n\|_{\mathfrak{S}_2}^2\big|\lesssim L^{1/2}\alpha(2j_0+1).$$

As $2(2j_0+1)\le\|Q_n\|_{\mathfrak{S}_2}^2\le 2(2j_0+1)\big(1-\alpha\pi/4\big)^{-1}$, then necessarily

$$\big|\|N_n\|_{\mathfrak{S}_2}^2-2(2j_0+1)\big|\lesssim\alpha(2j_0+1), \tag{7.86}$$

and for α sufficiently small, the upper bound is smaller than 4. This proves

$$\mathrm{Dim\,Ran}\,P_n\cap\mathrm{Ran}\,\boldsymbol{\pi}^n_+=2j_0+1.$$

Remark 7.21. There exists a unitary $\psi_{a;n}$ such that

$$\Phi_{\mathrm{SU}}\,\psi_{a;n} = \operatorname{Ran} P_n \cap \operatorname{Ran} \boldsymbol{\pi}^n_+.$$

We can assume that $\psi_{a;n} \in \operatorname{Ker}\big(\mathrm{J}_3 - j_0\big)$. Then we have

$$N_n := \operatorname{Proj} \Phi_{\mathrm{SU}}\,\psi_{a;n} - \operatorname{Proj} \Phi_{\mathrm{SU}}\,\mathrm{C}\psi_{a;n}. \tag{7.87}$$

Equivalently writing $\psi_{w;n} := \mathrm{C}\psi_{a;n}$ there holds $\Phi_{\mathrm{SU}}\,\psi_{w;n} = \operatorname{Ran}(1-P_n) \cap \operatorname{Ran} \boldsymbol{\pi}^n_-$.

– We have :

$$P_n = \operatorname{Proj} \Phi_{\mathrm{SU}}\,\psi_{a;n} - \operatorname{Proj} \Phi_{\mathrm{SU}}\,\psi_{w;n} + \boldsymbol{\pi}^n_-. \tag{7.88}$$

We thus write

$$Q_n = N_n + \gamma_{vac;n}. \tag{7.89}$$

As $\operatorname{Ran} P_n$ is $\widetilde{D}_{Q_n}$ invariant and that $\widetilde{D}_{Q_n}$ is bounded (with a bound that depends on Λ), necessarily

$$\widetilde{D}_{Q_n}\psi_{a;n} = \mu_n \psi_{a;n},\ \mu_n \in \mathbb{R}_+.$$

As in [Sok14d], studying the Hessian we have

$$m - \mu_n + 2\eta_n \geq 0.$$

– As for ψ_n, there is no vanishing for $(\psi_{a,n})_n$ for α sufficiently small : decomposing $\psi_+ \in \operatorname{Ran} P_n$:

$$\psi_+ = a\psi_{a;n} + \phi,\ \phi \in \operatorname{Ran} P_n \cap \operatorname{Ran} \boldsymbol{\pi}^n_-,$$

we have

$$|a|^2 \geq \frac{1}{\mu}\big(m + \langle|\widetilde{D}_{Q_n}|\phi\,,\,\phi\rangle - K(\alpha^2 j_0 + \eta_n \|\Gamma_n\|_{\mathfrak{S}_2})\big).$$

Provided that μ_n is close to m, the absence of vanishing for ψ_n implies that of $\psi_{a;n}$.

By Kato's inequality (7.37) :

$$\begin{aligned}\widetilde{D}^2_{Q_n} &\geq |\mathcal{D}^0|\big(1 - 2\alpha\|R_{Q_n}|\mathcal{D}^0|^{-1}\|_{\mathcal{B}} - 4\eta_n\|\Gamma_n\|_{\mathcal{B}}\big)|\mathcal{D}^0| \\ &\geq |\mathcal{D}^0|^2\big(1 - \alpha\|Q_n\|_{\mathrm{Ex}} - 4\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big)\end{aligned}$$

Thus

$$\big|\widetilde{D}_{Q_n}\big| \geq |\mathcal{D}^0|\big(1 - \alpha\|Q_n\|_{\mathrm{Ex}} - 2\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big) \text{ and } \mu_n \geq 1 - K(\alpha^2 j_0 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2}).$$

In the same way we can prove that

$$|\mu_n - m| \lesssim \alpha^2 j_0 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2}$$

So

$$\psi_{a,n} \rightharpoonup \psi_a \neq 0.$$

– We decompose $\gamma_{vac;n} = \boldsymbol{\pi}^n_- - \mathcal{P}^0_- \in \mathscr{W}_0 - \mathcal{P}^0_-$ as in (7.64) : using Cauchy's expansion (7.53)-(7.54), we have

$$\boldsymbol{\pi}^n_- - \mathcal{P}^0_- = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\omega}{\mathcal{D}^0 + i\omega}\big(2\eta_n\Gamma_n - \alpha\Pi_\Lambda R_{Q_n}\Pi_\Lambda + 2\eta_n\Gamma_n\big)\frac{1}{\widetilde{D}_{Q_n} + i\omega}\Pi_\Lambda. \tag{7.90}$$

To justify this equality, we remark that $|\widetilde{D}_{Q_n}|$ is uniformly bounded from below, it follows that the r.h.s. of (7.90) is well-defined provided that $\alpha \leq \alpha_{j_0}$:

$$\Pi_\Lambda R_{Q_n}\Pi_\Lambda^2 \lesssim |\nabla|\|Q_n\|^2_{\mathrm{Ex}} \lesssim \alpha(2j_0+1)|\nabla| \leq \alpha(2j_0+1)|\mathcal{D}^0|^2.$$

We must ensure that $\alpha\sqrt{\alpha(2j_0+1)}$ is sufficiently small.

Integrating the norm of bounded operator in (7.90), we obtain

$$\|\boldsymbol{\pi}^n_- - \mathcal{P}^0_-\|_{\mathcal{B}} \lesssim \alpha\|Q_n\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2} < 1.$$

We also expand in power of $Y_n := -\alpha\Pi_\Lambda R_{Q_n}\Pi_\Lambda + 2\eta_n\Gamma_n$ as in (7.54)

$$\boldsymbol{\pi}_-^n - \mathcal{P}_-^0 \quad = \quad \sum_{j\geq 1}\alpha^j M_j[Y_n]. \tag{7.91}$$

We have

$$\|\gamma_{vac;n}\|_{\mathfrak{S}_2} \lesssim \alpha\|Q_n\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2} \lesssim \alpha^2. \tag{7.92}$$

We take the norm $\||\mathcal{D}^0|^{1/2}(\cdot)\|_{\mathfrak{S}_2}$:

$$\||\mathcal{D}^0|^{1/2}\gamma_{vac;n}\|_{\mathfrak{S}_2} \lesssim \sqrt{L\alpha}\|Q_N\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2} \lesssim L^{1/2}\alpha j_0. \tag{7.93}$$

– We thus write

$$\gamma_{vac;n} \quad = \quad \sum_{j\geq 1}\lambda_{j;n}q_{j;n},$$

where $q_{j;n}$ has the same form as the one in (7.64).

Up to a subsequence, we may assume all weak convergence as in Remark (7.16) : the sequence of eigenvalues $(\lambda_{j;n})_n$ tends to $(\mu_j)_j \in \ell^2$ and each $(e_{j;n}^\star)_n$ (with $\star \in \{a, b\}$) tends to $e_{j;\infty}^\star$, $(\psi_{e;n})_n$ tends to ψ_e. We can also assume that the sequence $(\mu_n)_n$ tends to μ with $0 \leq \mu \leq m$.

Notation 7.16. For shot we write $\psi_v := \mathrm{C}\psi_e$.

Furthermore, we write $\overline{P} := Q_\infty + \mathcal{P}_-^0$ and $\boldsymbol{\pi} := \chi_{(-\infty,0)}(D_{Q_\infty}^{(\Lambda)})$.

– We will prove that

1. $\big[D_{Q_\infty}^{(\Lambda)}, \overline{P}\big] = 0,$
2. $D_{Q_\infty}^{(\Lambda)}\psi_a = \mu\psi_a$ and so $\overline{\boldsymbol{\pi}}\psi_a = 0$.

   Moreover $D_{Q_\infty}^{(\Lambda)}\mathrm{C}\psi_a = -\mu\mathrm{C}\psi_a$ and $\langle \mathrm{C}\psi_a\,,\,\psi_a\rangle = 0$.
3. $$\overline{\boldsymbol{\pi}} = \overline{P} - \mathrm{Proj}\,\Phi_{\mathrm{SU}}(\psi_a) + \mathrm{Proj}\,\Phi_{\mathrm{SU}}(\mathrm{C}\psi_a) =: \overline{P} - N. \tag{7.94}$$

These results follow from the strong convergence

$$\mathrm{s.}\lim_n R_{Q_n} = R_{Q_\infty}. \tag{7.95}$$

This fact enables us to show

$$\left|\begin{array}{l}\lim_n R_{Q_n}\psi_{a;n} = R_{Q_\infty}\psi_a \text{ in } L^2,\\ \mathrm{s.op.}\ \lim_n\big(\boldsymbol{\pi}_-^n - \mathcal{P}_-^0\big) = \overline{\boldsymbol{\pi}} - \mathcal{P}_-^0 \text{ in } \mathcal{B}(\mathfrak{H}_\Lambda),\\ \mathrm{w.op.}\ \lim_n P_n = \overline{\boldsymbol{\pi}} - \mathcal{P}_-^0 + \mathrm{Proj}\,\Phi_{\mathrm{SU}}\,\psi_a - \mathrm{Proj}\,\Phi_{\mathrm{SU}}\psi_w \text{ in } \mathcal{B}(\mathfrak{H}_\Lambda),\\ \lim_n \psi_{a;n} = \psi_a \text{ in } L^2.\end{array}\right. \tag{7.96}$$

Remark 7.22. We only write in this paper the proof of

$$R_{Q_n}\psi_{a;n} \underset{n\to+\infty}{\overset{L^2}{\longrightarrow}} R_{Q_\infty}\psi_a \text{ and } \psi_{a;n} \underset{n\to+\infty}{\overset{L^2}{\longrightarrow}} \psi_a.$$

The convergence in the weak-topology can be proved using the same method as in [Sok14d]. For the first limit this follows from the convergence of R_{Q_n} in the strong topology. For the proof of this fact and of the strong convergence of $\gamma_{vac;n} = \boldsymbol{\pi}_-^n - \mathcal{P}_-^0$, we refer the reader to [Sok14d].

For R_{Q_n}, it suffices to remark that $Q_n(x,y)$ converges in L^2_{loc} and *a.e.*. To estimate the mass at infinity, we simply use the term $\frac{1}{|x-y|}$ in $\frac{Q_n(x,y)}{|x-y|}$.

The strong convergence of $\gamma_{vac;n}$ follows from that of R_{Q_n} and the Cauchy expansion (7.91).

Then, assuming all these convergences, the convergence of Q_n resp. $\big[\widetilde{D}_{Q_n}^{(\Lambda)}; P_n\big]$ in the weak operator topology to Q_∞ resp. $\big[D_{Q_\infty}^{(\Lambda)}, \overline{P}\big]$ are straightforward.

Similarly, using (7.95), it is clear that

$$\widetilde{D}_{Q_n}\psi_{a;n} \underset{n\to+\infty}{\rightharpoonup} D_{Q_\infty}\psi_a,$$

and that

$$D^{(\Lambda)}_{Q_\infty}\psi_a = \mu\psi_a.$$

To get the existence of minimizer, it suffices to prove that $\|\psi_a\|_{L^2} = 1$ or equivalently $\lim_n \psi_{a;n} = \psi_a$ in L^2.

– To prove the norm convergence of $\psi_{a;n}$ to ψ_a, we need a uniform upper bound of μ_n, or precisely, we need the following :

$$\limsup_n (m - \mu_n) > 0. \tag{7.97}$$

Indeed, we then get

$$(\mathcal{D}^0 - \mu_n)\psi_{a;n} = \alpha R_{Q_n}\psi_{a;n} - 2\eta_n\Gamma_n\psi_{a;n} \text{ and } \psi_{a;n} = \frac{\alpha}{\mathcal{D}^0 - \mu_n}\big(R_{Q_n}\psi_{a;n} - 2\eta_n\Gamma_n\psi_{a;n}\big). \tag{7.98}$$

Provided that (7.97) holds and that we have norm convergence of $R_{Q_n}\psi_{a;n}$ we obtain the norm convergence of $\psi_{a;n}$.

– To prove the norm convergence of $R_{Q_n}\psi_{a;n}$ to $R_{Q_\infty}\psi_a$, we use the fact that the element of $\Phi_{\mathrm{SU}}\,\psi_{a;n}$ are "almost radial" (see in Remark 7.20). We recall (7.84) holds. In the following, we write $\delta Q_n := Q_n - Q_\infty$ and $\delta\psi_n := \psi_{a;n} - \psi_a$ and use Cauchy-Schwartz inequality : for any $A > 0$ there hold

$$\begin{aligned}
\int_{|x|\geq A}\Big|\int \frac{\delta Q_n(x,y)}{|x-y|}\psi_{a;n}(y)dy\Big|^2 dx &\leq \|\delta Q_n\|^2_{\mathrm{Ex}}\frac{K(j_0)}{A},\\
\int_{|x|\leq A}\Big|\int \frac{\delta Q_n(x,y)}{|x-y|}\psi_{a;n}(y)dy\Big|^2 dx &\leq \frac{2\pi}{2}\langle|\nabla|\psi_{a;n}\,,\,\psi_{a;n}\rangle \iint_{B(0,A)\times B(0,2A)}\frac{|\delta Q_n(x,y)|^2}{|x-y|}dxdy\\
&\quad + \frac{2}{A^2}\|\delta Q_n\|^2_{\mathfrak{S}_2}\|\psi_{a;n}\|^2_{L^2}.
\end{aligned}$$

Thus

$$\limsup_n \|R[Q_n - Q_\infty]\psi_{a;n}\|_{L^2} = 0.$$

Similarly

$$\begin{aligned}
\int_{|x|\geq A}\Big|\frac{Q_\infty(x,y)}{|x-y|}\delta\psi_n(y)dy\Big|^2 dx &\leq \frac{2}{A-\frac{A}{2}}\|Q_\infty\|^2_{\mathfrak{S}_2}\|\delta\psi_n\|^2_{L^2} + 2\|\delta\psi_n\|^2_{L^2}\frac{2}{A}\|Q_\infty\|^2_{\mathrm{Ex}},\\
\int_{|x|\leq A}\Big|\frac{Q_\infty(x,y)}{|x-y|}\delta\psi_n(y)dy\Big|^2 dx &\leq \frac{2\pi}{2}\langle|\nabla|\delta\psi_n\,,\,\delta\psi_n\rangle \iint_{B(0,A)\times B(0,2A)}\frac{|\delta Q_n(x,y)|^2}{|x-y|}dxdy\\
&\quad + \frac{2}{A^2}\|Q_\infty\|^2_{\mathfrak{S}_2}\|\delta\psi_n\|^2_{L^2},
\end{aligned}$$

and

$$\limsup_n \|R_{Q_\infty}(\psi_{a;n} - \psi_a)\|_{L^2} = 0.$$

This proves that

$$\lim_{n\to+\infty}\|R_{Q_n}\psi_{a;n} - R_{Q_\infty}\psi_a\|_{L^2} = 0.$$

– Let us prove (7.97). We have :

$$\begin{aligned}
2\mu_n(2j_0+1) &= \mathrm{Tr}\Big(\widetilde{D}_{Q_n}N_n\Big),\\
&= \mathrm{Tr}\Big(\widetilde{D}_{\gamma_{vac;n}}N_n\Big) - \alpha\|N_n\|^2_{\mathrm{Ex}},\\
&= \mathcal{E}^0_{\mathrm{BDF}}(Q_n) - \mathcal{E}^0_{\mathrm{BDF}}(\gamma_{vac;n}) - \tfrac{\alpha}{2}\|N_n\|^2_{\mathrm{Ex}},\\
&< 2m(2j_0+1) - K(j_0)\alpha^2.
\end{aligned} \tag{7.99}$$

This upper bound holds provided that $\alpha \leq \alpha_{j_0}$ thanks to the upper bound of $E_{j_0,\varepsilon}$ obtained in the previous section.

7.3.5 Lower bound of $E_{j_0,\pm}$

Our aim is to prove the estimate of Proposition 7.2. We consider the minimizer $Q_\infty = N + \gamma_{vac}$ found in the previous subsection. It satisfies Eq. (7.94) where

$$\overline{P} = \mathcal{P}^0_- + Q_\infty \text{ and } \gamma_{vac} = \chi_{(-\infty,0)}(D^{(\Lambda)}_{Q_infty}) - \mathcal{P}^0_-. \tag{7.100}$$

– The proof is the same as that in [Sok14b, Sok14d] and relies on estimates on the Sobolev norms $\|\,|\nabla|^s N_+\|_{\mathfrak{S}_2}$ where we write

$$N_+ := \text{Proj}\,\Phi_{\text{SU}}\,\psi_a = \text{Ker}\,(D^{(\Lambda)}_{Q_\infty} - \mu). \tag{7.101}$$

Using (7.101), we get

$$\begin{aligned}\text{Tr}\big(|\mathcal{D}^0|^2 N_+\big) &= 2(2j_0+1)\mu^2 + 2\alpha\mu\text{Tr}\big(R_{Q_\infty}N_+\big) + \alpha^2\text{Tr}\big(R^2_{Q_\infty}N_+\big),\\ &\le 2(2j_0+1)\mu^2 + 4\alpha\mu\|Q_\infty\|_{\mathfrak{S}_2}\|\nabla N_+\|_{\mathfrak{S}_2} + 4\alpha^2\|Q_\infty\|^2_{\mathfrak{S}_2}\|\nabla N_+\|^2_{\mathfrak{S}_2}\end{aligned}$$

and provided that $\alpha \le \alpha_{j_0}$, we get

$$\text{Tr}\big((-\Delta)N_+\big) \lesssim \frac{\alpha^2(2j_0+1)}{1-4\alpha^2(2j_0+1) - 2\|g_0\|_{L^\infty}\|g_0''\|_{L^\infty}}. \tag{7.102}$$

We have used Hardy's inequality :

$$\frac{1}{4|\cdot|^2} \le -\Delta \text{ in } \mathbb{R}^3. \tag{7.103}$$

We recall that

$$0 \le \|g_0\|_{L^\infty} - 1 \lesssim \alpha\log(\Lambda) \text{ and } \|g_0''\|_{L^\infty} \lesssim \alpha.$$

See (7.32) (or [Sok14b, Appendix A] for more details).

Thus for sufficiently small α, we have

$$\forall\,\psi \in \mathbb{S}\text{Ran}\,N_+,\ \|\nabla\psi\|^2_{L^2} \lesssim \frac{\alpha^2}{1-4\alpha^2(2j_0+1) - 2\|g_0\|_{L^\infty}\|g_0''\|_{L^\infty}} \lesssim \alpha^2. \tag{7.104}$$

– By *bootstrap argument*, we can estimate $\|\,\Delta N_+\|_{\mathfrak{S}_2}$. We have :

$$\forall\,\psi \in \mathbb{S}\text{Ran}\,N_+,\ \|\,|\nabla|^{3/2}\psi\|^2_{L^2} \lesssim \alpha^3\sqrt{2j_0+1} \text{ and } \|\Delta\psi\|_{L^2} \lesssim \alpha^4(2j_0+1)^{3/2}. \tag{7.105}$$

We prove this result below.

Furthermore, using the Cauchy expansion (7.54) and (7.51), we get

$$\Big|\ \|\,|\mathcal{D}^0|^{1/2}\gamma_{vac}\|_{\mathfrak{S}_2} \quad\lesssim\quad \alpha\|\nabla N\|_{\mathfrak{S}_2} + \sqrt{L\alpha}\|\gamma_{vac}\|_{\text{Ex}} + \alpha^2\|Q_\infty\|^2_{\text{Ex}}\big(\|\nabla N\|_{\mathfrak{S}_2} + \|\gamma_{vac}\|_{\text{Ex}}\big),$$

hence

$$\|\,|\mathcal{D}^0|^{1/2}\gamma_{vac}\|_{\mathfrak{S}_2} \lesssim \alpha^2\sqrt{2j_0+1}. \tag{7.106}$$

Now, if we assume (7.105)-(7.106), then we get

$$\text{For } \alpha \le \alpha_{j_0},\ \mathcal{E}^0_{\text{BDF}}\big(Q_\infty\big) = 2m(2j_0+1) + \frac{\alpha^2 m}{g_1'(0)^2}E^{nr}_{\mathbf{t}X^{\ell_0}} + \mathcal{O}\big(\alpha^3 K(j_0)\big).$$

We do not prove this fact : the method is the same as in [Sok14b, Sok14d] (in the proof of the lower bound of $E^0_{\text{BDF}}(1)$ resp. $E_{1,1}$).

We just recall how we get (7.105).

Proof of (7.105) We scale the wave functions of (7.104) by $\lambda := \frac{g_1'(0)^2}{\alpha m}$:

$$\forall\, x \in \mathbb{R}^3,\ U_\lambda \psi(x) = \underline{\psi}(x) := \lambda^{3/2}\psi(\lambda x),$$

and we split ψ (resp. $\underline{\psi}$) into the upper spinor φ (resp. $\underline{\varphi}$) and the lower spinor χ (resp. $\underline{\chi}$). Thanks to (7.99), we have

$$\alpha^{-2}(m-\mu) =: \alpha^{-2}\delta m \geq K(j_0) > 0$$

provided that α is sufficiently small ($\alpha \leq \alpha_{j_0}$).

We write

$$\forall\, Q_0 \in \mathfrak{S}_2,\ \underline{Q_0} := U_\lambda Q_0 U_\lambda^{-1} = U_\lambda Q_0 U_{\lambda^{-1}}.$$

For all ψ in $\mathbb{S}\mathrm{Ran}\underline{N_+}$ we have

$$\begin{cases} \lambda^2 \delta m \underline{\varphi} &= i\lambda\boldsymbol{\sigma}\cdot\nabla\underline{\chi} + \alpha\lambda\big(R_{\underline{Q_\infty}}\underline{\psi}\big)_\uparrow, \\ \underline{\chi} &= \frac{-i\lambda\boldsymbol{\sigma}\cdot\nabla\underline{\varphi}}{\lambda(m+\mu)} - \frac{\alpha}{\lambda}\big(R_{\underline{Q_\infty}}\underline{\psi}\big)_\downarrow. \end{cases} \tag{7.107}$$

– We recall

$$\forall\, Q_0 \in \mathfrak{S}_2,\ \|\big[\nabla, R_{Q_0}\big]\tfrac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}}^2 \lesssim \iint |p-q|^2|p+q||\widehat{Q_0}(p,q)|^2 dpdq. \tag{7.108}$$

This result was previously proved in [Sok14d] and follows from the fact that a (scalar) Fourier multiplier $F(\mathbf{p}-\mathbf{q}) = F(-i\nabla_x + i\nabla_y)$ commutes with the operator $R[\cdot] : Q(x,y) \mapsto \frac{Q(x,y)}{|x-y|}$. Then it suffices to use Hardy's inequality (7.103) :

$$\|\big[\nabla, R_{\underline{Q_\infty}}\big]\underline{\psi}\|_{L^2}^2 \lesssim \lambda^2 \iint |p-q|^2|\widehat{Q}_\infty(p,q)|^2 dpdq \times \|\nabla\underline{\psi}\|_{L^2}^2.$$

By Hardy's inequality (7.103) and (7.108), the following holds :

$$\left|\begin{array}{rcl} \|\underline{\chi}\|_{\mathfrak{S}_2}^2 &\leq& \frac{2}{4\lambda^2 m^2}\|\nabla\underline{\varphi}\|_{\mathfrak{S}_2}^2 + 2\alpha^2\|R_{\underline{Q_\infty}}\underline{\psi}\|_{\mathfrak{S}_2}^2 \lesssim \alpha^2, \\ \|\nabla\underline{\chi}\|_{\mathfrak{S}_2}^2 &\leq& 2(\lambda\delta m)^2 + 2\alpha^2\|R_{\underline{Q_\infty}}\underline{\psi}\|_{\mathfrak{S}_2}^2 \lesssim \frac{(\delta m)^2}{\alpha^2} + \alpha^2(2j_0+1), \\ \|\Delta\underline{\varphi}\|_{\mathfrak{S}_2}^2 &\leq& 2\lambda^2 m\|\nabla\underline{\chi}\|_{L^2}^2 + 2\alpha^2(\|\big[\nabla, R_{\underline{Q_\infty}}\big]\underline{\psi}\|_{L^2} + \|R_{Q_\infty}\|_{L^2}\nabla\underline{\psi})^2 \\ &\lesssim& \frac{(\delta m)^2}{\alpha^4} + (2j_0+1) + \alpha^2(2j_0+1)^{3/2}, \\ \|\Delta\underline{\chi}\|_{\mathfrak{S}_2}^2 &\leq& 2\lambda^2(\delta m)^2\|\nabla\underline{\varphi}\|_{L^2} + 2\alpha^2(\|\big[\nabla, R_{\underline{Q_\infty}}\big]\underline{\psi}\|_{L^2} + \|R_{Q_\infty}\|_{L^2}\nabla\underline{\psi})^2 \\ &\lesssim& \frac{(\delta m)^2}{\alpha^2} + (2j_0+1) + \alpha^2(2j_0+1)^{3/2}. \end{array}\right. \tag{7.109}$$

– There remains to estimate

$$\iint |p-q|^2|\widehat{Q_0}(p,q)|^2 dpdq,\ \text{for } Q_0 = N \text{ and } \gamma_{vac}.$$

For $Q_0 = N$, we just have to estimate $\mathrm{Tr}\big(|\nabla|^2 N_+\big)$.

The case $Q_0 = \gamma_{vac}$ is dealt with as in [Sok14b, Sok13] : by a *fixed-point* argument (valid for $\alpha \leq \alpha_{j_0}$), we prove that

$$\Big\{\iint |p-q|^2|\widehat{\gamma_{vac}}(p,q)|^2 dpdq\Big\}^{1/2} \lesssim \alpha \min\big(\|\Delta N\|_{\mathfrak{S}_2}, \|\,|\nabla|^{3/2}N\|_{\mathfrak{S}_2}\big).$$

Now, we can prove that

$$\mathrm{Tr}\big(|\nabla|^3 N_+\big) \lesssim \alpha^{5/2}(2j_0+1)^{3/2}.$$

For a unitary ψ in $\mathrm{Ran}\, N_+$, there holds

$$\begin{array}{rcl} \|\,|\nabla|^{1/2}\mathcal{D}^0\psi\|_{L^2}^2 &\leq& \mu^2\langle|\nabla|\psi\,,\,\psi\rangle + \alpha K\|\,|\nabla|^{1/2}\psi\|_{L^2}\|R_{Q_\infty}\psi\|_{L^2} \\ && +\alpha^2\big(\|[R_{Q_\infty}, |\nabla|^{1/2}]\psi\|_{L^2} + 2\|Q_\infty\|_{\mathfrak{S}_2}\|\,|\nabla|^{3/2}\|_{L^2}\big)^2. \end{array} \tag{7.110}$$

Similarly, in Fourier space we have :

$$\Big|\mathscr{F}\big([R_{Q_\infty}, |\nabla|^{1/2}]; p, q\big)\Big| \lesssim |p-q|^{1/2}|\widehat{R}_{Q_\infty}(p,q)|,$$

and by Hardy's inequality

$$\|[R_{Q_\infty}, |\nabla|^{1/2}]\psi\|_{L^2}^2 \lesssim \iint |p-q||\widehat{Q_\infty}(p,q)|^2 dpdq \|\nabla\psi\|_{L^2}^2 \lesssim \mathrm{Tr}\big(|\nabla| Q_\infty^2\big)\|\nabla\psi\|_{L^2}^2.$$

Substituting in (7.110), we get

$$\langle |\nabla|^3\psi\,,\,\psi\rangle \lesssim \alpha^{5/2}\sqrt{2j_0+1},\ \text{hence}\ \mathrm{Tr}\big(|\nabla|^3 N_+\big) \lesssim \alpha^{5/2}(2j_0+1)^{3/2}.$$

7.3.6 Proof of Lemmas 7.3 and 7.4

Proof of Lemma 7.3

We consider a trial state $P_\psi \in \mathscr{M}_{\mathscr{J}}^1$:

$$Q_\psi := P_\psi - \mathcal{P}_-^0 = |\psi\rangle\langle\psi| - |\mathrm{I_s}\psi\rangle\langle \mathrm{I_s}\psi|,\ \mathcal{P}_+^0\psi = \psi \in \mathbb{S}\,\mathfrak{H}_\Lambda.$$

Its BDF energy is

$$\begin{aligned}\mathcal{E}_{\mathrm{BDF}}^0(Q_\psi) &= 2\langle |\mathcal{D}^0|\psi\,,\,\psi\rangle - \frac{\alpha}{2}\iint \frac{|\psi\wedge \mathrm{I_s}\psi(x,y)|^2}{|x-y|}dxdy\\ &\geq 2m + 2\langle\big(|\mathcal{D}^0| - m\big)\psi\,,\,\psi\rangle - \alpha D\big(|\psi|^2,\psi^2\big) =: 2m + \mathcal{G}_{\mathrm{I_s}}(\psi).\end{aligned}$$

We recall the following

$$|\mathcal{D}^0| - m = \frac{1}{|\mathcal{D}^0|+m}\big((g_0(-i\nabla)-m)(g_0(-i\nabla)+m) + g_1(-i\nabla)^2\big).$$

Thanks to Estimates (7.32) and Kato's inequality (7.37), we have

$$\mathcal{G}_{\mathrm{I_s}}(\psi) \leq (1-K\alpha)\langle \tfrac{-\Delta}{2|\mathcal{D}^0|}\psi\,,\,\psi\rangle - \alpha\frac{\pi}{4}\langle |\nabla|\psi\,,\,\psi\rangle$$

We split ψ into two with respect to the frequency cut-off $\Pi_{\alpha K_0}$: we get

$$\psi = \Pi_{\alpha K_0}\psi + \psi_2 = \psi_1 + \psi_2.$$

The constant K_0 is chosen such that

$$\frac{\alpha^2 K_0^2}{2\widetilde{E}\,(\alpha K_0)} \gtrsim \alpha\pi\alpha K_0.$$

Then we have

$$\begin{aligned} D\big(|\psi|^2,|\psi|^2\big) &= D\big(|\psi_1|^2,|\psi_1|^2\big) + \mathcal{O}\big(\langle |\nabla|\psi_2\,,\,\psi_2\rangle + \||\psi_1|^2\|_{\mathcal{C}}\|\,|\nabla|^{1/2}\psi_2\|_{L^2}\big)\\ &= D\big(|\psi_1|^2,|\psi_1|^2\big) + \mathcal{O}\big(\langle |\nabla|\psi_2\,,\,\psi_2\rangle + \sqrt{\alpha}\|\,|\nabla|^{1/2}\psi_2\|_{L^2}\big),\end{aligned}$$

where we recall that $\|\rho\|_{\mathcal{C}}^2 = D(\rho,\rho)$. This gives

$$\begin{aligned}\tfrac{1}{2}\mathcal{G}_{\mathrm{I_s}}(\psi) &= \langle \tfrac{g_1(-i\nabla)^2}{|\mathcal{D}^0|+m}\psi_1\,,\,\psi_1\rangle - \alpha\tfrac{\pi}{2}D\big(|\psi_1|^2,|\psi_1|^2\big)\\ &\quad + K\langle \tfrac{g_1^2(-i\nabla)}{|\mathcal{D}^0|}\psi_2\,,\,\psi_2\rangle + \mathcal{O}(\alpha^3),\\ &\geq \tfrac{\alpha^2 g_1'(0)^2}{2m}\|\nabla\psi_1\|_{L^2}^2 - \tfrac{\alpha}{2}D\big(|\psi_1|^2,|\psi_1|^2\big) + \mathcal{O}(\alpha^3),\\ &\geq \tfrac{\alpha^2 m}{2g_1'(0)^2}E_{\mathrm{PT}}(1) + \mathcal{O}(\alpha^3).\end{aligned} \tag{7.111}$$

We have obtained a lower bound. Let us prove that it is attained up to an error $\mathcal{O}(\alpha^3)$. That is let us prove there exists a unitary $\psi_0 \in \mathrm{Ran}\mathcal{P}_+^0$ such that

$$\begin{aligned}\mathcal{E}_{\mathrm{BDF}}^0(Q_{\psi_0}) - 2m &= \mathcal{G}_{\mathrm{I_s}}(\psi_0) + \mathcal{O}(\alpha^3)\\ &= \tfrac{\alpha^2 m}{g_1'(0)^2}E_{\mathrm{PT}}(1) + \mathcal{O}(\alpha^3).\end{aligned} \tag{7.112}$$

As in [Sok14d], we consider the unique positive radially symetric Pekar minimizer $\phi_{\rm PT}$ in $L^2(\mathbb{R}^3,\mathbb{C})$. We form

$$\phi_1 := \begin{pmatrix} \phi_{\rm PT} \\ 0 \\ 0 \\ 0 \end{pmatrix} \in L^2(\mathbb{R}^3,\mathbb{C}^4), \tag{7.113}$$

which is a Pekar minimizer in the space of spinors. We scale this wave function by $\lambda^{-1} := \frac{\alpha m}{g_1'(0)^2}$:

$$\forall\, x \in \mathbb{R}^3,\ \phi_{\lambda^{-1}}(x) := \lambda^{-3/2}\phi_1(\lambda^{-1}x). \tag{7.114}$$

To get a proper $\psi_0 \in \mathrm{Ran}\,\mathcal{P}_+^0$, we form

$$\psi_0 := \frac{1}{\|\mathcal{P}_+^0\phi_{\lambda^{-1}}\|_{L^2}}\mathcal{P}_+^0\phi_{\lambda^{-1}}. \tag{7.115}$$

Our trial state is :

$$Q_0 := |\psi_0\rangle\langle\psi_0| - |\mathrm{I_s}\psi_0\rangle\langle\mathrm{I_s}\psi_0|. \tag{7.116}$$

We do not compute its energy : the method is as in [Sok14d] (except that instead of $\mathrm{I_s}$, the operator C is considered in [Sok14d], but that does not change anything). Eventually we refer the reader to the proof of the upper bound of $E_{\mathbf{t}X^{\ell_0}}$ above in Section 7.3.2 for the ideas.

Proof of Lemma 7.4

We remark the following fact.

Lemma 7.6. *Let $\mathbb{S}_{\mathrm{I_s}} \subset \mathfrak{H}_\Lambda$ be the set*

$$\mathbb{S}_{\mathrm{I_s}} = \big\{f \in \mathfrak{H}_\Lambda,\ \|f\|_{L^2} = 1,\ \langle f\,,\,\mathrm{I_s}f\rangle = 0\big\} = \big\{f \in \mathfrak{H}_\Lambda,\ \|f\|_{L^2} = 1,\ \mathfrak{Im}\langle\mathcal{P}_-^0 f\,,\,\mathrm{I_s}\mathcal{P}_+^0 f\rangle = 0\big\}.$$

There exists a smooth angle operator $\mathcal{A} : \mathbb{S}_{\mathrm{I_s}} \to \mathbb{R}/\pi\mathbb{Z}$.
For two $\mathbb{C}$-colinear wave functions f_1, f_2 in $\mathbb{S}_{\mathrm{I_s}}$ we have $\mathcal{A}(f_1) = \mathcal{A}(f_2)$.
Furthermore we have $\mathcal{A}^{-1}(0) = \mathrm{Ran}\,\mathcal{P}_-^0$ and $\mathcal{A}^{-1}(\frac{\pi}{2}) = \mathrm{Ran}\,\mathcal{P}_+^0$.

Proof : Let f be in $\mathbb{S}_{\mathrm{I_s}}$: the space $\mathrm{Span}_{\mathbb{C}}(f,\mathrm{I_s}f)$ is spanned by the eigenvectors $g_- := \frac{f+i\mathrm{I_s}f}{\|f+i\mathrm{I_s}f\|_{L^2}}$ and $g_+ := \frac{f-i\mathrm{I_s}f}{\|f-i\mathrm{I_s}f\|_{L^2}}$. We have

$$\mathrm{Span}_{\mathbb{C}}(f,\mathrm{I_s}f) = \mathrm{Span}(\mathcal{P}_-^0 g_\pm, \mathcal{P}_+^0 g_\pm).$$

It follows that $\mathcal{P}_\pm^0 f \parallel \mathcal{P}_\pm^0 g_+$ and $\mathcal{P}_-^0 f \parallel \mathrm{I_s}\mathcal{P}_+^0 f$. As $f \in \mathbb{S}_{\mathrm{I_s}}$, for $\varepsilon \in \{+,-\}$ with $\mathcal{P}_\varepsilon^0 f \neq 0$, we have

$$\mathcal{P}_{-\varepsilon}^0 f \in \mathrm{Span}_{\mathbb{R}}(\mathcal{P}_\varepsilon^0 f).$$

Thus we have with

$$\mathrm{Span}_{\mathbb{R}}(f,\mathrm{I_s}f) = \mathrm{Span}_{\mathbb{R}}(e_-,\mathrm{I_s}e_-),\ e_- \in \mathrm{Ran}\,\mathcal{P}_-^0 \text{ and } \|e_-\|_{L^2} = 1. \tag{7.117}$$

Indeed if $\mathcal{P}_-^0 f \neq 0$ we can choose $e_- := \frac{\mathcal{P}_-^0 f}{\|\mathcal{P}_-^0 f\|_{L^2}}$, else we can choose $e_- := \mathrm{I_s}\frac{\mathcal{P}_+^0 f}{\|\mathcal{P}_+^0 f\|_{L^2}}$.

Then we decompose f w.r.t. the basis $(e_-,\mathrm{I_s}e_-)$ and there exists $\theta \in \mathbb{R}/(2\pi\mathbb{Z})$ with $f = \cos(\theta)e_- + \sin(\theta)\mathrm{I_s}e_-$. In fact the function $f \mapsto (e_-,\mathrm{I_s}e_-)$ that maps f to a basis (7.117) is bi-valued : if $(e_-,\mathrm{I_s}e_-)$ is a possibility, then $(-e_-,-\mathrm{I_s}e_-)$ is another possibility. It follows that the angle θ is defined up to π : we thus obtain a function

$$\mathcal{A} : \mathbb{S}_{\mathrm{I_s}} \to \mathbb{R}/\pi\mathbb{Z}.$$

The smoothness of $\mathcal{A}$ is straightforward. The end of the proof is also clear.

□

We use the angle operator to get a mountain pass argument : see Lemma 7.7 below.

We use and Theorem 7.3 and Proposition 7.6.

– Let $\mathscr{U} \subset \mathscr{M}_{\mathscr{I}}$ be the *open* subset

$$\mathscr{U} \subset \mathscr{M}_{\mathscr{I}} := \Big\{ P = Q + \mathcal{P}^0_- \in \mathscr{M}_{\mathscr{I}},\ \dim \operatorname{Ker}(Q - \|Q\|_{\mathcal{B}}) = 1 \Big\}.$$

For all $P = Q + \mathcal{P}^0_- \in \mathscr{U}$, the eigenspace $\operatorname{Ker}(Q - \|Q\|_{\mathcal{B}})$ is spanned by a unitary vector f_0. By $\mathrm{I_s}$-symmetry, we have

$$\mathrm{I_s}\operatorname{Ker}(Q - \|Q\|_{\mathcal{B}}) = \operatorname{Ker}(Q + \|Q\|_{\mathcal{B}}),$$

and we have $\langle f_0\,,\, \mathrm{I_s} f_0\rangle = 0$. By Proposition 7.6, the plane $\operatorname{Span}_{\mathbb{C}}(f, \mathrm{I_s} f)$ is spanned by $f_- \in \operatorname{Ran} P$ and $f_+ \in \operatorname{Ran}(1-P)$.

By $\mathrm{I_s}$-symmetry, we have $\mathrm{I_s} f_- \in \mathbb{R} f_+$. In other words :

the wave function f_- is in $\mathbb{S}_{\mathrm{I_s}}$.

Definition 7.4. Let $Q + \mathcal{P}^0_- \in \mathscr{U} \subset \mathscr{M}_{\mathscr{I}}$ and f_- as above. We define the smooth function $\mathcal{A}_U$ as follows :

$$\mathcal{A}_U : Q + \mathcal{P}^0_- \in \mathscr{U} \subset \mathscr{M}_{\mathscr{I}} \mapsto \mathcal{A}(f_-).$$

It is clear it does not depend on the choice of f_- but is a function of $\mathbb{C} f_-$. Furthermore, we have

$$\forall\, P \in \mathscr{U},\ \nabla \mathcal{A}_U(P) \neq 0$$

The following Lemma is an application of classical results in geometry.

Lemma 7.7. *Let $\mathscr{M}_{U,\mathrm{I_s}}$ be the subset*

$$\mathscr{M}_{U,\mathrm{I_s}} := \big\{ Q + \mathcal{P}^0_- \in \mathscr{U},\ \|Q\|_{\mathcal{B}} = 1 \big\} = \mathcal{A}_U^{-1}\big(\{\frac{\pi}{2}\}\big),$$

in other words the set of projectors in $\mathscr{U}$ whose range intersects nontrivially $\operatorname{Ran}\mathcal{P}^0_+$. For any differentiable function $c : (-\varepsilon, \varepsilon) \to \mathscr{M}_{\mathscr{I}}$ such that $\varepsilon > 0$, $c(0) \in \mathscr{M}_{U,\mathrm{I_s}}$ and

$$\operatorname{Tr}\big(\nabla \mathcal{A}_U(c(0))^* \frac{d}{ds} c(0)\big) \neq 0,$$

the following holds : any sufficiently small smooth perturbation

$$c + \delta c : (-\varepsilon, \varepsilon) \to \mathscr{M}_{\mathscr{I}},$$

in the norm

$$\|\widetilde{c}\| := \sup_{s \in (-\varepsilon,\varepsilon)} \|\widetilde{c}(s) - \mathcal{P}^0_-\|_{\mathfrak{S}_2} + \sup_{s \in (-\varepsilon,\varepsilon)} \|\tfrac{d}{ds}\widetilde{c}(s)\|_{\mathfrak{S}_2}$$

still intersects $\mathscr{M}_{U,\mathrm{I_s}}$ at some $s(\delta c)$.

– Let us now prove Lemma 7.4. We recall that we have defined a loop $c_\psi = c_0$ that crosses $\mathscr{M}_{U,\mathrm{I_s}}$ at $s = \frac{1}{2}$ and we can easily check that $\operatorname{Tr}\big(\mathcal{A}_U(c(2^{-1}))^* \frac{d}{ds} c(2^{-1})\big) = 1 \neq 0$.

Furthermore we have defined the family $(c_t)_{t \geq 0}$ by $c_t := \Phi_{\mathrm{BDF};t}(c_\psi)$ where $\Phi_{\mathrm{BDF};t}$ is the gradient flow of the BDF energy.

– By Lemma 7.7, the loop c_t still intersects $\mathscr{M}_{U,\mathrm{I_s}}$ for sufficiently small t. We must ensure that this fact holds for all $t \geq 0$ to end the proof.

We use a continuation principle and set

$$t_\infty := \sup \Big\{ t \geq 0,\ \forall\, 0 \leq \tau \leq t, \exists s_0 \in [0,1] c_\tau \text{ crosses } \mathscr{M}_{U,\mathrm{I_s}} \text{ at } s = s_0 \Big\}.$$

We also define for all $0 \le \tau < t_\infty$:

$$\left| \begin{array}{lcl} s_-(\tau) & = & \sup\{s \in [0,1],\ \forall\, s' \le s,\ \|c_\tau(s')\|_{\mathcal{B}} < 1\} > 0, \\ s_+(\tau) & = & \inf\{s \in [0,1],\ \forall\, s' \ge s,\ \|c_\tau(s')\|_{\mathcal{B}} < 1\} < 1. \end{array} \right.$$

– We assume that $t_\infty < +\infty$ and prove this implies a contradiction.

The initial loop c_0 induces

$$\mathcal{L}_0 : s \in [0,1] \mapsto \mathcal{A}_U(c_0(s)) = \pi s \in \mathbb{T},$$

and we notice that $\mathcal{L}_0$ has a non-trivial homotopy.

Thus, at least for τ close to 0, the following holds.

1. There exist $0 < \eta_\tau, \eta'_\tau \ll 1$ such that

$$\mathcal{A}_U\left[c_\tau\big((s_-(\tau) - \eta_\tau, s_-(\tau))\big)\right] \cap \left(\tfrac{\pi}{2}, \tfrac{\pi}{2} + \eta'_\tau\right) = \varnothing. \tag{7.118}$$

2. There exist $0 < \eta_\tau, \eta'_\tau \ll 1$ such that

$$\mathcal{A}_U\left[c_\tau\big((s_+(\tau), s_+(\tau) + \eta_\tau)\big)\right] \cap \left(\tfrac{\pi}{2} - \eta'_\tau, \tfrac{\pi}{2}\right) = \varnothing. \tag{7.119}$$

The functions $\tau \ge 0 \mapsto s_\pm(\tau)$ are well-defined and continuous in a neighbourhood of 0 with $s_-(0) = s_+(0) = \frac{1}{2}$.

– We prove that by continuity in τ we have

$$\forall\, s \in [0,1],\ \|c_\tau(s)\|_{\mathcal{B}} = 1 \Rightarrow c_\tau(s) + \mathcal{P}^0_- \in \mathscr{M}_{U,\mathrm{I_s}} \tag{7.120}$$

and in particular

$$c_\tau(s_\pm(\tau)) \in \mathscr{M}_{U,\mathrm{I_s}} - \mathcal{P}^0_-. \tag{7.121}$$

If not, this implies that as τ increases, the second highest eigenvalue of $c_\tau(s_0)$ also increases to reach 1 where (7.118) becomes false, at some (τ_0, s_0).

This cannot occurs because of the energy condition : if this was true, we would have by Kato's inequality (7.37)

$$\mathcal{E}^0_{\mathrm{BDF}}\big(c_{\tau_0}(s_0)\big) \ge (1 - \alpha\tfrac{\pi}{4})\mathrm{Tr}\big(|\mathcal{D}^0| c_{\tau_0}(s_0)^2\big) \ge 4m(1 - \alpha\tfrac{\pi}{4}) > 2m.$$

Thus (7.120)-(7.121) hold for all $0 \le \tau < t_\infty$.

– Thanks to this fact, by continuity for all $0 \le \tau < t_\infty$, (7.118)-(7.119) hold : if we follow the point $s_\pm(\tau)$ from $\tau = 0$, we see that there cannot exist τ_0 such that (7.118) or (7.119) becomes false, because the set $\{t \ge 0,\ \forall\, 0 \le \tau < t,\ (7.118)\ (\text{resp. } (7.119)) \text{ holds for } \tau\}$ is non-empty and open.

– Up to an isomorphism of $[0,1]$, we can suppose that for all $0 \le \tau \le t_\infty$,

$$\forall\, s \in [0,1],\ \|\partial_s c_\tau(s_0)\|_{\mathfrak{S}_2} \lesssim 1.$$

Remark 7.23. In $\mathfrak{S}_2$, the function $\partial_s c_t(s_0)$ satsifies the following equation :

$$\frac{d}{dt}\partial_s c_t(s_0) = \partial_s \nabla \mathcal{E}^0_{\mathrm{BDF}}(c_t(s_0)) \in \mathfrak{S}_2.$$

These new loops are written $\widetilde{c}_\tau$ and have the same range as the c_τ's and define the same arc length.

Studying the limit of $\widetilde{c}_\tau$ as τ tends to t_∞, we get that at $t = t_\infty$, (7.118)-(7.119) still holds for the loop $\widetilde{c}_{t_\infty}$ at some $0 < s_-(t_\infty) \le s_+(t_\infty) < 1$.

Then necessarily, the loop $\widetilde{c}_{t_\infty}$ crosses $\mathscr{M}_{U,\mathrm{I_s}}$ at some $s \in [s_-(t_\infty), s_+(t_\infty)]$. Going back to c_{t_∞}, this proves that the same holds for c_{t_∞}, which contradicts the definition of t_∞.

7.4 Proofs on results on the variational set

7.4.1 Proof of Lemma 7.1

Let

$$\Phi'_{\rm SU}:\mathbf{SU}(2)\to\mathbf{U}(E),\ E\subset\mathfrak{H}_\Lambda$$

be an irreducible representation of $\Phi_{\rm SU}$. As $\mathbf{J}^2$ and $\mathbf{S}$ commutes with the action of $\mathbf{SU}(2)$, then necessarily E is an eigenspace for $\mathbf{J}^2$ and $\mathbf{S}$, associated to $j(j+1)$ and $\kappa_j=\varepsilon(j+\frac12)$ where $j\in\frac12+\mathbb{Z}_+$ and $\varepsilon=\pm$. The eigenspaces are known [Tha92, p. 126] : they are spanned by wave functions of type

$$\forall\, x=r\omega_x\in\mathbb{R}^3,\ \psi(x):=a(r)\Phi^{\pm}_{m,\kappa_j},\ m=-j,-j+1,\dots,j, \tag{7.122}$$

where

$$a(r)\in L^2(\mathbb{R}_+,r^2dr), \tag{7.123a}$$

$$\Phi^+_{m,\pm(j+\frac12)}:=\begin{pmatrix} i\Psi^m_{j\pm\frac12}\\ 0\end{pmatrix}\text{ and }\Phi^-_{m,\pm(j+\frac12)}:=\begin{pmatrix}0\\ \Psi^m_{j\mp\frac12}\end{pmatrix} \tag{7.123b}$$

$$\Psi^m_{j-\frac12}=\frac{1}{\sqrt{2j}}\begin{pmatrix}\sqrt{j+m}\,Y^{m-\frac12}_{j-\frac12}\\ \sqrt{j-m}\,Y^{m+\frac12}_{j-\frac12}\end{pmatrix}\text{ and }\Psi^m_{j+\frac12}=\frac{1}{\sqrt{2j+2}}\begin{pmatrix}\sqrt{j+1-m}\,Y^{m-\frac12}_{j+\frac12}\\ -\sqrt{j+1+m}\,Y^{m+\frac12}_{j+\frac12}\end{pmatrix}. \tag{7.123c}$$

We recall that the Y^m_ℓ are the spherical harmonics (eigenvectors of $\mathbf{L}^2$).

Hence E is spanned by a wave function which is a linear combination of that of type (7.122).

We recall that for any integer $n\geq 1$ there is but one irreducible representation of $\mathbf{SU}(2)$ of dimension n up to isomorphism. They can be found by the number of eigenvalues of J'_3, the infinitesimal "rotation" around the z axis which induces a representation of $\mathbf{SO}(3)$.. Here J'_3 corresponds to J_3.

Thus we get that for $\varepsilon\in\{+,-\}$

$$E_\varepsilon:=\Phi_{\rm SU}\,a(r)\Phi^\varepsilon_{j,\kappa_j}$$

is irreducible with respect to $\Phi_{\rm SU}$. By unicity of the irreducible representation of dimension $2j+1$, there exists an isomorphism from E_- to E_+. As there must be a correspondence between the eigenspace of $J_3(E_-)$ and that of $J_3(E_+)$, necessarily $\mathbb{C}a\Phi^-_{m,\kappa_j}$ is sent to $\mathbb{C}a\Phi^+_{m,\kappa_j}$.

In particular as $P_\uparrow E$ and $P_\downarrow E$ are also representation of $\mathbf{SU}(2)$ with same eigenvalues of $\mathbf{J}^2,\mathbf{S}$ (or $=\{0\}$). If one of them is zero then E is of type $E_\pm$. If both are non-zero, then there exists $a_\uparrow(r),a_\downarrow(r)$ such that

$$P_\uparrow E=\Phi_{\rm SU}a_\uparrow(r)\Phi^+_{j,\kappa_j}\text{ and }P_\downarrow E=\Phi_{\rm SU}a_\downarrow(r)\Phi^-_{j,\kappa_j}.$$

Both $P_\uparrow E$ and $P_\downarrow E$ are irreducible. We can suppose that there exists $f\in E$ with

$$P_\uparrow f=a_\uparrow(r)\Phi^+_{j,\kappa_j}\text{ and }P_\downarrow f=a_\downarrow(r)\Phi^-_{j,\kappa_j}.$$

The isomorphism between the two representations implies that

$$E=\Phi_{\rm SU}\big(a_\uparrow(r)\Phi^+_{j,\kappa_j}+a_\downarrow(r)\Phi^-_{j,\kappa_j}\big).$$

7.4.2 Proof of Proposition 7.5

We have to prove that $\mathscr{M}_{\mathscr{J}}$ and $\mathscr{W}$ are submanifold of $\mathscr{M}$. The method is similar to the one used in [Sok14d] to prove that $\mathscr{M}_{\mathscr{C}}$ is a submanifold of $\mathscr{M}$.

Let $P_0=Q_0+\mathcal{P}^0_-\in\mathscr{M}$. We will prove that in a neighbourhood of P_0 in $\mathcal{P}^0_-+\mathfrak{S}_2$, the projectors P_1 in $\mathscr{M}_{\mathscr{J}}$ (resp. $\mathscr{W}$) can be written as

$$P_1=e^AP_0e^{-A},$$

where $A\in\mathfrak{m}^{\mathscr{J}}_{P_0}$ (resp. $\mathfrak{m}^{\mathscr{W}}_{P_0}$).

– If we assume this point, then it is clear that the two sets are submanifolds of $\mathscr{M}$. Indeed e^A is a global linear isometry of $\mathfrak{H}_\Lambda$, whose restriction to the $\mathfrak{m}^{\cdot}_P$'s maps $\mathfrak{m}^{\cdot}_{P_0}$ onto $\mathfrak{m}^{\cdot}_{P_1}$.

Equivalently it maps the first tangent plane onto the other :

$$\{[a,P_0],\ a\in\mathfrak{m}^{\cdot}_{P_0}\}\underset{\simeq}{\to}\{[a,P_1],\ a\in\mathfrak{m}^{\cdot}_{P_1}\}.$$

– We use Theorem 7.3 to write

$$Q_0=\sum_{j=1}^{+\infty}\lambda_j\big(|f_j\rangle\langle f_j|-|f_{-j}\rangle\langle f_{-j}|\big) \tag{7.124}$$

where $(\lambda_i)_i\in\ell^2$ is non-increasing and the f_i's form an orthonormal basis of $\operatorname{Ran}Q$. Provided that

$$\|P_1-P_0\|_{\mathfrak{S}_2}<1,$$

then $\lambda_1<1$ and there is no j such that f_j or f_{-j} is in the range of $\mathcal{P}^0_+$ or $\mathcal{P}^0_-$.

We decompose with respect with the eigenvalues $\mu_1>\mu_2>\cdots>0$ as follows :

$$Q_0=\sum_{k=1}^{+\infty}\mu_k\big(\text{Proj Ker}(Q_0-\mu_k)-\text{Proj Ker}(Q_0+\mu_k)\big).$$

For short we write $\mu_{-k}:=-\mu_k$, and

$$M_k:=\text{Proj Ker}(Q_0-\mu_k)\text{ and }E^{Q_0}_{\mu_k}:=\text{Ker}(Q_0-\mu_k). \tag{7.125}$$

As any $\mathrm{Y}\in\{\mathrm{C},\mathrm{I_s}\}$ is an isometry (linear or antilinear) and as the eigenvalues are the sine of the angles between vectors in P_0 and $\mathcal{P}^0_-$, for any k we have

$$\mathrm{Y}E^{Q_0}_{\mu_k}=E^{Q_0}_{-\mu_k} \tag{7.126}$$

and the eigenspaces $E^{Q_0}_{\mu_k}\oplus E^{Q_0}_{-\mu_k}=\text{Ker}(Q_0^2-\mu_k^2)$ are invariant under Y.

Case of $\mathscr{W}$ – In the case $\mathrm{Y}=\mathrm{C}$ and $P_0\in\mathscr{W}$, each eigenspace $\text{Ker}(Q_0^2-\mu_k^2)$ is also invariant under the action of Φ_{SU}. In other words, $\text{Ker}(Q_0^2-\mu_k^2)$ is a finite dimensional representation of Φ_{SU}, and we can decompose it into irreducible representations $E^{(\ell)}_{\mu_k}$, where $0\le\ell\le\ell_k$.

By C-symmetry, we have

$$\mathrm{C}E^{(\ell_1)}_{\mu_k}=E^{(\ell_1')}_{-\mu_k},$$

there is a one-to-one correspondence between irreducible representations of type $E^{(\ell)}_{\mu_k}$ and that of type $E^{(\ell)}_{-\mu_k}$. Up to changing indices ℓ_j', we can suppose that

$$\mathrm{C}E^{(\ell)}_{\mu_k}=E^{(\ell)}_{-\mu_k},\ 0\le\ell\le\ell_k.$$

Decomposing $E^{(\ell)}_{\mu_k}$ with respect with $\mathcal{P}^0_-$ and $\mathcal{P}^0_+$, we see that

$$\mathcal{P}^0_\pm E^{(\ell)}_{\mu_k}\text{ is irreducible,}$$

and from the spectral decomposition of Q_0

$$\mathcal{P}^0_-E^{(\ell)}_{\mu_k}\oplus\mathcal{P}^0_+E^{(\ell)}_{\mu_k}=E^{(\ell)}_{\mu_k}\oplus F_{-\mu_k},$$

where $F_{-\mu_k}$ is an irreducible subset of $\text{Ker}(Q_0+\mu_k)$.

– Let us show that

$$F_{-\mu_k}\cap\mathrm{C}E^{(\ell)}_{\mu_k}=\{0\}. \tag{7.127}$$

Indeed, from Lemma 7.1 and the expression of the $\Phi^\pm_{m,\kappa}$, we see that

$$\mathrm{C}\text{Ker}\big(J_3-m\big)=\text{Ker}\big(J_3+m\big).$$

Thus if the intersection is non-zero, then we have by C-symmetry and Φ_{SU}-symmetry :

$$F_{-\mu_k} = \mathrm{C}E^{(\ell)}_{\mu_k}.$$

But as shown in [Sok14d], this cannot happen : let us say that $E^{(\ell)}_{\mu_k}$ is associated to the eigenvalues $j_0(j_0+1), \kappa$ of $\mathbf{J}^2$ resp. $\mathbf{S}$. We consider :

$$\mathrm{Ker}(J_3 - m) \cap \mathcal{P}^0 \pm E^{(\ell)}_{\mu_k} = \mathbb{C}e_{\pm;m},\ -j_0 \le m \le j_0,\ \|e_{\pm;m}\|_{L^2} = 1.$$

We would have

$$\mathrm{C}e_{\pm;m} = \exp i\theta(\pm;m) e_{\mp;-m}.$$

The constant $\theta(\pm;m)$ does not depend on m by Φ_{SU}-symmetry. Moreover, if

$$\mathrm{Ker}(J_3 - m) \cap E^{(\ell)}_{\mu_k} = \mathbb{C}f_m,$$

then

$$\mathcal{P}^0_{\pm} f_m \parallel e_{\pm;m}.$$

As in [Sok14d] for $\mathscr{M}_{\mathscr{C}}$, the condition $\mathrm{C}^2 = 1$ implies $\theta_+ - \theta_- \equiv 0[2\pi]$ while

$$-\mathrm{C}Q_0\mathrm{C} = Q_0$$

implies $\theta_+ - \theta_- \equiv \pi[2\pi]$, which cannot occur.

Similarly, we can prove that (7.127) holds and that in fact $F_{-\mu_k}$ is orthogonal to $\mathrm{C}E^{(\ell)}_{\mu_k}$.

As a consequence, the number of $E^{(\ell)}_{\mu_k}$'s is even, or equivalently, the number of $\mathcal{P}^0_- E^{(\ell)}_{\mu_k}$ is even.

– The fact that

$$P_1 = e^A P_0 e^{-A},\ \text{with } \Phi_{\mathrm{SU}}A = A,\ \mathrm{C}A\mathrm{C} = A,\ \|A\|_{\mathfrak{S}_2} < +\infty, \tag{7.128}$$

follows from Theorem 7.3 and the different symmetries.

The f_j's in (7.124) can be written as ($\lambda_j = \sin(\theta_j)$)

$$f_j = \sqrt{\frac{1-\lambda_j}{2}} e_{-;j} + \sqrt{\frac{1+\lambda_j}{2}} e_{+;j},\ \mathcal{P}^0_{\pm} e_{\pm;j} = e_{\pm;j}.$$

We also have

$$f_{-j} = -\sqrt{\frac{1+\lambda_j}{2}} e_{-;j} + \sqrt{\frac{1-\lambda_j}{2}} e_{+;j}.$$

Then we define

$$A = \sum_{j=1}^{+\infty} \theta_j \big(|e_{+;j}\rangle\langle e_{-;j}| - |e_{-;j}\rangle\langle e_{+;j}|\big). \tag{7.129}$$

It is easy to check that A satisfies (7.128). In fact, we can assume that f_j spans an irreducible representation of $\mathbf{SU}(2)$, and in this case the same holds for $e_{+;j}$ and $e_{-;j}$.

As in Section 7.4.1, the correspondence $e_{-;j} \mapsto e_{+;j}$ induces an isomorphism between $\Phi_{\mathrm{SU}}e_{-;j}$ and $\Phi_{\mathrm{SU}}e_{+;j}$. This fact together with the Φ_{SU}-symmetry implies that

$$\forall U \in \mathrm{Ran}\,\Phi_{\mathrm{SU}},\ UAU^{-1} = A.$$

The fact that $\mathrm{C}A\mathrm{C} = A$ was proved in [Sok14d] in the case $P_0, P_1 \in \mathscr{M}_{\mathscr{C}}$. Here this remains true because

$$\mathscr{W} \subset \mathscr{M}_{\mathscr{C}}.$$

– We can now determine the connected component of $\mathscr{W}$. Let P_0, P_1 be in $\mathscr{W}$ and let $Q = P_1 - P_0$.

We consider

$$E^Q_1 := \mathrm{Ker}(Q-1).$$

If $E^Q_1 = \{0\}$, then we can write $P_1 = e^A P_0 e^{-A}$ as in (7.129). And we see that the path in ℓ^2 :

$$t \in [0,1] \mapsto (t\theta_j)_j \in \ell^2$$

induces a path connecting P_0 and P_1.

If $E_1^Q \neq \{0\}$, we count the number of irreducible representation in E_1^Q : let b_{j,κ_j} be the number of irr. rep. in

$$\mathrm{Ker}\big(\mathbf{J}^2 - j(j+1)\big) \cap \mathrm{Ker}\big(\mathbf{S} - \kappa_j\big).$$

If all the b_{j,κ_j}'s are even, we can still write P_1 as $P_1 = e^A P_0 e^{-A}$ with A as in (7.129) with the first θ_j equal to $\frac{\pi}{2}$. In particular the two projectors can be connected by a path in $\mathscr{W}$.

Let us say that $b_{j_0,\kappa_0} \equiv 1[2]$ for some j_0, κ_0. We have shown that for $P \in \mathscr{W}$ with $\|P - P_0\|_{\mathcal{B}} < 1$, the number of planes Π_j's in the decomposition of Theorem 7.3 is even. Precisely, due to the C-symmetry, there exists a sequence $(\ell_\mu(j,\kappa))_j$ in $\mathbb{N}$, with

$$\begin{aligned}&\mathrm{Ker}\big((P - P_0) - \mu\big) \cap \mathrm{Ker}\big(\mathbf{J}^2 - j(j+1)\big) \cap \mathrm{Ker}\big(\mathbf{S} - \kappa\big)\\ &\quad= \bigoplus_{1 \le \ell \le \ell_\mu(j,\kappa)} E_\mu^{(\ell)},\end{aligned}$$

where each $E_\mu^{(\ell)}$ is irreducible as a representation of Φ_{SU} and $\ell_\mu(j,\kappa)$ is *even*.

We show that there cannot exist a continuous path linking P_0 and P_1 by a contradiction argument.

Let us say that $\gamma : t \in [0,1] \to \mathscr{W}$ is a continuous path with $\gamma(0) = P_0$ and $\|\gamma(1) - P_0\|_{\mathcal{B}} = 1$.

Then by the previous remarks, we have by continuity :

$$\begin{aligned}&\forall t \in [0,1], \forall\, j \in \tfrac12 + \mathbb{Z}_+,\ \forall \kappa \in \big\{\pm\big(j + \tfrac12\big)\big\},\\ &\ell_1(Q_t = \gamma(t) - P_0; j, \kappa) \equiv 0[2].\end{aligned}$$

In particular it is not possible to have $\gamma(1) = P_1$.

Case of $\mathscr{M}_{\mathscr{I}}$ For $\mathrm{Y} = \mathrm{I_s}$ and $P_0 \in \mathscr{M}_{\mathscr{I}}$, we use (7.126). For each $f \in E_\mu^Q$, we have $\mathrm{I_s} \in E_{-\mu}^Q$ where $\mu \in \sigma(Q)$. We may assume that $\mu > 0$.

Thus the plane

$$\Pi := \mathrm{Span}\big(f, \mathrm{I_s} f\big)$$

is invariant under Q and $\mathrm{I_s}$. We decompose f and $\mathrm{I_s} f$ with respect to P_0 and $1 - P_0$. By a dimension argument :

1. either $\mu = 1$, $P_0 f = 0$ and $(1 - P_0)\mathrm{I_s} f = 0$,
2. or $0 < \mu < 1$ and
$$\mathbb{C}P_0 f = \mathbb{C}P_0 \mathrm{I_s} f \text{ and } \mathbb{C}(1 - P_0) f = \mathbb{C}(1 - P_0)\mathrm{I_s} f.$$

In each case, we write e_- a unitary vector in $\mathrm{Ran}\, P_0 \cap \Pi$ and $e_+ = \mathrm{I_s} e_-$.

If we consider the sequence $(\mu_i)_i$ of positive eigenvalues of Q (counted with multiplicities), we get the correspondent sequences $(e_{-;j})_j$ and $(e_{+;j})$. Moreover by Theorem 7.3, we know that $\mu_j = \sin(\theta_j)$ where $\theta_j \in [0, \frac{\pi}{2}]$ is the angle between the two lines $\mathbb{C}e_{-;j}$ and $\mathbb{C}f_j$.

Provided that we take $-\theta_j$ instead of θ_j and up to a phase, we can suppose that

$$f_j = \cos(\theta_j) e_{-;j} + \sin(\theta_j)\mathrm{I_s} e_{-;j}.$$

In particular we have

$$P_1 = e^A P_0 e^{-A},$$

with

$$A = \sum \theta_j \big(|e_{+;j}\rangle\langle e_{-;j}| - |e_{-;j}\rangle\langle e_{+;j}|\big).$$

It is straightforward to check that $\mathrm{I_s} A \mathrm{I_s}^{-1} = A$.

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Quatrième partie

Appendices

Chapitre 8

Espace de Fock et hamiltonien

Nous soulignons que cette partie est très technique et que sa compréhension n'est pas nécessaire pour saisir le propos de cette thèse.

8.1 Espace de Fock

L'espace de Fock peut se définir comme la «C^*-algèbre» engendrée par l'algèbre CAR contenant un état du vide[Tha92, p. 280]. C'est-à-dire :

1. $\mathcal{F}_{el}$ est un espace de Hilbert dont l'espace d'opérateurs unitaires $\mathbf{U}\big(\mathcal{F}_{el}\big)$ contient l'algèbre CAR.
2. L'algèbre CAR est engendrée par des opérateurs $a(f), b(g)$ où
   (a) $f \in \mathfrak{H}_+ \mapsto a(f)$ est antilinéaire et $g \in \mathfrak{H}_- \mapsto b(g)$ est linéaire.
   (b) Ces opérateurs satisfont les «relations canoniques d'anticommutation»
   $$\{a(f_1), a(f_2)\} = \{a^*(f_1), a^*(f_2)\} = 0, \quad \{a(f_1), a^*(f_2)\} = \langle f_1\,,\, f_2\rangle_{\mathfrak{H}}\mathbf{1},$$
   $$\{b(g_1), b(g_2)\} = \{b^*(g_1), b^*(g_2)\} = 0, \quad \{b(g_1), b^*(g_2)\} = \overline{\langle g_1\,,\, g_2\rangle_{\mathfrak{H}}}\mathbf{1},$$
   $$\{a^{\times}(f), b^{\diamond}(g)\} = 0,$$
   où les deux symboles $\times$ et $\diamond$ dénotent l'étoile d'adjonction $*$ ou son absence.

   L'opérateur $a(f)$ annihile une particule d'état f et $b(g)$ une antiparticule d'état g. Leurs adjoints respectifs créent une particule (resp. antiparticule) d'état f (resp. g).
3. L'espace $\mathcal{F}_{el}$ contient un état $\Omega \in \mathcal{F}_{el}\backslash\{0\}$ qui vérifie
   $$\forall (f,g) \in \mathfrak{H}_+ \times \mathfrak{H}_-,\ a(f)\Omega = b(g)\Omega = 0.$$
4. L'espace $\mathcal{F}_{el}$ est minimal pour toutes ces propriétés. En particulier, une base hilbertienne de $\mathcal{F}_{el}$ est $(e_{I,J})_{I,J}$, définie par
   $$e_{I,J} := \prod_{i\in I} a^*(f_i) \prod_{j\in J} b^*(g_j)\Omega,\ I,J \subset \mathbb{N},\ |I|,|J| < +\infty, \tag{8.2}$$
   où (f_i) et (g_j) sont des bases orthonormées respectivement de $\mathfrak{H}_+$ et $\mathfrak{H}_-$.

À isomorphisme près, on peut choisir l'espace précédemment décrit (2.1) : dans ce cas l'état Ω est donné par un vecteur unitaire de $\mathcal{F}^{(0,0)} \simeq \mathbb{C}$.

L'opérateur de champ Ψ décrit l'annihilation d'une particule et la création d'une antiparticule :
$$\forall\, f \in \mathfrak{H},\ \Psi(f) = a\big(\mathrm{Proj}(\mathfrak{H}_+)f\big) + b^*\big(\mathrm{Proj}(\mathfrak{H}_-)f\big).$$
On peut également définir formellement l'opérateur $\Psi(x)$ qui annihile une particule et crée une antiparticule au point $x \in \mathbb{R}^3$.

Soit $(f_i)_i$ resp. $(g_i)_i$ une base orthonormée de $\mathfrak{H}_+$ resp. $\mathfrak{H}_-$, on écrit

$$\begin{array}{rclrclrcl} a(x) & := & \sum_i a(f_i)f_i(x), & b^*(x) & := & \sum_i b^*(g_i)g_i(x), & \Psi(x) & := & a(x)+b^*(x), \\ a^*(x) & = & \sum_i a^*(f_i)f_i^*(x) & b(x) & := & \sum_i b(f_i)g_i^*(x), & \Psi^*(x) & := & a^*(x)+b(x). \end{array} \tag{8.3}$$

La nature de ces objets n'est pas évidente, on peut les considérer comme des distributions à valeurs opérateurs. Par exemple :

$$\forall\, \phi \in \mathcal{D}(\mathbb{R}^3, \mathbb{C}^4),\ \langle a(x)\,,\, \phi\rangle_{\mathcal{D}'\times\mathcal{D}} = \sum_i a(f_i)\langle \phi\,,\, f_i\rangle_{\mathfrak{H}} \quad \text{et} \quad \langle a^*(x)\,,\, \phi\rangle_{\mathcal{D}'\times\mathcal{D}} = \sum_i a^*(f_i)\langle f_i\,,\, \phi\rangle_{\mathfrak{H}}. \tag{8.4}$$

8.2 État BDF

Un état BDF Ω_P est défini comme suit [HLS05a, appendice]. Soit un projecteur P définissant une nouvelle décomposition orthogonale

$$\mathfrak{H} = \mathrm{Ker}(P) \oplus \mathrm{Im}(P). \tag{8.5}$$

Notons $P_+ = 1 - P$ et $P_- = P$. Suivant cette décomposition on peut réaliser l'algèbre CAR *relativement à* P et *dans* $\mathcal{F}_{el}$ en définissant

$$a_P(f) := \Psi(P_+f) \text{ et } b_P(f) := \Psi^*(P_-f),\ f \in \mathfrak{H}. \tag{8.6}$$

Ce projecteur définit un état BDF si et seulement si il existe un état unitaire $\Omega_P \in \mathcal{F}_{el}$ satisfaisant

$$\forall (f, g) \in \mathrm{Ker}(P) \times \mathrm{Im}(P),\ a_P(f)\Omega_P = b_P(g)\Omega_P = 0.$$

L'espace de Fock associé à la décomposition (8.5) «vit» alors dans celui associé à la décomposition $\mathfrak{H} = \mathfrak{H}_+ \oplus \mathfrak{H}_-$.

Une application du théorème de Shale-Stinespring [Tha92, chapitre 10] permet d'affirmer que cela n'est possible que lorsque la différence des projecteurs

$$P - \mathrm{Proj}\big(\mathfrak{H}_+\big)$$

est Hilbert-Schmidt.

8.2.1 Hamiltonien

L'hamiltonien de la QED $\mathbb{H}_{\mathrm{QED}}$ rend compte des interactions du champ d'électrons et positrons et du champ des photons au sein d'un champ électromagnétique externe.

Dans le modèle BDF on néglige les photons et on suppose que le champ magnétique externe est nul. On ne prend en considération que les interactions électrostatiques des particules. Notant V_{ext} le potentiel électrostatique externe, l'hamiltonien $\mathbb{H}$ s'écrit[Gra11, p. 73]

$$\mathbb{H}(\Psi) = \int \Psi^*(x) D_0 \Psi(x) dx + \int V_{ext} \rho_\Psi(x) dx + \frac{\alpha}{2} \iint \frac{\rho_\Psi(x)\rho_\Psi(y)}{|x-y|} dxdy, \tag{8.7}$$

où $\Psi(x)$ est l'opérateur de champ (8.3) et ρ_Ψ est l'opérateur de densité défini par

$$\rho_\Psi(x) = \frac{1}{2} \sum_{\sigma=1}^{4} \Big(\Psi^*(x)_\sigma \Psi(x)_\sigma - \Psi(x)_\sigma \Psi^*(x)_\sigma \Big).$$

Chapitre 9

Preuves de résultats techniques

9.1 End of the proof of [Sok14b, Lemma B.3]

9.1.1 Reminder

Let (Q_0, ρ_0) be in $\mathfrak{S}_2 \times \mathcal{C}$. We consider the Cauchy expansion of

$$\chi_{(-\infty,0)}\Big(\Pi_\Lambda\big(\mathcal{D}^0 + \alpha\big(\rho_0 * \frac{1}{|\cdot|} - R_{Q_0}\big)\big)\Pi_\Lambda\Big) = \sum_{\ell=1}^{+\infty} \alpha^\ell Q_\ell(Q_0, \rho_0), \tag{9.1}$$

$$= \sum_{\ell=1}^{+\infty} \alpha^\ell \sum_{j+k=\ell} \alpha^\ell Q_{j,k}(Q_0, \rho_0). \tag{9.2}$$

The density of $Q_{j,k}(Q_0, \rho_0)$ is written $\rho_{j,k}(Q_0, \rho_0)$. We recall [1] that

$$Q_\ell(Q_0, \rho_0) = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\eta}{\mathcal{D}^0 + i\eta}\Big(\Pi_\Lambda(R_Q - \rho_0 * \tfrac{1}{|\cdot|})\Pi_\Lambda \frac{1}{\mathcal{D}^0 + i\eta}\Big)^\ell$$

and that $Q_{j,k}$ is the part of Q_{j+k} which is polynomial in R_{Q_0} (resp. $\rho_0 * \frac{1}{|\cdot|}$) of degree j (resp. k).

In the definition of $Q_{j,k}$, we write

$$\frac{\Pi_\Lambda}{\mathcal{D}^0 + i\eta} = \frac{\mathcal{P}^0_+\Pi_\Lambda}{\mathcal{D}^0 + i\eta} + \frac{\mathcal{P}^0_-\Pi_\Lambda}{\mathcal{D}^0 + i\eta}.$$

For a $(\ell+1)$-tuple $\varepsilon \in \{+,-\}^{\ell+1}$, we write $Q^\varepsilon_{j,k}$ and $\rho^\varepsilon_{j,k}$ the corresponding terms.

A simple computation shows that

$$Q^{+\cdots+}_{j,k} = Q^{-\cdots-}_{j,k} = 0.$$

Remark 9.1. Let $f : \mathbb{R}^3 \to [1, +\infty)$ such that there exists $K(f) \geq 1$ satisfying

$$\forall\, p,q,r \in \mathbb{R}^3,\ \sqrt{f(p-q)} \leq K(f)\Big(\sqrt{f(p-r)} + \sqrt{f(r-q)}\Big).$$

We have introduced the two norms $\|\cdot\|_{\mathcal{Q}_f}$, $\|\cdot\|_{\mathfrak{C}_f}$ based on f.

For short, we write $v_{\rho_0} := \rho_0 * \frac{1}{|\cdot|}$.

We prove in this part estimates on the norms of $\rho_{k,j}$ for $k+j \geq 2$ in terms of that of $\|Q_0\|_{\mathcal{Q}_f}$ and $\|\rho_0\|_{\mathfrak{C}_f}$. From an algebraic point of view the proof is essentially the same as for [HLS05a, Lemmas 13 and 15].

1. one more time

9.1.2 Proof

We just have to deal with the following cases :

1. $(j,k)=(j,k)$ with $j\geq 2$.
2. $(j,k)=(1,k)$ with $k\geq 2$.
3. $(j,k)\in\big\{(1,1),(0,3)\big\}$.

We have already dealt with the case $(j,k)=(0,k)$ with $k\geq 5$. We recall that by Furry's Theorem the densities $\rho_{0,2k}(Q_0,\rho_0)$ vanish.

Below the letter ℓ always denotes $k+j$.

We use the *duality* : we consider a Schwartz function $\zeta\in\mathcal{S}(\mathbb{R}^3,\mathbb{C})$ and prove that

$$\Big|\mathrm{Tr}(Q_{j,k}\zeta)\Big|\leq\binom{\ell}{k}(K(f)C)^{\ell}\|Q_0\|_{\mathcal{Q}_f}^{j}\|\rho_0\|_{\mathfrak{C}_f}^{k}\sqrt{\int_{\mathbb{R}^3}\frac{|p|^2}{f(p)}|\widehat{\zeta}(p)|^2dp}.$$

In fact we go in Fourier space and use both the KSS inequalities and Hölder inequalities for Schatten operators.

If $j\geq 2$, then $Q_{j,k}$ is already trace-class. Else we show $Q_{j,k}\zeta$ is trace-class : thanks to the cut-off we have

$$\|Q_{j,k}|D_0|^{1/2}\tfrac{\Pi_\Lambda}{|D_0|^{1/2}}\zeta\|_{\mathfrak{S}_1}\lesssim\Lambda\|Q_{j,k}|D_0|^{1/2}\|_{\mathfrak{S}_2}\|\zeta\|_{L^2}.$$

By symmetry we can just deal with the term $O_{j,k}$ of $Q_{j,k}$ that has first the j terms R_{Q_0} at the beginning.

Remark 9.2. Below we will introduce constants $C_0,C_1,\ \widetilde{C}_1$ and so on. They are constants that depend on the dimension and *not* on the parameters Q_0,ρ_0,j,k.

We just do not want to precise their values.

First case We have

$$\begin{array}{rcl}\Big|\mathrm{Tr}(O_{j,k}\zeta)\Big| & \leq & \frac{1}{(2\pi)^{1+3(\frac{k+1}{2})}}\displaystyle\int_{\mathbb{R}}\int_{(B(0,\Lambda))^{\ell}}\tfrac{dp_1\cdots dp_\ell}{\sqrt{\widetilde{E}(p_0)^2+\eta^2}}\prod_{i=1}^{j}\tfrac{|\widehat{R}_{Q_0}(p_{i-1},p_i)|}{\sqrt{\widetilde{E}(p_i)+\eta^2}}\\ & & \times\prod_{i=j+1}^{\ell}\tfrac{|\widehat{v}_{\rho_0}(p_{i-1}-p_i)|}{\sqrt{\widetilde{E}(p_i)^2+\eta^2}}\tfrac{|\widehat{zeta}(p_\ell-p_0)|}{\sqrt{f(p_\ell-p_0)}}\sqrt{f(p_\ell-p_0)}.\end{array}\tag{9.3}$$

We have

$$\sqrt{f(p_\ell-p_0)}\leq K(f)^{\ell-1}\sum_{i=1}^{\ell}\sqrt{f(p_i)-p_{i-1}}.\tag{9.4}$$

For $\widehat{v}(\cdot)\in\{|\widehat{v}_\rho(\cdot)|,\sqrt{f(\cdot)}|\widehat{v}_{\rho_0}(\cdot)|,\frac{|\widehat{\zeta}(\cdot)|}{\sqrt{f(\cdot)}}\}$ and $d_\eta:=\sqrt{|\mathcal{D}^0|^2+\eta^2}$, we have

$$\|d_\eta^{-1/2}\Pi_\Lambda v\Pi_\Lambda d_\eta^{-1/2}\|_{\mathfrak{S}_6}\leq\frac{C_0}{E(\eta)^{1/2}}\|v\|_{L^6},\tag{9.5}$$

By Sobolev's inequality we have $\|v\|_{L^6}\leq\widetilde{C}_1\|\nabla v\|_{L^2}$ hence the terms $\|\rho_0\|_{\mathcal{C}}\leq\|\rho_0\|_{\mathfrak{C}_f}$ and $\|\zeta\|_{\mathfrak{C}'_f}$ for the three different v.

Moreover we have

$$\sqrt{f(p-q)}|\widehat{R}_{Q_0}(p,q)|=|\widehat{R}_{\widetilde{Q}_0}(p-q)|,\ \widetilde{Q}_0(p',q'):=\sqrt{f(p'-q')}\widehat{Q}_0(p',q');\tag{9.6}$$

and for $Q\in H^{1/2}(\mathbb{R}^3\times\mathbb{R}^3)$ we have

$$\|\tfrac{1}{|\nabla|^{1/2}}R_Q\|_{\mathfrak{S}_2}\leq\widetilde{C}_2\sqrt{\mathrm{Tr}(Q^*R_Q)}\lesssim C_2\sqrt{\iint(\widetilde{E}\,(p)^{1/2}+\widetilde{E}\,(q)^{1/2})|\widehat{Q}(p,q)|^2dpdq}.\tag{9.7}$$

These estimates give rise to the terms $\|Q_0\|_{\mathcal{Q}_f}$.

Thus using the tricks (9.4)-(9.7), we get

$$\Big(\mathrm{Tr}(Q_{j,k}(Q_0,\rho_0)\zeta)\Big|\leq K(f)^{\ell-1}\binom{\ell}{k}(C_0C_1)^{k+1}C_2^j\int_{\mathbb{R}}\frac{d\eta}{E(\eta)^{(\ell+1)/2}}\|Q_0\|_{\mathcal{Q}_f}^{j}\|\rho_0\|_{\mathfrak{C}_f}^{k}\|\zeta\|_{\mathfrak{C}'_f}.\tag{9.8}$$

Second case We use the same tricks (9.4)-(9.7). The operator $Q_{j,k}\zeta$ is trace-class by Hölder's inequalies :

$$\frac{1}{2}+3\times\frac{1}{6}=1.$$

We get the same estimate as in (9.8).

Last case Unfortunately for $(j,k)\in\big\{(1,1);(0,3)\big\}$, we have to compute the terms.

The term $\rho_{1,1}(Q_0,\rho_0)$ By symmetry, we can just estimate the norms of $\rho^{\varepsilon}_{1,1}(Q_0,\rho_0)$ with

$$\varepsilon\in\{(+-+);(++-);(-++)\}.$$

Furthermore we can only treat the term $\widetilde{Q}_{1,1}$ where the term R_{Q_0} appears first (reading from left to right).
1. We have

$$\begin{aligned}&\mathrm{Tr}_{\mathbb{C}^4}(\widehat{\widetilde{Q}^{+-+}_{1,1}\zeta}(p,p))\\&=(2\pi)^{-3}\iint\limits_{B(0,\Lambda)^2}dp_1dp_2\mathrm{Tr}_{\mathbb{C}^4}\Big(\tfrac{\widehat{\mathcal{P}^0_+}(p)\widehat{R}_{Q_0}(p,p_1)\widehat{\mathcal{P}^0_-}(p_1)\widehat{v}_{\rho_0}(p_1-p_2)\widehat{\mathcal{P}^0_+}(p_2)}{(\widetilde{E}(p)+\widetilde{E}(p_1))(\widetilde{E}(p_1)+\widetilde{E}(p_2))}\zeta(\widehat{p_2-p_0})\Big).\end{aligned}\tag{9.9}$$

We first take the absolute value in (9.9). Then we use trick (9.4) and (9.6)-(9.7). Then we remark that

$$\begin{aligned}&\Big\|\int_{p_1}dp_1\frac{\sqrt{f(p_1-p_2)}|\widehat{v}_{\rho_0}(p_1-p_2)||\widehat{\mathcal{P}^0_-}(p_1)\widehat{\mathcal{P}^0_+}(p_2)|}{\widetilde{E}\,(p_1)^{1/2+1/4}}\times\frac{|\widehat{\zeta}(p_2-p)|}{\widetilde{E}\,(p_2)^{3/4}\sqrt{f(p_2-p)}}\Big\|_{L^2((\mathbb{R}^3)^2,dp_1dp)}\\&\lesssim\|\rho_0\|_{\mathfrak{C}_f}\|\zeta\|_{\mathfrak{C}'_f}.\end{aligned}$$

The first part is the integral kernel of a Hilbert-Schmidt operator while the second part is the one of an operator in the Schatten class $\mathfrak{S}_6$.
2. We have

$$\begin{aligned}&\mathrm{Tr}_{\mathbb{C}^4}(\widehat{\widetilde{Q}^{++-}_{1,1}\zeta}(p,p))\\&=(2\pi)^{-3}\iint\limits_{B(0,\Lambda)^2}dp_1dp_2\mathrm{Tr}_{\mathbb{C}^4}\Big(\tfrac{\widehat{\mathcal{P}^0_+}(p)\widehat{R}_{Q_0}(p,p_1)\widehat{\mathcal{P}^0_+}(p_1)\widehat{v}_{\rho_0}(p_1-p_2)\widehat{\mathcal{P}^0_-}(p_2)}{(\widetilde{E}(p)+\widetilde{E}(p_2))(\widetilde{E}(p_1)+\widetilde{E}(p_2))}\zeta(\widehat{p_2-p_0})\Big).\end{aligned}\tag{9.10}$$

As there holds

$$\big((\widetilde{E}\,(p)+\widetilde{E}\,(p_2))(\widetilde{E}\,(p_1)+\widetilde{E}\,(p_2))\big)^{-1}\le\widetilde{E}\,(p)^{-1/2}\,\widetilde{E}\,(p_1)^{-3/4}\,\widetilde{E}\,(p_2)^{-3/4},$$

we get a similar estimate as above : indeed we have

$$\Big\||\widehat{\mathcal{P}^0_+}(p_1)\widehat{\mathcal{P}^0_-}(p_2)|\widetilde{E}\,(p_1)^{-3/4}\,|\sqrt{f(p_1-p_2)}|\widehat{v}_{\rho}(p_1-p_2)|\Big\|_{L^2(dp_1dp_2)}\lesssim\|\rho_0\|_{\mathfrak{C}_f}.$$

3. Finally we have

$$\begin{aligned}&\mathrm{Tr}_{\mathbb{C}^4}(\widehat{\widetilde{Q}^{-++}_{1,1}\zeta}(p,p))\\&=(2\pi)^{-3}\iint\limits_{B(0,\Lambda)^2}dp_1dp_2\mathrm{Tr}_{\mathbb{C}^4}\Big(\tfrac{\widehat{\mathcal{P}^0_-}(p)\widehat{R}_{Q_0}(p,p_1)\widehat{\mathcal{P}^0_+}(p_1)\widehat{v}_{\rho_0}(p_1-p_2)\widehat{\mathcal{P}^0_+}(p_2)}{(\widetilde{E}(p)+\widetilde{E}(p_1))(\widetilde{E}(p)+\widetilde{E}(p_2))}\zeta(\widehat{p_2-p_0})\Big).\end{aligned}\tag{9.11}$$

We have

$$\big((\widetilde{E}\,(p)+\widetilde{E}\,(p_1))(\widetilde{E}\,(p)+\widetilde{E}\,(p_2))\big)^{-1}\le\widetilde{E}\,(p_1)^{-1/2}\,\widetilde{E}\,(p)^{-3/4}\,\widetilde{E}\,(p_2)^{-3/4},$$

This time we use both

$$\|\widetilde{E}\,(p_1)^{-1/2}\sqrt{f(p-p_1)}|\widehat{R}_{Q_0}(p,p_1)|\|_{L^2(dpdp_1)}\lesssim\|Q_0\|_{\mathcal{Q}_f},$$

and

$$\Big\||\widehat{\mathcal{P}^0_+}(p_2)\widehat{\mathcal{P}^0_-}(p)|\frac{|\widehat{\zeta}(p_2-p)|}{\sqrt{f(p_2-p)}}\widetilde{E}\,(p)^{-3/4}\Big\|_{L^2(dp_2dp)}\lesssim\|\zeta\|_{\mathfrak{C}'_f}.$$

The term $\rho_{0,3}(\rho_0)$ By symmetry we only treat the two cases $+---$ and $++--$. The method is the same as for $\rho_{1,1}$. 1. The residuum formula gives a term

$$\frac{\mathrm{Tr}_{\mathbb{C}^4}\big(\widehat{\mathcal{P}^0_+}(p)\widehat{\mathcal{P}^0_-}(p_1)\widehat{\mathcal{P}^0_-}(p_2)\widehat{\mathcal{P}^0_-}(p_3)\big)}{(\widetilde{E}\,(p)+\widetilde{E}\,(p_1))(\widetilde{E}\,(p)+\widetilde{E}\,(p_2))(\widetilde{E}\,(p)+\widetilde{E}\,(p_3))},$$

its norm is lesser than

$$\frac{|\widehat{\mathcal{P}^0_+}(p)\widehat{\mathcal{P}^0_-}(p_1)|}{\widetilde{E}\,(p)^{2/3}\,\widetilde{E}\,(p_1)^{7/9}\,\widetilde{E}\,(p_2)^{7/9}\,\widetilde{E}\,(p_3)^{7/9}}.$$

Then we have

$$\Big\|\widetilde{E}\,(p)^{-2/3}\,|\widehat{\mathcal{P}^0_+}(p)\widehat{\mathcal{P}^0_-}(p_1)|\sqrt{f(p-p_1)}|\widehat{v}_{\rho_0}(p-p_1)|\Big\|_{L^2(dpdp_1)} \lesssim \|\rho_0\|_{\mathfrak{C}_f}.$$

Furthermore for

$$\widehat{v}(p)\in\Big\{\sqrt{f(p)}|\widehat{v}_{\rho_0}(p)|;\,\frac{|\widehat{\zeta(p)}|}{\sqrt{f(p)}}\Big\}, \tag{9.12}$$

we have

$$\|v\tfrac{\Pi_\Lambda}{|\mathcal{D}^0|^{7/9}}\|_{\mathfrak{S}_6}\lesssim\|\nabla v\|_{L^2}.$$

2. The residuum formula gives a term

$$\begin{aligned}&\mathrm{Tr}_{\mathbb{C}^4}\big(\widehat{\mathcal{P}^0_+}(p)\widehat{\mathcal{P}^0_+}(p_1)\widehat{\mathcal{P}^0_-}(p_2)\widehat{\mathcal{P}^0_-}(p_3)\big)\times\Big\{\big((\widetilde{E}\,(p)+\widetilde{E}\,(p_2))(\widetilde{E}\,(p_1)+\widetilde{E}\,(p_2))(\widetilde{E}\,(p_1)+\widetilde{E}\,(p_3))\big)^{-1}\\&\quad+\big((\widetilde{E}\,(p)+\widetilde{E}\,(p_2))(\widetilde{E}\,(p)+\widetilde{E}\,(p_3))(\widetilde{E}\,(p_1)+\widetilde{E}\,(p_3))\big)^{-1}\Big\}.\end{aligned}$$

Taking the norm of the above term, we get

$$\begin{aligned}&|\widehat{\mathcal{P}^0_+}(p_1)\widehat{\mathcal{P}^0_-}(p_2)|\times\Big\{\big(\widetilde{E}\,(p)^{2/3}\,\widetilde{E}\,(p_1)^{1/3+2/3}\,\widetilde{E}\,(p_2)^{1/3+1/3}\,\widetilde{E}\,(p_3)^{2/3}\big)^{-1}\\&\quad+\big(\widetilde{E}\,(p)^{1/4+1/2}\,\widetilde{E}\,(p_1)^{3/4}\,\widetilde{E}\,(p_2)^{3/4}\,\widetilde{E}\,(p_3)^{1/4+1/2}\big)^{-1}\Big\}.\end{aligned}$$

We then compute

$$\big\|\widetilde{E}\,(p_1)^{-3/4}\,|\widehat{\mathcal{P}^0_+}(p_1)\widehat{\mathcal{P}^0_-}(p_2)|\sqrt{f(p_1-p_2)}|\widehat{v}_{\rho_0}(p_1-p_2)|\big\|_{L^2(dp_1dp_2)}\lesssim\|\rho_0\|_{\mathfrak{C}_f}$$

and

$$\|\tfrac{\Pi_\Lambda}{|\mathcal{D}^0|^{2/3}}v\|_{\mathfrak{S}_6}\lesssim\|\nabla v\|_{L^2},$$

where v is as in (9.12).

This ends the proof.

9.2 On the function f_Λ

The functions g_0, g_1 are defined in the previous chapters (see [Appendix, Chapter 3] for instance). For short, we write

$$\mathbf{g}_1(p):=\frac{g_1(p)}{|p|}p\in\mathbb{R}^3 \text{ and } \mathbf{g}(p):=\begin{pmatrix}g_0(p)\\ \mathbf{g}_1(p)\end{pmatrix}\in\mathbb{R}^4.$$

We have $\widetilde{E}\,(p)=|\mathbf{g}(p)|$ and $\mathbf{s}_p:=\widetilde{E}\,(p)^{-1}\,(g_0(p)\beta+\boldsymbol{\alpha}\cdot\mathbf{g}_1(p))$.

We end the study of f_Λ initiated in the Appendix of Chapter 4. We recall that f_Λ is defined as a series :

$$\forall p\in B(0,\Lambda),\;\; f_\Lambda(p)=f_\Lambda(|p|)=\sum_{j=0}^{+\infty}\alpha^{j+1}f_{\Lambda,j-1}, \tag{9.13}$$

where the radial functions $f_{\Lambda,j}$ are defined as follows.

For $\mathbf{e}\in\mathbb{S}^2$ we write
$$B(r) := B(-\tfrac{r}{2}\mathbf{e},\Lambda)\cap B(\tfrac{r}{2}\mathbf{e},\Lambda)\subset B(0,\Lambda) \text{ and } k = r\mathbf{e}.$$
We have
$$f_{\Lambda,0}(p) := \frac{1}{\pi^2|p|^2}\int\limits_{B(|p|)} du \frac{\widetilde{E}\left(u-\frac{p}{2}\right)\widetilde{E}\left(u+\frac{p}{2}\right) - \langle \mathbf{g}(u-\frac{p}{2}), \mathbf{g}(u-\frac{p}{2})\rangle_{\mathbb{R}^4}}{\widetilde{E}\left(u-\frac{p}{2}\right)+\widetilde{E}\left(u+\frac{p}{2}\right)}.$$

For $j\geq 2$ we have :
$$f_{\Lambda,j-1}(r) = \frac{1}{(2\pi)^{2(j-1)}r^2}\int\limits_{B(r)^j}\frac{du_1\cdots du_j}{\prod\limits_{2\leq \ell\leq j}|u_\ell-u_{\ell-1}|^2}\frac{\mathrm{Tr}_{\mathbb{C}^4}(M_j((u_\ell)_{\ell=1}^j))}{\prod\limits_{1\leq\ell\leq j}(\widetilde{E}\left(u_\ell+\frac{k}{2}\right)+\widetilde{E}\left(u-\frac{k}{2}\right))}, \tag{9.14}$$
where we define $M_j:\mathbb{R}^3\to\mathrm{End}(\mathbb{C}^4)$ by induction over j :
$$\begin{cases} M_1(v_1) & := \mathbf{s}_{v_1+\frac{k}{2}}\mathbf{s}_{v_1-\frac{k}{2}} - 1,\\ M_i((v_\ell)_{1\leq\ell\leq i}) & := \mathbf{s}_{v_1+\frac{k}{2}} M_{i-1}((v_\ell)_{2\leq\ell\leq i})\mathbf{s}_{v_1-\frac{k}{2}} - M_{i-1}((v_\ell)_{2\leq\ell\leq i}).\end{cases}$$

We already know that $\mathrm{supp} f_\Lambda\subset B(0,2\Lambda)$ and that f_Λ is twice differentiable in $B(0,2\Lambda)$. We have to prove that
$$\lim_{r_0\to(2\Lambda)^-}\partial_r^2 f_\Lambda(r_0) = 0. \tag{9.15}$$

We refer the reader to [Appendix, Chapter 4] for the formula of $\partial_r^2 f_\Lambda$ (in particular for the use of the co-area formula).

We emphasize the following. Each $f_{\Lambda,j}$ can be written as a composition of $r\mapsto(r,\dots,r)\in\mathbb{R}^{2(j+1)}$
$$((x_0,y_0),\dots,(x_j,y_j))\mapsto \mathcal{L}_{\Lambda,j}(x_0,y_0,\dots,x_j,y_j) \tag{9.16}$$
where
$$\mathcal{L}_{\Lambda,j}(x_0,y_0,\dots,x_j,y_j) = \int\cdots\int\limits_{\prod B(y_j)} dv_0\dots dv_j(\mathrm{Fct})_{\Lambda,j}(v_0\pm\frac{x_0}{2}\mathbf{e},\dots,v_j\pm\frac{x_j}{2}\mathbf{e}). \tag{9.17}$$
Thus for any $r_0\in(0,2\Lambda)$ and $0<\delta r\ll 1$, we have
$$\mathcal{L}_{\Lambda,j}(r_0+\delta r,\dots,r_0+\delta r) = f_{\Lambda,j}(r_0)+\delta r(\partial_r f_{\Lambda,j}(r_0)) + \frac{(\delta r)^2}{2}(\partial_r^2 f_{\Lambda,j}(r_0)) + o((\delta r)^2). \tag{9.18}$$
In fact we showed that f_Λ was twice differentiable by proving such an expansion (the summability of the expansion is clear for α sufficiently small).

In (9.18), each δr comes from the expansion w.r.t. a term $x_k = r_0+\delta r$ or $y_k = r_0+\delta r$. A careful study of [Appendix, Chapter 4] enables us to say that the coefficient in coeff $\times(\delta r)^2$ coming from the expansion w.r.t.

1. either a term x_k and a term $x_{k'}$,
2. or a term x_k and a term $y_{k'}$,
3. or a term y_k and a term $y_{k'}$ with $|k-k'|\geq 2$

vanishes as r tends to 2Λ.

Indeed we have $B(r)\subset B_{\mathbb{R}^3}(0,\sqrt{\Lambda^2-\frac{r^2}{4}})$. Thus as r tends to 2Λ this set shrinks down to $\{0\}$ and its volume is $\mathcal{O}_{r\to2\Lambda}\big((\Lambda-\frac{r}{2})^{3/2}\big)$.

We use the method explained in Chapter 3.

For $j\geq 1$, integrating w.r.t. y_0, then w.r.t. $B(y_1)$ up to y_j or first w.r.t. y_j then w.r.t. y_{j-1} down to y_0, we can assume that the last integral is an integral over $B(r_0)$ of kind
$$\int_{B(r_0)}\frac{du}{\widetilde{E}\left(u+\frac{r_0}{2}\mathbf{e}\right)+\widetilde{E}\left(u-\frac{r_0}{2}\mathbf{e}\right)}\frac{1}{\max_\varepsilon(|u+\varepsilon\frac{r_0}{2}\mathbf{e}|^2)} = \underset{r_0\to2\Lambda}{o}(1).$$

Remark 9.3. Similarly the area of $\partial B(r)$ is $\mathcal{O}_{r\to 2\Lambda}\big(\Lambda-\frac{r}{2}\big)$ and the length of the curve $\{|u\pm\frac{r}{2}\mathbf{e}|=\Lambda\}$ is $\mathcal{O}_{r\to 2\Lambda}\big((\Lambda-\frac{r}{2})^{1/2}\big)$.

For $j=0$, it is easy to see that $\partial_r^2 f_{\Lambda,0}(r)$ tends to 0 as $r\to 2\Lambda$ by the previous Remark (and by the formulae of Chapter 4).

There remains to study the coefficient in coeff $\times(\delta r)^2$ corresponding to the expansion w.r.t. y_k and y_{k+1} together with that coming from the expansion w.r.t. y_k only.

We write $\partial B(r)=S(r)$ and $S_\pm(r):=S(r)\cap B(\mp\frac{r}{2}\mathbf{e},\Lambda)$. As $B(r)$ shrinks down to $\{0\}$, we see from the formulae of Chapter 4 that we just have to prove the following :

$$\frac{1}{\Lambda^4}\iint\limits_{\left(S_\pm(r)\right)^2}\frac{d\mathcal{H}_2(u)d\mathcal{H}_2(v)}{|u-v|}=\underset{r\to 2\Lambda}{o}(1), \tag{9.19a}$$

$$\frac{1}{\Lambda^4}\iint\limits_{S_+(r)\times S_-(r)}\frac{d\mathcal{H}_2(u)d\mathcal{H}_2(v)}{|u-v|^2}=\underset{r\to 2\Lambda}{o}(1). \tag{9.19b}$$

The first estimate (9.19a) is straightforward : a rough upper bound is

$$\int_{S_+(r)}d\mathcal{H}_2(u)\int_{\Lambda\mathbb{S}^2}\frac{d\mathcal{H}_2(v)}{|u-v|}\lesssim\mathcal{H}_2(S_+(r))\Lambda\int_{-1}^1\frac{dy}{\sqrt{1-y}}.$$

We prove the second estimate.

For short, we write $x:=\frac{r}{2\Lambda}$ and $\theta_0:=\arccos(x)$. We also write $c_a:=\cos(a)$ and $s_a:=\sin(a)$ for $a\in\mathbb{R}$.

The l.h.s. of (9.19b) is equal to

$$\frac{2\pi}{\Lambda^2}\iiint\limits_{\substack{0\le\theta_1\le\theta_0\\ \pi-\theta_0\le\theta_{-1}\le\pi\\ -\pi\phi\le\pi}}\frac{s_{\theta_1}d\theta_1\sin_{\theta_{-1}}d\theta_{-1}d\phi}{(c_{\theta_1}-c_{\theta_{-1}}-2x)^2+(s_{\theta_1}-s_{\theta_{-1}}c_\phi)^2+s_{\theta_{-1}}^2s_\phi^2}. \tag{9.20}$$

We define ϕ_1,ϕ_{-1} by :

$$0\le\theta_1=:\theta_0-\phi_1\le\theta_0 \text{ and } \pi-x\le\theta_{-1}=:\phi_{-1}+\pi-\theta_0\le\pi$$

Writing $\phi:=\phi_1+\phi_{-1}=\mathcal{O}_{x\to 1}(\sqrt{1-x})$, we have :

$$\begin{aligned}c_{\theta_1}-c_{\theta_{-1}}-2x&=\sqrt{1-x^2}(\phi_1+\phi_{-1})-\frac{1}{2}(\phi_1^2+\phi_{-1}^2)+\mathcal{O}_{x\to 1}\big((1-x)\phi^2+\sqrt{1-x}\phi^3+\phi^4\big),\\ &\ge\frac{\sqrt{1-x^2}}{3}(\phi_1+\phi_{-1})\end{aligned}$$

where the lower bound holds for x sufficiently close to 1.

Furthermore we have :

$$(s_{\theta_1}-s_{\theta_{-1}}c_\phi)^2+s_{\theta_{-1}}^2s_\phi^2=(s_{\theta_1}-s_{\theta_{-1}})^2+2(1-c_\phi)s_{\theta_1}s_{\theta_{-1}}.$$

In the integral of (9.20), we first integrate over ϕ. For $A,B>0$ we have

$$\int\limits_{-\pi\le\phi\le\pi}\frac{d\phi}{A^2+B^2(1-c_\phi)}\le 2\int_0^\pi\frac{d\phi}{A^2+\frac{4}{\pi^2}B^2\phi^2}\lesssim\frac{1}{AB}.$$

Up to a constant, we get the following upper bound :

$$\begin{aligned}\frac{1}{\Lambda^2\sqrt{1-x}}\iint\limits_{\phi_1,\phi_{-1}\le\theta_0}\frac{\sqrt{s_{\theta_1}s_{\theta_{-1}}}d\phi_1d\phi_{-1}}{\phi_1+\phi_{-1}}&\lesssim\frac{1}{\Lambda^2}\iint\limits_{\phi_1,\phi_{-1}\le\theta_0}\frac{d\phi_1d\phi_{-1}}{\phi_1+\phi_{-1}},\\ &\lesssim\frac{\theta_0}{\Lambda^2}\int_0^1\log\big(1+\frac{1}{\varepsilon}\big)d\varepsilon=\underset{x\to 1}{\mathcal{O}}\Big(\frac{\sqrt{1-x}}{\Lambda^2}\Big).\end{aligned}$$

9.3 Proof of [Sok14a, Theorem 1]

– The proof of (2.) ⇒ (1.) is an easy adaptation of [CDL08, HLS05b, HLS09].

If there is equality for some k : $E^{\nu}_{\mathrm{BDF}}(q) = E^{\nu}_{\mathrm{BDF}}(q-k) + E^{0}_{\mathrm{BDF}}(k)$, then we construct as in [HLS09] a minimizing sequence $(Q_n)_n$ of trial functions which decouple in two clusters whose distance from each other becomes infinite as n tends to infinity.

– Let us prove (1.) ⇒ (2.) : we prove it by contraposition, following [HLS09].

For any minimizing sequence $(Q_n)_n$ of $E^{\nu}_{\mathrm{BDF}}(q)$ weakly-$\star$ converging to $Q_\infty \in \mathcal{K}$, norm-convergence in $\mathcal{K}$ is equivalent to charge conservation : $\mathrm{Tr}_{P^0_-}(Q) = q$ [HLS09].

Let $(Q_n)_n$ be a minimizing sequence for $E^{\nu}_{\mathrm{BDF}}(q)$ that is not precompact in the strong topology of $\mathcal{K}$. We have to show that $E^{\nu}_{\mathrm{BDF}}(q) \ge E^{\nu}_{\mathrm{BDF}}(q-k) + E^{0}_{\mathrm{BDF}}(k)$.

Up to a subsequence we assume $(Q_n)_n$ weakly-$*$ converges to $Q_\infty \in \mathcal{Q}(q-k)$.

Localisation operators We define localizations operators Y_A and X_A for any $A > 0$ [CDL08]. Let χ_1 be in $\mathscr{C}^\infty_0(\mathbb{R}^3)$ such that

$$\chi_{B(0,1)} \le \chi_1 \le \chi_{B(0,2)},$$

and $\eta_1 \ge 0$ be defined by $\eta_1 := \sqrt{1-\chi_1^2}$. Then :

$$\begin{array}{ll|ll} \eta_A(x) & := \eta_1\big(x/A\big), & Y_A & := P^0_+\eta_A P^0_+ + P^0_-\eta_A P^0_- \\ \chi_A(x) & := \chi_1\big(x/A\big), & X_A & := \sqrt{1-Y_A^2}. \end{array}$$

In fact we will need more : we suppose that $\nabla\sqrt{\eta_1(1-\eta_A)} \in L^p$ for $p \ge 3$.

For instance if η_1 is chosen such that in the annulus $A(0,\frac{7}{4},2)$: $\eta_1(x) = \exp(-\frac{1}{4-|x|^2})$ and in $A(0,1,\frac{5}{4})$: $\eta_1(x) = \exp(-\frac{1}{|x|^2-1})$, then :

$$|\nabla\theta_A^{1/2}(x)| \quad \lesssim \chi_{B(0,2A)}(x)A^{-1}.$$

– By the duality definition of ρ_Q, it is clear that $\rho_{Q_n} \rightharpoonup_{\mathcal{C}} \rho_Q$. It is easy to adapt [CDL08, Lemmas 10 and 11]. We will write $w_A = Y_A - \eta_A \in \mathfrak{S}_p$, $Y_A^2 = \eta_A^2 + W_A$, $W_A = w_A\eta_A + Y_A w_A \in \mathfrak{S}_p$.

We will add the following estimate :

Lemma 9.1. *for any $A > 0, p > 3$ and $3/p < t < 1, 0 < a < 2$:*

$$\|X_A - \chi_A\|_{\mathfrak{S}_p} \quad \le K\big(\tfrac{1}{1-t}\|w_A\|_{\mathfrak{S}_{tp}}\|w_A\|_{\mathfrak{S}_p}^{a(1-t)/2} + \|w_A\|_{\mathfrak{S}_p}^{1-a/2}\big)$$

Proof : We use : $\sqrt{x} = \frac{1}{\pi}\int_0^{+\infty} s^{-1/2}ds(x+s)^{-1}$.

$$\begin{aligned} \pi(X_A - \chi_A) \quad &= \pi(\sqrt{1-Y_A^2} - \sqrt{1-\eta_A^2}) = \int_0^{+\infty}\frac{ds}{\sqrt{s}}\Big\{\frac{\eta_A^2 + W_A}{\eta_A^2 + W_A + s} - \frac{\eta_A^2}{\eta_A^2 + s}\Big\} \\ &= \int_0^{+\infty}\frac{ds}{\sqrt{s}}\Big\{(\eta_A^2 + W_A + s)^{-1}W_A - \big((\eta_A^2 + W_A + s)^{-1} - (\eta_A^2 + s)^{-1}\big)\eta_A^2\Big\} \\ &= \int_0^{+\infty}\frac{ds}{\sqrt{s}}\Big\{(Y_A^2 + s)^{-1}W_A(1 - \tfrac{\eta_A^2}{\eta_A^2+s})\Big\} = \int_0^{+\infty}\frac{ds}{\sqrt{s}}\frac{1}{Y_A^2 + s}W_A\frac{s}{\eta_A^2 + s}. \end{aligned}$$

We remark that $w_A = \eta_A^{+-} + \eta_A^{-+}$ and by the Cauchy-Schwartz inequality :

$$-Y_A \le w_A \le Y_A,$$

Then we split at level $M = \|w_A\|^a_{\mathfrak{S}_p}$: $\int_0^{+\infty} = \int_0^M + \int_M^{+\infty}$.

For the first integral we have $W_A = w_A\eta_A + Y_A w_A$ and it follows that :

$$\begin{aligned} \|\tfrac{Y_A}{Y_A^2+s}w_A\tfrac{s}{s+\eta_A^2}\|_{\mathfrak{S}_p} \quad &\le 2\|\tfrac{Y_A}{Y_A^2+s}|w_A|^{1-t}\|_{\mathfrak{S}_\infty}\||w_A|^t\|_{\mathfrak{S}_p} \quad \le 2s^{-t/2}\|w_A\|_{\mathfrak{S}_{tp}} \\ \|\tfrac{\sqrt{s}}{Y_A^2+s}w_A\tfrac{\eta_A\sqrt{s}}{\eta_A^2+s}\|_{\mathfrak{S}_p} \quad &\le 2\|\tfrac{\sqrt{s}}{Y_A^2+s}|w_A|^{1-t}\|_{\mathfrak{S}_\infty}\||w_A|^t\|_{\mathfrak{S}_p} \quad \le 2s^{-t/2}\|w_A\|_{\mathfrak{S}_{tp}}. \end{aligned}$$

So :

$$\int_0^{\|w_A\|_{\mathfrak{S}_p}^a} \|\cdot\|_{\mathfrak{S}_p} \le \frac{8}{1-t}\|w_A\|_{\mathfrak{S}_{tp}}\|w_A\|_{\mathfrak{S}_p}^{(1-t)a/2}.$$

For the second integral, we have :

$$\begin{array}{ll} \|\frac{Y_A}{Y_A^2+s}w_A\frac{s}{s+\eta_A^2}\|_{\mathfrak{S}_p} & \le \|\frac{1}{Y_A^2+s}\|_{\mathfrak{S}_\infty}\|Y_Aw_A\|_{\mathfrak{S}_p}\|\frac{s}{\eta_A^2+s}\|_{\mathfrak{S}_\infty} \le s^{-1}\|w_A\|_{\mathfrak{S}_p}\\ \|\frac{1}{Y_A^2+s}w_A\eta_A\frac{s}{\eta_A^2+s}\|_{\mathfrak{S}_p} & \le \|\frac{1}{Y_A^2+s}\|_{\mathfrak{S}_\infty}\|w_A\eta_A\|_{\mathfrak{S}_p}\|\frac{s}{\eta_A^2+s}\|_{\mathfrak{S}_\infty} \le s^{-1}\|w_A\|_{\mathfrak{S}_p}; \end{array}$$

and

$$\int_{\|w_A\|_{\mathfrak{S}_p}^a}^{+\infty} \|\cdot\|_{\mathfrak{S}_p} \le 4\|w_A\|_{\mathfrak{S}_p}^{1-a/2}.$$

As $\|w_A\|_{\mathfrak{S}_p} = \mathcal{O}(A^{-1+3/p})$ we choose for instance : $tp-3 = (p-3)/2$ and $(1-a/2) = (1-t)a/2$ that is

$$t = \frac{3+p}{2p},\ a = \frac{2}{1+(1-t)/2},$$

but of course it can be optimized in a, t. □

Kinetic energy

We write

$$\widetilde{Q}_n := |\mathbf{D}|^{1/2}(Q_n^{++} - Q_n^{--})|\mathbf{D}|^{1/2} =: \widetilde{Q}_n^+ - \widetilde{Q}_n^-.$$

We have :

$$\begin{array}{ll} \mathrm{Tr}(|\mathbf{D}|^{1/2}(Q_n^{++}-Q_n^{--})|\mathbf{D}|^{1/2}) & = \mathrm{Tr}(X_A^2\widetilde{Q}_n) + \mathrm{Tr}(Y_A\widetilde{Q}_nY_A)\\ \mathrm{Tr}(X_A^2\widetilde{Q}_n^+) & = \mathrm{Tr}\big\{(X_A^2-\chi_A^2)\widetilde{Q}_n^+\big\} + \mathrm{Tr}(\chi_A\widetilde{Q}_n^+\chi_A)\\ \mathrm{Tr}(Y_A\widetilde{Q}_n^+Y_A) & = \mathrm{Tr}\big\{[Y_A,|\mathbf{D}|^{1/2}]Q_n^{++}|\mathbf{D}|^{1/2}Y_A\big\} + \mathrm{Tr}\big\{|\mathbf{D}|^{1/2}Y_AQ_n^{++}[|\mathbf{D}|^{1/2},Y_A]\big\}\\ & \quad +\mathrm{Tr}\big\{|\mathbf{D}|^{1/2}(Y_AQ_nY_A)^{++}|\mathbf{D}|^{1/2}\big\}, \end{array}$$

where :

$$\begin{array}{ll} \|[Y_A,|\mathbf{D}|^{1/2}]\frac{1}{|\mathbf{D}|^{1/2}}|\mathbf{D}|^{1/2}Q_n^{++}|\mathbf{D}|^{1/2}\|_{\mathfrak{S}_1} & \le \|[Y_A,|\mathbf{D}|^{1/2}]\frac{1}{|\mathbf{D}|^{1/2}}\|_{\mathcal{B}}\||\mathbf{D}|^{1/2}Q_n^{++}|\mathbf{D}|^{1/2}\|_{\mathfrak{S}_1}\\ & \lesssim \|[Y_A,|\mathbf{D}|^{1/2}]\frac{1}{|\mathbf{D}|^{1/2}}\|_{\mathcal{B}} = \underset{A\to\infty}{o}(1)\\ \|(X_A^2-\chi_A^2)|\mathbf{D}|^{1/2}Q_n^{++}|\mathbf{D}|^{1/2}\|_{\mathfrak{S}_1} & \lesssim \|X_A^2-\chi_A^2\|_{\mathcal{B}} = \mathcal{O}(A^{-1})\\ \liminf\limits_{n\to+\infty}\ \mathrm{Tr}(\chi_A|\mathbf{D}|^{1/2}(Q_n^{++}-Q_n^{--})|\mathbf{D}|^{1/2}\chi_A) & \ge \mathrm{Tr}(\chi_A|\mathbf{D}|^{1/2}(Q_\infty^{++}-Q_\infty^{--})|\mathbf{D}|^{1/2}\chi_A). \end{array}$$

The last inequality is just Fatou's Lemma.

Exchange term

As there hold $|\mathbf{D}|^{1/2}Q_n \underset{\mathfrak{S}_2}{\rightharpoonup} |\mathbf{D}|^{1/2}Q_\infty$ and $\Lambda^2|\mathbf{D}|^{1/2} \ge |D_0|^{3/2}$, the sequence $(Q_n)_n$ is $H^1(\mathbb{R}^3\times\mathbb{R}^3)$-bounded. Up to a subsequence, $(Q_n)_n$ tends to Q_∞ in L^2_{loc} and $(Q_n(x,y))_n$ tends *a.e.* to $Q_\infty(x,y)$ in $\mathbb{R}^3\times\mathbb{R}^3$.

We write

$$\delta_n = Q_n - Q_\infty. \tag{9.21}$$

First we have

$$\begin{array}{ll} \mathrm{Tr}(Q_nR(Q_n)) & = \mathrm{Tr}(Q_\infty R(Q_\infty)) + \mathrm{Tr}((Q_n-Q_\infty)R(Q_n-Q_\infty)) + 2\mathfrak{Re}\ \mathrm{Tr}((Q_n-Q_\infty)R(Q_\infty));\\ \mathrm{Tr}((\delta_n)R(\delta_n)) & = \iint \frac{|Y_A\delta_nY_A(x,y)|^2}{|x-y|}dxdy + \iint \frac{|(\delta_n-Y_A\delta_nY_A)(x,y)|^2}{|x-y|}dxdy\\ & \quad +2\mathfrak{Re}\ \mathrm{Tr}((\delta_n-Y_A\delta_nY_A)R(Y_A\delta_nY_A));\\ \mathrm{Tr}(Y_A\delta_nY_AR(Y_A\delta_nY_A)) & = \mathrm{Tr}(Y_AQ_nY_AR(Y_AQ_nY_A)) + \mathrm{Tr}(Y_AQ_\infty Y_AR(Y_AQ_\infty Y_A))\\ & \quad -2\mathfrak{Re}\mathrm{Tr}(Y_AQ_\infty Y_AR(Y_AQ_nY_A))\\ & \le \mathrm{Tr}(Y_AQ_nY_AR(Y_AQ_nY_A)) + C_1\mathrm{Tr}(Y_AQ_\infty Y_AR(Y_AQ_\infty Y_A)) \end{array}$$

where the last inequality holds because there is a uniform bound for $\mathrm{Tr}(Y_A Q_n Y_A R(Y_A Q_n Y_A))$.

By weak-$*$ convergence, it is clear that :

$$\lim_{n\to+\infty} \mathfrak{Re}\ \mathrm{Tr}((Q_n - Q_\infty)R(Q_\infty)) = \lim_{n\to+\infty} \mathfrak{Re}\ \mathrm{Tr}((Q_n - Q_\infty)R(Q_\infty)) = 0,$$

it suffices to remark that $|\mathbf{D}|^{-1/2}R(Q_\infty) \in \mathfrak{S}_2$. There remains to estimate

$$M_n^R := \iint \frac{|(\delta_n - Y_A\delta_n Y_A)(x,y)|^2}{|x-y|}dxdy,$$

for the last term we just use the Cauchy-Schwartz inequality.

– There holds :

$$1 - Y_A = \chi_A^2 + \eta_A^2 - \eta_A + \eta_A - Y_A = \chi_A^2 + (\eta_A^2 - \eta_A) + (\eta_A^{+-} + \eta_A^{-+}) = \chi_A^2 + \underbrace{\eta_A(1-\eta_A)}_{\theta_A} + w_A. \tag{9.22}$$

It is clear that supp χ_A, supp $\theta_A \subset B(0,2A)$. By [CDL08], $\|w_A\|_{\mathfrak{S}_p} = \mathcal{O}(A^{-1+3/p})$ for any $p > 3$:

$$\begin{aligned} \delta_n - Y_A\delta_n Y_A &= (1-Y_A)\delta_n + Y_A\delta_n(1-Y_A) \\ &= (1-Y_A)\delta_n(\chi_A^2 + \eta_A^2) + (Y_A - \eta_A)\delta_n(1-Y_A) + \eta_A\delta_n(1-Y_A) \\ &= (\chi_A^2 + \theta_A + w_A)\delta_n(\chi_A^2 + \eta_A^2) + (Y_A - \eta_A)\delta_n(1-Y_A) + \eta_A\delta_n(\chi_A^2 + \theta_A + w_A) \\ &=: (\chi_A^2 + \theta_A)\delta_n\chi_A^2 + (\chi_A^2+\theta_A)\delta_n\eta_A^2 + \eta_A\delta_n(\chi_A^2 + \theta_A) + \delta\delta_n \end{aligned} \tag{9.23}$$

Let us prove $\limsup_{n\to+\infty} \mathrm{Tr}(\delta\delta_n R(\delta\delta_n)) = \underset{A\to+\infty}{o}(1)$. We have $\|R(Q)\|_{\mathfrak{S}_2} \lesssim \|\nabla Q\|_{\mathfrak{S}_2}$. For any $\widetilde{B} \in \mathcal{B}$ there holds

$$\partial_j \eta_A^{+-}\delta_n\widetilde{B} = P_+^0(\partial_j\eta_A)P_-^0\delta_n\widetilde{B} + \eta_A^{+-}(\partial_j\delta_n)\widetilde{B}.$$

For the term $q_n^1 := (\chi_A^2 + \theta_A)\delta_n\chi_A^2$ in (9.23) we use the Cauchy-Schwartz inequality :

$$|\mathrm{Tr}(q_n^1 R(q_n^1))| \le 4\|q_n^1\|_{\mathfrak{S}_2}\|\nabla q_n^1\|_{\mathfrak{S}_2} \lesssim \|q_n^1\|_{\mathfrak{S}_2}\sup_n\|\sqrt{1-\Delta}Q_n\|_{\mathfrak{S}_2}.$$

By L^2_{loc} convergence of (Q_n), we have $\lim_n\|q_n^1\|_{\mathfrak{S}_2} = 0$ and

$$\lim_{n\to+\infty}\mathrm{Tr}(q_n^1 R(q_n^1)) = 0.$$

For $q_n^2 := (\chi_A^2 + \theta_A)\delta_n\eta_A^2 + \eta_A\delta_n(\chi_A^2+\theta_A)$ we split the domain of integration in two :

$$\begin{aligned} \iint \frac{|q_n^2(x,y)|^2}{|x-y|}dxdy &= \iint_{|x-y|>A} \frac{|q_n^2(x,y)|^2}{|x-y|}dxdy + \iint_{|x-y|\le A} \frac{|q_n^2(x,y)|^2}{|x-y|}dxdy \\ &\le \frac{\|q_n^2\|_{\mathfrak{S}_2}^2}{A} + \iint_{|x|,|y|\le 3A} \frac{|q_n^2(x,y)|^2}{|x-y|}dxdy \\ &\le \frac{\|q_n^2\|_{\mathfrak{S}_2}^2}{A} + \|R(q_n^2)\|_{\mathfrak{S}_2}\Big(\iint_{|x|,|y|\le 3A}|q_n^2(x,y)|^2dxdy\Big)^{1/2}. \end{aligned}$$

As before

$$\limsup_{n\to+\infty}\iint\frac{|q_n^2(x,y)|^2}{|x-y|}dxdy = \mathcal{O}(A^{-1}).$$

Finally :

$$M_n^R \le 3\big(\mathrm{Tr}(q_n^1R(q_n^1)) + \mathrm{Tr}(q_n^2R(q_n^2)) + \mathrm{Tr}(\delta\delta_nR(\delta\delta_n))\big)$$

and

$$\limsup_{n\to+\infty} M_n^R = \underset{A\to+\infty}{o}(1).$$

Direct term

As for the exchange term :

$$D(\rho_{Q_n},\rho_{Q_n}) = D(\rho_{Q_\infty},\rho_{Q_\infty}) + D(\rho(Q_n-Q_\infty),\rho(Q_n-Q_\infty)) + 2\mathfrak{Re}\; D(\rho(Q_n-Q_\infty),\rho(Q_\infty))$$

with $\lim_{n\to+\infty} D(\rho(Q_n-Q_\infty),\rho(Q_\infty)) = 0$ by weak convergence of $\rho(Q_n)$ to $\rho(Q_\infty)$.

There remains to estimate : $M_n^d := D(\rho(Q_n-Q_\infty),\rho(Q_n-Q_\infty))$. We write $\delta_n = Q_n - Q_\infty$ and

$$\begin{aligned} \|\rho(\delta_n)\|_{\mathcal{C}}^2 &= \|\rho(Y_A\delta_nY_A)\|_{\mathcal{C}}^2 + 2\mathfrak{Re}\; D(\rho(\delta_n),\rho(\delta_n - Y_A\delta_nY_A)) + \|\rho(\delta_n - Y_A\delta_nY_A)\|_{\mathcal{C}}^2 \\ \|\rho(Y_A\delta_nY_A)\|_{\mathcal{C}}^2 &= \|\rho(Y_AQ_nY_A)\|_{\mathcal{C}}^2 + \|Y_AQ_\infty Y_A\|_{\mathcal{C}}^2 - 2\mathfrak{Re}\; D(\rho(Y_AQ_nY_A),\rho(Y_AQ_\infty Y_A)) \\ &\geq \|\rho(Y_AQ_nY_A)\|_{\mathcal{C}}^2 - C_2\|Y_AQ_\infty Y_A\|_{\mathcal{C}}^2. \end{aligned} \tag{9.24}$$

The last inequality holds because there is a uniform bound for $\|\rho(Y_AQ_nY_A)\|_{\mathcal{C}}^2$, following from the uniform bound for $(\||D_0|^{a[\Lambda]}Q_n^{\pm\pm}\|_{\mathfrak{S}_1} + \||D_0|^{a[\Lambda]}Q_n\|_{\mathfrak{S}_2})_n$ where $a[\Lambda] := \frac{1+(\log(\Lambda))^{-1}}{2}$.

Remark 9.4. We estimate $\|\rho(Y_AQ_nY_A)\|_{\mathcal{C}}$ with the help of the duality formula.

We write

$$\delta_n - Y_A\delta_nY_A = -(1-Y_A)\delta_n(1-Y_A) + (1-Y_A)\delta_n + \delta_n(1-Y_A) = q_n^3 + q_n^4 + q_n^5 \tag{9.25}$$

and by the Cauchy-Schwarz inequality :

$$D(q_n^3+q_n^4+q_n^5, q_n^3+q_n^4+q_n^5) \leq 3(D(q_n^3,q_n^3) + D(q_n^4,q_n^4) + D(q_n^5,q_n^5)).$$

Remark 9.5. We recall that $[Y_A, P_+^0] = 0$. For all $0<\varepsilon<1$, we write $a = (1+\varepsilon)/2$. There holds :

$$\|\rho_Q\|_{\mathcal{C}} \leq C_\varepsilon(\||D_0|^aQ^{\pm\mp}\|_{\mathfrak{S}_2} + \||D_0|^aQ^{\pm\pm}\|_{\mathfrak{S}_1}).$$

In particular, for $\varepsilon_1,\varepsilon_2\in\{+,-\}$ we have :

$$|D_0|^aY_AQ_n^{\varepsilon_1,\varepsilon_2}Y_A = [|D_0|^a, Y_A]|D_0|^{-a}|D_0|^aQ_n^{\varepsilon_1,\varepsilon_2}Y_A + Y_A|D_0|^aQ_n^{\varepsilon_1,\varepsilon_2}Y_A,$$

and taking either the trace-class norm ($\varepsilon_1=\varepsilon_2$) or the Hilbert-Schmidt norm ($\varepsilon_1=-\varepsilon_2$) we obtain a uniform bound independant of n and $A\geq 1$.

There holds for $0<\varepsilon\leq 1$:

$$\big\|[|D_0|^{(1+\varepsilon)/2}, 1-Y_A]\big\|_{\mathcal{B}} \leq \big\|[\eta_A^{++}, |D_0|^{(1+\varepsilon)/2}]\big\|_{\mathcal{B}} + \big\|[\eta_A^{--}, |D_0|^{(1+\varepsilon)/2}]\big\|_{\mathcal{B}} \lesssim 1/A.$$

We use the same method as in [CDL08, Lemma 11] but with the following formula : $x^a = \text{Cnst}\displaystyle\int_0^{+\infty}\frac{x}{x+s}\frac{ds}{s^{a-1}}$ to $x=|D_0|$ and $a=\frac{1+\varepsilon}{2}$. We apply (9.22) to $(1-Y_A)|D_0|^{(1+\varepsilon)/2}\delta_n^{(++)}$ and so on. The term with w_A is easily dealt with :

$$\begin{aligned} \|w_A|D_0|^aQ_n^{(++)}B\|_{\mathfrak{S}_1} &\leq \|w_A\|_{\mathcal{B}}\||D_0|^a\delta_n^{(++)}\|_{\mathfrak{S}_1}\|B\|_{\mathcal{B}} \\ \|w_A|D_0|^aQ_nB\|_{\mathfrak{S}_2} &\leq \|w_A\|_{\mathcal{B}}\||D_0|^a\delta_n\|_{\mathfrak{S}_2}\|B\|_{\mathcal{B}} \end{aligned}$$

where we recall : $|D_0|^{3/2}\leq\Lambda^2|\mathbf{D}|\leq\Lambda^2|D_0|^{3/2}$. For the other terms (with $\chi_A^2+\theta_A$) we use the following :

$$\rho((\chi_A^2+\theta_A)Q) = (\chi_A^2+\theta_A)\rho(Q) = \rho(\chi_AQ\chi_A + \theta_A^{1/2}Q\theta_A^{1/2}). \tag{9.26}$$

Indeed the two equalities are true for any $Q\in\mathfrak{S}_1$. We conclude by density.

Finally for $a=\frac{1+\varepsilon}{2}$ with $0<\varepsilon<1$ to be chosen and $\xi_A = \chi_A, \theta_A^{1/2}$ there holds :

$$\begin{aligned} \|\xi_AQ\xi_A\|_{\mathcal{C}} &\leq C_\varepsilon\big\{\||D_0|^a(\xi_AQ\xi_A)^{\pm\mp}\|_{\mathfrak{S}_2} + \||D_0|^a(\xi_AQ\xi_A)^{\pm\pm}\|_{\mathfrak{S}_1}\big\} \\ |D_0|^aP_+^0\xi_AQ\xi_AP_+^0 &= |D_0|^a\big\{\xi_A^{+-}Q^{-+}\xi_A^{++} + \xi_A^{+-}Q^{--}\xi_A^{-+} + \xi_A^{++}Q^{+-}\xi_A^{-+} + \xi_A^{++}Q^{++}\xi_A^{++}\big\} \\ |D_0|^aP_+^0\xi_AQ\xi_AP_-^0 &= |D_0|^a\big\{\xi_A^{+-}Q^{-+}\xi_A^{+-} + \xi_A^{+-}Q^{--}\xi_A^{--} + \xi_A^{++}Q^{+-}\xi_A^{--} + \xi_A^{++}Q^{++}\xi_A^{+-}\big\} \end{aligned}$$

Let us treat $|D_0|^a P_+^0 \xi_A Q \xi_A P_+^0$. The second term is much simpler because it suffices to estimate it in the Hilbert-Schmidt norm.

We *choose* $0 < \varepsilon < 4^{-1}$ (say 2^{-3}) and $a = (1+\varepsilon)/2$, $b_1 = 3/4 - \varepsilon, b_2 = 3/4 + \varepsilon$.

We use : (*cf* [GLS09] for the second equality)

$$\begin{aligned} K[|D_0|^a, \xi_A^{+-}] &= -i \int_0^{+\infty} \frac{ds}{s^{1-a}} \frac{1}{|D_0|+s} \big\{ P_+^0 \boldsymbol{\alpha} \cdot \nabla \xi_A P_-^0 + 2\xi_A^{+-} D_0 \big\} \frac{1}{|D_0|+s} \\ \xi_A^{+-} = P_+^0 [\xi_A, P_-^0] &= -\frac{i}{2\pi} P_+^0 \int_{-\infty}^{+\infty} \frac{1}{D_0 + i\eta} \boldsymbol{\alpha} \cdot \nabla \xi_A \frac{d\eta}{D_0 + i\eta} \\ K[|D_0|^a, \xi_A^{++}] |D_0|^{-b_1} &= -i \int_0^{+\infty} \frac{ds}{s^{1-a}} \frac{1}{|D_0|+s} \boldsymbol{\alpha} \cdot \nabla \xi_A \frac{1}{|D_0|^{b_1}} \frac{1}{|D_0|+s}, \end{aligned} \tag{9.27}$$

leading to

$$\begin{aligned} [|D_0|^a, \xi_A^{+-}] |D_0|^{-b_1} &\in \mathfrak{S}_4 \text{ provided } \varepsilon < 3/5, \\ [|D_0|^a, \xi_A^{++}] |D_0|^{-b_1} &\in \mathfrak{S}_4 \text{ provided } \varepsilon < 3/5. \end{aligned}$$

In particular for all $\varepsilon_1, \varepsilon_2 = +/-$:

$$[|D_0|^a, \xi_A^{+,\varepsilon_1}] |D_0|^{-b_1} \ |D_0|^{b_1} Q^{\varepsilon_1,\varepsilon_2} |D_0|^{b_2} \ |D_0|^{-b_2} \xi_A^{\varepsilon_2,+} \in \mathfrak{S}_1$$

and by local compactness in Schatten spaces [Sim79, LR12], as $|D_0|^{b_1} \delta_n^{\varepsilon_1,\varepsilon_2} |D_0|^{b_2} \underset{\mathfrak{S}_2}{\rightharpoonup} 0$, the following norm-convergence holds :

$$[|D_0|^a, \xi_A^{+,\varepsilon_1}] |D_0|^{-b_1} \ |D_0|^{b_1} \delta_n^{\varepsilon_1,\varepsilon_2} |D_0|^{b_2} \ |D_0|^{-b_2} \xi_A^{\varepsilon_2,+} \underset{n\to+\infty}{\overset{\mathfrak{S}_1}{\longrightarrow}} 0.$$

There remains terms of type $\xi_A^{+,\varepsilon_1} |D_0|^a \delta_n^{\varepsilon_1,\varepsilon_2} \xi_A^{\varepsilon_2,+}$:

$$\begin{array}{rl|rl} |D_0|^{-\frac{3}{4}} \xi_A^{++} & \in \mathfrak{S}_p \, \forall \, p > 4 & \xi_A^{++} |D_0|^{-\frac{1}{4}+\frac{\varepsilon}{2}} & \in \mathfrak{S}_\infty \\ \xi_A^{+-} |D_0|^{-\frac{1}{4}+\frac{\varepsilon}{2}} & \in \mathfrak{S}_p \, \forall \, p > \frac{12}{5-\varepsilon} & |D_0|^{-\frac{3}{4}} \xi_A^{-+} & \in \mathfrak{S}_2, \end{array}$$

the first row treats the case of $q'_{1;n} = \xi_A^{+-} |D_0|^a \delta_n^{-+} \xi_A^{++}$ and the second that of $q'_{2;n} = \xi_A^{++} |D_0|^a \delta_n^{+-} \xi_A^{-+}$. As $2^{-1} + 4^{-1} + \frac{4^+}{12} = 1^+$ (that is the choice $\varepsilon = \frac{1}{4^+}$), it is clear that if $\varepsilon < 4^{-1}$, the sequence $(q'_{1;n})_n$ converges in the trace-class norm to 0. The same holds for $(q'_{2;n})_n$. Then as before :

$$\begin{aligned} \xi_A^{+-} |D_0|^a \delta_n^{--} \xi_A^{-+} &= \xi_A^{+-} |D_0|^{-1/4+\varepsilon/2} \big\{ |D_0|^{3/4} \delta_n^{--} |D_0|^{3/2} \big\} |D_0|^{-3/2} \xi_A^{-+} \underset{n\to+\infty}{\overset{\mathfrak{S}_1}{\longrightarrow}} 0 \\ \xi_A^{++} |D_0|^a \delta_n^{++} \xi_A^{++} &= \xi_A^{++} |D_0|^{-1/4+\varepsilon/2} \big\{ |D_0|^{3/4} \delta_n^{++} |D_0|^{3/2} \big\} |D_0|^{-3/2} \xi_A^{++} \underset{n\to+\infty}{\overset{\mathfrak{S}_1}{\longrightarrow}} 0. \end{aligned}$$

We have to use here the additional assumption on η_1.

– Let us come back to (9.25) : what we have done enable us to deal with $(1-Y_A)\delta_n$ and $\delta_n(1-Y_A)$.

There remains but $(1-Y_A)\delta_n(1-Y_A)$. We write $1 - Y_A = \chi_A^2 + \theta_A + w_A$. The term

$$w_A \delta_n (1-Y_A) + (\chi_A^2 + \theta_A) \delta_n w_A$$

is treated like $w_A \delta_n$. There remains $(\chi_A^2 + \theta_A)\delta_n(\chi_A^2 + \theta_A)$ which is treated like $\chi_A \delta_n \chi_A$.

– Finally we have :

$$\liminf_{n\to+\infty} \|\rho(\delta_n - Y_A \delta_n Y_A)\|_{\mathcal{C}}^2 \geq \underset{A\to+\infty}{o}(1). \tag{9.28}$$

Conclusion

There holds :

$$\left\{ \begin{aligned} \mathrm{Tr}(|\mathbf{D}|^{1/2}(Q_n^{++} - Q_n^{--})|\mathbf{D}|^{1/2}) &= \mathrm{Tr}(\chi_A |\mathbf{D}|^{1/2}(Q_n^{++} - Q_n^{--})|\mathbf{D}|^{1/2} \chi_A) \\ &\quad + \mathrm{Tr}(|\mathbf{D}|^{1/2}(Y_A Q_n Y_A)^{++} |\mathbf{D}|^{1/2}) + \varepsilon_T^A(n) \\ \iint \frac{|Q_n(x,y)|^2}{|x-y|} dx dy &\leq \mathrm{Tr}(Q_\infty R(Q_\infty)) + \mathrm{Tr}(Y_A Q_n Y_A R(Y_A Q_n Y_A)) \\ &\quad + \varepsilon_R^A(n) + C_1 \mathrm{Tr}(Y_A Q_\infty Y_A R(Y_A Q_\infty Y_A)) \\ D(\rho_{Q_n}, \rho_{Q_n}) &\geq \|\rho_{Q_\infty}\|_{\mathcal{C}}^2 + \|\rho(Y_A Q_n Y_A)\|_{\mathcal{C}}^2 + \varepsilon_\rho^A(n) - C_2 \|\rho(Y_A Q_\infty Y_A)\|_{\mathcal{C}}^2 \end{aligned} \right.$$

where $\limsup_{n\to+\infty}\{|\varepsilon_T^A(n)|+|\varepsilon_R^A(n)|+|\varepsilon_\rho^A(n)|\}=\varepsilon_\infty^A=o_{A\to+\infty}(1)$. Therefore :

$$\begin{aligned}\liminf_{n\to+\infty}\mathcal{E}_{\rm BDF}^\nu(Q_n) \quad & \geq \mathrm{Tr}(\chi_A|\mathbf{D}|^{1/2}(Q_\infty^{++}-Q_\infty^{--})|\mathbf{D}|^{1/2}\chi_A)-\alpha D(\rho_{Q_\infty},\nu)\\ &+\tfrac{\alpha}{2}\Big\{\|\rho_{Q_\infty}\|_{\mathcal{C}}^2-\mathrm{Tr}(Q_\infty R(Q_\infty))\Big\}-\varepsilon_\infty^A-C_2\|\rho(Y_AQ_\infty Y_A)\|_{\mathcal{C}}^2\\ &+E_{\rm BDF}^0(q-\mathrm{Tr}_{P_-^0}(X_AQ_\infty X_A))-C_1\iint\frac{|Y_AQ_\infty Y_A(x,y)|^2}{|x-y|}dxdy,\end{aligned} \tag{9.29}$$

where we used the fact that

$$\mathrm{Tr}((Q_n^{++}-Q_n--)(X_A^2-\chi_A^2+|D_0|^{3/2}|D_0|^{-3/2}\chi_A^2)\underset{n\to+\infty}{\longrightarrow}\mathrm{Tr}(X_A(Q_\infty^{++}-Q_\infty^{--})X_A)$$

by weak-$*$ convergence and the continuity of the map $E_{\rm BDF}^0(\cdot):\mathbb{R}\to\mathbb{R}$ [HLS09, Corollary 3 *mutatis mutandis*].
– At last, let us prove that in the limit $A\to+\infty$, we have :

$$\liminf_{n\to+\infty}\mathcal{E}_{\rm BDF}^\nu(Q_n)=E_{\rm BDF}^\nu(q)\geq E_{\rm BDF}^\nu(q-k)+E_{\rm BDF}^0(k). \tag{9.30}$$

Indeed with the help of (9.27), we can prove that $\rho(Y_AQ_\infty Y_A)\underset{A\to+\infty}{\overset{\mathcal{C}}{\longrightarrow}}0$.
We write $Y_A=\eta_A^{++}+\eta^{--}$ and for $a=(1+2^{-3})/2$ and $b=3/4$:

$$\begin{aligned}(Y_AQ_\infty Y_A)^{++} \quad & =\eta_A^{++}Q_\infty^{++}\eta_A^{++}\\ |D_0|^a(Y_AQ_\infty Y_A)^{++} \quad & =[|D_0|^a,\eta_A^{++}]|D_0|^{-b}|D_0|^bQ_\infty^{++}\eta_A^{++}+\eta_A^{++}|D_0|^aQ^{++}\eta_A^{++}\\ \big\||D_0|^a(Y_AQ_\infty Y_A)^{++}\big\|_{\mathfrak{S}_1} \quad & \leq \big\|[|D_0|^a,\eta_A^{++}]|D_0|^{-b}\big\|_{\mathcal{B}}\big\||D_0|^bQ_\infty^{++}\big\|_{\mathfrak{S}_1}+\big\|\eta_A|D_0|^aQ^{++}\eta_A\big\|_{\mathfrak{S}_1}\\ \big\||D_0|^a(Y_AQ_\infty Y_A)^{++}\big\|_{\mathfrak{S}_1} \quad & \underset{A\to+\infty}{\longrightarrow}0;\end{aligned}$$

similarly :

$$\begin{aligned}(Y_AQ_\infty Y_A)^{+-} \quad & =\eta_A^{++}Q_\infty^{+-}\eta_A^{--}\\ |D_0|^a(Y_AQ_\infty Y_A)^{+-} \quad & =[|D_0|^a,\eta_A^{++}]|D_0|^{-a}|D_0|^aQ_\infty^{+-}\eta_A^{--}+\eta_A^{++}|D_0|^aQ^{+-}\eta_A^{--}\\ \big\||D_0|^a(Y_AQ_\infty Y_A)^{+-}\big\|_{\mathfrak{S}_2} \quad & \leq \big\|[|D_0|^a,\eta_A^{++}]|D_0|^{-a}\big\|_{\mathcal{B}}\big\||D_0|^aQ_\infty^{+-}\big\|_{\mathfrak{S}_2}+\big\|\eta_A|D_0|^aQ^{+-}\eta_A\big\|_{\mathfrak{S}_2}\\ \big\||D_0|^a(Y_AQ_\infty Y_A)^{+-}\big\|_{\mathfrak{S}_2} \quad & \underset{A\to+\infty}{\longrightarrow}0,\end{aligned}$$

where we use the fact that $\eta_A|f_1\rangle\langle f_2|\eta_A=|\eta_Af_1\rangle\langle\eta_Af_2|\underset{A\to+\infty}{\longrightarrow}0$ in the trace-class norm. That $\|\eta_A|D_0|^aQ^{+-}\eta_A\|_{\mathfrak{S}_2}$ tends to 0 is easier for $D_0|^aQ^{+-}\in\mathfrak{S}_2$: it suffices to use the dominated convergence.

Then as before, by Hardy's inequality :

$$\begin{aligned}\mathrm{Tr}\big\{Y_AQ_\infty Y_AR(Y_AQ_\infty Y_A)\big\} \quad & \leq 2\|Y_AQ_\infty Y_A\|_{\mathfrak{S}_2}\|\nabla Y_AQ_\infty Y_A\|_{\mathfrak{S}_2}\\ \mathrm{Tr}\big\{Y_AQ_\infty Y_AR(Y_AQ_\infty Y_A)\big\} \quad & \underset{A\to+\infty}{\longrightarrow}0.\end{aligned}$$

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Résumé

Les modèles de champ moyen en QED apparaissent naturellement dans la modélisation du nuage électronique des atomes lourds. Cette modélisation joue un rôle croissant en physique et chimie quantique, les effets relativistes ne pouvant pas être négligés pour ces atomes. En physique quantique relativiste, le vide est un milieu polarisable, susceptible de réagir à la présence de champ électromagnétique.

On se place dans le cadre du modèle variationnel de Bogoliubov-Dirac-Fock (BDF) qui est une approximation de champ moyen de la QED sans photon (en particulier, les interactions considérées sont purement électrostatiques).

Il est à noter que pour donner un sens au modèle BDF, il est nécessaire d'introduire une régularisation ultra-violette. Il se produit un phénomène de renormalisation de charge due à la polarisation du vide : la charge « observée » de l'électron dépend de sa charge « nue » et du paramètre de régularisation. On étudie rigoureusement ce phénomène ainsi que le problème de la renormalisation de la masse. Cette dernière est en lien avec l'existence d'un état fondamental pour le système d'un électron dans le vide, en l'absence de tout champ extérieur. En revanche, on montre l'absence de minimiseurs dans le cas de deux électrons.

Enfin, on exhibe des points critiques de l'énergie BDF, interprétés comme des états excités du vide. On met en évidence le positronium, système métastable d'un électron et de son antiparticule le positron, ainsi que le dipositronium, molécule métastable constituée de deux électrons et de deux positrons.

Les méthodes utilisées sont variationnelles (concentration-compacité, lemme de Borwein et Preiss).

Astract

In QED, mean-field models appear in the modelling of the electron clouds of heavy atoms. This modelling plays a increasing role in physics and in quantum chemistry : relativistic effects cannot be neglected in these atoms. In relativistic quantum physics the vacuum is a polarizable medium that can react to the presence of an electromagnetic field.

We consider the so-called Bogoliubov-Dirac-Fock (BDF) model, a variational model which is a mean-field approximation of no-photon QED (in particular the interactions are purely electrostatic).

We point out that an ultraviolet regularisation is necessary to properly define the BDF model. The vacuum polarisation leads to a *renormalisation* phenomenon, the "observed" charge of the electron depends on its "bare" charge and the regularisation parameter. We rigorously study both the problem of charge renormalisation and mass renormalisation. This last one is linked to the existence of ground state in the case of an electron in the vacuum, without any external field. In contrast, we show there is no ground state in the case of two electrons.

Finally we exhibit some critical points of the BDF energy which are interpreted as vacuum excited states. In particular, there are the positronium (a metastable system constituted by an electron and its antiparticle called the positron) and the dipositronium (a metastable molecule constituted by two electrons and two positrons).

The methods that we use are variational (concentration-compactness, Borwein and Preiss's Lemma).