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Properties of Ground States in the Bogoliubov-Dirac-Fock Model

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Abstract

We study the Bogoliubov-Dirac-Fock model that allows to consider relativistic electrons interacting with the vacuum in the presence of an external electrostatic field. It can be seen as a Hartree-Fock approximation of QED, where photons are neglected. A state is described by its one-body density matrix: an infinite rank, self-adjoint operator which is a compact perturbation of the negative spectral projector of the free Dirac operator.

We are interested in the properties of minimizers of the BDF-energy in the presence of an external field with charge density $\nu \geq 0$ in the regime α , $\alpha \log(\Lambda)$ and $\alpha\nu$ (in some norms) small where α is the coupling constant and Λ the ultraviolet cut-off. We prove that the density of such minimizer is integrable and compute the effective charge of the system. We also ensure the existence of minimizers under charge constraint $M \in \mathbf{N}^*$ provided that there holds $M - 1 < \int \nu$ close to the nonrelativistic limit $\alpha \rightarrow 0$ with $\alpha \log(\Lambda)$ fixed to a small value. This contrasts with the assumptions of [Arch. Ration. Mech. Anal, 192(3):453-499(2009)] where Λ is fixed. As a consequence, the nonrelativistic model we obtain in the limit keeps track of the charge renormalisation: it is different from the Hartree-Fock model obtained.

1 Introduction

The relativistic quantum theory of electrons is based on the Dirac operator [22]: $mc^2\beta - \sum_{j=1}^3 i\hbar c\alpha_j \cdot \partial_j$. Here c is the speed of light, m the mass of electron, \hbar the Planck's constant,

$$\beta := \begin{pmatrix} \text{id}_{\mathbf{C}^2} & 0 \\ 0 & -\text{id}_{\mathbf{C}^2} \end{pmatrix}, \quad \alpha_j := \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix} \in \text{End}(\mathbf{C}^4),$$

where the σ_j 's are the Pauli matrices:

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

The Dirac operator acts on $\mathfrak{H} := L^2(\mathbf{R}^3, \mathbf{C}^4)$, it is self-adjoint with domain $H^1(\mathbf{R}^3, \mathbf{C}^4)$. In the one-particle theory of Dirac, the energy of a free particle (with wave function $\psi \in L^2(\mathbf{R}^3, \mathbf{C}^4)$) is $\langle D_0\psi, \psi \rangle$. The spectrum of D_0 is $(-\infty, -mc^2] \cup [mc^2, +\infty)$ and one cannot exclude negative energy state a priori. To explain why electrons with negative energies are not observed, Dirac postulated 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 can be seen as a mean-field approximation of Quantum Electrodynamics (QED) and which was introduced by Chaix and Iracane. It enables us to consider a system of relativistic electrons interacting with the vacuum in the presence of an electrostatic field (*e.g.* that one created by some nucleus). This paper is a continuation of previous works by Hainzl, Gravejat, Lewin, Séré, Solovej [9, 10, 12, 11, 7] and Sok (unpublished work arxiv.1211.3830). In this paper we will extend some results of [7].

This model is derived from full QED by making several approximations: the starting point is the full Hamiltonian \mathbb{H} defined on the Fock space $\mathcal{F}_{el} \otimes \mathcal{F}_{pho}$ (the tensor product of that one of the electrons and that one of the photons) and the first approximation is to neglect the photons and work only with \mathcal{F}_{el} (see [2] for more details).

We use relativistic units $\hbar = c = 1$ and set the bare particle mass equal to 1. The fine structure constant is written α . We write $D^0 = -i\boldsymbol{\alpha} \cdot \nabla + \beta$ the free Dirac operator acting on the Hilbert space $\mathfrak{H} = L^2(\mathbf{R}^3, \mathbf{C}^4)$ and P_-^0 (resp. P_+^0) the negative (resp. positive) spectral projector of D_0 .

In the BDF model a system is described by a "Hartree-Fock" state in the Fock space, fully characterized by its one-body density matrix (1pdm) P , an orthogonal projector of $L^2(\mathbf{R}^3, \mathbf{C}^4)$. The projector P_-^0 is the one-body density matrix of the free vacuum Ω_0 of the Fock space \mathcal{F}_{el} . In fact we rather consider the reduced 1pdm $Q := P - P_-^0$. These BDF states are defined in the appendix of [9], it can be shown that a projector P is the 1pdm of a BDF state Ω_P iff Q is Hilbert-Schmidt. By algebraic computation, it can be shown that the formal difference of the energy $\langle \Omega_P | \mathbb{H} | \Omega_P \rangle$ of the state Ω_P and that of Ω_0 is a function of Q , the so-called BDF energy.

We assume there is an external density of charge ν (real-valued) of finite Coulomb norm:

$$D(\nu, \nu) = \|\nu\|_C^2 := \frac{4\pi}{(2\pi)^3} \int \frac{|\widehat{\nu}(k)|^2}{|k|^2} dk = \iint \frac{\nu(x)\nu(y)^*}{|x-y|} dx dy.$$

The last equality holds for suitable ν (for instance $\nu \in \mathcal{C} \cap L^{6/5}(\mathbf{R}^3)$).

Formally the BDF energy for a BDF state with reduced 1pdm Q is:

$$\begin{cases} \text{Tr}_{P_-^0}(D_0 Q) - \alpha D(\rho_Q, \nu) + \frac{\alpha}{2} (D(\rho_Q, \rho_Q) - \text{Ex}[Q]), \\ \text{Tr}_{P_-^0}(D_0 Q) := \text{Tr}\{P_-^0(D_0 Q)P_-^0 + P_+^0(D_0 Q)P_+^0\}, \\ \text{Ex}[Q] := \iint \frac{|Q(x, y)|^2}{|x-y|} dx dy. \end{cases} \quad (2)$$

Here, $\alpha > 0$ is the coupling constant, $Q(x, y)$ the integral kernel of the operator Q and ρ_Q is its density: $\rho_Q(x) = \text{Tr}_{\mathbf{C}^4}(Q(x, x))$. We recognize the kinetic energy, the interaction energy with ν , the direct term and the exchange term as in Hartree-Fock theory. This expression does not always make sense even if Q is Hilbert-Schmidt (that is if $\iint |Q(x, y)|^2 dx dy < +\infty$), in particular it is not always possible to define ρ_Q .

An ultraviolet cut-off $\Lambda > 0$ is needed: in [9, 10, 12, 11], the authors have considered a sharp cut-off, that is they replaced $L^2(\mathbf{R}^3, \mathbf{C}^4)$ by its subspace \mathfrak{H}_Λ consisting of functions whose Fourier transforms vanish outside a ball $B(0, \Lambda)$. Moreover an operator \mathcal{D}^0 different from D_0 is introduced in [12] with projectors

$$\mathcal{P}_-^0 := \chi_{(-\infty, 0)}(\mathcal{D}^0) \text{ and } \mathcal{P}_+^0 := \chi_{(0, +\infty)}(\mathcal{D}^0).$$

In fact Hainzl *et al.* studied the periodized hamiltonian \mathbb{H}_L in a finite box $[-\frac{L}{2}, \frac{L}{2}]$ (with periodic boundary conditions). For L large enough they prove there exists a unique ground state which tends to $\gamma^0 := \mathcal{P}_-^0 - \frac{1}{2}$ as L tends to $+\infty$. Defining the BDF energy with respect to this minimizer ("subtracting $\langle \Omega_{\mathcal{P}_0} | \mathbb{H} | \Omega_{\mathcal{P}_0} \rangle$ ") gives a more relevant model. There holds $\mathcal{D}^0 := \boldsymbol{\alpha} \cdot \mathbf{w}_1(-i\nabla) + \beta w_0(-i\nabla)$ and \mathcal{D}^0 satisfies the following equation:

$$\mathcal{D}^0 = D_0 + \frac{\alpha}{2} \frac{\text{sgn}(\mathcal{D}^0)(x, y)}{|x-y|}. \quad (3)$$

This operator \mathcal{D}^0 was first studied by Lieb and Siedentop in [18] in another context. We know $\mathbf{w}_1(-i\nabla) = \frac{-i\nabla}{|-i\nabla|} w_1(-i\nabla)$ and w_0, w_1 are radial functions satisfying

$$\forall p \in B(0, \Lambda), |p| \leq w_1(p) \leq w_0(p)|p| \text{ and } 1 \leq w_0(p) \leq 1 + \text{Cst} \times \alpha \log(\Lambda). \quad (4)$$

Useful estimates on w_0, \mathbf{w}_1 are proved in arxiv.1211.3830.

Remark 1. Our convention for the Fourier transform \mathcal{F} is the following:

$$\forall f \in L^2(\mathbf{R}^3) \cap L^1(\mathbf{R}^3) : \widehat{f}(p) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbf{R}^3} f(x) e^{-ip \cdot x} dx.$$

Given that, it is possible to define properly a functional $\mathcal{E}_{\text{BDF}}^\nu$ out of (2), defined on a subspace \mathcal{K} of

$$\mathcal{I} = \{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), Q^* = Q, -\mathcal{P}_-^0 \leq Q \leq \mathcal{P}_+^0\}.$$

The set \mathcal{I} is the convex hull in $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ of the reduced 1pdm's and \mathcal{K} is defined in the next section. In the BDF energy we replace the kinetic energy $\text{Tr}_{\mathcal{P}_-^0}(D_0 Q)$ by $\text{Tr}_0(\mathcal{D}^0 Q)$ defined by:

$$\text{Tr}_0(\mathcal{D}^0 Q) := \text{Tr}\{\mathcal{P}_-^0(\mathcal{D}^0 Q)\mathcal{P}_-^0 + \mathcal{P}_+^0(\mathcal{D}^0 Q)\mathcal{P}_+^0\}, \quad (5)$$

A global minimizer of $\mathcal{E}_{\text{BDF}}^\nu$ is interpreted as the polarized vacuum in the presence of an external density ν . To describe a physical system with M electrons, we consider the sector charge of \mathcal{K} defined by the condition $\text{Tr}_0(Q) = M$. We define then the energy functional for $q \in \mathbf{R}$:

$$\begin{cases} E_{\text{BDF}}^\nu(q) & := \inf \{ \mathcal{E}_{\text{BDF}}^\nu(Q), Q \in \mathcal{Q}(q) \}, \\ \mathcal{Q}(q) & := \{ Q \in \mathcal{K}, \text{Tr}_0(Q) = q \}. \end{cases}$$

An important question is that of the existence of a minimizer for $E_{\text{BDF}}^\nu(q)$. In [11], it was shown that a sufficient condition for it is the validity of binding inequalities at level q :

$$\forall q' \in \mathbf{R} \setminus \{0, q\}, E_{\text{BDF}}^\nu(q) < E_{\text{BDF}}^\nu(q - q') + E_{\text{BDF}}^0(q'). \quad (6)$$

A much more difficult task is to check that these inequalities hold. In [11], the authors showed that, given a density $\nu \in L^1(\mathbf{R}^3, \mathbf{R}_+) \cap \mathcal{C}$, an integer $0 \leq M < \int \nu + 1$ and a cut-off level $\Lambda_0 > 0$, then there exists a minimizer of $E_{\text{BDF}}^\nu(M)$ provided $\alpha \leq \varepsilon_0(\nu, \Lambda_0)$ for some number $\varepsilon_0(\nu, \Lambda_0)$. It was proved in arxiv.1211.3830 that $E_{\text{BDF}}^0(1)$ admits a minimizer provided $\alpha, \Lambda^{-1}, L := \alpha \log(\Lambda)$ are small enough which shows that an electron can bind alone in the Dirac sea without any external density. In both cases the results hold in the nonrelativistic regime $\alpha \ll 1$.

We know a minimizer for $E_{\text{BDF}}^\nu(M)$ should satisfy a self-consistent equation of the form [11, 7]

$$Q + \mathcal{P}_-^0 = \chi_{(-\infty, \mu)} \left(\mathcal{D}^0 + \alpha((\rho_Q - \nu) * \frac{1}{|\cdot|} - \frac{Q(x, y)}{|x - y|}) \right) =: \chi_{(-\infty, \mu)}(D_Q). \quad (7)$$

Here, μ is a Lagrange multiplier due to the charge constraint M , interpreted as a chemical potential. For $M > 0, \Lambda_0 > 0$ we have $\mu > 0$ and as $\alpha \rightarrow 0$, a scaling by α^{-1} of $\chi_{(0, \mu)}(D_Q)$ tends - up to translation and extraction of a subsequence - to a minimizer of the Hartree-Fock energy $\mathcal{E}_{\text{HF}}^Z$ for M electrons with $Z := \int \nu$. In arxiv.1211.3830, it is shown that in the case of $\mathcal{E}_{\text{BDF}}^0(1)$ the nonrelativistic limit with L fixed gives the Choquard-Pekar model [15].

In this paper we show that, provided $L = \alpha \log(\Lambda) \leq L_0$, there exists a minimizer for $E_{\text{BDF}}^\nu(M)$ as soon as $M < \int \nu + 1$ and $\alpha \leq \varepsilon_1(\nu, L)$ for some constant $\varepsilon_1(\nu, L)$. The nonrelativistic limit is a perturbed Hartree-Fock model: writing $Z = \int \nu$ and $a = (\frac{2}{3\pi}L)/(1 + \frac{2}{3\pi}L) < 1$ the energy is

$$\begin{aligned} \forall \Gamma \in \mathfrak{S}_1(L^2(\mathbf{R}^3, \mathbf{C}^4)), 0 \leq \Gamma \leq 1, \text{Tr}(\Gamma) = M : \\ \mathcal{E}_{nr}^Z(\Gamma) := \frac{1}{2} \text{Tr}(-\Delta \Gamma) - Z(1 - a) \text{Tr}\left(\frac{1}{|\cdot|} \Gamma\right) + \frac{1}{2} \left\{ \|\rho_\Gamma\|_{\mathcal{C}}^2 - \text{Ex}[\Gamma] \right\} - a \|\rho_\Gamma\|_{\mathcal{C}}^2. \end{aligned}$$

The last term must be thought of as $-a\text{Tr}(\rho_\Gamma * \frac{1}{|\cdot|}\Gamma)$. The vacuum polarizes due to the presence of ν and the electrons, the positive charge ν attracts a cloud of virtual charges 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 $-a\|\rho_\Gamma\|_{\mathcal{C}}^2$ like in a polaron model). Our result gives a wider range of existence of ground state in the space of parameters (α, Λ) compared to that of [11], where the quantity $\alpha \log(\Lambda_0)$ is neglected and considered as $\underset{\alpha \rightarrow 0}{o}(1)$.

To prove this existence result it is necessary to have a good understanding of a minimizer Q_0 and of its density ρ_{Q_0} . In [7] the authors proved that, in the simplified model without the exchange term, the density of a minimizer is integrable. This is a natural result: in the presence of a finite number of charged particles with finite Coulomb energy the vacuum should polarize accordingly and its density should be finite.

Mathematically speaking however this is a non-trivial result because a minimizer of $E_{\text{BDF}}^\nu(M)$ is *not* trace-class. As in [7] we prove in this paper that if Q is such a minimizer, provided L is small enough and $M, \|\nu\|_{\mathcal{C}}^2 \lesssim \log(\Lambda)$, then $\rho_Q \in L^1 \cap \mathcal{C}$ and $\text{Tr}_{\mathcal{P}_\pm}(Q) = M \neq \int \rho_Q$. Moreover, the following *charge renormalisation* formula holds:

$$\int (\rho_Q - \nu) =: Z_3(M - Z) \simeq \frac{M - Z}{1 + \frac{2}{3\pi}L}, \quad (8)$$

where Z_3 is interpreted as the *renormalization constant* [8]. 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 [7] that the density ρ_Q of a minimizer of the reduced energy $E_{\text{rBDF}}^\nu(M)$ is radial as soon as ν is radial and that, in this case, away from the origin, the electrostatic potential of the system is

$$\alpha(\rho_Q - \nu) * \frac{1}{|\cdot|}(x) \underset{x \rightarrow +\infty}{\sim} \frac{\alpha Z_3(M - Z)}{|x|}.$$

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 . It cannot be easily obtained from [7], the presence of the exchange term complicates the study. In our results, we were unable to remove the technical conditions $M, \|\nu\|_{\mathcal{C}}^2 \lesssim \log(\Lambda)$. We emphasize here that we can prove the same results with another choice of cut-off considered in [7], the one consisting in replacing \mathcal{D}^0 by $D_0(1 - \frac{\Delta}{\Lambda^2})$ in $L^2(\mathbf{R}^3, \mathbf{C}^4)$.

The paper is organized as follows: in the next section we properly define the variational problem $\mathcal{E}_{\text{BDF}}^\nu$ and states the main results. In Section 3, we derive from the Cauchy expansion of a minimizer the two fixed point schemes we use. Moreover *a priori* estimates are proved in Subsection 3.2. In Section 4 we prove important estimates on a term of the Cauchy expansion (" $Q_{1,0}$ ") and prove Theorem 1. Section 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 2) and the existence of minimizers close to the nonrelativistic limit (Theorem 3) in Section 6. The nonrelativistic energy is studied in Appendix B. The very technical Appendix C is devoted to prove Proposition 1. We prove Lemma 8 which is used for Sections 4 and 5 in Appendix A.

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 ($\|\nu\|_{\mathcal{C}} < +\infty$).

First let us introduce the ultraviolet cut-off $\Lambda > 0$ used: following the choice of [7], we replace D_0 by \mathcal{D}^0 . Let us recall $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ is the Schatten class of compact operators

A in \mathfrak{H}_Λ such that $\text{Tr}(|A|^p) < +\infty$ [21]. As in [7] and [11] we will deal with

$$\mathfrak{S}_1^{\mathcal{P}^0} := \{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), Q^{++}, Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\} \quad (9)$$

where $Q^{\varepsilon_1 \varepsilon_2} := \mathcal{P}_{\varepsilon_1}^0 Q \mathcal{P}_{\varepsilon_2}^0$. We recall the kinetic energy functional is $\text{Tr}_0(|\mathcal{D}^0|(Q^{++} - Q^{--}))$. We will work in a subset of this space, namely

$$\mathcal{K} := \{Q, -\mathcal{P}_-^0 \leq Q \leq \mathcal{P}_+^0\} \cap \mathfrak{S}_1^{\mathcal{P}^0} \subset \{Q, Q^* = Q\} \cap \mathfrak{S}_1^{\mathcal{P}^0}, \quad (10)$$

the closed convex hull (under that norm) of the difference of two orthogonal projections of type $P - \mathcal{P}_-^0 \in \mathfrak{S}_1^{\mathcal{P}^0}$.

We would like to define the density ρ_Q such that it coincides with the usual density when Q is (locally) trace-class: $\rho_Q(x) = \text{Tr}_{\mathbb{C}^4}(Q(x, x))$ and such that it is of finite Coulomb energy.

Let Q be in $\mathfrak{S}_1^{\mathcal{P}^0}$, then ρ_Q is well defined by duality:

$$\forall V \in \mathcal{C}', QV \in \mathfrak{S}_1^{\mathcal{P}^0} \text{ and } \text{Tr}_0(QV) = \mathcal{C}'\langle V, \rho_Q \rangle_{\mathcal{C}}. \quad (11)$$

and the map: $Q \in \mathfrak{S}_1^{\mathcal{P}^0} \mapsto \rho_Q \in \mathcal{C}$ is continuous [7]. Furthermore $\rho_Q(x)$ is well defined for Q is locally trace-class.

Finally the exchange term is well defined: thanks to Kato's inequality [1, 12, 9]

$$\begin{aligned} \frac{2}{\pi} \iint \frac{|Q(x, y)|^2}{|x - y|} dx dy &\leq \text{Tr}(|\nabla|Q^2) \leq \text{Tr}(|D_0|Q^2) = \text{Tr}\{|D_0|^{1/2}Q^2|D_0|^{1/2}\} \\ \text{and for } Q \in \mathcal{K} : &\leq \text{Tr}\{|D_0|^{1/2}(Q^{++} - Q^{--})|D_0|^{1/2}\} \leq \text{Tr}_{\mathcal{P}_-^0}(\mathcal{D}^0 Q), \end{aligned} \quad (12)$$

Notation 2. For a density $\rho \in \mathcal{C}$ we write: $v_\rho = v[\rho] := \rho * \frac{1}{|\cdot|}$.

For an operator $Q \in \mathfrak{S}_1^{\mathcal{P}^0}$ 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 $\text{Ex}[Q] = \text{Tr}(R_Q^* Q) =: \|Q\|_{\text{Ex}}^2$.

Moreover we write

$$B_Q := v[\rho_Q] - R_Q.$$

The BDF energy is defined as follows:

$$\mathcal{E}_{\text{BDF}}^\nu(Q) := \text{Tr}_{\mathcal{P}_-^0}(\mathcal{D}^0 Q) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2} \left(D(\rho_Q, \rho_Q) - \iint \frac{|Q(x, y)|^2}{|x - y|} dx dy \right), \quad Q \in \mathcal{K}. \quad (13)$$

As said in the introduction we define the energy functional $E_{\text{BD}}^\nu(q)$ by the infimum over $\mathcal{Q}(q) = \{Q \in \mathcal{K}, \text{Tr}_{\mathcal{P}_-^0}(Q) = q\}$.

Notation 3. We write \mathfrak{s}_p for $\frac{\widehat{\mathcal{D}^0}(p)}{\sqrt{w_0(p)^2 + w_1(p)^2}}$ the action of $\text{sign}(\mathcal{D}^0)$ in the Fourier space.

The function $\sqrt{1 + |p|^2}$ is also written $E(p)$ and $\tilde{E}(p) := \sqrt{w_0(p)^2 + w_1(p)^2}$.

Remark 4. We will work in the regime

$$\alpha \leq \alpha_0 \ll 1 \text{ and } L := \alpha \log(\Lambda) \leq L_0 \ll 1. \quad (14)$$

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 we will use the letter K to denote 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 $m > 1$ is some integer, then as in [9] we write

$$K_m := \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^m}.$$

For $M \in \mathbf{N}^*$, let us say that the problem $E_{\text{BDF}}^\nu(M)$ has a minimizer: as pointed out in [11, 7] such a minimizer $\gamma' = \gamma + N$ must be of the following form:

$$\begin{cases} \gamma + P^0 = \chi_{(-\infty, 0)} \{ \mathcal{D}^0 + \alpha((\rho[\gamma'] - \nu) * \frac{1}{|\cdot|} - R[\gamma']) \} =: \chi_{(-\infty, 0)}(D_{\gamma'}), \\ N = \chi_{(0, \mu]} \{ \mathcal{D}^0 + \alpha((\rho_{\gamma'} - \nu) * \frac{1}{|\cdot|} - (R_{\gamma'})) \} = \sum_{j=1}^{M_0} |\psi_j\rangle\langle\psi_j|, \\ \text{so } D_{\gamma'}\psi_j = \mu_j\psi_j \text{ and we write: } n := \rho_N = \sum_j |\psi_j|^2. \end{cases} \quad (15)$$

We choose $0 \leq \mu_1 \leq \mu_2 \leq \dots \leq \mu_{M_0} = \mu < 1$. *A priori* $M_0 \neq M$ but in our regime they are equal (Lemma 3). Indeed in the spirit of [9] 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

$$\|Q\|_{\mathbf{Q}_1}^2 = \|Q\|_{\mathcal{T}}^2 := \iint (\tilde{E}(p) + \tilde{E}(q)) |\widehat{Q}(p, q)|^2 dpdq.$$

Cauchy's expansion: Let $\gamma' = \gamma + N$ be a minimizer for $E_{\text{BDF}}^\nu(M)$, the decomposition is explained in (15).

Notation 5. Throughout this paper $n := \rho_N$, moreover we write ρ'_γ for $\rho_{\gamma'}$ and the double prime means $-\nu$ is added:

$$\rho''_\gamma := \rho_\gamma + n - \nu, \quad n'' = n - \nu.$$

We also write $B'_\gamma = B_{\gamma'} := \rho''_\gamma * \frac{1}{|\cdot|} - R[\gamma']$.

Notation 6. From now on, for any $g : \mathbf{R}^3 \rightarrow [1, +\infty)$ satisfying the condition

$$\exists K_{(g)} > 0 \quad \forall p, q, p_1 \in \mathbf{R}^3, \quad g(p - q) \leq K_{(g)}(g(p - p_1) + g(p_1 - q)),$$

we define two Hilbert spaces:

$$\begin{aligned} \mathbf{Q}_g &:= \{Q \in \mathfrak{S}_2, \iint (\tilde{E}(p) + \tilde{E}(q)) g(p - q) |\widehat{Q}(p, q)|^2 dpdq < +\infty\}, \\ \mathfrak{C}_g &:= \{\rho \in \mathcal{S}'(\mathbf{R}^3), \int \frac{g(k)}{|k|^2} |\widehat{\rho}(k)|^2 dk < +\infty\}. \end{aligned} \quad (16)$$

The letter g always refers to a function of this kind. The case $g \equiv 1$ gives the space \mathbf{Q}_1 of operators Q with $\text{Tr}(|\mathcal{D}^0||Q|^2 + Q^*|\mathcal{D}^0|Q) < +\infty$ and $\mathfrak{C}_1 = \mathcal{C}$. As an example of such functions g one can take $g(p - q) := E(p - q)^a$ for $a > 1$.

Writing the Cauchy expansion [9] in (15) we get:

$$\begin{cases} \gamma + N = N - \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \left(\frac{1}{D_{\gamma'} + i\eta} - \frac{1}{\mathcal{D}^0 + i\eta} \right) = \sum_{j=1}^{+\infty} \alpha^j Q_j(\gamma', \rho''_\gamma), \\ Q_j(\gamma', \rho''_\gamma) := -\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \frac{1}{\mathcal{D}^0 + i\eta} \left(B_{\gamma'} \frac{1}{\mathcal{D}^0 + i\eta} \right)^j. \end{cases} \quad (17)$$

Notation 7. We define $Q_{k,l}$ as the part of $Q_{k+l}(Q, \rho)$ which is polynomial of degree k in R_Q and polynomial of degree l in ρ and $\rho_{k,l}(Q, \rho)$ as its density. For $\ell \geq 1$ and $(Q, \rho) \in \mathfrak{S}_2(H^{1/2}) \in \mathcal{C}$, $\tilde{Q}_\ell[Q, \rho]$ is the operator:

$$\tilde{Q}_\ell[Q, \rho] := \sum_{j=\ell}^{+\infty} \alpha^{j-\ell} Q_j[Q, \rho].$$

Moreover for $(\varepsilon_1, \dots, \varepsilon_{J+1}) \in \{+, -\}^{J+1}$ we define $Q_J^{\varepsilon_1 \dots \varepsilon_{J+1}}$ with the same formula as in (17) save we replace $(\mathcal{D}^0 + i\eta)^{-1}$ by $P_{\varepsilon_j}^0 / (\mathcal{D}^0 + i\eta)$ in the same order. The same holds for $Q_{k,\ell}^{\varepsilon_1 \dots \varepsilon_{J+1}}$. At last we write $Q_{k,\ell}^{\varepsilon_1 a_1 \varepsilon_2 \dots a_J \varepsilon_{J+1}}$ with $a_j \in \{v, R\}$ for the operator

$$-\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \frac{P_{\varepsilon_1}^0}{\mathcal{D}^0 + i\eta} A_1 \frac{P_{\varepsilon_2}^0}{\mathcal{D}^0 + i\eta} \dots A_J \frac{P_{\varepsilon_{J+1}}^0}{\mathcal{D}^0 + i\eta},$$

where $A_j = v = \rho''_\gamma * \frac{1}{|\cdot|}$ if $a_j = v$ or $A_j = -R(\gamma')$ if $a_j = R$.

As shown in [9, 7] we have

$$\rho_{0,1}[\rho] = -\mathcal{F}^{-1}(B_\Lambda) * \rho \quad (18)$$

where $\mathcal{F}^{-1}(B_\Lambda)$ is a radial L^1 function. Going further, we see $Q_{1,0}[\cdot]$ is a very specific operator.

Lemma 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 it is in $L(\mathfrak{S}_p)$ for $1 < p = 1 + \varepsilon < 2$ with norm $\mathcal{O}((\log(\Lambda))^{1-\frac{\varepsilon}{2}})$. Moreover $F_{1,0}$ is also a bounded operator in $L(\mathbf{Q}_g)$ with norm $\mathcal{O}(1)$, and the function

$$\rho F_{1,0} : Q \in \mathbf{Q}_g \mapsto \rho(F_{1,0}[Q]) \in \mathfrak{C}_g$$

is bounded with norm $\mathcal{O}(\sqrt{\log(\Lambda)})$. Provided $\alpha \log(\Lambda)$ is sufficiently small, the operator $(\text{Id} - \alpha F_{1,0})$ is invertible with inverse \mathbf{T} in all those Banach spaces with norm $\mathcal{O}(1)$. The function $\mathfrak{t} : Q \in \mathbf{Q}_g \mapsto \rho(\mathbf{T}[Q] - Q) \in \mathfrak{C}_g$ is bounded and

$$\|\mathfrak{t}_Q\|_{\mathfrak{C}_g} \lesssim \sqrt{L\alpha} \|Q\|_{\mathbf{Q}_g}.$$

This Lemma is proved in Section 4. We write

$$\mathfrak{T} := \mathbf{T} - \text{Id}, \quad \tau_Q := \rho_{\mathbf{T}(Q)}, \quad \tau_{j,k} := \rho_{\mathbf{T}(Q_{j,k})} \quad \text{and} \quad \mathfrak{t}_Q := \rho_{\mathfrak{T}(Q)}. \quad (19)$$

If $Q \in \mathbf{Q}_g \cap \mathfrak{S}_1^{P_0}$ we obtain that $\tau_Q \in \mathcal{C}$. If $\rho_Q \in \mathfrak{C}_g$ then $\tau_Q \in \mathfrak{C}_g$.

The self-consistent equation (15) is rewritten:

$$(\text{Id} - \alpha F_{1,0})(\gamma') = N + \alpha Q_{0,1}(\rho''_\gamma) + \sum_{j=2}^{+\infty} Q_j(\gamma', \rho''_\gamma).$$

Taking the inverse \mathbf{T} , we get:

$$\gamma' = \mathbf{T} \left\{ N + \alpha Q_{0,1}(\rho''_\gamma) + \sum_{j=2}^{+\infty} Q_j(\gamma', \rho''_\gamma) \right\}. \quad (20)$$

The important proposition holds:

Proposition 1. For $\rho \in \mathcal{C}$ we have $\alpha \tau_{0,1}(\rho) = -\check{f}_\Lambda * \rho$ where \check{f}_Λ is a radial L^1 function whose L^1 -norm is $\mathcal{O}(\alpha \log(\Lambda))$.

Its technical proof is in Appendix C.

We also need a theorem in the same spirit of Furry's one [6, 9]:

Theorem 1. *There exists $K > 0$ such that for any ρ_0, ρ_1 (say in \mathcal{C}) and $\alpha \sqrt{\log(\Lambda)} \leq K$ there holds:*

$$\rho \left\{ \mathbf{T}(Q_{0,2}(\rho_0)) \right\} = \rho \left\{ \mathbf{T}(Q_{1,1}(\mathbf{T}Q_{0,1}(\rho_1), \rho_0)) \right\} = 0. \quad (21)$$

Remark 8. $\mathbf{T}(Q_{0,2}(\rho_0))$ 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 $\text{Tr}_{\mathbb{C}^4}$ is taken. The smallness of $\alpha \sqrt{\log(\Lambda)}$ is to ensure the \mathbf{T} operator is well defined on \mathbf{Q}_1 .

Computation of $\int_{\mathbb{R}} \rho_\gamma(x) dx$:

Theorem 2. *Let M be in \mathbf{N} and $\gamma' = \gamma + N$ be a minimizer of $E_{BDF}^\nu(M)$ and assume $M, \|\nu\|_{\mathcal{C}}^2 \lesssim \log(\Lambda)$ and (14), the decomposition of γ' is that of (15). Then $\rho_\gamma \in L^1$ and*

$$\int \rho_\gamma(x) dx = -\frac{\alpha f_\Lambda(0)}{1 + \alpha f_\Lambda(0)} (M - Z) \quad (22)$$

Existence of minimizers.

Theorem 3. *There exists $L_0 > 0$ satisfying the following result: for any non-negative function $\nu \in \mathcal{C} \cap L^1$ with $Z = \int \nu$ and $0 < L \leq L_0$, there exists $\alpha_1 = \alpha_1(\nu, L) > 0$ such that if $\alpha \leq \alpha_1$ and $\frac{f_\Lambda(0)}{1+f_\Lambda(0)} = a$ then for any integer $0 \leq M < Z + 1$ the problem $E_{\text{BDF}}^\nu(M)$ admits a minimizer.*

Let $\gamma' = \chi_{(0, \mu]}(D_{\gamma'})$ be a minimizer, decomposed as in (15) and let U_α be defined as follows:

$$U_\alpha : \begin{array}{ccc} L^2(\mathbf{R}^3, \mathbf{C}^4) & \rightarrow & L^2(\mathbf{R}^3, \mathbf{C}^4) \\ \phi(x) & \mapsto & \alpha^{-3/2} \phi(\frac{x}{\alpha}) \end{array} .$$

Then as α tends to 0, $U_\alpha^ \chi_{(0, \mu]}(D_{\gamma'}) U_\alpha$ tends to a minimizer of*

$$\begin{aligned} \mathcal{E}_{nr}^Z(\Gamma) &:= \frac{1}{2} \text{Tr}(-\Delta \Gamma) - Z(1-a) \text{Tr}\left(\frac{1}{|\cdot|} \Gamma\right) \\ &\quad + \frac{1}{2} (D(\rho_\Gamma, \rho_\Gamma) - \text{Ex}[\Gamma]) - aD(\rho_\Gamma, \rho_\Gamma), \quad 0 \leq \Gamma \leq 1, \quad \text{Tr}(\Gamma) = M. \end{aligned}$$

Remark 9. Thanks to Section C and [7] we know that

$$\frac{f_\Lambda(0)}{1+f_\Lambda(0)} = \frac{\frac{2}{3\pi} \alpha \log(\Lambda)}{1 + \frac{2}{3\pi} \alpha \log(\Lambda)} + \mathcal{O}(\alpha + (\alpha \log(\Lambda))^2).$$

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 [21]. The norm of bounded linear operator in \mathfrak{H} is written $\|\cdot\|_{\mathcal{B}}$. We recall $\|\cdot\|_{\text{Ex}}$ and $\|\cdot\|_{\mathcal{C}}$ have already been defined in Sections 1 and 2 and $\|\cdot\|_{\mathbf{Q}_g}, \|\cdot\|_{\mathfrak{C}_g}$ are defined in Remark 6.

With the fixed point method we would like to estimate together

- $\|F_Q(Q, \rho)\|_{\mathcal{T}}$ and $\|F_\rho(Q, \rho)\|_{\mathcal{C}}$,
- In general $\|F_Q(Q, \rho)\|_{\mathbf{Q}_g}$ and $\|F_\rho(Q, \rho)\|_{\mathfrak{C}_g}$. We define $\mathcal{X}_g := \mathbf{Q}_g \times \mathfrak{C}_g$

Remark 10. Throughout the paper we write:

$$\forall p \in B(0, \Lambda), \quad \mathfrak{s}_p := \widehat{\text{sign}(\mathcal{D}^0)}(p) = \frac{\widehat{\mathcal{D}^0}(p)}{\widetilde{E}(p)}. \quad (23)$$

3 Description of minimizers

3.1 Minimizers and fixed point schemes

Let $\gamma' = \gamma + N$ be a minimizer for $E_{\text{BDF}}^\nu(M)$. From Eq. (17) and (18), it is possible to define a fixed-point scheme in the spirit of [9]: we define

$$F^{(1)} = F_Q^{(1)} \times F_\rho^{(1)} : \mathcal{X}_1 \rightarrow \mathcal{X}_1,$$

$$F_Q^{(1)}(Q', \rho'') = N + \sum_{\ell=1}^{\infty} \alpha^\ell Q_\ell(Q', \rho''), \quad (24a)$$

$$\mathcal{F}(F_\rho^{(1)}(Q', \rho''); k) = \frac{1}{1 + \alpha B_\Lambda(k)} \widehat{n}''(k) + \frac{1}{1 + \alpha B_\Lambda(k)} \left(\alpha \widehat{\rho}_{1,0}(Q'; k) + \sum_{\ell=2}^{\infty} \alpha^\ell \widehat{\rho}_\ell(Q', \rho''); k \right) \quad (24b)$$

To prove $F^{(1)}$ is well-defined we use the following Lemma proved in Section 5.

Lemma 2. Let g be some function satisfying (6), with constant $K_{(g)} > 0$. There exists $C_0 > 0$ such that for any $J \geq 2$, the linear operator:

$$(Q, \rho) \in \mathbf{Q}_g \times \mathfrak{C}_g \mapsto (Q_J(Q, \rho), \rho_J(Q, \rho)) \in \mathbf{Q}_g \times \mathfrak{C}_g$$

is bounded with norm lesser than $2K_{(g)}^J C_0^J J^{1/2}$.

This gives:

Lemma 3. Let $\gamma' = \gamma + N$ be a minimizer for $E_{\text{BDF}}^\nu(M)$. In the regime of Remark 4 the following holds:

1. $F^{(1)} : B_{\mathcal{X}_1}(0, R_0) \rightarrow B_{\mathcal{X}_1}(0, R_0)$ 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 as γ is a difference of an orthogonal projector and \mathcal{P}^0 , we get $|\text{Tr}_0(\gamma)| \lesssim \|\gamma\|_{\mathfrak{S}_2}^2 = o(1)$. As shown in [9], this must be an integer: $\text{Tr}_0(\gamma) = 0$ and

$$\text{Tr}(N) = \text{Tr}_0(N) = \text{Tr}_0(\gamma') - \text{Tr}_0(\gamma) = M.$$

□

It is more subtle to prove ρ_γ is in L^1 : 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 defined in (a ball of) $\mathcal{C} \cap L^1$, namely:

$$\begin{cases} h_2 &= \alpha^2 \tau_{1,1} \left\{ \mathbf{T}[N] + \alpha^2 \{ \alpha \mathbf{T} \tilde{Q}_3(\gamma', \rho_\gamma'') + \mathbf{T} Q_{2,0}(\gamma', \rho_\gamma'') \}, \rho_\gamma'' \right\} + \alpha^2 \tau_{2,0}(\gamma') \\ F_2^{(2)}(\rho'') &= \alpha^2 (\tau_{1,1} \{ \alpha^2 [\mathbf{T} Q_{1,1}(\gamma', \rho'') + \mathbf{T} Q_{0,2}(\rho'')], \rho'' \}) \\ h_3 &= \alpha^4 \tau(\tilde{Q}_4(\gamma', \rho_\gamma'')) + \alpha^3 \{ \tau_{3,0}(\rho_\gamma'') + \tau_{2,1}(\gamma', \rho_\gamma'') \} \\ F_3^{(2)}(\rho'') &= \alpha^3 \tau_{0,3}(\rho'') + \alpha^3 \tau_{1,2}(\gamma', \rho'') \end{cases} \quad (25)$$

$$\mathcal{F}\{F^{(2)}(\rho'')\} = \frac{1}{1 + f_\Lambda(\cdot)} \tilde{n}'' + \frac{1}{1 + f_\Lambda(\cdot)} \left\{ \hat{h}_2 + \mathcal{F}\{F_2^{(2)}\} + \hat{h}_3 + \mathcal{F}\{F_3^{(2)}\} \right\}(\rho'') \quad (26)$$

Remark 11. The definition of $F^{(2)}$ may appear complicated. It is built on the self-consistent equation:

$$\rho_\gamma' = \tau \left\{ N + \alpha Q_{0,1}(\rho_\gamma'') + \alpha^2 (\tilde{Q}_2(\gamma', \rho_\gamma'') - Q_{1,1}(\gamma', \rho_\gamma'')) \right\} + \alpha^2 \tau [Q_{1,1}(F_Q^{(1)}(\gamma', \rho_\gamma''), \rho_\gamma'')].$$

Notation 12. We introduce the function $F_\Lambda := \frac{f_\Lambda}{1 + f_\Lambda}$, studied in Appendix C: among other results we prove there that $\tilde{F}_\Lambda \in L^1$.

Lemma 4. Let $\gamma' = \gamma + N$ be a minimizer for $E_{\text{BDF}}^\nu(M)$ and $F^{(2)}$ the function built on it. In the regime of Remark 4, this is a well-defined function in \mathcal{C} and $\mathcal{C} \cap L^1$.

There exists $R_0 > 0$ such that $B(0, R_0)$ is $F^{(2)}$ -invariant and on which $F^{(2)}$ is a contraction; ρ_γ'' is the only fixed point in both Banach spaces. In particular $\rho_\gamma \in L^1$.

Remark 13. The study of $Q_{1,0}$ enables us to give the *linear* response of the vacuum to the presence of electrons N and the external potential ν :

$$\begin{cases} \gamma &= \alpha \mathbf{T}[Q_{0,1}((\delta_0 - \tilde{F}_\Lambda) * (n - \nu + \mathbf{t}_N))] + \mathfrak{T}_N + \dots \\ \rho_\gamma &= -\tilde{F}_\Lambda * (n - \nu) + (\delta_0 - \tilde{F}_\Lambda) * \mathbf{t}_N + \dots \end{cases}$$

Remark 14. Results of Lemma 2 and 3 are already in arxiv.1211.3830 but we have chosen to rewrite a simplified proof here because we use the same estimates to prove Lemma 4 in a more difficult way.

3.2 *A priori* estimates

Lemma 5. Let $M \in \mathbf{N}$ and Q a test function Q for $E_{\text{BDF}}^\nu(M)$ and assume $\mathcal{E}_{\text{BDF}}^\nu(Q) \leq E_{\text{BDF}}^\nu(M) + \varepsilon$ where $0 < \varepsilon = o(\alpha \|\nu\|_{\mathcal{C}}^2)$. Then we have $\|Q\|_{\mathfrak{S}_2}^2 \lesssim M + \alpha \|\nu\|_{\mathcal{C}}^2$ and

$$\begin{aligned} \text{Tr}(|\nabla|Q^2) &\lesssim \alpha \|\nu\|_{\mathcal{C}}^2 + \alpha^{1/2} M + \sqrt{\alpha M} \|\nu\|_{\mathcal{C}}, \\ \alpha \|\rho_Q - \nu\|_{\mathcal{C}}^2 &\lesssim \alpha \|\nu\|_{\mathcal{C}}^2 + \alpha^{3/2} M + \sqrt{\alpha M} \alpha \|\nu\|_{\mathcal{C}}. \end{aligned}$$

As a corollary we get the following result.

Lemma 6. Assume we are in the regime of Remark 4 and let Q be as in Lemma 5. Let D_Q be $D_Q := \mathcal{D}^0 + \alpha B = \mathcal{D}^0 + \alpha((\rho_Q - \nu) * \frac{1}{|\cdot|} - R_Q)$. In the sense of self-adjoint operator we have

$$(1 - o(1))|\mathcal{D}^0| \leq |\mathcal{D}^0 + \alpha B_Q| \leq (1 + o(1))|\mathcal{D}^0|, \quad (27)$$

where the $o(1)$ is $\mathcal{O}(\alpha \|\nu\|_{\mathcal{C}} + \alpha^{5/4} M^{1/2} + (\alpha M)^{1/4} \alpha \|\nu\|_{\mathcal{C}}^{1/2})$.

Proof of Lemma 5: It is known [11] that $E_{\text{BDF}}^\nu(M) \leq M$. There holds:

$$\begin{aligned} M + \varepsilon + \frac{\alpha}{2} \|\nu\|_{\mathcal{C}}^2 &\geq \mathcal{E}_{\text{BDF}}^\nu(Q) + \frac{\alpha}{2} \|\nu\|_{\mathcal{C}}^2 \geq (1 - \alpha \frac{\pi}{4}) \text{Tr}_0(\mathcal{D}^0 Q) + \frac{\alpha}{2} \|\rho_Q - \nu\|_{\mathcal{C}}^2 \\ &\geq (1 - \alpha \frac{\pi}{4}) \|Q\|_{\mathfrak{S}_2}^2 + \frac{\alpha}{2} \|\rho_Q - \nu\|_{\mathcal{C}}^2. \end{aligned}$$

We can say more. Indeed:

$$\begin{aligned} \text{Tr}_0(\mathcal{D}^0 Q) - M &= \text{Tr}(|\mathcal{D}^0|^{1/2} (Q^{++} - Q^{--}) |\mathcal{D}^0|^{1/2}) - \text{Tr}_0(Q) \\ &\geq \text{Tr}(|\mathcal{D}^0|^{1/2} Q^2 |\mathcal{D}^0|^{1/2}) - \text{Tr}(Q^2) \\ &\geq \frac{1}{(2\pi)^3} \iint (\tilde{E}(p) - 1) |\hat{Q}(p, q)|^2 dp dq, \end{aligned} \quad (28)$$

and $\tilde{E}(p) - 1 \geq \frac{1}{2} \frac{p^2}{E(p)}$. Then thanks to Kato's inequality (56):

$\text{Tr}(QR_Q) \leq \frac{\pi}{2} \text{Tr}(|\nabla|Q^2)$ which leads to:

$$\frac{1}{2} \text{Tr} \left(\frac{-\Delta}{|D_0|} Q^2 \right) + \frac{\alpha}{2} \|\rho_Q - \nu\|_{\mathcal{C}}^2 \leq \varepsilon + \alpha \left(\frac{\|\nu\|_{\mathcal{C}}^2}{2} + \frac{\pi}{4} \text{Tr}(|\nabla|Q^2) \right).$$

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:

$$\text{Tr} \left(\frac{-\Delta}{|D_0|} Q^2 \right) \lesssim \alpha (\|\nu\|_{\mathcal{C}}^2 + M), \quad (29)$$

thus by the Cauchy-Schwartz inequality:

$$\text{Tr}(|\nabla|Q^2) \lesssim \alpha \|\nu\|_{\mathcal{C}}^2 + \sqrt{\alpha M} + \sqrt{\alpha M} \|\nu\|_{\mathcal{C}}. \quad (30)$$

Proof of Lemma 6:

For all $f \in \mathfrak{H}_\Lambda$ we have:

$$\langle |\mathcal{D}^0|^2 f, f \rangle (1 - \alpha \| |\mathcal{D}^0|^{-1} B \|_{\mathfrak{B}})^2 \leq \langle |\mathcal{D}^0 + \alpha B|^2 f, f \rangle \leq \langle |\mathcal{D}^0|^2 f, f \rangle (1 + \alpha \| |\mathcal{D}^0|^{-1} B \|_{\mathfrak{B}})^2. \quad (31)$$

However thanks to (53) and second point of Lemma 8: $\|R_Q |\nabla|^{-1/2}\|_{\mathfrak{B}} \lesssim \sqrt{\text{Tr}(QR_Q)}$ and

$$\|(\rho_Q - \nu) * \frac{1}{|\cdot|} |\nabla|^{-1/2}\|_{\mathfrak{B}} \lesssim \|(\rho_Q - \nu) * \frac{1}{|\cdot|}\|_{L^6} \lesssim \|\rho_Q - \nu\|_{\mathcal{C}}.$$

As the square root is monotone, there holds

$$(1 - \alpha \| |\mathcal{D}^0|^{-1} B_Q \|_{\mathfrak{B}}) |\mathcal{D}^0| \leq |\mathcal{D}^0 + \alpha B_Q| \leq (1 + \alpha \| |\mathcal{D}^0|^{-1} B_Q \|_{\mathfrak{B}}) |\mathcal{D}^0|, \quad (32)$$

and in the regime precised in Remark 4, this gives $(1 - o(1))|\mathcal{D}^0| \leq |\mathcal{D}^0 + \alpha B_Q| \leq (1 + o(1))|\mathcal{D}^0|$. 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 $\mathcal{O}(\alpha \|\nu\|_{\mathcal{C}} + \alpha^{5/4} M^{1/2} + (\alpha M)^{1/4} \alpha \|\nu\|_{\mathcal{C}}^{1/2})$. \square

***A priori* estimates of a minimizer**

Lemma 7. Let us take $\gamma' = \gamma + N$ a minimizer of $E_{\text{BDF}}^\nu(M)$, decomposed as in (15). Then we have in the regime (14)

$$\begin{aligned} \text{Tr}(|\mathcal{D}^0|N) &\lesssim \log(\Lambda), & \|\gamma\|_{\text{T}} &\lesssim L, \\ \|n''\|_{\mathcal{C}} &\lesssim \sqrt{\log(\Lambda)}, & \|\rho_\gamma\|_{\mathcal{C}} &\lesssim L\sqrt{\log(\Lambda)}. \end{aligned}$$

Proof: For $E_{\text{BDF}}^\nu(M)$ with $M, \|\nu\|_{\mathcal{C}}^2 \lesssim \log(\Lambda)$, we have thanks to Lemma 5:

$$\alpha(\|\rho_\gamma''\|_{\mathcal{C}} + \sqrt{\text{Tr}(|\nabla|\gamma')}) \lesssim \sqrt{\alpha}(\alpha^{1/2}\|\nu\|_{\mathcal{C}} + \alpha^{3/4}M^{1/2} + (\alpha M)^{1/4}\alpha^{1/2}\|\nu\|_{\mathcal{C}}^{1/2}) =: \alpha^{1/2}\ell.$$

We have $\ell = O(\sqrt{L})$. Using Eq. (20) and assuming Lemma 2 and Proposition 1 above we get that:

$$\|\rho_\gamma\|_{\mathcal{C}} \leq \|\check{F}_\Lambda * n''\|_{\mathcal{C}} + \|(\delta_0 - \check{F}_\Lambda) * (\mathfrak{t}_N + \sum_{j \geq 2} \alpha^j \tau_j)\|_{\mathcal{C}} \lesssim L\|n''\|_{\mathcal{C}} + \sqrt{L\alpha}\|N\|_{\text{T}} + O(L\alpha).$$

As $\|n''\|_{\mathcal{C}} \leq \|\rho_\gamma''\|_{\mathcal{C}} + \|\rho_\gamma\|_{\mathcal{C}}$ 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:

$$\text{Tr}(|\mathcal{D}^0|N) \lesssim M(1 + O(\sqrt{\alpha}\ell)) \lesssim \log(\Lambda).$$

Finally we have

$$\begin{aligned} \|\gamma\|_{\text{T}} &\lesssim \sqrt{L\alpha}\|n''\|_{\mathcal{C}} + \alpha\sqrt{\text{Tr}(|\nabla|Q^2)} + O(L\alpha) \lesssim L + O(L\alpha) \lesssim L \\ \|\rho_\gamma\|_{\mathcal{C}} &\lesssim L\|n''\|_{\mathcal{C}} + \sqrt{L\alpha M} + O(L\alpha) \lesssim L\sqrt{\log(\Lambda)}. \end{aligned} \quad (33)$$

□

4 The operator $Q_{1,0}(\cdot)$

Remark 15. • 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:

$$[\partial_j, R_Q] = R([\partial_j, Q]). \quad (34)$$

Lemma 8. Let Q be in $\mathcal{S}(\mathbf{R}^3 \times \mathbf{R}^3)$.

1. We have:

$$\|\nabla|^{-1/2}R_Q\|_{\mathfrak{S}_2} \lesssim \sqrt{\text{Tr}(R_Q^*Q)}.$$

In particular for any $g \geq 1$ there holds:

$$\iint \frac{g(p - q)}{|p|} |\widehat{R}_Q(p, q)|^2 dp dq \lesssim \iint |p + q|g(p - q)|\widehat{Q}(p, q)|^2 dp dq.$$

2. There exists $K > 0$ such that for all $0 < \varepsilon \leq 1$

$$\begin{aligned} \||D_0|^{-\frac{1+\varepsilon}{2}}R_Q|D_0|^{-\frac{1+\varepsilon}{2}}\|_{\mathfrak{S}_1} &\leq \frac{K}{\varepsilon}\|Q\|_{\mathfrak{S}_1}, \\ \||D_0|^{-(1+\varepsilon)}R_Q\|_{\mathfrak{S}_2} &\leq \frac{K}{\sqrt{\varepsilon}}\|Q\|_{\mathfrak{S}_2}. \end{aligned}$$

Taking $|\mathcal{D}^0|^{-1/2}$ instead of $|D_0|^{-(1+\varepsilon)/2}$ we get the same estimates above provided $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ and ε^{-1} is replaced by $\log(\Lambda)$.

We extend all those inequalities by density in the corresponding Banach spaces.

We prove this Lemma in Appendix A.

4.1 Proof of Lemma 1

In the Schatten norms Let us consider the operator $\mathbf{Q}_{1,0}$ defined as:

$$\mathbf{Q}_{1,0} : Q \mapsto Q_{1,0}(Q) := -\frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \frac{1}{\mathcal{D}^0 + i\eta} R_Q \frac{1}{\mathcal{D}^0 + i\eta}. \quad (35)$$

We recall \mathfrak{s} is defined in (23). There holds [9]:

$$\widehat{Q}_{1,0}(p, q) = \frac{1}{2} \frac{1}{\widetilde{E}(p) + \widetilde{E}(q)} \left(\widehat{R}(p, q) - \mathfrak{s}_p \widehat{R}(p, q) \mathfrak{s}_q \right) \quad (36)$$

which is a difference of two operators who are in \mathfrak{S}_2 (resp. \mathfrak{S}_1) if Q is in \mathfrak{S}_2 (resp. \mathfrak{S}_1). By interpolation it is in \mathfrak{S}_p ($1 \leq p \leq 2$) if Q is so. 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, so is

$$\int_{s=0}^{+\infty} \frac{\mathcal{D}^0}{|\mathcal{D}^0|} \mathcal{F}^{-1}(e^{-s\widetilde{E}(\cdot)}) R_Q \mathcal{F}^{-1}(e^{-s\widetilde{E}(\cdot)}) \frac{\mathcal{D}^0}{|\mathcal{D}^0|} ds :$$

it is a sum of nonnegative operators. We can rewrite $Q_{1,0}$ (and $Q_{0,1}$) as

$$\mathcal{J}_t(x - y) := \mathcal{F}^{-1}(\exp(-t\widetilde{E}(p)))(x - y) \quad (37a)$$

$$\begin{cases} Q_{1,0}(Q) &= \frac{1}{2} \int_{t=0}^{+\infty} (\mathcal{J}_t R_Q \mathcal{J}_t - \mathcal{J}_t \frac{\mathcal{D}^0}{|\mathcal{D}^0|} R_Q \frac{\mathcal{D}^0}{|\mathcal{D}^0|} \mathcal{J}_t) dt \\ Q_{0,1}(\rho) &= -\frac{1}{2} \int_{t=0}^{+\infty} (\mathcal{J}_t(\rho * \frac{1}{|\cdot|}) \mathcal{J}_t - \mathcal{J}_t \frac{\mathcal{D}^0}{|\mathcal{D}^0|} (\rho * \frac{1}{|\cdot|}) \frac{\mathcal{D}^0}{|\mathcal{D}^0|} \mathcal{J}_t) dt \end{cases} \quad (37b)$$

Then we remark that $(\widetilde{E}(p) + \widetilde{E}(q))^{-1} \leq \widetilde{E}(p)^{-1/2} \widetilde{E}(q)^{-1/2}$ and that

$$\begin{aligned} \|\mathcal{D}^0\|^{-\frac{1}{2}} R(\mathcal{F}^{-1}(|\widehat{Q}(p, q)|)) \|\mathcal{D}^0\|^{-\frac{1}{2}} \|_{\mathfrak{S}_2} &\leq K \sqrt{\log(\Lambda)} \|\mathcal{F}^{-1}(|\widehat{Q}(p, q)|)\|_{\mathfrak{S}_2} \\ &= K \sqrt{\log(\Lambda)} \|\widehat{Q}\|_{\mathfrak{S}_2} = K \sqrt{\log(\Lambda)} \|Q\|_{\mathfrak{S}_2}. \end{aligned}$$

By interpolation ($1 < p = 1 - \varepsilon + 2\varepsilon < 2$), there exists $K_{(1,0)}^{\mathfrak{S}} > 0$

$$\|Q_{1,0}(Q)\|_{\mathfrak{S}_p} \leq K_{(1,0)}^{\mathfrak{S}} (\log(\Lambda))^{1 - \frac{\varepsilon}{2}} \|Q\|_{\mathfrak{S}_p}, \quad (38)$$

$\rho[Q_{1,0}(\cdot)]$ We show here inequalities needed to estimate $\mathbf{T}(Q_\ell(Q, \rho))$ and $\tau_\ell(Q, \rho)$ in norms $\|\cdot\|_{\mathbf{Q}_g}, \|\cdot\|_{\mathfrak{e}_g}$. There exists a constant C_R (defined in [9]) such that for any function $g \geq 0$

$$\iint (\widetilde{E}(p) + \widetilde{E}(q)) g(p - q) |\widehat{Q}_{1,0}(Q, p, q)|^2 dp dq \leq C_R^2 \iint g(p - q) E(p + q) |\widehat{Q}(p, q)|^2 dp dq. \quad (39)$$

By Cauchy-Schwartz inequality: (cf [9] and inequality (95))

$$|\widehat{\rho}_{1,0}(Q, k)|^2 \leq |k|^2 \int_{B(0, \Lambda)} \frac{|\widehat{R}(u + \frac{k}{2}, u - \frac{k}{2})|^2}{1 + \widetilde{E}(u, k/2)} du \int_{B(0, \Lambda)} \frac{du}{1 + \widetilde{E}(u, k/2)} \frac{1}{1 + |u|^2 + |k|^2/4}, \quad (40)$$

where $\widetilde{E}(u, k/2) := \max(\widetilde{E}(u + k/2), \widetilde{E}(u - k/2))$. So the following upper bound holds:

$$|\widehat{\rho}_{1,0}(Q, k)|^2 \leq C_{(1,0)} \int E(2u) |\widehat{Q}(u + \frac{k}{2}, u - \frac{k}{2})|^2 du, \quad (41)$$

where $0 < C_{(1,0)} = C_{(1,0)}(\Lambda)$ satisfies $C_{(1,0)} \lesssim \log(\Lambda)$.

Well-definedness of \mathbf{T} and τ

Thanks to (38) we can prove Lemma 1: for $\alpha \log(\Lambda)$ sufficiently small the function \mathbf{T} is a linear bounded operator in $L(\mathfrak{S}_p)$ for $1 \leq p = 1 + \varepsilon \leq 2$ with norm lesser than

$$C_{\mathbf{T}, \mathfrak{S}}^{(p)} := \sum_{\ell=0}^{+\infty} (\alpha K_{(1,0)}^{\mathfrak{S}} (\log(\Lambda))^{1-\frac{\varepsilon}{2}})^{\ell} = \frac{1}{1 - \alpha (\log(\Lambda))^{1-\frac{\varepsilon}{2}} K_{(1,0)}^{\mathfrak{S}}}$$

which is finite as soon as $\alpha \log(\Lambda)$ is sufficiently small. We write $C_{\mathbf{T}, \mathfrak{S}} := C_{\mathbf{T}, \mathfrak{S}}^{(1)}$.

As $\mathbf{T} = (\text{Id} - \alpha \mathbf{Q}_{1,0})^{-1} = \sum_{\ell=0}^{+\infty} \alpha^{\ell} Q_{1,0}^{\circ(\ell)}(\cdot)$ it suffices to show that $\alpha Q_{1,0}^{\circ(\cdot)}$ is a bounded operator with norm lesser than 1. Thanks to inequality (39) we see that it is bounded with norm lesser than αC_R . And \mathbf{T} is a bounded linear operator with norm lesser than

$$C_{\mathbf{T}, \mathbf{Q}_g} := \frac{1}{1 - \alpha C_R}. \quad (42)$$

Then inequalities (39) and (41) enable us to say that for $\ell \geq 1$:

$$|\widehat{\rho}(G_{1,0}^{\circ(\ell)}(Q); k)|^2 \leq \alpha^{2\ell} C_{(1,0)}^{\ell} |k|^2 \int E(2u) |\widehat{Q}(u + \frac{k}{2}, u - \frac{k}{2})|^2 du$$

Therefore:

$$\int \frac{g(k)}{|k|^2} |\widehat{\rho}(G_{1,0}^{\circ(\ell)}(Q); k)|^2 \leq \alpha^{2\ell} C_{(1,0)}^{\ell} \iint g(p-q) E(p+q) |\widehat{Q}(p, q)|^2 dp dq \quad (43)$$

and \mathfrak{t} is a bounded linear operator with norm lesser than

$$C_{\mathfrak{t}, \mathfrak{e}} := \sum_{\ell=1}^{+\infty} (\alpha \sqrt{C_{(1,0)}})^{\ell} = \mathcal{O}(\alpha \sqrt{\log(\Lambda)}) \quad (44)$$

for $\alpha \sqrt{\log(\Lambda)}$ sufficiently small.

Notation 16. Let us define for $1 \leq p = 1 + \varepsilon \leq 2$:

$$Y_{\alpha, \Lambda}(p) = Y(p) \lesssim C_{\mathbf{T}, \mathfrak{S}}^{(p)}, \quad (45)$$

which is an upper bound of the $L(\mathfrak{S}_p)$ -norm of $Q \mapsto |D_0|^{-7/12} R(\mathbf{T}[Q]) |D_0|^{-7/12}$: cf Lemma 8 in Appendix A.1.

We have thus proved:

$$\begin{cases} \|\mathbf{T}(Q)\|_{\mathbf{Q}_g} & \leq C_{\mathbf{T}, \mathbf{Q}_g} \|Q\|_{\mathbf{Q}_g} = \frac{\|Q\|_{\mathbf{Q}_g}}{1 - \alpha C_R}, \\ \|\tau Q\|_{\mathfrak{e}_g} & \leq C_{\mathfrak{t}, \mathfrak{e}} \|Q\|_{\mathbf{Q}_g}. \end{cases} \quad (46)$$

4.2 Proof of Theorem 1

Before the proof let us define recursively the function $A_j^{(\ell_j)_{j=1}^J}$ by:

$$\begin{cases} A_1^{\ell_1} \widehat{Q}(p, q) & := \widehat{Q}(p - \ell_1, q - \ell_1) - \mathbf{s}_p \widehat{Q}(p - \ell_1, q - \ell_1) \mathbf{s}_q, \\ A_j^{(\ell_1, \mathbf{L})} \widehat{Q}(p, q) & := A_1^{\ell_1} (A_{j-1}^{\mathbf{L}} Q)(p, q) \text{ with } j \in \mathbf{N}^*, \ell_j \in \mathbf{R}^3. \end{cases} \quad (47)$$

It appears in the Fourier transform of $Q_{1,0}^{\circ J}[Q]$ (see Appendix C), \mathbf{s} is defined in (23).

Proof: The proof is based upon the following fact:

Lemma 9. The trace $\text{Tr}_{\mathcal{C}^4}$ of the product of an *odd* number of Dirac matrices (that is $\alpha_1, \alpha_2, \alpha_3, \beta$) vanishes.

Taking $\langle \cdot \rangle$ in the sense of algebra we define:

$$\begin{cases} \mathcal{A}_D & := \langle \alpha_1, \alpha_2, \alpha_3, \beta \rangle, \\ \mathcal{A}_D^+ & := \langle \text{Id}, (1 - \delta_{jk}) \alpha_j \alpha_k, \beta \alpha_j \rangle \\ \mathcal{A}_D^- & := \alpha_1 \mathcal{A}_D^+ + \alpha_2 \mathcal{A}_D^+ + \alpha_3 \mathcal{A}_D^+ + \beta \mathcal{A}_D^+ \end{cases} \quad (48)$$

It is clear that $\mathcal{A}_D = \mathcal{A}_D^+ + \mathcal{A}_D^-$ and Lemma 9 just says that

$$\forall M \in \mathcal{A}_D^- : \text{Tr}_{\mathbb{C}^4}(M) = 0.$$

Remark 23 and Appendix C implies that for almost all $(p, q) \in \mathbf{R}^3 \times \mathbf{R}^3$:

- $\widehat{G}_{1,0}^{\circ J}(Q_{0,1}(\rho); p, q) \in \mathcal{A}_D^+$,
- if $\widehat{Q}(p, q) \in \mathcal{A}_D^\varepsilon$ then so is $\widehat{G}_{1,0}^{\circ J}(Q; p, q)$.

Now let us study $Q_{0,2}(\rho)$:

$$Q_{0,2} = -\frac{1}{2\pi} \int_{\eta=-\infty}^{+\infty} \frac{d\eta}{\mathcal{D}^0 + i\eta} v_\rho \frac{1}{\mathcal{D}^0 + i\eta} v_\rho \frac{1}{\mathcal{D}^0 + i\eta}.$$

We recall $Q_{0,2}^{\varepsilon_1, \varepsilon_2, \varepsilon_3}$ and $Q_{1,2}^{\varepsilon_1, R, \varepsilon_2, v, \varepsilon_3}$ are defined in Section 2. By the residuum formula we have $Q_{0,2}^{\varepsilon, \varepsilon} = 0$ for any $\varepsilon \in \{+, -\}$. We then look at $Q_{0,2}^{+-}$ and $Q_{0,2}^{++}$ together, $Q_{0,2}^{+ -}$ and $Q_{0,2}^{- +}$, $Q_{0,2}^{- +}$ and $Q_{0,2}^{+ -}$. Those pairs are chosen such that:

$$\begin{aligned} A &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \int_{p_1} dp_1 \frac{P_+^0(p)}{\widetilde{E}(p) + i\eta} \widehat{v}(p - p_1) \frac{P_-^0(p_1)}{-\widetilde{E}(p_1) + i\eta} \widehat{v}(p_1 - q) \frac{P_-^0(q)}{\widetilde{E}(q) + i\eta} \\ &= \int_{p_1} \frac{dp_1}{8} \frac{1}{\widetilde{E}(p) + \widetilde{E}(p_1)} \frac{1}{\widetilde{E}(p) + \widetilde{E}(q)} (1 + \mathbf{s}_p) \widehat{v}(p - p_1) (1 - \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 - \mathbf{s}_q), \\ B &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \int_{p_1} dp_1 \frac{P_-^0(p)}{\widetilde{E}(p) + i\eta} \widehat{v}(p - p_1) \frac{P_+^0(p_1)}{-\widetilde{E}(p_1) + i\eta} \widehat{v}(p_1 - q) \frac{P_+^0(q)}{\widetilde{E}(q) + i\eta} \\ &= - \int_{p_1} \frac{dp_1}{8} \frac{1}{\widetilde{E}(p) + \widetilde{E}(p_1)} \frac{1}{\widetilde{E}(p) + \widetilde{E}(q)} (1 - \mathbf{s}_p) \widehat{v}(p - p_1) (1 + \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 + \mathbf{s}_q), \end{aligned}$$

However

$$\begin{aligned} &\frac{1}{2} (1 + \mathbf{s}_p) \widehat{v}(p - p_1) (1 - \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 - \mathbf{s}_q) - (1 - \mathbf{s}_p) \widehat{v}(p - p_1) (1 + \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 + \mathbf{s}_q) \\ &= \mathbf{s}_p \widehat{v}(p - p_1) \mathbf{s}_{p_1} \widehat{v}(p_1 - q) \mathbf{s}_q + \mathbf{s}_p \widehat{v}(p - p_1) \widehat{v}(p_1 - q) - \widehat{v}(p - p_1) \widehat{v}(p_1 - q) \mathbf{s}_q - \widehat{v}(p - p_1) \mathbf{s}_{p_1} \widehat{v}(p_1 - q). \end{aligned} \quad (49)$$

Remark 17. Thinking of $Q_{1,2}(Q, \rho)$ we have done as if $\widehat{v}(p - p_1)$ and $\widehat{v}(p_1 - q)$ were matrices.

In (49) there only remains matrices in \mathcal{A}_D^- . Symmetrically:

$$\begin{aligned} &\bullet \frac{1}{2} (1 + \mathbf{s}_p) \widehat{v}(p - p_1) (1 - \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 + \mathbf{s}_q) - (1 - \mathbf{s}_p) \widehat{v}(p - p_1) (1 + \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 - \mathbf{s}_q) \\ &= -\mathbf{s}_p \widehat{v}(p - p_1) \mathbf{s}_{p_1} \widehat{v}(p_1 - q) \mathbf{s}_q + \mathbf{s}_p \widehat{v}(p - p_1) \widehat{v}(p_1 - q) + \widehat{v}(p - p_1) \widehat{v}(p_1 - q) \mathbf{s}_q - \widehat{v}(p - p_1) \mathbf{s}_{p_1} \widehat{v}(p_1 - q), \\ &\bullet \frac{1}{2} (1 - \mathbf{s}_p) \widehat{v}(p - p_1) (1 - \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 + \mathbf{s}_q) - (1 + \mathbf{s}_p) \widehat{v}(p - p_1) (1 + \mathbf{s}_{p_1}) \widehat{v}(p_1 - q) (1 - \mathbf{s}_q) \\ &= \mathbf{s}_p \widehat{v}(p - p_1) \mathbf{s}_{p_1} \widehat{v}(p_1 - q) \mathbf{s}_q - \mathbf{s}_p \widehat{v}(p - p_1) \widehat{v}(p_1 - q) + \widehat{v}(p - p_1) \widehat{v}(p_1 - q) \mathbf{s}_q - \widehat{v}(p - p_1) \mathbf{s}_{p_1} \widehat{v}(p_1 - q). \end{aligned} \quad (50)$$

Therefore for almost all (p, q) : $\widehat{Q}_{0,2}(\rho; p, q) \in \mathcal{A}_D^-$: its trace $\text{Tr}_{\mathbb{C}^4}$ vanishes and for all $J \geq 1$:

$$\widehat{\rho}(G_{1,0}^{\circ J}(Q_{0,2}(\rho)); k) = \text{Cst} \iint_{u, \ell_1} \dots \int \frac{dud\ell}{\prod_{\ell_j, 1 \leq j \leq J} |\ell_j|^2} \text{Tr}_{\mathbb{C}^4} \frac{A_J^{(\ell_j)_{j=1}^J} \widehat{Q}_{0,2}(\rho)(u + \frac{k}{2}, u - \frac{k}{2})}{\prod_{0 \leq j \leq J} (\widetilde{E}(u + k/2 - L_j) + \widetilde{E}(u - k/2 - L_j))} \quad (51)$$

where for almost all (p, q, ℓ_j) : $\text{Tr}_{\mathbb{C}^4} \left\{ A_J^{(\ell_j)_{j=1}^J} \widehat{Q}_{0,2}(\rho; p, q) \right\} = 0$ for those matrices are in \mathcal{A}_D^- .

Thus $\widehat{\rho}(G_{1,0}^{\circ J}(Q_{0,2}(\rho)); k) = 0$ for almost all $k \in \mathbf{R}^3$ and so $\widehat{\tau}_{0,2}(\rho; k) = 0$ for almost all $k \in \mathbf{R}^3$, that is $\widehat{\tau}_{0,2}(\rho) = 0$.

It remains to prove that $\tau_{1,1}(\alpha \mathbf{T}(Q_{0,1}(\rho_0)), \rho_1) = 0$. It suffices to show that for all $J, J' \geq 0$: $\rho \left\{ G_{1,0}^{\circ J} [Q_{1,1}(\alpha G_{1,0}^{\circ J'} [Q_{0,1}(\rho_0)], \rho_1)] \right\}$ vanishes. Once again we look at

- $Q_{1,1}^{+R-v-}(G_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)), \rho_1)$ and $Q_{1,1}^{-R+v+}(G_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)), \rho_1)$,

- then $Q_{1,1}^{+v-R-}(G_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)), \rho_1)$ and $Q_{1,1}^{-v+R+}(G_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)), \rho_1)$, and so on.

As $\widehat{G_{1,0}^{\circ J'}}(Q_{0,1}(\rho_0); p, q) \in \mathcal{A}_D^+$ for almost all p, q , then $\widehat{Q_{1,1}^{+R-v-}}(G_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)); p, q), \rho_1) + \widehat{Q_{1,1}^{-R+v+}}(G_{1,0}^{\circ J'}(Q_{0,1}(\rho_0)), \rho_1; p, q) \in \mathcal{A}_D^-$ for almost all p, q thanks to (49) and (50). So its trace $\text{Tr}_{\mathcal{C}^4}$ vanishes. The same result holds for the other cases: $Q_{1,1}^{+v-R-} + Q_{1,1}^{-v+R+}$, $Q_{1,1}^{+-+} + Q_{1,1}^{-+-}$, $Q_{1,1}^{-+-} + Q_{1,1}^{+-+}$ and as in (51):

$$\widehat{\rho}(G_{1,0}^{\circ J}(Q_{1,1}(G_{1,0}^{\circ J'}(\rho_0), \rho_1)); k) = 0 \text{ for almost all } k.$$

□

5 The fixed point method

We give here proofs of Lemmas 2, 3 and 4.

5.1 Tools

- Let us now recall some Sobolev inequalities in \mathbf{R}^3 . For suitable f -say H^1 - we have

$$\begin{aligned} \|f\|_{L^6} &\leq \|\nabla f\|_{L^2}, & \|f\|_{L^4} &\leq \|\nabla|f|^{3/4}\|_{L^2}, \\ \|f\|_{L^3} &\leq \|\nabla|f|^{1/2}\|_{L^2} \end{aligned} \quad (52)$$

In particular, we use them to the following inequalities: for $\rho \in \mathcal{C}$, $v_\rho := \rho * \frac{1}{|\cdot|}$ and $\phi \in H^{1/2}$:

$$\|v_\rho \phi\|_{L^2} \lesssim \|v_\rho\|_{L^6} \|\phi\|_{L^3} \lesssim \|\rho\|_{\mathcal{C}} \|\nabla|f|^{1/2}\|_{L^2}. \quad (53)$$

$$\|\rho * \frac{1}{|\cdot|}\|_{L^4} \lesssim \|\nabla|f|^{3/4}\|_{L^2} \|\rho * \frac{1}{|\cdot|}\|_{L^2} \lesssim \sqrt{\int \frac{|\widehat{\rho}(k)|^2}{|k|^{5/2}} dk} \lesssim \left(\inf_{\varepsilon > 0} \left\{ 2\pi\varepsilon^{1/2} \|\widehat{\rho}\|_{L^\infty}^2 + \varepsilon^{-1/2} \|\rho\|_{\mathcal{C}}^2 \right\} \right)^{1/2}. \quad (54)$$

With $v_\rho := \rho * \frac{1}{|\cdot|}$ equation (54) will be used in:

$$\|\frac{1}{\mathcal{D}^{0+i\eta}} v_\rho\|_{\mathfrak{S}_4}, \|\frac{1}{|\mathcal{D}^{0+i\eta}|^{1/2}} v_\rho \frac{1}{|\mathcal{D}^{0+i\eta}|^{1/2}}\|_{\mathfrak{S}_4} \leq \frac{K_2^{1/4}}{E(\eta)^{1/4}} \|\rho * \frac{1}{|\cdot|}\|_{L^4} \quad (55)$$

We recall Kato's and Hardy's inequalities for $\phi \in L^2(\mathbf{R}^3)$:

$$\begin{cases} \int_{\mathbf{R}^3} \frac{|\varphi(x)|^2}{|x|} dx &\leq \frac{\pi}{2} \langle |\nabla| \varphi, \varphi \rangle, \\ \int_{\mathbf{R}^3} \frac{|\varphi(x)|^2}{|x|^2} dx &\leq 4 \langle (-\Delta) \varphi, \varphi \rangle, \end{cases} \quad (56)$$

and the Kato-Seiler-Simon's inequality (KSS) for compact operators in $\mathcal{B}(L^2(\mathbf{R}^3))$:

$$\forall 2 \leq p \leq +\infty : \|f(-i\nabla)g(x)\|_{\mathfrak{S}_p} \leq (2\pi)^{-3/p} \|f\|_{L^p} \|g\|_{L^p}. \quad (57)$$

- We recall that for any $p, q \in B(0, \Lambda)$ we have (see arxiv.1211.3830.)

$$|\widehat{\mathcal{P}}_-^0(p) - \widehat{\mathcal{P}}_-^0(q)| = |\widehat{\mathcal{P}}_+^0(p) - \widehat{\mathcal{P}}_+^0(q)| \lesssim \frac{|p - q|}{\max(\widetilde{E}(p), \widetilde{E}(q))}. \quad (58)$$

By (58) we get the following result.

Lemma 10. Let $\rho \in \mathcal{C}$, then there exists $K > 0$ such that for any $a > 1/2$ and $\varepsilon \in \{+, -\}$ we have:

$$\|\mathcal{P}_\varepsilon^0 v_\rho \mathcal{P}_{-\varepsilon}^0 |D_0|^{-a}\|_{\mathfrak{S}_2} \leq \frac{K}{\sqrt{2a-1}} \|\rho\|_{\mathcal{C}}.$$

Proof: It is obvious once we have seen the integral kernel of its Fourier transform is lesser than:

$$K \frac{|\widehat{\rho}(p-q)|}{|p-q|} \frac{1}{E(q)^a \max(E(q), E(p))}.$$

□

- For $m > 1$ we define the constant K_m as follows:

$$K_m = \frac{1}{2\pi} \int_{\mathbf{R}} \frac{dx}{E(x)^m}. \quad (59)$$

By Laplace's method [3], we have

$$\mathcal{O}_{m \rightarrow +\infty}(m^{-1/2}). \quad (60)$$

5.2 $Q_{0,1}$

We estimate $\|Q_{0,1}\|_{\mathbf{Q}_g}$ as in [9], we remark that:

$$\begin{aligned} \int_{B(0,\Lambda)} \frac{du}{E(u+\varepsilon k/2)^2} \frac{\widetilde{E}(u+k/2) + \widetilde{E}(u-k/2)}{(\widetilde{E}(u+k/2) + \widetilde{E}(u-k/2))^2} &\leq 4\pi \int_0^\Lambda \frac{du}{\sqrt{1+r^2}} \\ &\leq 4\pi(1 + \log(\Lambda)) \lesssim \log(\Lambda), \end{aligned} \quad (61)$$

leading to:

$$\iint g(p-q)(\widetilde{E}(p) + \widetilde{E}(q)) |\widehat{Q}_{0,1}(\rho; p, q)|^2 dpdq \lesssim (1 + \log(\Lambda)) \|\rho\|_{\mathfrak{E}_g}^2, \quad (62)$$

where we have used (58).

5.3 Proof of Lemma 2

We recall that for $J \geq 1$:

$$Q_J := \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\eta}{\mathcal{D}^0 + i\eta} \prod_{1 \leq j \leq J} \left(B \frac{1}{\mathcal{D}^0 + i\eta} \right)$$

where $B = v_\rho - R_Q$.

We write

$$\mathfrak{a}(Q) := \mathcal{F}^{-1}(|\widehat{Q}|) \text{ and } \mathfrak{a}(\rho) := \mathcal{F}^{-1}(|\widehat{\rho}|).$$

It is clear that $|\widehat{Q}_{k,\ell}(p, q)|$ is lesser than the integral kernel of the Fourier transform of

$$\mathfrak{a}(Q_{k,\ell}) := \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{d\eta}{\sqrt{|\mathcal{D}^0|^2 + \eta^2}} \left(\mathfrak{a}(\rho) * \frac{1}{|\cdot|} + R[\mathfrak{a}(Q)] \right)^J.$$

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:

$$\left| \begin{array}{lll} \|\mathfrak{a}(v_\rho)\|_{L^6} & \lesssim \|\nabla \mathfrak{a} v_\rho\|_{L^2} & \lesssim \|\mathfrak{a}(\rho)\|_c = \|\rho\|_c, \\ \|\mathfrak{a}(v_\rho)\|_{L^4} & \lesssim \|\nabla^{3/2} \mathfrak{a}(v_\rho)\|_{L^2} & \lesssim \|\widehat{\mathfrak{a}(\rho)}\|_{L^\infty} + \|\mathfrak{a}(\rho)\|_c = \|\widehat{\rho}\|_{L^\infty} + \|\rho\|_c, \\ \|\frac{1}{|\cdot|^{1/2}} \mathfrak{a}(R_Q)\|_{\mathfrak{E}_2} & \lesssim \|\mathfrak{a}(R_Q)\|_{\mathfrak{E}_x} & \lesssim \|\mathfrak{a}(Q)\|_{\mathfrak{T}} = \|Q\|_{\mathfrak{T}}. \end{array} \right.$$

By the KSS inequality, there exist $C_6, C_4 > 0$:

$$\begin{aligned} \|d_\eta^{-1/2} v_\rho d_\eta^{-1/2}\|_{\mathfrak{E}_6} &\leq C_6 E(\eta)^{-1/2} \|\rho\|_c, \\ \|d_\eta^{-5/12} v_\rho d_\eta^{-7/12}\|_{\mathfrak{E}_4} &\leq C_4 E(\eta)^{-1/4} \|v_\rho\|_{L^4}. \end{aligned} \quad (63)$$

As g satisfies (6), we have:

$$g(p-q) \widehat{\mathfrak{a}}(Q_J(Q, \rho); p, q) \leq JK_{(g)}^J \widehat{\mathfrak{a}}\left(Q_J[\mathcal{F}^{-1}(g(p'-q')\widehat{Q}(p', q')), \mathcal{F}^{-1}(\rho)]; p, q\right).$$

It suffices to check that for $p_0 = p, p_{J+1} = q$ and $p_1, \dots, p_J \in \mathbf{R}^3$ we have:

$$g(p - q) \leq \sum_{j=1}^{J+1} K_{(g)}^j g(p_{j-1} - p_j) \leq JK_{(g)}^J \prod_{j=1}^{J+1} g(p_{j-1} - p_j).$$

In the definition of $\|\cdot\|_{\mathbf{Q}_g}$, there remains to multiply by $\tilde{E}(p)^{1/2} + \tilde{E}(q)^{1/2}$. We use the first or the last d_η^{-1} to get:

$$\frac{\tilde{E}(r)^{1/2}}{\sqrt{\tilde{E}(r)^2 + \eta^2}} \leq \frac{1}{(\tilde{E}(r)^2 + \eta^2)^{1/4}} \text{ with } r \in \{p, q\}.$$

For all the terms $Q_J(Q, \rho)$ with $J \geq 3$ we get that:

$$\|\mathfrak{a}Q_J(Q, \rho)\|_{\mathbf{Q}_g} \leq \frac{JK_{(g)}^J}{2\pi} \left(\left\| \frac{1}{|\cdot|^{1/2}} R[\mathfrak{a}(Q)] \right\|_{\mathfrak{S}_2} + C_6 \|\rho\|_c \right)^J \int_{-\infty}^{+\infty} \frac{d\eta}{\tilde{E}(\eta)^{(J+1)/2}}.$$

For $J = 2$, there is a problem for $Q_{0,2}(\rho)$ because the product of two operators in \mathfrak{S}_6 is not necessarily Hilbert-Schmidt. By the Cauchy expansion we have [9]

$$Q_J^{+\dots+} = Q_J^{-\dots-} = 0.$$

So it suffices to treat $Q_{0,2}^{\varepsilon_1, \varepsilon_2, \varepsilon_3}$ with $(\varepsilon_1, \varepsilon_2, \varepsilon_3) \neq (+ + +), (- - -)$. In particular we have a change of sign $+-$ or $-+$. By Hölder inequality and Lemma 10 we have for $\varepsilon \in \{+, -\}$:

$$\|d_\eta^{-1/2} v^{\varepsilon, -\varepsilon} d_\eta^{-1/4}\|_{\mathfrak{S}_2} \lesssim \|\rho\|_c \left\{ \int \frac{dq}{E(q)^{7/2}} \right\}^{1/2} \lesssim \|\rho\|_c.$$

Hence using the above inequality and (63) we get:

$$\|Q_{0,2}(\rho)\|_{\mathbf{Q}_g} \lesssim \|\rho\|_c^2 \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^{1+4^{-1}}}.$$

By (60), there exists $K > 0$ such that

$$\|Q_J(Q, \rho)\|_{\mathbf{Q}_g} \leq J^{1/2} (K \times K_{(g)} (\|Q\|_F + \|\rho\|_{\mathfrak{e}_g}))^J.$$

To deal with ρ_J , we use the same method as in [9] and estimate $\|\rho_J\|_c$ by duality. We consider $\zeta \in \mathcal{S}(\mathbf{R}^3)$ a Schwartz function and prove that for any $k, \ell \geq 0$ with $k + \ell \geq 2$ we have:

$$|\text{Tr}(Q_{k,\ell}\zeta)| \leq \text{Cst}(Q, \rho, k, \ell) \sqrt{\int \frac{|p|^2 |\widehat{\zeta}(p)|^2}{g(p)^2} dp} = \text{Cst}(Q, \rho, k, \ell) \|\zeta\|_{\mathfrak{e}_g}.$$

We emphasize that by Furry's Theorem [6, 9] we have $\rho_{0,2J} = 0$ for any $J \in \mathbf{N}^*$.

First we must prove that $Q_{k,\ell}\zeta$ is trace-class. We use Hölder's inequalities for \mathfrak{S}_2 and do as in [9]:

$$\|Q_{k,\ell}\zeta\|_{\mathfrak{S}_1} \leq \|Q_{k,\ell}|D^0|\|_{\mathfrak{S}_2} \left\| \frac{1}{|\cdot|^{2\ell}} \zeta \right\|_{\mathfrak{S}_2} \lesssim E(\Lambda)^2 \|Q_{k,\ell}\|_{\mathfrak{S}_2} \|\zeta\|_{L^2}.$$

It is clear that

$$|\widehat{Q_{k,\ell}\zeta}(p, p)| \leq |\mathfrak{a}(\widehat{Q_{k,\ell}})\zeta|.$$

Writing $d_\eta(p) := \sqrt{\tilde{E}(p)^2 + \eta^2}$, $p_0 = p$ and $\mathbf{m} = (m_1, \dots, m_J) \in \{v_\rho, R_Q\}^J$ we have:

$$2\pi |\mathfrak{a}(\widehat{Q_{k,\ell}^{\mathbf{m}}})\zeta(p, p)| \leq \int_{\mathbf{R}} d\eta \int_{(B(0,\Lambda))^J} \frac{d\mathbf{p}}{d_\eta(p)} \prod_{j=1}^J |\widehat{m}_j(p_j, p_{j-1})| d_\eta(p_j)^{-1} |\widehat{\zeta}(p_J - p)|$$

We replace $|\widehat{\zeta}(p_J - p)|$ by:

$$|\widehat{\zeta}(p_J - p)| \times \frac{g(p_J - p)}{g(p_J - p)} \leq JK_{(g)}^J \frac{|\widehat{\zeta}(p_J - p)|}{g(p_J - p)} \prod_{j=1}^J g(p_j - p_{j-1}) =: JK_{(g)}^J |\widehat{\zeta}'(p_J - p)| \prod_{j=1}^J g(p_j - p_{j-1}). \quad (64)$$

We write $R' := R[\mathcal{F}^{-1}(g(p - q)|\widehat{Q}(p, q)|)]$ and $V' := v[\mathcal{F}^{-1}(g(p)|\widehat{\rho}(p)|)]$. For (k, ℓ) different from $(0, 3), (1, 1), (0, 2J)$ we get that:

$$\begin{aligned} |\mathrm{Tr}(Q_{k, \ell} \zeta)| &\leq \frac{(k + \ell) K_{(g)}^{k + \ell}}{2\pi} \binom{k + \ell}{k} \int_{\mathbf{R}} d\eta \|d_\eta^{-1/2} \zeta' d_\eta^{-1/2}\|_{\mathfrak{S}_6} \|d_\eta^{-1/2} R' d_\eta^{-1/2}\|_{\mathfrak{S}_2}^k \|d_\eta^{-1/2} V' d_\eta^{-1/2}\|_{\mathfrak{S}_6}^\ell \\ &\leq \frac{(k + \ell) K_{(g)}^{k + \ell}}{2\pi} \binom{k + \ell}{k} K^{k + \ell} \int_{\mathbf{R}} \frac{d\eta}{E(\eta)^{(1+j+\ell)/2}} \|Q\|_{\mathbf{Q}_g}^k \|\rho\|_{\mathfrak{C}_g}^\ell. \end{aligned}$$

To deal with $\rho_{1,1}, \rho_{0,3}$ we use the same method as for $\|Q_{0,2}\|_{\mathbf{Q}_g}$. We treat the case of $\rho[Q_{1,1}^{+R-v-}]$ as an example and the other terms are dealt with in the thesis of the author (to appear in 2014). We have:

$$|\mathrm{Tr}_{\mathbf{C}^4}(\widehat{Q}_{1,1}^{+R-v-}(p_0, p_2) \widehat{\zeta}(p_2 - p_0))| \leq \int_{\mathbf{R}} \int_{(B(0, \Lambda))^3} \frac{d\eta dp_1 dp_2 |\widehat{R}_Q(p_0, p_1)| |\widehat{v}(p_1 - p_2)|}{d_\eta(p_0) d_\eta(p_1) d_\eta(p_2)} |\widehat{\zeta}^{+}(p_2 - p_0)|.$$

Using Lemma 10 and (64) we get that:

$$|\mathrm{Tr}(Q_{1,1}^{+R-v-} \zeta)| \lesssim \|Q\|_{\mathbf{Q}_g} \|\rho\|_{\mathfrak{C}_g} K_{5/4} \|\zeta\|_{\mathfrak{C}'_g}.$$

□

5.4 Estimates for $F^{(2)}$

Let us look at (26): that is let us take $\gamma' = \gamma + N$ a minimizer of $E_{\mathrm{BDF}}^\nu(M)$ and define the function $F^{(2)}$. Two Banach spaces will be considered: first \mathcal{C} and then $\mathcal{C} \cap L^1$. We recall that for $\eta \in \mathbf{R}$ we write $d_\eta = \sqrt{|\mathcal{D}^0|^2 + \eta^2}$.

5.4.1 Estimates in the \mathcal{C} -norm

Thanks to previous estimates (Lemmas 5, 6, *a priori* estimates (33) and estimates in the $\|\cdot\|_{\mathfrak{C}_g}$ -norm), in the regime $M, \|\nu\|_{\mathcal{C}} \lesssim \log(\Lambda)$ there hold the following *non-sharp* estimates:

$$\begin{cases} \|h_2\|_{\mathcal{C}} &\leq \alpha^2 \left\{ \|\rho''\|_{\mathcal{C}} [|\mathcal{N}|_{\mathbf{T}} + \alpha^2 (\|\gamma'\|_{\mathbf{T}} + \|\rho''\|_{\mathcal{C}})^2] + \|\gamma'\|_{\mathbf{T}}^2 \right\} \\ &\leq \alpha^2 \times \log(\Lambda) = L\alpha \\ \|h_3\|_{\mathcal{C}} &\leq \alpha^3 (\|\gamma'\|_{\mathbf{T}} + \|\rho''\|_{\mathcal{C}})^3 \lesssim (L\alpha)^{3/2}. \end{cases} \quad (65)$$

Then $F_2^{(2)}(\rho'')$ and $F_3^{(2)}(\rho'')$ are at most cubic in ρ'' :

$$\begin{cases} \|F_2^{(2)}(\rho')\|_{\mathcal{C}} &\leq \alpha^4 (\|\gamma'\|_{\mathbf{T}} + \|\rho''\|_{\mathcal{C}}) \|\rho''\|_{\mathcal{C}}^2 \\ \|F_3^{(2)}(\rho')\|_{\mathcal{C}} &\leq \alpha^3 (\|\rho''\|_{\mathcal{C}} + \|\gamma'\|_{\mathbf{T}}) \|\rho''\|_{\mathcal{C}}^2 \\ \|\mathrm{d}F_2^{(2)}(\rho')\|_{\mathcal{L}(\mathcal{C})} &\leq \alpha^4 (\|\gamma'\|_{\mathbf{T}} \|\rho''\|_{\mathcal{C}} + \|\rho''\|_{\mathcal{C}}^2) \\ \|\mathrm{d}F_3^{(2)}(\rho')\|_{\mathcal{L}(\mathcal{C})} &\leq \alpha^3 (\|\gamma'\|_{\mathbf{T}} \|\rho''\|_{\mathcal{C}} + \|\rho''\|_{\mathcal{C}}^2). \end{cases} \quad (66)$$

5.4.2 Estimates in the L^1 -norm

Our aim in this part is to prove Lemma 11 below which states that $F^{(2)}$ is a well-defined \mathcal{C}^1 function of $\mathcal{C} \cap L^1$.

- First let us prove that $h_2, h_3 \in L^1$ (we recall they are defined in (25)). In fact they are densities of trace-class operators, to see this we use the methods in the proof of Lemma 2 above.

1. $N = \sum_j |\psi_j\rangle\langle\psi_j| \in \mathfrak{S}_1$ so $\mathbf{T}[N] \in \mathfrak{S}_1$ and

$$\|\tau_N\|_{L^1} \leq \|\mathbf{T}[N]\|_{\mathfrak{S}_1} \leq C_{\mathbf{T},\mathfrak{S}}\|N\|_{\mathfrak{S}_1}. \quad (67)$$

2. $Q_{2,0}(\gamma') \in \mathfrak{S}_1$: We have:

$$\|Q_{2,0}(\gamma')\|_{\mathfrak{S}_1} \lesssim \|\gamma'\|_{\mathbb{E}_x}^2 K_2. \quad (68)$$

3. $Q_{0,\ell}(\rho''_\gamma)$ with $\ell \geq 4$. As $Q_{0,\ell}^{+\dots+} = Q_{0,\ell}^{-\dots-} = 0$ there is at least one change of sign $+-$ or $-+$. Then with the help of Lemma 10 and (63) we have

$$\|Q_{0,\ell}(\rho''_\gamma)\|_{\mathfrak{S}_1} \lesssim \|\rho''_\gamma\|_c^\ell K_{(\ell+1)/2+1/4},$$

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 $\ell \geq 3$:

$$\|Q_{k,\ell}(\gamma', \rho''_\gamma)\|_{\mathfrak{S}_1} \lesssim \binom{k+\ell}{k} (K\|\gamma'\|_{\mathbb{T}})^k (K\|\rho''_\gamma\|_c)^\ell K_{1+(k+\ell)/2}. \quad (69)$$

5. Thanks to Furry's Theorem and Theorem 1:

$$\tau\{Q_{0,2}(\rho''_\gamma)\} = \tau_{1,1}\{\mathbf{T}[Q_{0,1}(\rho''_\gamma)], \rho''_\gamma\} = 0. \quad (70)$$

6. With the same methods: $Q_{0,3}(\rho''_\gamma), Q_{1,2}(\gamma', \rho''_\gamma) \in \mathfrak{S}_{6/5}$:

$$\|Q_{0,3}(\rho''_\gamma)\|_{\mathfrak{S}_{6/5}} \lesssim \|\rho''_\gamma\|_c^3 K_{2+1/4} \quad \text{and} \quad \|Q_{1,2}(\gamma', \rho''_\gamma)\|_{\mathfrak{S}_{6/5}} \lesssim \|\gamma'\|_{\mathbb{T}} \|\rho''_\gamma\|_c^2 K_{1+3/2}.$$

We use (45) and the inequalities:

$$\|d_\eta^{-3/8} v_\rho d_\eta^{-5/8}\|_{\mathfrak{S}_6} \lesssim E(\eta)^{-1/2} \|\rho\|_c \quad \text{and} \quad \|d_\eta^{-5/8} R(\mathbf{T}[Q]) d_\eta^{-5/8}\|_{\mathfrak{S}_{6/5}} \lesssim Y(\frac{6}{5}) \|Q\|_{\mathfrak{S}_{6/5}}.$$

Thus:

$$\begin{cases} \|\mathbf{T}_{1,1}\{\mathbf{T}Q_{0,3}(\rho''_\gamma), \rho''_\gamma\}\|_{\mathfrak{S}_1} & \lesssim 2C_{\mathbf{T},\mathfrak{S}} K_{5/4} \|\rho''_\gamma\|_c (Y(\frac{6}{5}) \|\rho''_\gamma\|_c^3 K_{2+1/4}), \\ \|\mathbf{T}_{1,1}\{\mathbf{T}Q_{1,2}(\gamma', \rho''_\gamma), \rho''_\gamma\}\|_{\mathfrak{S}_1} & \lesssim 2C_{\mathbf{T},\mathfrak{S}} K_{5/4} \|\rho''_\gamma\|_c (3Y(\frac{6}{5}) \|\gamma'\|_{\mathbb{T}} \|\rho''_\gamma\|_c^2 K_{1+3/2}) \\ \|\mathbf{T}_{1,1}\{\mathbf{T}N, \rho''_\gamma\}\|_{\mathfrak{S}_1} & \lesssim 2C_{\mathbf{T},\mathfrak{S}} K_{5/4} \|\rho''_\gamma\|_c Y(\frac{6}{5}) M. \end{cases} \quad (71)$$

7. We apply \mathbf{T} , h_2 is the density of $Q(h_2)$ and h_3 of $Q(h_3)$ with

$$\begin{cases} Q(h_2) & = \alpha^2 \left\{ \mathbf{T}Q_{1,1}[\mathbf{T}N + \alpha^2 \mathbf{T}[Q_{2,0}(\gamma') + \tilde{Q}_3(\gamma', \rho''_\gamma)]; \rho''_\gamma \right\} + \mathbf{T}Q_{2,0}(\gamma') \\ Q(h_3) & = \alpha^3 \left\{ \mathbf{T}Q_{3,0}(\gamma') + \mathbf{T}Q_{2,1}(\gamma', \rho''_\gamma) + \alpha \tilde{Q}_4(\gamma', \rho''_\gamma) \right\} \end{cases}$$

The previous estimates leads to a sequence of numbers $(b_\ell)_{\ell \geq 2}$ with the following asymptotic behaviour:

$$b_\ell = \mathcal{O}_{\ell \rightarrow +\infty}(\ell^{1/2}) \quad (72)$$

and a constant $C_0 > 0$ such that:

$$\begin{aligned} & \left\| \alpha^2 Q_{2,0}(\gamma') + \alpha^3 [Q_{3,0} + Q_{2,1}](\gamma', \rho''_\gamma) + \alpha^4 \tilde{Q}_4(\gamma', \rho''_\gamma) \right\|_{\mathfrak{S}_1} \\ & + \alpha^3 \left\| Q_{0,3}(\rho''_\gamma) + Q_{1,2}(\gamma', \rho''_\gamma) \right\|_{\mathfrak{S}_{6/5}} \leq \sum_{\ell=2}^{+\infty} b_\ell (\alpha C_0)^\ell (\|\rho''_\gamma\|_c + \|\gamma'\|_{\mathbb{T}})^\ell =: A_{h,\mathfrak{S}}. \end{aligned} \quad (73)$$

We have:

$$\|Q(h_2)\|_{\mathfrak{S}_1} \lesssim \alpha^2 C_{\mathbf{T},\mathfrak{S}} (2K_{5/4} Y(\frac{6}{5}) (M + A_{h,\mathfrak{S}}) + \|\gamma'\|_{\mathbb{Q}_g}^2) \quad (74)$$

and write $B_{h_2,\mathfrak{S}}$ this upper bound. Similarly:

$$\|Q(h_3)\|_{\mathfrak{S}_1} \leq C_{\mathbf{T},\mathfrak{S}} \sum_{\ell=3}^{+\infty} b_\ell (\alpha C_0)^\ell (\|\rho''_\gamma\|_c + \|\gamma'\|_{\mathbb{T}})^\ell =: B_{h_3,\mathfrak{S}_1}. \quad (75)$$

Remark 18. The introduced numbers $A_{h,\mathfrak{S}}, B_{h_2,\mathfrak{S}_1}, B_{h_3,\mathfrak{S}}$ are *not* constants: they all depend on α and the minimizer γ' . As we have *a priori* estimates (Lemma 5) we know that these upper bounds are small provided we are in the regime of Remark 4. Indeed we have

$$\left(1 - \frac{\alpha\pi}{4}\right)\|\gamma'\|_{\mathbb{T}}^2 + \frac{\alpha}{2}\|\rho''\|_{\mathcal{C}}^2 \leq \frac{\alpha}{2}\|\nu\|_{\mathcal{C}}^2 + M,$$

so $\alpha(\|\gamma'\|_{\mathbb{T}} + \|\rho''\|_{\mathcal{C}}) \leq \alpha\|\nu\|_{\mathcal{C}} + \sqrt{\alpha M} = \mathcal{O}((L\alpha)^{1/4})$. In particular those upper bounds are $o(1)$.

• Let us estimate $F_2^{(2)}(\rho'')$ and $F_3^{(2)}(\rho'')$ in the L^1 -norm for $\rho'' \in \mathcal{C} \cap L^1$. To this end we use (55) and (54) at level $\varepsilon = 1$ for instance: there exists $K_{L^4}^{(v)} > 0$ such that:

$$\|v_{\rho''}\|_{L^4} \leq K_{L^4}^{(v)}\{\|\rho''\|_{L^1} + \|\rho''\|_{\mathcal{C}}\}. \quad (76)$$

We use the second inequality of (63) and Lemma 10 with $a = 7/12$. Following the method used to prove Lemma 2.

Lemma 11. Let ρ'' be in $\mathcal{C} \cap L^1$ and γ' a minimizer for $E_{\text{BDF}}'(M)$ with density ρ'_γ . We have:

$$\begin{aligned} \|\mathbf{T}Q_{0,3}(\rho'')\|_{\mathfrak{S}_1} &\lesssim 6K_{13/12}C_{\mathbb{T},\mathfrak{S}}\{\|\rho''\|_{L^1} + \|\rho''\|_{\mathcal{C}}\}^2\|\rho''\|_{\mathcal{C}} \\ \|\mathbf{T}Q_{1,2}(\gamma', \rho'')\|_{\mathfrak{S}_1} &\lesssim \binom{3}{1}K_2C_{\mathbb{T},\mathfrak{S}}\|\gamma'\|_{\mathbb{T}}\{\|\rho''\|_{L^1} + \|\rho''\|_{\mathcal{C}}\}^2 \\ \|Q_{0,2}(\rho'')\|_{\mathfrak{S}_{4/3}} &\lesssim 4K_{7/3}\|\rho''\|_{\mathcal{C}}\{\|\rho''\|_{L^1} + \|\rho''\|_{\mathcal{C}}\} \\ \|Q_{1,1}(\gamma', \rho'')\|_{\mathfrak{S}_{4/3}} &\lesssim 2K_{7/4}\|\gamma'\|_{\mathbb{T}}\{\|\rho''\|_{L^1} + \|\rho''\|_{\mathcal{C}}\} \\ \|\mathbf{T}Q_{1,1}\{\mathbf{T}Q_{0,2}(\rho''), \rho''\}\|_{\mathfrak{S}_1} &\lesssim 2K_{13/12}Y\left(\frac{4}{3}\right)C_{\mathbb{T},\mathfrak{S}}\|Q_{0,2}(\rho'')\|_{\mathfrak{S}_{4/3}}\{\|\rho''\|_{L^1} + \|\rho''\|_{\mathcal{C}}\} \\ \|\mathbf{T}Q_{1,1}\{\mathbf{T}Q_{1,1}(\gamma', \rho''), \rho''\}\|_{\mathfrak{S}_1} &\lesssim 2K_{13/12}Y\left(\frac{4}{3}\right)C_{\mathbb{T},\mathfrak{S}}\|Q_{1,1}(\gamma', \rho'')\|_{\mathfrak{S}_{4/3}}K_{L^4}^{(v)}\{\|\rho''\|_{L^1} + \|\rho''\|_{\mathcal{C}}\} \end{aligned} \quad (77)$$

Similarly we can estimate $\|dF_j^{(2)}\|_{\mathbb{L}(\mathcal{C} \cap L^1)}$. As $\|\gamma'\|_{\mathbb{T}} \lesssim \sqrt{\log(\Lambda)}$ we have:

$$\begin{cases} \|F_2^{(2)}(\rho'')\|_{\mathcal{C} \cap L^1} &\lesssim \alpha^4\|\rho''\|_{\mathcal{C} \cap L^1}^2\{\sqrt{\log(\Lambda)} + \|\rho''\|_{\mathcal{C} \cap L^1}\} \\ \|F_3^{(2)}(\rho'')\|_{\mathcal{C} \cap L^1} &\lesssim \alpha^3\|\rho''\|_{\mathcal{C} \cap L^1}^2\{\sqrt{\log(\Lambda)} + \|\rho''\|_{\mathcal{C} \cap L^1}\}, \\ \|dF_2^{(2)}(\rho'')\|_{\mathbb{L}(\mathcal{C} \cap L^1)} &\lesssim \alpha^4\|\rho''\|_{\mathcal{C} \cap L^1}^2\{\sqrt{\log(\Lambda)} + \|\rho''\|_{\mathcal{C} \cap L^1}\}, \\ \|dF_3^{(2)}(\rho'')\|_{\mathbb{L}(\mathcal{C} \cap L^1)} &\lesssim \alpha^3\|\rho''\|_{\mathcal{C} \cap L^1}^2\{\sqrt{\log(\Lambda)} + \|\rho''\|_{\mathcal{C} \cap L^1}\}. \end{cases} \quad (78)$$

5.5 Application of the Banach fixed point theorem

5.5.1 $F^{(1)}$

With *exactly* the same method of [9] 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.

Let us define (where $K_{(g)} > 0$ is defined in (6) and $C_0 > 0$ is the constant of Lemma 2)

$$\mathcal{X}_g := \mathbf{Q}_g \times \mathfrak{C}_g, \quad \text{with } \|(Q, \rho)\|_{\mathcal{X}_g} := K_{(g)}C_0(\|Q\|_{\mathbf{Q}} + \|\rho\|_{\mathfrak{C}_g}). \quad (79)$$

Thanks to the previous estimates we can say that the function $F^{(1)}$ is well defined in a ball $B_{\mathcal{X}_g}(0, \bar{R})$ with $\bar{R} = \mathcal{O}(\sqrt{\log(\Lambda)})$, say $\bar{R} = K_0\sqrt{\log(\Lambda)}$. Indeed:

$$\|F^{(1)}(Q', \rho'')\|_{\mathcal{X}_g} \leq \|(N, n'')\|_{\mathcal{X}_g} + \alpha\kappa_1(\Lambda)\|(Q', \rho'')\|_{\mathcal{X}_g} + \sum_{\ell=2}^{+\infty} \alpha^\ell \kappa_\ell \|(Q', \rho'')\|_{\mathcal{X}_g}^\ell, \quad (80)$$

where

$$\begin{cases} \kappa_1(\Lambda) &= \mathcal{O}_{\Lambda \rightarrow +\infty}(\sqrt{\log(\Lambda)}) \\ \kappa_\ell &= \mathcal{O}_{\ell \rightarrow +\infty}(\ell^{1/2}), \end{cases} \quad (81)$$

in particular 1 is the radius of convergence of the power series $f(x) = \sum_{\ell=2}^{+\infty} \kappa_\ell x^\ell$ and:

$$\|dF^{(1)}(Q', \rho'')\|_{L(\mathcal{X}_g)} \leq \alpha \kappa_1(\Lambda) + \alpha f'(\alpha \| (Q', \rho'') \|_{\mathcal{X}_g}). \quad (82)$$

For $\|(N, n'')\|_{\mathcal{X}_g} \neq (0, 0)$ it is clear that $F^{(1)}(0, 0) = (N, \mathcal{F}^{-1}(-\frac{1}{1+\alpha B_\Lambda(\cdot)} \widehat{n}'')) \neq 0$. So

$$\sup_{(Q', \rho'') \in B_{\mathcal{X}_g}(0, \overline{R})} \|dF^{(1)}(Q', \rho'')\|_{L(\mathcal{X}_g)} \leq \alpha \kappa_1(\Lambda) + \alpha f'(\alpha \overline{R}) =: \nu(\overline{R}). \quad (83)$$

For $(Q', \rho'') \in B_{\mathcal{X}_g}(0, \overline{R})$ we have

$$\begin{aligned} \|F^{(1)}(Q', \rho'')\|_{\mathcal{X}_g} &\leq \|F^{(1)}(Q', \rho'') - F^{(1)}(0, 0)\|_{\mathcal{X}_g} + \|F^{(1)}(0, 0)\|_{\mathcal{X}_g} \\ &\leq \nu(\overline{R}) \|(Q', \rho'')\|_{\mathcal{X}_g} + \|F^{(1)}(0, 0)\|_{\mathcal{X}_g}. \end{aligned}$$

Thus a sufficient condition for $B_{\mathcal{X}_g}(0, \overline{R})$ being invariant under $F^{(1)}$ is:

$$\|F^{(1)}(0, 0)\|_{\mathcal{X}_g} \leq (1 - \nu(\overline{R}))\overline{R}. \quad (84)$$

As $F^{(1)}(0, 0) \neq 0$ this gives $\nu(\overline{R}) < 1$.

Let us say that $\|(N, n'')\|_{\mathcal{X}_g} = \varepsilon_0 \overline{R} = \varepsilon_0 K_0 \sqrt{\log(\Lambda)}$, $\varepsilon_0 < 1$. We have:

$$\|F^{(1)}(0, 0)\|_{\mathcal{X}_g} \leq \varepsilon_0 \overline{R}, \quad (85)$$

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.

5.5.2 $F^{(2)}$

We work with $(\mathcal{C}, \|\cdot\|_{\mathcal{C}})$ and $(\mathcal{C} \cap L^1, \max(\|\cdot\|_{\mathcal{C}}, \|\cdot\|_{L^1}))$. In Appendix C it is proved that $\|\check{f}_\Lambda\|_{L^1} \leq K\alpha B_\Lambda(0)$ where we can choose $K = 2$ for $\alpha \log(\Lambda)$ sufficiently small. Thus:

$$\mathcal{F}^{-1}(F_\Lambda) = \mathcal{F}^{-1} \left\{ \frac{f_\Lambda}{1 + f_\Lambda} \right\} = \sum_{\ell=1}^{+\infty} (-1)^{\ell+1} \check{f}_\Lambda^{\ast \ell} \in L^1$$

and its L^1 -norm is lesser than $\frac{2\alpha B_\Lambda(0)}{1-2\alpha B_\Lambda(0)} \leq 4\alpha B_\Lambda(0)$ as soon as $\alpha B_\Lambda(0) \leq 4^{-1}$. Moreover we can write

$$\frac{1}{1 + f_\Lambda} = 1 - \frac{f_\Lambda}{1 + f_\Lambda};$$

therefore if $\rho \in L^1$ then $\mathcal{F}^{-1}\{\frac{1}{1+f_\Lambda}\widehat{\rho}\}^{-1} \in L^1$ and its L^1 -norm is lesser than

$$(1 + 4\alpha B_\Lambda(0))\|\rho\|_{L^1} \leq 2\|\rho\|_{L^1}.$$

In particular:

$$\|\mathcal{F}^{-1}(\frac{1}{1+f_\Lambda}\widehat{n}'')\|_{L^1} \leq 2(M + Z).$$

So we have:

$$\begin{cases} \|F^{(2)}(\rho'')\|_{\mathcal{C} \cap L^1} &\leq 2(M + Z) + \|h_2 + h_3\|_{\mathcal{C} \cap L^1} + K\alpha^3(\sqrt{\log(\Lambda)} + \|\rho''\|_{\mathcal{C} \cap L^1})\|\rho''\|_{\mathcal{C} \cap L^1}^2 \\ \|dF^{(2)}(\rho'')\|_{L(\mathcal{C} \cap L^1)} &\leq K\alpha^3\|\rho''\|_{\mathcal{C} \cap L^1}(2\sqrt{\log(\Lambda)} + 3\|\rho''\|_{\mathcal{C} \cap L^1}). \end{cases} \quad (86)$$

where the constants K can be chosen independently of $\alpha \leq \alpha_0$ and $\alpha \log(\Lambda) \leq L_0$ for α_0, L_0 sufficiently small. The term $\sqrt{\log(\Lambda)}$ is due to $\|\gamma'\|_{\mathcal{T}} \lesssim \sqrt{\log(\Lambda)}$ (Lemma 5). 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 $F^{(2)}$; then this function will be a contraction and we will be able to apply the fixed point theorem. Then:

- There is exactly only one fixed point of $F^{(2)}$ in $B_{\mathcal{C}}(0, \overline{R})$ by the Banach-Picard Theorem, $\rho_\gamma + n - \nu$ is such a fixed point. Indeed by Section 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 (14) and is a fixed point of $F^{(1)}$. So it is a fixed point of $F^{(2)}$ (which is derived from $F^{(1)}$).

- There is exactly only one fixed point of $F^{(2)}$ in $B_{C \cap L^1}(0, \overline{R})$ by the same theorem. In particular it is also a fixed point of $F^{(2)}$ in $B_C(0, \overline{R})$ as $B_{C \cap L^1}(0, \overline{R}) \subset B_C(0, \overline{R})$. By unicity $\rho_\gamma \in L^1$.

6 Proofs of Theorems 2 and 3

6.1 Proof of Theorem 2

Proof: The fact that $\rho_\gamma \in L^1$ is a result of Section 5.5. We recall that if $Q \in \mathfrak{S}_1$, then $\int \rho_Q = \text{Tr}(Q) = \text{Tr}_{P_-^0}(Q)$. Writing

$$\begin{aligned} A &:= \alpha \mathbf{T}[Q_{0,1}(\rho''_\gamma)] & C &:= \alpha^3 \mathbf{T}\{Q_{1,1}[\mathbf{T}[Q_{0,1}(\rho''_\gamma)], \rho''_\gamma]\} \\ B &:= \alpha^2 \mathbf{T}(Q_{0,2}(\rho''_\gamma)) & S &:= \gamma - (A + B + C) \end{aligned} \quad (87)$$

it has been shown in Section 5 that $S \in \mathfrak{S}_1$. Theorem 1 says $\rho_B = \rho_C = 0$.

Let us show that $B^{++}, B^{--}, C^{++}, C^{--}$ are trace-class. As for any Q (say in \mathfrak{S}_2), we have

$$P_-^0 Q_{1,0}(Q) P_-^0 = P_+^0 Q_{1,0}(Q) P_+^0 = 0,$$

there only remains $\alpha^2 Q_{0,2}(\rho''_\gamma)^{\varepsilon, \varepsilon}$ for B and $\alpha^3 Q_{1,1}(\mathbf{T}Q_{0,1}(\rho''_\gamma), \rho''_\gamma)^{\varepsilon, \varepsilon}$ for C . 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 10 with $a = \frac{3}{4}$ and Cauchy-Schwartz inequality we get

$$\left\| \frac{1}{|D_0|^{3/8}} P_\varepsilon^0 v_\rho P_{-\varepsilon}^0 \frac{1}{|D_0|^{3/8}} \right\|_{\mathfrak{S}_2} \lesssim \|\rho\|_C \lesssim \|\rho\|_C \quad (88)$$

We recall that $\left\| \frac{1}{|\nabla|^{1/2}} R_Q \right\|_{\mathfrak{S}_2} \lesssim \|Q\|_{\text{Ex}}$. These two estimates enables us to prove the following inequalities ($\varepsilon \in \{+, -\}$):

$$\begin{aligned} \|Q_{0,2}^{\varepsilon, -\varepsilon, \varepsilon}(\rho''_\gamma)\|_{\mathfrak{S}_1} &\lesssim K_{3/2} \|\rho''_\gamma\|_C^2, \\ \|Q_{1,1}^{\varepsilon, -\varepsilon, \varepsilon}(\gamma', \rho''_\gamma)\|_{\mathfrak{S}_1} &\lesssim K_{7/4} \|\gamma'\|_{\text{Ex}} \|\rho''_\gamma\|_C. \end{aligned}$$

As shown in Sections 5 and C we have $Q_{0,1}^{++} = Q_{0,1}^{--} = 0$ and that $\rho_A = -\check{f}_\Lambda * (\rho'_\gamma) \in L^1$.

$$\begin{aligned} \int \rho_\gamma &= \int (\rho_{\gamma^{++}} + \rho_{\gamma^{--}}) + \int \{\rho_{A^{+-}} + \rho_{A^{-+}} + \rho_{B^{+-}} + \rho_{B^{-+}} + \rho_{C^{+-}} + \rho_{C^{-+}}\} \\ &= \text{Tr}_{P_-^0}(\gamma) - \alpha f_\Lambda(0) \int \{\rho_\gamma + n - \nu\} - \int \{\rho_{B^{++}} + \rho_{B^{--}} + \rho_{C^{--}} + \rho_{C^{++}}\} \\ &= 0 - \alpha f_\Lambda(0) \left\{ \int \rho_\gamma + M - Z \right\} - \text{Tr}_{P_-^0}(B) - \text{Tr}_{P_-^0}(C). \end{aligned}$$

So it suffices to show that $\text{Tr}(B^{++} + B^{--}) = \text{Tr}(C^{++} + C^{--}) = 0$. This is straightforward when written in Fourier space [9]. \square

6.2 Proof of Theorem 3

We follow the method of [11]. Thanks to a result of Borwein and Preiss (Theorem 4.[11]), we consider an approximate minimizer $\gamma'_0 = \gamma_0 + N_0$ of $E^\nu(M)$. Indeed, we can extend \mathcal{E}_{BDF}^ν to $\mathfrak{K} = \cap \{Q \in \mathfrak{S}_2 : Q^* = Q, 0 \leq Q + P_-^0 \leq 1\}$ by setting $\mathcal{E}_{BDF}^\nu(Q) := +\infty$ whenever $Q \notin \mathfrak{K}$. This extension is lower semi-continuous and bounded from below in the \mathfrak{S}_2 -topology and the set

$$\mathcal{M} := \{Q \in \mathfrak{K}, (Q + P_-^0)^2 = Q + P_-^0, \text{Tr}_0(Q) = M\}$$

is closed in the same topology. Its convex closure in \mathfrak{S}_2 is

$$\mathfrak{K}(M) := \{Q \in \mathfrak{K}, \text{Tr}_0(Q) = M\}.$$

Applying the theorem, 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 $\mathcal{E}_{\text{BDF}}^\nu + \varepsilon \text{Tr}((A - \cdot)^2)$ on \mathcal{M} and

$$\mathcal{E}_{\text{BDF}}^\nu(\gamma'_0) \leq E_{\text{BDF}}^\nu(M) + \varepsilon^2, \quad \|\gamma'_0 - A\|_{\mathfrak{S}_2} \leq \sqrt{\varepsilon}.$$

As in [11], γ'_0 satisfies the self-consistent equation

$$\begin{aligned} \gamma'_0 + P_-^0 &= \chi_{(-\infty, \mu_0]}(D_{\gamma'_0} + 2\varepsilon(\text{sgn}(D_0) - A)) \\ &= \chi_{(-\infty, \mu_0]}(\tilde{D} + \alpha B_{\gamma'_0} - 2\varepsilon A) \end{aligned} \quad (89)$$

where $\mu_0 \in \mathbf{R}$ and $\tilde{D} := \mathcal{D}^0 + D_0 \frac{2\varepsilon}{|D_0|}$. We choose $\varepsilon = \lambda^{-1}$ small *e.g.* $\varepsilon = \Gamma(\frac{\Lambda}{\alpha})^{-1}$: using the proof of Lemma 5 we show the following *a priori* estimate holds for γ'_0 :

$$\text{Tr}(|\nabla|(\gamma'_0)^2) + \alpha \|\rho_{\gamma'_0}''\|_{\mathcal{C}}^2 \lesssim \alpha \|\nu\|_{\mathcal{C}}^2 + \sqrt{\alpha} M + \sqrt{\alpha} M \|\nu\|_{\mathcal{C}}.$$

Using the Cauchy expansion we have

$$\gamma_0 = \sum_{j=0}^{+\infty} \alpha^j Q_j(\rho_{\gamma_0}'', \gamma'_0) + \frac{2}{\lambda} W_\lambda(A, \alpha B(\gamma'_0)),$$

where \tilde{Q}_j has the same formula as Q_j with \tilde{D} instead of \mathcal{D}^0 . By the same method as in Section 5 we have:

$$\|\mathcal{D}^0|^{1/2} W_\lambda\|_{\mathfrak{S}_2} + \|\rho[W_\lambda]\|_{\mathcal{C}} \lesssim \|A\|_{\mathfrak{S}_2} (1 + \alpha[\|\rho_{\gamma_0}''\|_{\mathcal{C}} + \|\nabla|^{1/2} \gamma'_0\|_{\mathfrak{S}_2}]),$$

indeed it suffices to replace $R[\gamma'_0]$ by A in the Q_j 's and notice $A \in \mathfrak{S}_2$. Replacing \mathcal{D}^0 by \tilde{D} is harmless; as before, by defining some function $\tilde{F}^{(1)}$ we can show $\text{Tr}_0(\gamma_0) = 0$ (but with an alternative B_Λ cf Section C). Let $(\psi_j)_{1 \leq j \leq M}$ be an orthonormal family of eigenvectors of $\tilde{D} + \alpha B_{\gamma'_0} + 2/\varepsilon(1 - P_-^0 - A)$ spanning $\text{Ran}(N_0)$ (with eigenvalues (μ_j)). In particular we can write

$$\rho_{\gamma_0} := -\mathcal{F}^{-1}(\tilde{F}_\Lambda) * n_0'' + (\delta_0 - \mathcal{F}^{-1}(\tilde{F}_\Lambda)) * \tau_{\text{rem}} \in \mathcal{C}$$

where $\|\tau_{\text{rem}}\|_{\mathcal{C}} \lesssim \|\mathfrak{t}[N_0]\|_{\mathcal{C}} + \alpha^2 \|\tilde{\tau}_2\|_{\mathcal{C}} + \|A\|_{\mathfrak{S}_2}/\lambda$ and \tilde{F}_Λ is defined in Section C. We write $\mathfrak{f}_\Lambda := \mathcal{F}^{-1}(\tilde{F}_\Lambda)$ for short. As in Section 5 we get:

$$\begin{cases} \|\gamma_0\|_{\mathfrak{S}_2} \lesssim \alpha(\|\rho_{\gamma_0}''\|_{\mathcal{C}} + \|\gamma'_0\|_{\text{T}}) \\ \|\rho_{\gamma_0} + \mathfrak{f}_\Lambda * n_0'' - (\delta_0 - \mathfrak{f}_\Lambda) * \mathfrak{t}[N_0]\|_{\mathcal{C}} \lesssim \alpha^2(\|\gamma'_0\|_{\text{T}} + \|\rho_{\gamma_0}''\|_{\mathcal{C}})^2. \\ \|\mathfrak{f}_\Lambda * n_0'' + (\delta_0 - \mathfrak{f}_\Lambda) * \mathfrak{t}[N_0]\|_{L^1} \lesssim L(Z + M). \end{cases} \quad (90)$$

We then scale γ'_0 by α^{-1} (we mark this procedure by an underline) as in [11] we get:

$$\left[\left(\frac{w_0(-i\alpha\nabla)\beta}{\alpha^2} - \frac{iw_1(-i\alpha\nabla)}{\alpha^2} \alpha \cdot \nabla \right) + \rho[\underline{\gamma}'_0] * \frac{1}{|\cdot|} - R[\underline{\gamma}'_0] + \frac{2}{\alpha^2 \lambda} \left(\frac{1}{2} - P_-^0 - A \right) \right] \underline{\psi}_j = \frac{\mu_j}{\alpha^2} \underline{\psi}_j. \quad (91)$$

Remark 19. We have $U_{\alpha^{-1}} \underline{\psi}(x) = \alpha^{\frac{3}{2}} \underline{\psi}(\alpha x) = \underline{\psi}(x)$ and for an operator S we have:

$$\underline{S} := U_{\alpha^{-1}}^* S U_{\alpha^{-1}}.$$

This mean-field operator $H_{\alpha^{-1}}$ can be decomposed as follows: $H_{\alpha^{-1}} = H_{\alpha^{-1}}^{(1)} + h_{\text{rem}}$ where

$$H_{\alpha^{-1}}^{(1)} := \frac{\mathcal{D}^0}{\alpha^2} + (\delta_0 - \mathfrak{f}_\Lambda) * \underline{n}_0'' - R[\underline{N}_0], \quad \underline{n}_0''(x) = \alpha^{-3} n''(x/\alpha), \quad \tilde{F}_\Lambda(k) = \tilde{F}_\Lambda(\alpha k).$$

As in Lemma 13 and 14 in [11] we can show that there exists $\varepsilon > 0$ such that $\limsup_{\alpha \rightarrow 0} (\alpha^{-2}(\mu_j - 1)) < -\varepsilon < 0$ for all $1 \leq j \leq M$ and that $(\underline{\psi}_j)_j$ is bounded in $H^1(\mathbf{R}^3, \mathbf{C}^4)^M$ (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 $-\underline{f}_\Lambda * (\underline{n}_0'') * \frac{1}{|\cdot|}$ and $(\delta_0 - \underline{f}_\Lambda) * \underline{t}_{N_0}$: we need the following lemma (proved below).

Lemma 12. Let χ be a Schwartz function and for $R > 0$: $\chi_R(x) := R^{-3/2}\chi(x/R)$. Then there holds:

$$\begin{aligned} \left| \langle \underline{f}_\Lambda * (\underline{n}_0'') * \frac{1}{|\cdot|} \chi_R - Z \tilde{F}_\Lambda(0) \frac{\chi_R}{|\cdot|}, \chi_R \rangle \right| &\lesssim \frac{ZL}{R^2} \|\nabla \chi\|_{L^2}^2 \\ &+ \frac{1}{R} \|\nabla \chi\|_{L^2} \|\chi\|_{L^2} \left(L \int_{|y| > \frac{1}{\alpha}} \nu(y) dy + Z \int_{|y| > \frac{1}{\alpha}} |\underline{f}_\Lambda(y)| dy \right), \end{aligned}$$

and $\int_{|y| > \frac{1}{\alpha}} |\underline{f}_\Lambda(y)| dy \lesssim L\alpha^{1/2}$. Moreover

$$\begin{aligned} \left| \langle (\delta_0 - \underline{f}_\Lambda) * \underline{t}_{N_0} * \frac{1}{|\cdot|} \chi_R, \chi_R \rangle \right| &\lesssim \frac{L^2 M}{R^2} \|\nabla \chi\|_{L^2}^2 \\ &+ \frac{1}{R} \|\nabla \chi\|_{L^2} \|\chi\|_{L^2} \left(L \int_{|y| > \frac{1}{\alpha}} |\underline{t}_{N_0}|(y) dy + LM \int_{|y| > \frac{1}{\alpha}} |\underline{f}_\Lambda(y)| dy \right). \end{aligned}$$

To prove $(\underline{\psi}_j)_j$ is H^1 -bounded we show that:

$$\frac{M}{\alpha^4} + \frac{\text{Tr}(-\Delta N_0)}{\alpha^2} \leq \frac{\text{Tr}(\mathcal{D}^{02} N_0)}{\alpha^4} \leq \frac{M}{\alpha^4} + K(M, \nu) \left\{ \text{Tr}(-\Delta N_0) + \frac{\|\nabla N_0\|_{\mathfrak{S}_2}}{\alpha^2} \right\}. \quad (92)$$

The lower bound is clear and for the upper bound we use (91), Lemma 5 and Proposition 5 (for estimations of $w_*(\alpha p)^2$, $\star \in \{0, 1\}$). We get:

$$\begin{aligned} \left| \rho[\underline{\gamma}_0] + \rho[\underline{f}_\Lambda * \underline{n}_0'' - (\delta_0 - \underline{f}_\Lambda) * \underline{t}_{N_0}] \underline{\psi}_j \right|_{L^2} &\lesssim \alpha^{3/2} (\|\rho''_{\gamma_0}\|_c + \|\gamma'_0\|_{\mathbb{T}})^2 \|\nabla^{1/2} \underline{\psi}_j\|_{L^2} \\ &\lesssim K(M, \nu) \|\nabla^{1/2} \underline{\psi}_j\|_{L^2}. \end{aligned}$$

Moreover:

$$\begin{aligned} &\left| \begin{aligned} \|R[\underline{\gamma}_0] \underline{\psi}_j\|_{L^2} &\lesssim \|\gamma_0\|_{\mathfrak{S}_2} \|\nabla \underline{\psi}_j\|_{L^2} \lesssim \alpha^{3/4} K(M, \nu) \|\nabla \underline{\psi}_j\|_{L^2} \\ \|v[\underline{f}_\Lambda * \underline{n}_0'' - (\delta_0 - \underline{f}_\Lambda) * \underline{t}_{N_0}] \underline{\psi}_j\|_{L^2}^2 &\leq 4 \|\nabla \underline{\psi}_j\|_{L^2}^2 \|\rho[\underline{f}_\Lambda * \underline{n}_0'' - (\delta_0 - \underline{f}_\Lambda) * \underline{t}_{N_0}]\|_{L^1}^2 \\ &\lesssim L^2 (Z + M)^2 \|\nabla \underline{\psi}_j\|_{L^2}^2 \\ |\langle v[\underline{f}_\Lambda * \underline{n}_0'' - (\delta_0 - \underline{f}_\Lambda) * \underline{t}_{N_0}] \underline{\psi}_j, \underline{\psi}_j \rangle| &\leq |D(\rho[\underline{f}_\Lambda * \underline{n}_0'' - (\delta_0 - \underline{f}_\Lambda) * \underline{t}_{N_0}], \underline{\psi}_j)| \\ &\lesssim L(Z + M) \langle |\nabla \underline{\psi}_j, \underline{\psi}_j \rangle. \end{aligned} \right. \quad (93) \end{aligned}$$

Summing over $1 \leq j \leq M$ the inequalities (93) we get (92):

$$\sum_{j=1}^M \|\nabla \underline{\psi}_j\|_{L^2}, \text{Tr}(|\nabla \bar{N}_0|) \leq \sqrt{M} \sqrt{\text{Tr}(-\Delta N_0)}.$$

We conclude as in [11] (the proof uses [20]) provided that there hold binding inequalities for the non-relativistic limit: this is the result of Proposition 2 in Appendix B.

In particular there holds

$$\lim_{\alpha \rightarrow 0} \alpha^{-2} (E_{BDF}^\nu(M) - M + \frac{\alpha}{2} D(\tilde{F}_\Lambda * \nu, \nu)) = E_{nr}(M), \quad (94)$$

where E_{nr} is the non-relativistic energy cf Appendix B.

Proof of Lemma 12 With $f(x) = |\chi_R|^2 * \mathcal{F}^{-1}(\tilde{F}_\Lambda)$, we first estimate $|\iint f(x) \nu(y) (1/|x - \alpha y| - 1/|x|) dx dy|$: it is lesser than

$$\iint |f(x)| \nu(y) |\alpha y| \frac{dx dy}{|x| |x - \alpha y|}.$$

Splitting at level α^{-1} for y , we use Hardy's and Kato's inequalities:

$$\left\{ \begin{array}{l} \int_{|y| \leq \frac{1}{\alpha}} \nu(y) dy \int \frac{|f(x)| dx}{|x||x-\alpha y|} \leq (4Z \|\tilde{F}_\Lambda\|_{L^1}) \frac{\|\nabla \chi\|_{L^2}^2}{R^2} \\ \int_{|y| > \frac{1}{\alpha}} \nu(y) dy \int |\alpha y| \frac{dx}{|x||x-\alpha y|} |f(x)| \leq \frac{2\pi}{2} \int_{|y| > \frac{1}{\alpha}} \nu(y) dy \|\tilde{F}_\Lambda\|_{L^1} \frac{\|\nabla \chi\|_{L^2} \|\chi\|_{L^2}}{R}. \end{array} \right.$$

We estimate $Z \left| \iint |\chi_{R^c}(x)|^2 f_\Lambda(y) (1/|x-\alpha y| - 1/|x|) dx dy \right|$ in the same way with the help of Lemma 15 in Appendix C. For the terms with \underline{t}_{N_0} we use the fact that:

$$\|\underline{t}_{N_0}\|_{L^1} = \|\underline{t}_{N_0}\|_{L^1} \lesssim LM \text{ and } \int \underline{t}_{N_0} = \int t_{N_0} = 0,$$

and use the same method. \square

A Estimates and inequalities

Notation 20. In Section A and C, \mathbf{e} refers to any unitary vector in \mathbf{R}^3 and for $p \in \mathbf{R}^3$, $\omega_p := \frac{p}{|p|}$.

We recall there exists $C_s > 0$ such that:

$$\left\{ \begin{array}{l} \mathbf{s}_p := \widehat{\text{sign}(\mathcal{D}^0)}(p) = \frac{\widehat{\mathcal{D}^0(p)}}{|\widehat{\mathcal{D}^0(p)}|}(p) = \frac{w_0(p)\beta + w_1(p)\boldsymbol{\alpha} \cdot \omega_p}{\widehat{E}(p)}. \\ \text{Id} - \mathbf{s}_p \mathbf{s}_q = \mathbf{s}_p (\mathbf{s}_p - \mathbf{s}_q) = (\mathbf{s}_p - \mathbf{s}_q) \mathbf{s}_q \\ |\text{Id} - \mathbf{s}_p \mathbf{s}_q| \leq |\mathbf{s}_p - \mathbf{s}_q| = \left| \widehat{\mathcal{P}^0_+}(p) - \widehat{\mathcal{P}^0_+}(q) \right| \leq C_s \frac{|p-q|}{\max(\widehat{E}(p), \widehat{E}(q))}. \end{array} \right. \quad (95)$$

A.1 Proof of Lemma 8

- We recall [16] $\frac{1}{|\nabla|}(x-y) = \text{Cst}/|x-y|^2$. By Cauchy-Schwartz inequality we have

$$\begin{aligned} \text{Tr}(R_Q^* |\nabla|^{-1} R_Q) &= \iiint \text{Tr}_{\mathbf{C}^4} {}^t \overline{Q}(x, y) \frac{\text{Cst}}{|x-y|} \frac{Q(z, x)}{|y-z|^2 |z-x|} dx dy dz \\ &\lesssim \iiint |Q(x, y)|^2 \frac{1}{|y-z|^2 |z-x|^2} dx dy dz \\ &\lesssim \iint \frac{|Q(x, y)|^2}{|x-y|} = \text{Tr}(R_Q^* Q). \end{aligned}$$

We write $m(|p+q|)$ the multiplication in Fourier space by $|p+q|$; R . and $\frac{1}{|\nabla|^{1/2}}$ commute with the multiplication in Fourier space by $g(p-q)$ (written $m(g)$). We get thanks to Kato's inequality that

$$\|m(g_s) \cdot \frac{1}{|\nabla|^{1/2}} R[Q]\|_{\mathfrak{S}_2} = \|\frac{1}{|\nabla|^{1/2}} R[m(g) \cdot Q]\|_{\mathfrak{S}_2} \lesssim \|m(|p+q|)m(g) \cdot Q\|_{\mathfrak{S}_2}.$$

Similarly for $a > 0$ the operator $|D_0|^{-a}$ acts in Direct space as a convolution operator with a *positive* function ϕ_a : indeed we have [16]:

$$\frac{1}{1-\Delta}(x-y) = \frac{e^{-|x-y|}}{4\pi|x-y|}$$

and for any $0 < \varepsilon < 1$ (see [17], footnote p. 87):

$$\frac{1}{|D_0|^{2\varepsilon}} = \frac{\sin(\varepsilon\pi)}{\pi} \int_0^{+\infty} t^{p-1} \frac{x}{t+x} dt.$$

Thus for $a = 1 + \varepsilon > 1$ we have by Cauchy-Schwarz inequality:

$$\begin{aligned} \text{Tr}(R_Q^* \frac{1}{|D_0|^{2a}} R_Q) &\leq \iint |Q(x, y)|^2 \frac{1}{|x-y|} * \phi_{2a}(x-y) dx dy, \\ &\leq \iint |Q(x, y)|^2 \|\frac{1}{|\cdot|} * \phi_{2a}\|_{L^\infty} \\ &\lesssim \iint |Q(x, y)|^2 dx dy \int \frac{dp}{|p|E(p)^{2a}} \lesssim \frac{\|Q\|_{\mathfrak{S}_2}^2}{2(a-1)}. \end{aligned}$$

Then let us take a finite rank operator $Q(x, y)$. As $Q = \frac{Q+Q^*}{2} + \frac{Q-Q^*}{2}$ one may suppose it is self-adjoint and writing $Q = Q_+ - Q_-$ one may suppose it is nonnegative; so is R_Q and $|D_0|^{-a/2} R_Q |D_0|^{-a/2}$.

There holds:

$$\begin{aligned} \int \frac{\text{Tr}_{\mathbb{C}^4}(\widehat{R}(p, p))}{E(p)^{2a}} dp &= \frac{1}{2\pi^2} \iint \frac{d\ell}{|\ell|^2} \text{Tr}(\widehat{Q}(p - \ell, p - \ell)) \frac{dp}{E(p)^{2a}} \\ &= \frac{1}{2\pi^2} \int dp \text{Tr}(\widehat{Q}(p, p)) \int \frac{d\ell}{|\ell|^2} \frac{1}{E(p + \ell)^{2a}} \\ &\lesssim \frac{\|\widehat{Q}\|_{\mathfrak{S}_1}}{2a - 2}. \end{aligned}$$

Going in Fourier space we have:

$$\mathcal{F}(|\mathcal{D}^0|^{-1/2}) : f(p) \mapsto \chi_{|p| < \Lambda} \frac{f(p)}{\widetilde{E}(p)^{1/2}},$$

thus writing Π_A the projection onto $\{f \in L^2, \text{supp } \widehat{f} \subset B(0, A)\}$ we have

$$\| |\mathcal{D}^0|^{1/2} R_Q \|_{\mathfrak{S}_2} \leq \| |\mathcal{D}^0|^{1/2} \Pi_{2\Lambda} R_Q \Pi_{3\Lambda} \|_{\mathfrak{S}_2}.$$

Then 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 get:

$$\text{Tr}(\Pi_{3\Lambda} R_{Q^*} \frac{\Pi_{2\Lambda}}{|\mathcal{D}^0|} R_Q \Pi_{3\Lambda}) \leq \text{Tr}(R_{Q^*} \frac{e}{|\mathcal{D}^0|^{\frac{1}{2} + \frac{1}{2 \log(\Lambda)}}} R_Q) \lesssim \log(\Lambda) \|Q\|_{\text{Ex}}^2.$$

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

$$\begin{aligned} \mathcal{E}_{nr}^Z(\Gamma) &:= \frac{1}{2} \text{Tr}(-\Delta \Gamma) - Z(1-a) \text{Tr}\left(\frac{1}{|\cdot|} \Gamma\right) \\ &\quad + \frac{1}{2} (D(\rho_\Gamma, \rho_\Gamma) - \text{Ex}[\Gamma]) - aD(\rho_\Gamma, \rho_\Gamma). \end{aligned} \tag{96}$$

If we drop the last term, this is exactly the Hartree-Fock energy \mathcal{E}_{HF} with a nucleus of charge $Z_0 := Z(1-a)$ and if we drop $\text{Tr}\left(\frac{1}{|\cdot|} \Gamma\right)$ we get the Pekar-Tomasevitch energy $\mathcal{E}_{nr}^0 = \mathcal{E}_{\text{PT}}[a, U = 1]$ (cf [5]): this last functional is what we obtain by putting the system at infinity.

We write $E_{\text{PT}} := E_{\text{PT}}[1, U = a^{-1}]$: putting any test function at infinity there holds: $E_{nr}(M) \leq a^2 E_{\text{PT}}(M)$ and $E_{\text{PT}}(M) = M E_{\text{PT}}(1)$ for sufficiently small a , we refer to Corollary 1 in [5]: there exists U_0 such that if $U \stackrel{\text{here}}{=} \frac{1}{a} \geq U_0$ then there is no binding for $E_{\text{PT}}(M)$, $M \geq 2$.

Remark 21. 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,

$$\begin{aligned} \mathcal{E}_{nr}^Z(\Gamma) &= \frac{x^2}{2} \text{Tr}(-\Delta \Gamma) + \frac{y^2}{2} (D(\rho_\Gamma, \rho_\Gamma) - \text{Ex}[\Gamma]) - Z(1-a) \text{Tr}\left(\frac{1}{|\cdot|} \Gamma\right) \\ &\quad + \frac{1-x^2}{2} \text{Tr}(-\Delta \Gamma) + \frac{1-y^2}{2} (D(\rho_\Gamma, \rho_\Gamma) - \text{Ex}[\Gamma]) - aD(\rho_\Gamma, \rho_\Gamma) \text{ with } 0 < x, y < 1. \end{aligned}$$

Optimizing in x and y we get a lower bound $\mathcal{O}(\text{Cst}(a)M)$ for $M \geq 2Z_0 + 1$.

We define

$$\mathcal{G}(x) = \{\Gamma \in \mathfrak{S}_1 : \Gamma^* = \Gamma, 0 \leq \Gamma \leq 1, \sqrt{-\Delta} \Gamma \in \mathfrak{S}_2 \text{ and } \text{Tr}(\Gamma) = x\} \text{ with } x \in \mathbf{R}_+^*.$$

$E_{nr}(M)$ corresponds to the infimum over $\mathcal{G}(M)$. We want to prove:

Proposition 2. For any $M < Z + 1$, the variational problem $E_{nr}^Z(M)$ admits a minimizer.

By Lieb's method in [15], it is easy to see that there is a minimizer for $E_{nr}^Z(1)$. To prove binding for $2 \leq M \leq Z(1-a)$ we can follow Lieb's and Simon's method [19, 20]. We will however prove it with the method of concentration-compactness. We prove the problem $E_{nr}^Z(M)$ admits a minimizer by induction over M by using:

Proposition 3. For each $m > 0$ the following assertions are equivalent

- $\forall 0 < k < m : E_{nr}^Z(m) < E_{nr}^Z(m-k) + E_{nr}^0(k)$.
- Each minimizing sequence for $E_{nr}^Z(m)$ is precompact in $H^1(\mathbf{R}^3 \times \mathbf{R}^3)$.

In the case $m \in \mathbf{N}^*$, it suffices to prove binding inequalities for $K \in (0, m) \cap \mathbf{N}$.

This proposition is standard and we will not give the proof here but refer to [14, 13, 20]. As $E_{nr}^0(M_0) = M_0 E_{nr}^0$ for $M_0 \in \mathbf{N}^*$ we need to show

$$E_{nr}^Z(M) < E_{nr}^Z(M-1) + E_{nr}^0(1).$$

To this end, one just needs to find a test function Q whose energy is lesser than $E_{nr}^Z(M-1) + E_{nr}^0(1)$. We can show that Lieb's variational principle holds (*cf* proposition 3 in [11]). In fact for any orthonormal family (ϕ_1, ϕ_2) , with $P_\phi := |\phi\rangle\langle\phi|$ and $0 < t < 1$, we have

$$\begin{aligned} \mathcal{E}_{nr}^Z(\Gamma + t(P_{\phi_1} - P_{\phi_2})) - \mathcal{E}_{nr}^Z(\Gamma) &= \frac{t}{2}(\|\nabla\phi_1\|_{L^2}^2 - \|\nabla\phi_2\|_{L^2}^2 + 2(1-a)D(\rho_\Gamma, |\phi_1|^2 - |\phi_2|^2)) \\ &\quad - t\Re[\text{Tr}(\Gamma R[P_{\phi_1} - P_{\phi_2}])] - t^2\{D(|\phi_1|^2, |\phi_2|^2) - D(\phi_1^*\phi_2, \phi_1^*\phi_2) + \frac{a}{2}\||\phi_1|^2 - |\phi_2|^2\|_C^2\}. \end{aligned} \quad (97)$$

This shows that $E_{nr}^Z(m)$ is also the infimum of \mathcal{E}_{nr}^Z over

$$\{\Gamma \in \mathcal{G}(m) : \Gamma = P + (m - [m])|\phi\rangle\langle\phi|, P^2 = P = P^*, \phi \in \text{Ker}(P)\}.$$

Taking $\phi_2 = 0$ in (97) shows that $E_{nr}^Z(\cdot)$ is concave in $[M_0, M_0 + 1]$ with $M_0 \in \mathbf{N}$. It is also clear that E_{nr}^Z is decreasing since large binding inequalities hold. We consider a minimizer of $E_{nr}^Z(M-1)$ 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 $H^2(\mathbf{R}^3)$ and fast decaying. We consider a minimizer of the problem at infinity: this is just a minimizer ϕ_{CP} of $E_{PT}(1)$ scaled by a : $\phi_0(x) = a^{3/2}\phi_{CP}(ax)$, we chose it to be radial [15]. Following [13], 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 consider for some $\mathbf{e} \in \mathbf{S}^2$:

$$\Gamma' := \chi_R \Gamma \chi_R + \tau_{-5R\mathbf{e}} |\chi_R \phi_0\rangle\langle\chi_R \phi_0| \tau_{5R\mathbf{e}}$$

where $\tau_{x_0}\psi(x) := \psi(x - x_0)$. We have $0 \leq \Gamma' \leq 1$ and $\text{Tr}(\Gamma') \leq M$, 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:

$$\begin{aligned} \mathcal{E}_{nr}^Z(\Gamma') &= \mathcal{E}_{nr}^Z(\Gamma) + \mathcal{E}_{nr}^0(\phi_0) + \int (\rho[\Gamma] * \frac{1}{|\cdot|}(x) - \frac{Z_0}{|x|}) |\tau_{5R\mathbf{e}}\phi_0(x)|^2 dx \\ &\quad - aD(\rho[\Gamma], |\tau_{5R\mathbf{e}}\phi_0|^2) + o(R^{-1}). \end{aligned}$$

As R tends to infinity we get:

$$\mathcal{E}_{nr}^Z(\Gamma') \leq E_{nr}^Z(M-1) + E_{nr}^0(1) + \frac{(M-1)(1-a) - Z_0}{5R} + o(R^{-1}) < E_{nr}(M-1) + E_{nr}^0(1).$$

C Proof of Proposition 1

Remark 22. We write:

$$\begin{aligned} E(u, k/2) &:= \max(E(u + k/2), E(u - k/2)) \geq \sqrt{1 + |u|^2 + \frac{|k|^2}{4}}, \\ \tilde{E}(u, k/2) &:= \max(\tilde{E}(u + k/2), \tilde{E}(u - k/2)) \geq E(u, k/2). \end{aligned}$$

Our aim is to prove Proposition 4 below.

Proposition 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 $f_\Lambda \in L^1$ is a radial function. Moreover

$$\begin{cases} f_\Lambda = \sum_{J=0}^{+\infty} \alpha^J f_{\Lambda,J} \\ f_{\Lambda,0} = \alpha\check{B}_\Lambda \text{ and } \check{g}_\Lambda := \sum_{J=1}^{+\infty} \alpha^J f_{\Lambda,J}, \end{cases}$$

with

$$\|f_\Lambda\|_{L^1} \lesssim L \text{ and } \|\check{g}_\Lambda\|_{L^1} \lesssim L\alpha.$$

In particular $\check{F}_\Lambda := \mathcal{F}^{-1}\left(\frac{f_\Lambda}{1+f_\Lambda}\right) \in L^1$.

We also study an alternative function F_Λ , needed for the proof of Theorem 3, at the end of this section.

We need the following proposition.

Proposition 5. The function $\widehat{\mathcal{D}}^0 : \overline{B(0, \Lambda)} \rightarrow \mathbf{R}^3$ is infinitely differentiable. In particular so is $\widehat{E}(\cdot)$ 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:

$$\|d^J w_0\|_{L^\infty} \leq \alpha C_J \text{ and } \|d^J \mathbf{w}_1\|_{L^\infty} \leq \chi_{J=1} + LC_J.$$

Proof: In the spirit of arxiv.1211.3830, we can prove it by induction over J : in [12] it is proved $\widehat{\mathcal{D}}^0$ is infinitely differentiable. Thus the function

$$|\widehat{\mathcal{D}}^0(p)| = \sqrt{w_0(p)^2 + \mathbf{w}_1(p) \cdot \mathbf{w}_1(p)},$$

is infinitely differentiable and does not vanish on $\overline{B(0, \Lambda)}$. Thanks to the self-consistent equation one has:

$$d^J \widehat{\mathcal{D}}^0(p) = d^J \widehat{D}_0(p) + \frac{\alpha}{4\pi^2} \frac{1}{|\cdot|^2} * d^J \left(\frac{\mathcal{D}^0}{|\mathcal{D}^0|} \right)(p).$$

□

Proof of Proposition 4: Throughout this proof we write $k := \mathbf{re}$.

1. Let us see:

$$\widehat{\tau}_{1,0}(\rho) = -f_\Lambda(\cdot)\widehat{\rho}(\cdot),$$

We recall (36) that for any $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ we have:

$$\widehat{Q}_{1,0}(Q, p, q) = \frac{1}{4\pi^2} \frac{1}{\widetilde{E}(p) + \widetilde{E}(q)} \int_\ell \frac{d\ell}{|\ell|^2} (\widehat{Q}(p - \ell, q - \ell) - \mathbf{s}_p \widehat{Q}(p - \ell, q - \ell) \mathbf{s}_q),$$

and (cf [9])

$$\widehat{Q}_{0,1}(\rho; p, q) = \frac{4\pi}{2^{5/2}\pi^{3/2}} \frac{\widehat{\rho}(p - q)}{|p - q|^2} \frac{1}{\widetilde{E}(p) + \widetilde{E}(q)} (\mathbf{s}_p \mathbf{s}_q - 1). \quad (98)$$

Let us recall the definition of $A_J^{(\ell_j)_{j=1}^J}$:

$$\begin{cases} A_1^{\ell_1} \widehat{Q}(p, q) & := \widehat{Q}(p - \ell_1, q - \ell_1) - \mathbf{s}_p \widehat{Q}(p - \ell_1, q - \ell_1) \mathbf{s}_q, \\ A_1^{(\ell_1, L)} \widehat{Q}(p, q) & := A_1^{\ell_1} (A_{L-1}^L \widehat{Q})(p, q). \end{cases} \quad (99)$$

For instance:

$$\begin{aligned} A_2^{(\ell_1, \ell_2)} \widehat{Q}(p, q) &= A_1^{\ell_1} (\widehat{Q}(\cdot_p - \ell_2, \cdot_q - \ell_2) - \mathbf{s}_p \widehat{Q}(\cdot_p - \ell_2, \cdot_q - \ell_2) \mathbf{s}_q)(p, q) \\ &= \left\{ \widehat{Q}(p - \ell_1 - \ell_2, q - \ell_1 - \ell_2) - \mathbf{s}_{p-\ell_1} \widehat{Q}(p - \ell_1 - \ell_2, q - \ell_1 - \ell_2) \mathbf{s}_{q-\ell_1} \right\} \\ &\quad - \mathbf{s}_p \left\{ \widehat{Q}(p - \ell_1 - \ell_2, q - \ell_1 - \ell_2) - \mathbf{s}_{p-\ell_1} \widehat{Q}(p - \ell_1 - \ell_2, q - \ell_1 - \ell_2) \mathbf{s}_{q-\ell_1} \right\} \mathbf{s}_q. \end{aligned}$$

Writing $L_J := \sum_{j=1}^J \ell_j$ with $L_0 := 0 \in \mathbf{R}^3$ we obtain:

$$\widehat{G}_{1,0}^{\circ J}(Q; p, q) = \frac{\alpha^J}{(4\pi^2)^J} \int_{\ell_1} \cdots \int_{\ell_J} \frac{d\ell}{\prod_{1 \leq j \leq J} |\ell_j|^2} \frac{A_J^{(\ell_j)_{j=1}^J} \widehat{Q}(p, q)}{\prod_{0 \leq j \leq J-1} (\widetilde{E}(p - L_j) + \widetilde{E}(q - L_j))}. \quad (100)$$

In particular the Fourier transform of the density of $G_{1,0}^{\circ J}(Q)$ is

$$\begin{aligned} \widehat{\rho}(G_{1,0}^{\circ J}(Q); k) &= \frac{1}{(2\pi)^{3/2}} \int_u \text{Tr}_{\mathbf{C}^4} \widehat{G}_{1,0}^{\circ J}(Q; u + \frac{k}{2}, u - \frac{k}{2}) du \\ &= \frac{\alpha^J}{(2\pi)^{3/2} (4\pi^2)^J} \iint_{u, \ell_1} \cdots \int_{\ell_J} \text{Tr}_{\mathbf{C}^4} \frac{dud\ell}{\prod_{1 \leq j \leq J} |\ell_j|^2} \frac{A_J^{(\ell_j)_{j=1}^J} \widehat{Q}(u + \frac{k}{2}, u - \frac{k}{2})}{\prod_{0 \leq j \leq J-1} (\widetilde{E}(u + \frac{k}{2} - L_j) + \widetilde{E}(u - \frac{k}{2} - L_j))} \\ &= \frac{\alpha^J}{(2\pi)^{3/2} (4\pi^2)^J} \iint_{u, \ell_1} \cdots \int_{\ell_J} \frac{dud\ell}{\prod_{1 \leq j \leq J} |\ell_j|^2} \frac{\text{Tr}_{\mathbf{C}^4} \left\{ (1 - \mathbf{s}_{u-\frac{k}{2}} \mathbf{s}_{u+\frac{k}{2}}) A_J^{(\ell_j)_{j=2}^{J-1}} \widehat{Q}(u + \frac{k}{2}, u - \frac{k}{2}) \right\}}{\prod_{0 \leq j \leq J-1} (\widetilde{E}(u + \frac{k}{2} - L_j) + \widetilde{E}(u - \frac{k}{2} - L_j))}. \end{aligned} \quad (101)$$

Above the domain of ℓ_j is:

$$\widetilde{B}_j(r) := \{\ell_j, |u - L_j \pm \frac{r}{2} \mathbf{e}| < \Lambda\}.$$

The domain of u is $\widetilde{B}_0(r) := \{u, |u \pm \frac{r}{2} \mathbf{e}| < \Lambda\}$. In particular

$$\text{supp } \widehat{\rho}(G_{1,0}^{\circ J}(Q)) \subset B(0, 2\Lambda).$$

Remark 23. We would like to apply (101) to the operator $Q_{0,1}(\rho)$ and by looking at (98) one may realize that $\widehat{Q}_{0,1}(p, q)$ is not a scalar matrix because of the term $\mathbf{s}_p \mathbf{s}_q - \text{Id}$. It is in the algebra spanned by the Dirac matrices $\alpha_1, \alpha_2, \alpha_3, \beta$ 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 1.

For any $J \geq 1$ and $\rho \in \mathcal{C}$ we get that $\widehat{\rho}(G_{1,0}^{\circ J}(Q_{0,1}[\rho]); k)$ is equal to:

$$\begin{aligned} &\frac{4\pi\alpha^J \widehat{\rho}(k)}{(2^5\pi^3)^{\frac{1}{2}} (2\pi)^{3/2} (4\pi^2)^J} \int_{\prod_{0 \leq j \leq J} \widetilde{B}_j(r)} \frac{dud\ell}{|k|^2 \prod_{1 \leq j \leq J} |\ell_j|^2} \frac{\text{Tr}_{\mathbf{C}^4} \left\{ (1 - \mathbf{s}_{u-\frac{k}{2}} \mathbf{s}_{u+\frac{k}{2}}) A_{J-1}^{(\ell_j)_{j=2}^{J-1}} (\mathbf{s}_{u-\frac{k}{2}} \mathbf{s}_{u+\frac{k}{2}} - 1) \right\}}{\prod_{0 \leq j \leq J} (\widetilde{E}(u + \frac{k}{2} - L_j) + \widetilde{E}(u - \frac{k}{2} - L_j))} \\ &= \widehat{\rho}(k) \int_{\prod_{0 \leq j \leq J} \widetilde{B}_j(r)} dud\ell S_J(u - L_j \pm \frac{k}{2}) T_J(u - L_j \pm \frac{k}{2}) \end{aligned} \quad (102)$$

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 $\text{Tr}_{\mathbf{C}^4}$ 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 this integral is well defined. The first problem is easily resolved:

$$\frac{1}{|k|^2} (\mathbf{s}_{u-L_j+k/2} \mathbf{s}_{u-L_j-k/2} - 1) (1 - \mathbf{s}_{u-k/2} \mathbf{s}_{u+k/2}) = \frac{(\mathbf{s}_{u-L_j+k/2} \mathbf{s}_{u-L_j-k/2} - 1) (1 - \mathbf{s}_{u-k/2} \mathbf{s}_{u+k/2})}{|k| |k|}$$

which is a smooth function by Taylor's formula (for $|k|$ or for k in $\mathbf{R}^3 \setminus \{0\}$). Moreover there holds the following estimate thanks to (95):

$$\begin{aligned} \left| \frac{\mathbf{S}_{u-L_J+k/2} \mathbf{S}_{u-L_J-k/2} - 1}{|k|} \frac{1 - \mathbf{S}_{u-k/2} \mathbf{S}_{u+k/2}}{|k|} \right| &\leq \frac{4C_s^2}{E(u-L_J, k/2)} \\ &\leq \frac{4C_s^2}{|u-L_J|E(u, k/2)}. \end{aligned}$$

Then we remark that for any U :

$$\begin{aligned} \int_{\ell} \frac{d\ell}{|\ell|^2} \frac{1}{|U-\ell| \tilde{E}(U-\ell, k/2)} &\leq \int_{\ell} \frac{d\ell}{|\ell|^2} \frac{1}{|U-\ell|^2}, \\ &\leq \frac{1}{|U|} \int \frac{d\ell}{|\ell|^2 |\mathbf{e}-\ell|^2}. \end{aligned}$$

Taking one after the other the U_j 's defined by $U_j = u - L_j$ for $1 \leq j \leq J-1$ and integrating over ℓ_{j+1} there remains but the integral over u :

$$\begin{aligned} \int_{u \in \tilde{B}_0(k)} \frac{2C_s^2 du}{\tilde{E}(u, k/2)} \frac{1}{|u|E(u, k/2)} &\times \left\{ 2 \int \frac{d\ell}{|\ell|^2 |\mathbf{e}-\ell|^2} \right\}^J \\ &\leq \left\{ 2 \int \frac{d\ell}{|\ell|^2 |\mathbf{e}-\ell|^2} \right\}^J \int_{u \in \tilde{B}_0(r)} \frac{2C_s^2 du}{|u|^2 \tilde{E}(u, k/2)} \\ &= (K \log(\Lambda)) \times (C'_{1,0})^J. \end{aligned}$$

At last we obtain:

$$\begin{aligned} \alpha |\widehat{\rho}(G_{1,0}^{\circ J}(Q_{0,1}(\rho)); k)| &\leq \frac{\alpha^{J+1}}{(2\pi)^{3/2} (4\pi^2)^J} 2^{J+1} C_s^2 \left\{ \int \frac{d\ell}{|\ell|^2 |\mathbf{e}-\ell|^2} \right\}^J \int_{u \in \tilde{B}_0(r)} \frac{du}{|u|^2 E(u)} |\widehat{\rho}(k)| \\ &\leq C_{1,0} (\alpha C'_{1,0})^J \alpha \log(\Lambda) |\widehat{\rho}(k)|. \end{aligned} \tag{103}$$

As a consequence there holds:

$$\alpha \widehat{\rho}(G_{1,0}^{\circ J}(Q_{0,1}(\rho)); k) = -g_{\Lambda; J}(k) \widehat{\rho}(k) \tag{104}$$

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:

$$\alpha \widehat{\tau_{0,1}}(\rho, k) = - \left(\alpha B_\Lambda(k) + \sum_{J=1}^{+\infty} g_{\Lambda; J}(k) \right) \widehat{\rho}(k) =: -f_\Lambda(k) \widehat{\rho}(k), \tag{105}$$

with

$$|f_\Lambda(k)| \leq \alpha B_\Lambda(k) + \alpha^2 \log(\Lambda) K = \mathcal{O}(\alpha \log(\Lambda)). \tag{106}$$

2. Let us prove this function is radial. Let \mathbf{e}_1 and \mathbf{e}_2 in \mathbf{S}^2 and $r > 0$. We must show that $f_\Lambda(r\mathbf{e}_1) = f_\Lambda(r\mathbf{e}_2)$. There exists $\mathcal{R} \in \text{SO}_3(\mathbf{R})$ such that $\mathbf{e}_2 = \mathcal{R}\mathbf{e}_1$. In (102) 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 $M_j = m_1 + \dots + m_j$, 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 \mathbf{R}^3 . We define

$$\alpha'_j := \alpha \cdot \mathcal{R}b_j.$$

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 can change variables:

$$\begin{cases} u_0 := u \text{ and for } 1 \leq j \leq J, u_j := u - L_j, l_j = u_j - u_{j-1}, \\ u_j \in B(|k|) := \{v \in B(0, \Lambda), |v \pm \frac{|k|}{2}\mathbf{e}| < \Lambda\}. \end{cases} \tag{107}$$

3. Now our purpose is to show that f_Λ is in $\mathcal{F}(L^1)$ with a (rather) precise bound on $\|\check{f}_\Lambda\|_{L^1}$. It is already known:

$$f_\Lambda(k) = \alpha B_\Lambda(k) + \mathcal{O}_{L^\infty}(\alpha^2 \log(\Lambda)) = \mathcal{O}(\alpha \log(\Lambda)).$$

As f_Λ is radial we take a fixed vector $\mathbf{e} \in \mathbf{S}^2$ 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 get then an upper bound of $\|\check{f}_\Lambda\|_{L^1}$. We will use the *co-area formula* [4].

Following the method of [7], we then 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 24. 1. As f_Λ is radial we have:

$$(-\Delta)f_\Lambda = (-\Delta_r)f_\Lambda = -(\partial_r^2 + \frac{2}{r}\partial_r)f_\Lambda. \quad (108)$$

2. For any $u \in \mathbf{R}^3$ and $r \geq 0$ Taylor's formula gives:

$$\left\{ \begin{array}{l} (1 - \mathbf{s}_{u+2^{-1}r\mathbf{e}}\mathbf{s}_{u-2^{-1}r\mathbf{e}}) = r\{\mathbf{s}_u m_1(-\frac{r}{2}) - m_1(\frac{r}{2})\mathbf{s}_u\} \\ \text{with } m_1(\frac{x}{2}) := \int_{t=0}^1 d\mathbf{s}_{u+tx\mathbf{e}/2} \cdot \left(\frac{\mathbf{e}}{2}\right) dt. \end{array} \right. \quad (109)$$

We write $\mathbf{w}(p) := \begin{pmatrix} w_0(p) \\ \mathbf{w}_1(p) \end{pmatrix} \in \mathbf{R}^4$ and $\sigma(p) := \frac{\mathbf{w}(p)}{E(p)}$.

As we have $\langle \sigma(u), d\sigma(u) \rangle = 0$, Taylor's Formula at order 2 gives

$$\left\{ \begin{array}{l} \frac{1 - \langle \sigma(u + r\frac{\mathbf{e}}{2}), \sigma(u - r\frac{\mathbf{e}}{2}) \rangle}{r^2} := \langle a(u), a(u) \rangle + \langle \sigma(u), m_2(r) + m_2(-r) \rangle \\ \quad + r\langle a(u), m_2(r) - m_2(-r) \rangle + r^2\langle m_2(r), m_2(-r) \rangle, \\ a(u) := d\sigma(u) \cdot \frac{\mathbf{e}}{2} \text{ and } m_2(\frac{x}{2}) := \iint_{[0,1]^2} d^2\sigma u + stx\mathbf{e}/2 \cdot \left(\frac{\mathbf{e}}{2}, \frac{\mathbf{e}}{2}\right) tdsdt. \end{array} \right. \quad (110)$$

3. For any $-\frac{1}{2} \leq x \leq \frac{1}{2}$:

$$\tilde{E}(u + x\mathbf{e}) \geq E(u + x\mathbf{e}) \geq \frac{E(u)}{2}. \quad (111)$$

In particular if one takes the modulus of the derivative over r in (109) or (110) for $0 \leq r \leq 1$, we get the following upper bounds:

- (a) $K/\tilde{E}(u)$ for the first derivative,
- (b) $K/\tilde{E}(u)^2$ for the second.

Lemma 13. The functions $\partial_r f_\Lambda$ and $\partial_r^2 f_\Lambda$ are well defined in \mathbf{R}^3 with support in $\overline{B}(0, 2\Lambda)$. Moreover we have for $J \in \mathbf{N}$:

$$\left\{ \begin{array}{l} |\partial_r f_{\Lambda, J}(p)| \lesssim J \frac{\alpha^{J+1} \log(\Lambda) K^{J+1} \log(\Lambda)}{E(p)} \chi_{|p| < 2\Lambda} \quad \left| \quad \right. \quad |\partial_r f_\Lambda(p)| \lesssim \frac{L}{E(p)} \chi_{|p| < 2\Lambda}, \\ |\partial_r^2 f_{\Lambda, J}(p)| \lesssim J \frac{\alpha^{J+1} \log(\Lambda) K^{J+1} \log(\Lambda)}{E(p)} \chi_{|p| < 2\Lambda} \quad \left| \quad \right. \quad |\partial_r^2 g_\Lambda| \lesssim \frac{\alpha^2 \log(\Lambda)}{E(r)^2} \chi_{r < 2\Lambda}. \end{array} \right. \quad (112)$$

As a consequence:

Lemma 14. For α sufficiently small, $\check{g}_\Lambda \in L^1$ and

$$\|\check{g}_\Lambda\|_{L^1} \lesssim (\alpha \log(\Lambda))^2. \quad (113)$$

Remark 25. At the very end of the proof of Lemma 13, we refer the reader to the thesis of the author for a (last) technical assumption: proving that $\lim_{|x| \rightarrow 2\Lambda^-} \partial_r^2 f_\Lambda(x) = 0$.

Proof of Lemma 14

We assume Lemma 13: as $(-\Delta_r) = -(\partial_r^2 + \frac{2}{r}\partial_r)$ we get that $f_\Lambda \in H^2(\mathbf{R}^3)$ with:

$$\|-\Delta f_\Lambda\|_{L^2} \lesssim L \quad (114)$$

since $\int \frac{dk}{|k|^2 E(k)^2} < +\infty$. Although $\partial_r^j g_\Lambda : \mathbf{R}_+^* \rightarrow \mathbf{R}$ has no singularity at 0, the function $-\Delta f_\Lambda$ has a singularity in $\frac{1}{r}$ because of the term $\frac{2}{r}\partial_r f_\Lambda$. The L^2 -norm remains finite since the domain is \mathbf{R}^3 . More generally, we have

$$-\Delta f_\Lambda \in L^{3/2}(\mathbf{R}^3) \cap L^2(\mathbf{R}^3).$$

Let $\frac{3}{2} < p < 2$ to be chosen and $q = \frac{2p}{3p-2}$. We use the generalized Young inequality: $\frac{1}{|\cdot|^{-3/4}} \in L_w^q(\mathbf{R}^3)$ and $\frac{1}{|\cdot|^{-3/4}} * (-\Delta f_\Lambda) \in L^2(\mathbf{R}^3)$. By Plancherel's Theorem this gives in Direct space the following result:

$$\frac{|\cdot|^{-2} \check{f}_\Lambda}{|\cdot|^{3-\frac{3}{q}}} \in L^2(\mathbf{R}^3), \text{ that is } |\cdot|^{-\frac{7p-6}{2p}} \check{f}_\Lambda \in L^2(\mathbf{R}^3).$$

We choose $\frac{3}{p} - \frac{3}{2} = 4^{-1}$, that is $p = \frac{12}{7}$, thus:

$$\int_{B(0,1)} |\check{f}_\Lambda(x)| dx \leq \sqrt{\int_{B(0,1)} |x|^{\frac{7}{4}} |\check{f}_\Lambda(x)|^2 dx} \int_{B(0,1)} \frac{dx}{|x|^{7/4}} \lesssim \|-\Delta f_\Lambda\|_{L^{\frac{12}{7}}} \left\| \frac{1}{|\cdot|^{11/4}} \right\|_{L_w^{11/12}} \lesssim L.$$

Then it is clear that

$$\int_{|x| \geq 1} |\check{f}_\Lambda(x)| \leq \|-\Delta f_\Lambda\|_{L^2} \sqrt{\int_{|x| \geq 1} \frac{dx}{|x|^4}} \lesssim L.$$

□

Proof of Lemma 13

• The idea of the proof is that each time one differentiates 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 sum.

We will often use the following inequality:

$$\int_{B(0,\Lambda)} \frac{dv}{|u-v|^2 (\tilde{E}(v + \frac{k}{2}) + \tilde{E}(v - \frac{k}{2})) |u + \varepsilon \frac{k}{2}|} \leq \frac{1}{|u + \varepsilon \frac{k}{2}|} \int \frac{dv}{|v|^2 |v - \mathbf{e}|^2}, \quad (115)$$

and for convenience we write:

$$u^\varepsilon := u + \varepsilon \frac{k}{2}, \quad \varepsilon \in \{1, -1\}. \quad (116)$$

That the function (and its derivatives) has an extension in 0 would be clear from (109) and (111): differentiating under the integral sign in the Taylor's formula, one gets:

$$\left| d^{J+1} \mathbf{s}_{u+t\mathbf{e}/2} \cdot ((t\mathbf{e}/2)^J, \frac{\mathbf{e}}{2}) \right| \leq K^J \frac{1}{E(u)^{J+1}}, \quad 0 < r, t < 1, \quad (117)$$

thus the problem of singularity at $r = 0$ drops thanks to (111).

More generally the variable r appears in two ways:

1. in the domains $B(r)^{J+1}$,
2. in a function of $v_j \pm r \frac{\mathbf{e}}{2}$.

One may write:

$$f_{\Lambda,J}(r) = \int_{B(r)^{J+1}} G_J(u_0 \pm r \frac{\mathbf{e}}{2}, \dots, u_J \pm r \frac{\mathbf{e}}{2}) d\mathbf{u}, \quad (118)$$

$$G_J = G_J^0(u_0 \pm r \frac{\mathbf{e}}{2}, \dots, u_J \pm r \frac{\mathbf{e}}{2}) \prod_{1 \leq j \leq J} \frac{1}{|u_j - u_{j-1}|^2}.$$

It is easy to see that $G_J^0 : (\mathbf{R}^3)^{2J+2} \rightarrow \mathbf{R}$ 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 gain a term $K(r^{-1} + \tilde{E}(u \pm \frac{k}{2})^{-1})$ for $r > 1$ or $K\tilde{E}(u)^{-1}$ for $r \leq 1$ (see Remark 24). 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 $1 < |k| < 2\Lambda$:

$$\left\{ \begin{array}{l} \int \frac{du_j}{|u_j - u_{j-1}|^2 \tilde{E}(u_j + \varepsilon k/2)^2} \leq \frac{1}{|u_{j-1} + \varepsilon k/2|} \int_{\mathbf{R}^3} \frac{du_j}{|u_j|^2 |u_j - \mathbf{e}|^2}, \\ \int \frac{du_i}{|u_i - u_{i-1}|^2 |u_i + \varepsilon k/2| \tilde{E}(u_i, k/2) \tilde{E}(u_i + \varepsilon' k/2)} \lesssim \frac{1}{|k|} \left(\frac{1}{|u_{i-1} + k/2|} + \frac{1}{|u_i - k/2|} \right) \int_{(\mathbf{R})^3} \frac{du_i}{|u_i - \mathbf{e}|^2 |u_i|^2}. \end{array} \right. \quad (119)$$

If one deals with the term with $(\partial_{u_0+k/2} - \partial_{u_0-k/2})G_0$ one has:

$$\int_{B(r)} \frac{du_0}{|u_0 - \varepsilon k/2| \tilde{E}(u_0 + \varepsilon k/2)} \left(\frac{1}{\tilde{E}(u_0 + \varepsilon k/2)^2} + \frac{1}{\tilde{E}(u_0 - \varepsilon k/2)^2} \right) \lesssim \frac{2}{|k|} \int_{B(0,2\Lambda)} \frac{du_0}{\tilde{E}(u_0)^2 |u_0|} \lesssim \frac{\log(\Lambda)}{|k|}. \quad (120)$$

If $r \leq 1$, Remark 24 enables us to say that

$$\int_{B(r)^{J+1}} \frac{|\partial_r G_J^0(u_j \pm r \mathbf{e}/2)|}{\prod_{1 \leq j \leq J} |u_j - u_{j-1}|^2} \lesssim \alpha^{J+1} J \left(K \int \frac{du}{|u|^2 |u - \mathbf{e}|^2} \right)^J \log(\Lambda).$$

For the second derivative: 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 $i(1) \neq i(2)$ then it suffices to apply twice (119),(120) and we get an upper bound of the form:

$$K J^2 (\chi_{|k| \leq 1} + \frac{\chi_{1 < |k| < 2\Lambda}}{|k|^2}) \alpha^{J+1} \left(K \int \frac{du}{|u|^2 |u - \mathbf{e}|^2} \right)^J \log(\Lambda),$$

If $i(1) = i(2)$, then as:

$$\int \frac{du}{|u - v|^2 |u| \tilde{E}(u, \frac{k}{2})} \left(\frac{1}{\tilde{E}(u + k/2)^2} + \frac{1}{\tilde{E}(u - k/2)^2} \right) \lesssim \frac{1}{|k|^2 |u|}, \quad (121)$$

we obtain an upper bound of the form

$$K J (\chi_{|k| \leq 1} + \frac{\chi_{1 < |k| < 2\Lambda}}{|k|^2}) \alpha^{J+1} \left(K \int \frac{du}{|u|^2 |u - \mathbf{e}|^2} \right)^J \log(\Lambda).$$

If $i(1) = i(2) = 0$, we integrate first over u_0 , then over u_1, u_2, \dots, u_J and use (121) with $u = u_0, v = u_1$: this gives

$$\text{for } 1 < r < 2\Lambda, \left| \partial_r^2 \frac{1 - \mathbf{s}_{u_0 + \frac{k}{2}} \mathbf{s}_{u_0 - \frac{k}{2}}}{r(\tilde{E}(u_0 + \frac{k}{2}) + \tilde{E}(u_0 - \frac{k}{2}))} \right| \lesssim \frac{r^{-2} + \tilde{E}(u_0 + \frac{k}{2})^{-2} + \tilde{E}(u_0 - \frac{k}{2})^{-2}}{|u| \tilde{E}(u, \frac{k}{2})}.$$

If $r \leq 1$ we use Remark 24 as before.

• There remains to deal with the terms corresponding to differentiation over r in the domain $B(r)^{J+1}$.

We rewrite (118) using the *co-area formula*. Indeed, let us write for $\varepsilon \in \{1, -1\}$ and $r \in [0, 2\Lambda]$:

$$B_\varepsilon(r) := \{p, |p + \frac{\varepsilon r}{2} \mathbf{e}| < \Lambda, \langle p, \varepsilon \mathbf{e} \rangle > 0\} \text{ and } B(r) := B_1(r) \cup B_{-1}(r) \subset B(0, \Lambda).$$

In particular $B(\Lambda) = \{p \in B(0, \Lambda), \langle p, \mathbf{e} \rangle \neq 0\}$. We define the function:

$$\begin{aligned} B(\Lambda) &\rightarrow [0, 2\Lambda] \\ z: p \in B_\varepsilon(\Lambda) &\mapsto r \text{ such that } \left|u + \frac{r\varepsilon\mathbf{e}}{2}\right| = \Lambda. \end{aligned}$$

We apply the co-area formula with the level function z . If $p \in B_{\varepsilon_0}$, we write $\varepsilon(p) := \varepsilon_0$ and

$$n(p) := \frac{p + \varepsilon(p)z(p)\frac{\mathbf{e}}{2}}{\left|p + \varepsilon(p)z(p)\frac{\mathbf{e}}{2}\right|} = \Lambda^{-1}(p + \varepsilon(p)z(p)\frac{\mathbf{e}}{2}).$$

For $0 \leq r < 2\Lambda$ 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 $B(0, \Lambda) \setminus B(\Lambda)$ is zero and the function z is differentiable with

$$\nabla z(p) = \frac{-2\varepsilon(p)}{\langle np, \mathbf{e} \rangle} n(p).$$

Thus for any integrable function $F : B(0, \Lambda) \rightarrow \mathbf{R}$ and $0 \leq r < 2\Lambda$ one has:

$$\int_{B(r)} F(p) dp = \int_{t=r}^{2\Lambda} dt \int_{S(t)} F(p) d\mathcal{H}_2(p), \quad (122)$$

where $d\mathcal{H}_2(p)$ is the Hausdorff measure on $S(r)$. If we take spherical coordinates with axis $\mathbf{R}\mathbf{e}$ in $S_\varepsilon(r)$ there holds $d\mathcal{H}_2(p) = \Lambda^2 \sin(\theta) d\theta d\phi$ in the domain:

$$M_\varepsilon(r) = \{(\theta, \phi) \in (0, \pi) \times (-\pi, \pi), \cos(\theta) \geq \frac{r}{2\Lambda}\}.$$

Notation 26. 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 may rewrite the integration over $u_i \in B(r)$. This enables us to get the full derivative $\partial_r f_{\Lambda, J}$. For each $0 \leq j \leq J$ we need to estimate

$$\int_{B(r)^{j-1} \times S(r) \times B(r)^{J-j}} \frac{du_0 \cdots \widehat{du_j} \cdots du_J d\mathcal{H}_2(u_j)}{\prod_{1 \leq j \leq J} |u_j - u_{j-1}|^2} |G_J^0(u_i \pm \frac{k}{2})|.$$

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, \dots, u_J . Using one gets (119) we have:

$$\begin{aligned} \int_{M_\varepsilon(r)} \frac{\Lambda^2 \sin(\theta) d\theta d\phi}{|v - \Lambda n|^2} \frac{1}{|\Lambda n|(\widetilde{E}(\Lambda n) + \widetilde{E}(\Lambda n - k))} &\leq \int_{\mathbb{S}^2} \frac{\sin(\theta) d\theta d\phi}{|v - \Lambda n|^2} \\ &\leq \frac{2\pi}{\Lambda|v|} \log\left(\frac{\Lambda+|v|}{\Lambda-|v|}\right). \end{aligned}$$

Then writing $v := u_{i-1} + \varepsilon \frac{k}{2}$ we have:

$$\begin{aligned} \int_{B(r)} \frac{du_i}{|u_i - u_{i-1}|^2 |u_i + \varepsilon \frac{k}{2}|} \log\left(\frac{\Lambda+|u_i + \varepsilon \frac{k}{2}|}{\Lambda-|u_i + \varepsilon \frac{k}{2}|}\right) \frac{1}{\widetilde{E}(u_i, k/2)} &= \int_{B(r) + \frac{\varepsilon k}{2}} \frac{du_i}{|u_i - v|^2 |u_i| \widetilde{E}(u_i)} \log\left(\frac{\Lambda+|u_i|}{\Lambda-|u_i|}\right) \\ &\leq \int_{B(0,1)} \frac{du}{|u - v\Lambda^{-1}|^2 |u| \widetilde{E}(\Lambda u)} \log\left(\frac{1+|u|}{1-|u|}\right) \leq 2\pi \int_{r=0}^1 \frac{\Lambda dr}{|v| \widetilde{E}(\Lambda r)} \log\left(\frac{1+r}{1-r}\right) \log\left|\frac{\Lambda^{-1}|v|+r}{\Lambda^{-1}|v|-r}\right| \\ &\leq 2\pi \int_0^1 \frac{\Lambda dr}{|v| \widetilde{E}(\Lambda r)} \left(\log^2\left(\frac{1+r}{1-r}\right) + \log^2\left|\frac{\Lambda^{-1}|v|+r}{\Lambda^{-1}|v|-r}\right|\right) \lesssim |v|^{-1}. \end{aligned}$$

Finally for sufficiently small α , we have

$$|\partial_r f_{\Lambda, J}(r)| \leq KL(\alpha K)^J (\chi_{r \leq 1} + \frac{\chi_{1 < r < 2\Lambda}}{r}).$$

By dominated convergence we get that as r tends to $(2\Lambda)^-$ then $\partial_r f_{\Lambda, J}$ tends to 0, thus $g_\Lambda \in H^1(\mathbf{R}^3)$.

• Let us deal now with the second derivative. There remains to deal with:

1. One derivative in $\tilde{B}(r)$ and one derivative in the integrand.
2. Two derivatives in two different $B(r)$.
3. Two derivatives in the same $B(r)$.

In fact, one has to deal with the last two cases together because each term alone is not well defined and only the sum gives a finite term. If we see the derivative as the coefficient of the second term in the Taylor series of $g_{\Lambda, J}(r + \delta r)$, then each term gives $\mathcal{O}(-\delta r \log(\delta r))$ but the sum is $\mathcal{O}(\delta r)$ due to some cancellation.

1.1. One derivative in $u_j \pm \frac{r}{2}\mathbf{e}$ and one in the domain of u_i with $i \neq j$. Up to integration over u_j from $j = 0$ to $j = J$, we can suppose that $j < i$. We split $S(r)$ between $S_+(r)$ and $S_-(r)$. In $S_\varepsilon(r)$, having used (115) (and (95) at the beginning) we get:

$$\begin{aligned} \int_{S_\varepsilon(r)} \frac{du_i}{|u_{i-1} - u_i|^2 \tilde{E}(u_i + \varepsilon \frac{k}{2}) |u_i + \varepsilon \frac{k}{2}|} &\leq \int_{\mathbf{S}^2} \frac{du_i}{\Lambda^2 \left| \frac{|u_{i-1}^\varepsilon|}{\Lambda} - u_i \right|^2} \\ &\lesssim \frac{1}{\Lambda |u_{i-1}^\varepsilon|} \log \left(\frac{1 + \frac{|u_{i-1}^\varepsilon|}{\Lambda}}{\Lambda - |u_{i-1}^\varepsilon|} \right). \end{aligned}$$

Taking spherical coordinates with respect with $-\varepsilon \frac{k}{2}$, we have for any $v \in B = B_+ \cup B_-$:

$$\begin{aligned} \int_{B(0, \Lambda)} \frac{du}{|u_{i-1} - v^\varepsilon|^2 |u_{i-1}| \tilde{E}(u_{i-1})} \log \left(\frac{1 + \frac{|u_{i-1}|}{\Lambda}}{1 - \frac{|u_{i-1}|}{\Lambda}} \right) &\lesssim \frac{1}{|v|} \int_0^1 dz \log \left(\frac{1+z}{1-z} \right) \log \left(\frac{\frac{|v^\varepsilon|}{\Lambda} + z}{\frac{|v^\varepsilon|}{\Lambda} - z} \right) \\ &\lesssim \frac{1}{|v^\varepsilon|} \int_0^2 \log \left(\frac{1+z}{1-z} \right)^2, \\ \int_{B(0, \Lambda)} \frac{du}{|u_{i-1}| \tilde{E}(u_{i-1}^2)} \log \left(\frac{1 + \frac{|u_{i-1}|}{\Lambda}}{1 - \frac{|u_{i-1}|}{\Lambda}} \right) &\lesssim \int_0^\Lambda \frac{dz}{E(z)} \log \left(\frac{1 + \frac{z}{\Lambda}}{1 - \frac{z}{\Lambda}} \right) \\ &\lesssim 1 + \Lambda^{-1}. \end{aligned}$$

We use the same method as for the first derivative: when integrating over u_j , we use $(\tilde{E}(u_j + \frac{k}{2}) + \tilde{E}(u_j - \frac{k}{2}))^{-1} \leq \tilde{E}(\frac{k}{2})^{-1}$. 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 $u_j \pm \frac{r}{2}\mathbf{e}$ and one in the domain of u_j . Splitting the integration over $S_+(r)$ and $S_-(r)$, and using (115), we have to estimate

$$\int_{S_\varepsilon(r)} \frac{du_i}{|u_i - v|^2 |u_i + \varepsilon \frac{k}{2}| \tilde{E}(u_i, k/2) \tilde{E}(u_i + \varepsilon' \frac{k}{2})} \leq \int_{S_\varepsilon(r)} \frac{du_i}{|u_i - v|^2 |u_i + \varepsilon \frac{k}{2}| \tilde{E}(u_i, k/2) \tilde{E}(u_i - \varepsilon \frac{k}{2})}. \quad (123)$$

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. Using (115) several times (starting with (95)) we get the term $|u_i + \varepsilon \frac{k}{2}| = |u_i^\varepsilon|$ in (123).

In (123), we use spherical coordinates and get the following upper bound:

$$\int_{\mathbf{S}^2} \frac{\Lambda^2 du}{\Lambda^2} \frac{1}{|\Lambda u - v^\varepsilon|^2 \tilde{E}(\Lambda u - r\mathbf{e})} \leq 2 \int_{\mathbf{S}^2} \frac{du}{|\Lambda u - |v^\varepsilon| \mathbf{e}|^2 E(u - r\mathbf{e})}. \quad (124)$$

We write

$$x := |v^\varepsilon|, \quad A := \Lambda^2 + x^2, \quad B := \sqrt{1 + \Lambda^2 + r^2}, \quad a := \frac{2x\Lambda}{x^2 + \Lambda^2} \quad \text{and} \quad b := \frac{2\Lambda r}{1 + \Lambda^2 + r^2}.$$

The upper bound is equal to

$$\frac{4\pi}{AB} \int_{-1}^1 \frac{dy}{(1-ay)\sqrt{1-by}} = \frac{4\pi}{ABa} \int_0^{\frac{2b}{\sqrt{1+b}+\sqrt{1-b}}} \frac{dz}{z^2 + 2z\sqrt{1-b} + b(\frac{1}{a}-1)}.$$

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 have:

$$\mathcal{O}\left(\frac{1}{AB} \int_{-1}^1 \frac{dy}{1-ay}\right) = \mathcal{O}\left(\frac{1}{\Lambda^2 E(v^\varepsilon)}\right).$$

If $\frac{1}{2} < a, b \leq 1$, we look at the second formula. 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

$$\frac{4\pi}{AaB} \left(\int_0^{2\sqrt{1-b}} \frac{dz}{2z\sqrt{1-b} + b(\frac{1}{a}-1)} + \int_{2\sqrt{1-b}}^{\frac{2b}{\sqrt{1+b}+\sqrt{1-b}}} \frac{dz}{z^2 + b(\frac{1}{a}-1)} \right)$$

The first integral 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 gives (without $4\pi/(AaB)$), with $X := (a^{-1}-1)^{-1}$:

$$\begin{aligned} \sqrt{\frac{X}{b}} \int_{2\sqrt{\frac{1-b}{b}X}}^{\frac{2\sqrt{bX}}{\sqrt{1-b}+\sqrt{1+b}}} \frac{dz}{z^2+1} &\lesssim \int_{2\sqrt{1-b}}^2 \frac{Xz^2}{1+Xz^2} \frac{dz}{z^2} \\ &\lesssim \frac{1}{\sqrt{1-b}} = \frac{\sqrt{1+\Lambda^2+r^2}}{\sqrt{1+(\Lambda-r)^2}}. \end{aligned}$$

We have:

$$\frac{\log(1-a)}{AB\sqrt{1-b}} = 2 \frac{\log\left|\frac{\sqrt{\Lambda^2+x^2}}{\Lambda-x}\right|}{(\Lambda^2+x^2)\sqrt{1+(\Lambda-x)^2}} \lesssim \frac{1 + \log(1 - \frac{|v^\varepsilon|}{\Lambda})}{(\Lambda^2 + |v^\varepsilon|^2)\sqrt{1+(\Lambda-|v^\varepsilon|)^2}}.$$

Let us emphasize that the condition $a > 2^{-1}$ is equivalent to

$$\frac{|v^\varepsilon|}{\Lambda} \geq 2 - \sqrt{3}.$$

Bringing all these results together, we get the following upper bound:

$$\frac{K}{\Lambda^2 |v^\varepsilon|} \left(1 - \chi_{|v^\varepsilon| > (2-\sqrt{3})\Lambda} \log\left(1 - \frac{|v^\varepsilon|}{\Lambda}\right)\right).$$

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:

$$\left\{ \begin{array}{l} \int_{B(0,\Lambda)} \frac{dv}{|v'-v|^2 \tilde{E}(v)|v|} \lesssim \frac{1}{|v'|} \int \frac{dv}{|v|^2 |v-\mathbf{e}|^2} \\ \int_{B(0,\Lambda)} \frac{dv}{|v| \tilde{E}(v)^2} \lesssim \log(\Lambda). \end{array} \right.$$

Moreover, writing $A_\Lambda := A(0, (2 - \sqrt{3})\Lambda, \Lambda)$ the annulus, we have:

$$\left\{ \begin{array}{l} \int_{A_\Lambda} \frac{\log(1 - \frac{|v|}{\Lambda}) dv}{|v'-v|^2 |v| \tilde{E}(v) (\Lambda^2 + |v|^2)} \lesssim \frac{1}{\Lambda^2 |v'|} \int_{2-\sqrt{3}}^1 \frac{-\log(1-z) dz}{z(1+z^2)} \log \left| \frac{\frac{|v'|}{\Lambda} + z}{\frac{|v'|}{\Lambda} - z} \right| \\ \int_{A_\Lambda} \frac{\log(1 - \frac{|v|}{\Lambda}) dv}{|v| \tilde{E}(v)^2 (\Lambda^2 + |v|^2)} \lesssim \frac{1}{\Lambda^2 |v'|}, \\ \int_{A_\Lambda} \frac{\log(1 - \frac{|v|}{\Lambda}) dv}{|v| \tilde{E}(v)^2 (\Lambda^2 + |v|^2)} \lesssim \frac{1}{\Lambda^2} \int_{2-\sqrt{3}}^1 \frac{-\log(1-z) dz}{z^3}. \end{array} \right.$$

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. Integration over u with u either u_j or u_i (and v either u_{j+1} or u_{i-1}) is:

$$\begin{aligned} \sum_{\varepsilon \in \{1, -1\}} \int_{S_\varepsilon(r)} \frac{du}{|u-v|^2} \frac{1}{|u + \varepsilon \frac{k}{2}| \tilde{E}\left(u + \varepsilon \frac{k}{2}\right)} &\lesssim \frac{1}{\Lambda^2} \sum_\varepsilon \int_{\frac{r}{2\Lambda}}^1 \frac{dy}{\Lambda^2 + |v^\varepsilon|^2 - 2\Lambda|v^\varepsilon|y} \\ &\lesssim \sum_\varepsilon \frac{1}{\Lambda|v^\varepsilon|} \log\left(\frac{\Lambda + |v^\varepsilon|}{\Lambda - |v^\varepsilon|}\right). \end{aligned} \quad (125)$$

If $j + 2 \leq i$ then, integrating over u_{j+1} we have:

$$\begin{aligned} &\int_{B(r)} \frac{du_{j+1}}{|u_{j+1} - u_{j+2}|^2} \frac{1}{|u_{j+1}^\varepsilon| (\tilde{E}(u_{j+1}^+) + \tilde{E}(u_{j+1}^-))} \log\left(\frac{\Lambda + |u_{j+1}^\varepsilon|}{\Lambda - |u_{j+1}^\varepsilon|}\right) \\ &\leq \frac{1}{\Lambda} \int_{B(0,1)} \frac{du}{|u|^2 |u - \Lambda^{-1} u_{j+2}^\varepsilon|^2} \log\left(\frac{1 + |u|}{1 - |u|}\right) \\ &\leq \int_0^1 \frac{dr}{|u_{j+2}^\varepsilon|} \log\left(\frac{1+r}{1-r}\right) \log\left(\frac{r + \frac{|u_{j+2}^\varepsilon|}{\Lambda}}{r - \frac{|v^\varepsilon|}{\Lambda}}\right) \lesssim \frac{1}{|u_{j+2}^\varepsilon|}, \end{aligned}$$

and we conclude as before. Else $j + 1 = i$ and we have:

$$\begin{aligned} \int_{B(r)} \frac{du_{j+1}}{|u_{j+1}^\varepsilon|^2} \frac{1}{\tilde{E}(u_{j+1}^+) + \tilde{E}(u_{j+1}^-)} \log\left(\frac{\Lambda + |u_{j+1}^\varepsilon|}{\Lambda - |u_{j+1}^\varepsilon|}\right)^2 &\leq \frac{1}{\Lambda} \int_{z=0}^\Lambda \frac{dz}{\tilde{E}(z)} \log\left(\frac{1 + \frac{z}{\Lambda}}{1 - \frac{z}{\Lambda}}\right)^2 \left(1 - \frac{r}{2\Lambda}\right) \\ &\lesssim \left(1 - \frac{r}{2\Lambda}\right) (\log(\Lambda) + 1). \end{aligned}$$

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

$$\begin{aligned} &\iint_{(u_j, u_{j+1}) \in B(r') \times S(r)} \frac{du_j du_{j+1}}{|u_j - u_{j+1}|^2} \frac{|\langle n(u_{j+1}), \mathbf{e} \rangle|}{2} \int_{B(r)^{J-1}} \frac{G_J^0(u_\ell \pm \frac{k}{2})}{\prod_{a \neq j+1} |u_a - u_{a+1}|^2} \\ =: &\iint_{(u_j, u_{j+1}) \in B(r') \times S(r)} \frac{du_j du_{j+1}}{|u_j - u_{j+1}|^2} \frac{|\langle n(u_{j+1}), \mathbf{e} \rangle|}{2} G_{J, j}(u_j, u_{j+1}). \end{aligned}$$

We subtract 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 $\mathbf{u}' = (u_0, \dots, \widehat{u}_j, \widehat{u}_{j+1}, \dots)$ and use the co-area formula. We get

$$\int_{r+\delta r}^r dt \int_{S(t)S(r)} \frac{du_j du_{j+1}}{|u_j - u_{j+1}|^2} \frac{|\langle n(u_j), \mathbf{e} \rangle|}{2} \frac{|\langle n(u_{j+1}), \mathbf{e} \rangle|}{2} G_{J,j}(u_j, u_{j+1}). \quad (126)$$

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:

$$\text{dist}(u_{j+1}, S(t)) \geq \Lambda \left| \sqrt{1 + \frac{\langle n_{u_{j+1}}, \mathbf{e} \rangle}{\Lambda} \delta r + \left(\frac{t-r}{2}\right)^2} - 1 \right| = \underset{\delta r \rightarrow 0}{\mathcal{O}}(\Lambda |t-r| \langle n_{u_{j+1}}, \mathbf{e} \rangle).$$

By the Theorem of projection onto a closed convex \mathbf{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 (126) is

$$\underset{\delta r \rightarrow 0}{\mathcal{O}} \left(\frac{(\alpha K)^J}{\Lambda^2} \int_r^{r+\delta r} dt \int_{\mathbf{S}^2} da |\langle a, \mathbf{e} \rangle| \log \left(1 + \frac{1}{|t-r|^2 |\langle a, \mathbf{e} \rangle|^2} \right) = \frac{(\alpha K)^J}{\Lambda^2} \delta r (1 - \log(\delta r)) \right).$$

The corresponding term is not Lipschitz because of the term $-\delta r \log(\delta r)$.

3. Let us write the expansion of

$$\int_{B(r')} \frac{|\langle n_{u_j}, \mathbf{e} \rangle| du_j}{2} \int_{B(r)^J} du_0 \cdots \widehat{du}_j \cdots du_J G_J(u_\ell \pm \frac{k}{2}) =: \int_{B(r')} F_{J,j}(u_j) du_j. \quad (127)$$

We subtract $\int_{B(r)} F_{J,j}(u_j) du_j$ in (127) and get

$$\int_{r+\delta r}^r dt \int_{S(t)} du_j F_{J,j}(u_j). \quad (128)$$

We split (128) between integration over $S_+(t)$ and $S_-(t)$. For any $t \in (r, r')$, we write $s := t - r$ and:

$$\Phi_t : \begin{array}{l} S(t) \rightarrow S(r) \\ u \in S_\varepsilon(t) \mapsto v(u) := u + z_t(u) n_u \in S_\varepsilon(r) \text{ where } |z(u)| = \underset{\delta r \rightarrow 0}{\mathcal{O}}(\delta r) \end{array} \quad (129)$$

From now on we assume $v \in S(r)$ and $u \in S(t)$ and write \bar{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 $z_t : S(t) \rightarrow \mathbf{R}$ satisfies the equation

$$\left| u + z_t(u) \bar{n}_u + \varepsilon \frac{r}{2} \mathbf{e} \right|^2 = \Lambda^2 \text{ that is } z_t \left(1 + \frac{z_t}{2\Lambda} - \frac{\varepsilon s \langle \bar{n}_u, \mathbf{e} \rangle}{2\Lambda} \right) = \frac{\varepsilon s \langle \bar{n}_u, \mathbf{e} \rangle}{2} - \frac{s^2}{8\Lambda}. \quad (130)$$

Changing variables in the integration over $S(t)$ we have:

$$\int_{S(t)} du_j F_{J,j}(u_j) = \int_{\Phi_t(S(t))} dv F_{J,j}(\Phi_t^{-1}(v)) J(\Phi_t; \Phi_t^{-1}(v))^{-1} dv.$$

We need to determine $\Phi_t^{-1}(v)$ and compute $J(\Phi_t; \Phi_t^{-1}(v))$.

First we have:

$$\bar{n}_u = \frac{v - z_t \bar{n}_u + \varepsilon \frac{r+s}{2} \mathbf{e}}{\Lambda} = n_v + \varepsilon \frac{s}{2\Lambda} \mathbf{e} - \frac{z_t}{\Lambda} \bar{n}_u,$$

thus

$$\bar{n}_u = \frac{1}{1 + \frac{z_t}{\Lambda}} (n_v + \varepsilon \frac{s}{2\Lambda} \mathbf{e}), \quad (131)$$

and

$$n_v = (1 + \frac{z_t}{\Lambda}) \bar{n}_u - \frac{\varepsilon s}{2\Lambda} \mathbf{e}. \quad (132)$$

Using the formula (131) in (130), we get that z_t satisfies:

$$z_t \left(1 + \frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda(1 + \frac{z_t}{\Lambda})} (\langle n_v, \mathbf{e} \rangle + \frac{\varepsilon s}{2\Lambda}) \right) = \frac{\varepsilon s}{2(1 + \frac{z_t}{\Lambda})} \left(\langle n_v, \mathbf{e} \rangle + \frac{\varepsilon s}{2\Lambda} \right) - \frac{s^2}{8\Lambda}. \quad (133)$$

In particular we have:

$$z_t(u) = \frac{\varepsilon s}{2\Lambda} \langle n_v, \mathbf{e} \rangle + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2). \quad (134)$$

We differentiate z_t in (130) and get:

$$\begin{aligned} \mathbf{T}_u S_\varepsilon(t) &\rightarrow \mathbf{R} \\ dz_t(u) : \quad h &\mapsto \frac{\varepsilon s}{2\Lambda} \frac{\langle h, \mathbf{e} \rangle (1 + \frac{z_t}{\Lambda})}{1 + \frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda} \langle \bar{n}_u, \mathbf{e} \rangle}. \end{aligned} \quad (135)$$

Thus differentiating in (129) and using (131) in (135) we get:

$$\begin{aligned} \mathbf{T}_u S_\varepsilon(t) &\rightarrow \mathbf{T}_v S_\varepsilon(r) \\ d\Phi_t(u) : \quad h &\mapsto (1 + \frac{z_t}{\Lambda}) h + \frac{\varepsilon s}{2\Lambda} \frac{\langle h, \mathbf{e} \rangle (1 + \frac{z_t}{\Lambda})}{1 + \frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda} \langle \bar{n}_u, \mathbf{e} \rangle} \frac{n_v + \frac{s}{2\Lambda} \mathbf{e}}{1 + \frac{z_t}{\Lambda}} \end{aligned} \quad (136)$$

Let (a, b) be an orthonormal basis of $\mathbf{T}_u S_\varepsilon(t)$ with $b \times \bar{n}_u = a$, then we have:

$$\begin{aligned} J(\Phi_t; u) &= \langle d\Phi_t(u)a \times d\Phi_t(u)b, n_v \rangle \\ &= \langle ([1 + \frac{z_t}{\Lambda}]a + \bar{n}_u dz_t(u)a) \times ([1 + \frac{z_t}{\Lambda}]b + \bar{n}_u dz_t(u)b), n_v \rangle \\ &= (1 + \frac{z_t}{\Lambda})^2 \langle \bar{n}_u, n_v \rangle - (1 + \frac{z_t}{\Lambda}) [\langle a, n_v \rangle dz_t(u)a + \langle b, n_v \rangle dz_t(u)b] \\ &= (1 + \frac{z_t}{\Lambda}) (1 + \frac{\varepsilon s}{2\Lambda} \langle n_v, \mathbf{e} \rangle) + \frac{\varepsilon s}{2\Lambda} (1 + \frac{z_t}{\Lambda}) (\langle a, \mathbf{e} \rangle dz_t(u)a + \langle b, \mathbf{e} \rangle dz_t(u)b) \\ &= (1 + \frac{z_t}{\Lambda}) (1 + \frac{\varepsilon s}{2\Lambda} \langle n_v, \mathbf{e} \rangle) + \frac{\varepsilon s}{2\Lambda} \left(1 - \frac{(\langle n_v, \mathbf{e} \rangle + \frac{\varepsilon s}{2\Lambda})^2}{(1 + \frac{z_t}{\Lambda})^2} \right) \times \\ &\quad \frac{1 + \frac{z_t}{\Lambda}}{1 + \frac{z_t}{\Lambda} - \frac{\varepsilon s}{2\Lambda(1 + \frac{z_t}{\Lambda})} (\langle n_v, \mathbf{e} \rangle + \frac{\varepsilon s}{2\Lambda})} \\ &= 1 + \frac{\varepsilon s}{2\Lambda} \left[1 - \frac{(\langle n_v, \mathbf{e} \rangle + \frac{\varepsilon s}{2\Lambda})^2}{(1 + \frac{z_t}{\Lambda})^2} + \langle n_v, \mathbf{e} \rangle (\frac{1}{\Lambda} + 1) \right] + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2). \end{aligned}$$

As $u = v - z_t \bar{n}_u = v + \frac{\varepsilon s}{2} \langle n_v, \mathbf{e} \rangle n_{v_j} + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2)$, we get:

$$\begin{aligned} \int_{S_\varepsilon(t)} du_j F_{J,j}(u_j) r &= \int_{\Phi_t(S_\varepsilon(t))} dv_j F_{J,j}(v_j + \frac{\varepsilon s}{2} \langle n_{v_j}, \mathbf{e} \rangle n_{v_j} + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2)) \times \\ &\quad \left(1 - \frac{\varepsilon s}{2\Lambda} \left[1 - \frac{(\langle n_v, \mathbf{e} \rangle + \frac{\varepsilon s}{2\Lambda})^2}{(1 + \frac{z_t}{\Lambda})^2} + \langle n_v, \mathbf{e} \rangle (\frac{1}{\Lambda} + 1) \right] + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2) \right) dv. \end{aligned} \quad (137)$$

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 $\mathbf{R}_+^3 \varepsilon \mathbf{e}$ we have

$$\Phi_t(S_\varepsilon(t)) \simeq \left\{ (\Lambda, \theta, \phi), \frac{rs}{2\Lambda \sqrt{1 - \frac{rs}{2\Lambda^2} + \frac{s^2}{4\Lambda^2}}} = \cos(\theta_t) \leq \cos(\theta) \leq 1 \right\}, \quad (138)$$

and $\cos(\theta_t) = \frac{r}{2\Lambda} - \frac{r^2}{8\Lambda^2} s + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2)$.

At this point, we need to differentiate $F_{J,j}$: we have

$$F_{J,j}(u_j) = \frac{|\langle n_{u_j}, \mathbf{e} \rangle|}{2} \int_{B(r)^J} du_0 \cdots \widehat{du_j} \cdots du_J \frac{G_J^0(u_\ell \pm \frac{k}{2})}{\prod_{1 \leq i \leq J} |u_i - u_{i-1}|^2}.$$

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

$$F_{J,j}(u_j) = \frac{|\langle n_{u_j}, \mathbf{e} \rangle|}{2} \int_{B(r; u_j)^J} dv_0 \cdots \widehat{dv_j} \cdots dv_J \frac{G_J^0(v_\ell + u_j \pm \frac{k}{2})}{\prod_{1 \leq i \leq J} |v_i - v_{i+1}|^2}, \quad (139)$$

with the convention $v_j = 0$. We differentiate the formula (139): 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 $\delta u \in \mathbf{R}^3$:

$$\int_{B_\varepsilon(r, u_j + \delta u)} F(v) dv - \int_{B_\varepsilon(r, u_j)} F(v) dv = \int_{S_\varepsilon(r; u_j)} F(v) (\langle n(v - u_j), \delta u \rangle + \mathcal{O}_{\delta u \rightarrow 0}(|\delta u|^2)) dv, \quad (140)$$

where $n(v - u_j)$ is the outward normal of $S_\varepsilon(r, u_j)$ at v . Substituting in (137), as in the part 2.2. we get terms which are $\mathcal{O}_{\delta u \rightarrow 0}(|\delta u|(1 - \log|\delta u|))$. Writing $u_j = u$ we have

$$\begin{aligned} F_{J,j}(v - \frac{\varepsilon s}{2} \langle n_v, \mathbf{e} \rangle n_v + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2)) &= \mathcal{O}_{\delta r \rightarrow 0}(-(\delta r)^2 \log(\delta r)) \\ + F_{J,j}(v) - \frac{\varepsilon s \langle n_v, \mathbf{e} \rangle}{2} \sum_{i \neq j} \int_{\substack{v_i \in S(r; v) \\ \mathbf{v}'_i \in B(r, v)^J}} \frac{du_i d\mathbf{v}'_i}{\prod_{1 \leq \ell \leq J} |v_\ell - v_{\ell-1}|^2} G_J^0(v_\ell \pm \frac{r}{2} \mathbf{e}) \langle n(v_i - u_j), n_v \rangle. \end{aligned} \quad (141)$$

We write $\mathcal{C}(r) := S_+(r) \cap S_-(r)$ (this is a curve): integrating $F_{J,j}(v_j)$ over $S_\varepsilon(r) \Delta \Phi_{\delta r}(S_\varepsilon(\delta r))$ gives rise to a term:

$$-\frac{2r^2}{8\Lambda^2} \int_{u_j \in \mathcal{C}(r), (u_i)_{i \neq j} \in B(r)^J} \frac{r}{4\Lambda} du_0 \cdots du_J G_J(u_\ell \pm \frac{k}{2}) + \mathcal{O}_{\delta r \rightarrow 0}((\delta r)^2).$$

Thus we get a term of order

$$-\frac{2r^2}{8\Lambda^2} \int_{u_j \in \mathcal{C}(r), (u_i)_{i \neq j} \in B(r)^J} \frac{r}{4\Lambda} du_0 \cdots du_J G_J(u_\ell \pm \frac{k}{2}) = \mathcal{O}\left(\frac{(\alpha K)^{J+1}}{\Lambda^2}\right).$$

Integrating the term $F_{J,j}(v) \times (J(\Phi_t; u_j)^{-1} - 1)$, we get a well defined number in the limit $\delta r \rightarrow 0$. Furthermore this term is

$$\mathcal{O}\left(\frac{1}{\Lambda} \int_{u_j \in S(r)} \int_{(u_0, \dots, \widehat{u_j}, \dots, u_J) \in B(r)^J} du_0 \cdots du_J |G_J(u_\ell \pm \frac{k}{2})|\right) = \mathcal{O}\left(\frac{(\alpha K)^{J+1} \log(\Lambda)}{\Lambda^2} \chi_{r < 2\Lambda}\right).$$

To conclude, we consider the term $F_{J,j}(\Phi_t^{-1}(v)) - F_{J,j}(v)$.

Up to a term $-\delta^2 \log(\delta r) = \mathcal{O}_{\delta r \rightarrow 0}(\delta r)$, we can take $S(r)$ instead of $\Phi_t(S_\varepsilon(t))$ and 1 instead of the full jacobian $J(\Phi_t; u)$. We have $\varepsilon \langle n_v, \mathbf{e} \rangle = |\langle n_v, \mathbf{e} \rangle|$. In (141) we take back the previous variables $u_i = v + v_j$, this gives

$$\delta r \int_{v \in S_\varepsilon(r)} \sum_{i \neq j} \int_{(u_i, \mathbf{u}') \in S(r) \times B(r)^{J-1}} du_0 \cdots du_J \frac{|\langle n_v, \mathbf{e} \rangle|}{2} \left(-\frac{|\langle n_v, \mathbf{e} \rangle| \langle n_v, n_{u_i} \rangle}{2} \right) G_J(u_\ell \pm \frac{k}{2}).$$

When we sum this term with that of (126), for each $i \neq j$ we have

$$\begin{aligned} \left| |\langle n_{u_i}, \mathbf{e} \rangle| - |\langle n_v, \mathbf{e} \rangle| |\langle n_v, n_{u_i} \rangle| \right| &= \left| \varepsilon(u_i) \langle n_{u_i}, \mathbf{e} \rangle - \varepsilon(v) \langle n_v, \mathbf{e} \rangle \times \varepsilon(v) \varepsilon(u_i) \langle n_v, n_{u_i} \rangle \right|, \\ &\leq \min(\sqrt{2} |n_{u_i} - n_v|, 2). \end{aligned}$$

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 (126) and get

$$\iint_{S(r) \times S(r)} \frac{|n_u - n_v| |\langle n_u, \mathbf{e} \rangle| dudv}{|u - v|^2} \frac{1}{\bar{E}(\Lambda)^2 \Lambda^2}.$$

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 $|n_u - n_v| \leq \frac{|u-v|}{\Lambda}$, and the integral is

$$\mathcal{O} \left(\int_{\mathbb{S}^2} \frac{du}{\Lambda^2 |u - \mathbf{e}|} \right) = \mathcal{O} \left(\frac{1}{\Lambda^2} \right).$$

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:

$$\begin{aligned} &\frac{2\pi}{\Lambda^2} \iiint_{(\theta_1, \theta_{-1}, \phi) \in (0, \theta_1^0) \times (-\pi, \theta_{-1}^0) \times (-\pi, \pi)} \frac{s(\theta_1) s(\theta_{-1}) d\theta_1 d\theta_{-1} d\phi}{(c(\theta_1) - c(\theta_{-1}) - 2x)^2 + s(\theta_{-1})^2 s_\phi^2 + (s(\theta_1) - s(\theta_{-1})) c_\phi^2} \\ &\lesssim \frac{1}{\Lambda^2} \iiint_{(\theta_1, \theta_{-1}, \phi) \in (0, \theta_1^0) \times (-\pi, \theta_{-1}^0) \times (-\pi, \pi)} \frac{s(\theta_1) s(\theta_{-1}) d\theta_1 d\theta_{-1} d\phi}{(c(\theta_1) - c(\theta_{-1}) - 2x)^2 + c(\theta_{-1})^2 \phi^2} =: \frac{A}{\Lambda^2}. \end{aligned}$$

We write $\theta_\varepsilon = \theta_\varepsilon^0 - \varepsilon \phi_\varepsilon$: we have

$$\begin{aligned} \varepsilon c(\theta_\varepsilon) - x &= x(c(\phi_\varepsilon) - 1) + \sqrt{1-x^2} s(\phi_\varepsilon), \\ x(c(\phi_\varepsilon) - 1) + \sqrt{1-x^2} s(\phi_\varepsilon) &\geq \phi_\varepsilon \left(\frac{2}{\pi} \sqrt{1-x^2} - x \frac{\phi_\varepsilon}{2} \right), \\ &\geq \frac{2\phi_\varepsilon}{\pi} \left(\sqrt{1-x^2} - \frac{\pi}{4} x \arccos(x) \right) \geq \frac{2\phi_\varepsilon \sqrt{1-x}}{\pi} \left(1 - \frac{x\pi}{4} \right) \\ &\geq \frac{2\phi_\varepsilon \sqrt{1-x}}{\pi} \left(1 - \frac{\pi}{4} \right) \geq \frac{\sqrt{1-x^2} \phi_\varepsilon}{\pi} \left(1 - \frac{\pi}{4} \right). \end{aligned}$$

Thus we have

$$\begin{aligned} A &\lesssim \iint_{\phi_1, \phi_{-1} \in (0, \theta_1^0)} \frac{\sin(\theta_1) d\phi_1 d\phi_{-1}}{\sqrt{1-x^2} \sqrt{\phi_1^2 + \phi_{-1}^2}} \\ &\lesssim \int_{\phi_1 \in (0, \theta_1^0)} \frac{d\phi_1}{\sqrt{1-x^2}} \log \left(1 + \frac{\arccos(x)}{\phi_1} \right) \\ &\lesssim \int_{\phi \in (0, 1)} \log(1 + \phi^{-1}) d\phi. \end{aligned}$$

Conclusion We obtain at last the following upper bound for the terms of 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). \square

Alternative F_Λ

In the proof of Theorem 3, one is lead to consider a perturbative 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 15 below for the proof of Lemma 12. We can write

$$\mathcal{D}^0 + \frac{2}{\lambda} \frac{\mathcal{D}^0}{|\mathcal{D}^0|} = \beta \tilde{w}_0(-i\nabla) + \boldsymbol{\alpha} \cdot \frac{-i\nabla}{|-i\nabla|} \tilde{w}_1(-i\nabla).$$

The formulae are the same with w_0, w_1 replaced by \tilde{w}_0, \tilde{w}_1 , estimates of the same kind hold. The alternative functions are marked with a tilde: \tilde{B}_Λ and \tilde{g}_Λ .

We can easily estimate $\int_{|x| \geq R} |\mathcal{F}^{-1}(\tilde{F}_\Lambda)(x)| dx$ for $R \geq 1$: writing $\mathfrak{f}_\Lambda := \mathcal{F}^{-1}(\tilde{F}_\Lambda)$ we have the following Lemma:

Lemma 15. For $\lambda, \Lambda \gg 1$ we have:

$$\alpha \int_{|x| \geq R} |\mathfrak{f}_\Lambda(x)| dx \leq \|-\Delta \tilde{F}_\Lambda\|_{L^2} \sqrt{4\pi R^{-1}} = \mathcal{O}(LR^{-1/2}). \quad (142)$$

In particular, with $R^{-1} = \alpha \ll 1$ and $L \leq L_0$ it is lesser than $KL\alpha^{1/2}$.

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