Existence of a stable polarized vacuum in the Bogoliubov-Dirac-Fock approximation

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Abstract

According to Dirac's ideas, the vacuum consists of infinitely many virtual electrons which completely fill up the negative part of the spectrum of the free Dirac operator D^0. In the presence of an external field, these virtual particles react and the vacuum becomes polarized.

In this paper, following Chaix and Iracane [5], we consider the Bogoliubov-Dirac-Fock model, which is derived from QED. The corresponding BDF-energy takes the polarization of the vacuum into account and is bounded from below. A BDF-stable vacuum is defined to be a minimizer of this energy. If it exists, such a minimizer is a solution of a self-consistent equation.

We show the existence of a minimizer of the BDF-energy in the presence of an external electrostatic field, by means of a fixed-point approach. This minimizer is interpreted as the polarized vacuum.

1 Introduction

The relativistic quantum theory of electrons and positrons is based on the free Dirac operator, which is defined by

$$D^0 = -i\sum_{k=1}^{3} \alpha_k \partial_k + \beta := -i\boldsymbol{\alpha}\cdot\nabla + \beta \tag{1}$$

where $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)$ and

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}, \qquad \alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix},$$

with

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

We follow here the notation of Thaller's book [30], and of [2]. We have chosen a system of units such that $\hbar = c = 1$, and also such that the mass m_e of the electron is normalized to 1.

The operator D^0 acts on 4-spinors, i.e. functions $\Psi \in \mathcal{H} := L^2(\mathbb{R}^3, \mathbb{C}^4)$. It is self-adjoint on $\mathcal{H}$, with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$ and form domain $H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Moreover, it is defined to ensure

$$(D^0)^2 = -\Delta + 1.$$

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The spectrum of D^0 is $(-\infty;-1]\cup[1;\infty)$. The fact that the spectrum of D^0 is not bounded from below is the main reason for all the problems that occur in this theory. To explain why a free electron does not dissolve into the lower continuum, Dirac's idea was to postulate that the vacuum contains infinitely many virtual electrons which completely fill up the negative part of the spectrum of D^0. This model of the vacuum is called the *Dirac Sea*.

In what follows, the projector associated with the negative part of the spectrum of D^0 will be denoted by P^0:

$$P^0 := \chi_{(-\infty;0)}(D^0).$$

We then have

$$D^0P^0 = P^0D^0 = -\sqrt{1-\Delta}P^0 = -P^0\sqrt{1-\Delta},$$
$$D^0(1-P^0) = (1-P^0)D^0 = \sqrt{1-\Delta}(1-P^0) = (1-P^0)\sqrt{1-\Delta},$$

and

$$\mathcal{H} = \mathcal{H}^0_- \oplus \mathcal{H}^0_+,$$

where $\mathcal{H}^0_- := P^0\mathcal{H}$ and $\mathcal{H}^0_+ := (1-P^0)\mathcal{H}$.

According to what we said above, we can identify P^0 with the vacuum since it projects onto the Dirac sea. It is often called the *bare vacuum* [5].

Let us now add the potential created by some nuclei of total charge Z. In our system of units, the Dirac operator with external potential φ is

$$D^{\alpha\varphi} := D^0 - \alpha\varphi, \tag{2}$$

where $\varphi = Zn * \frac{1}{|\cdot|}$ is the Coulomb potential created by the smeared out nuclei of total density $Zn \geq 0$ such that $\int_{\mathbb{R}^3} n = 1$. The constant α is often called the *Sommerfeld fine structure constant*, and its physical value is approximately $\frac{1}{137}$. Nevertheless in the present paper it will rather play the role of a small dimensionless coupling parameter.

Dirac postulated that the charge of the Dirac sea is not measurable. However, in the presence of the external field created by the nuclei, the virtual electrons should react, by occupying the negative energy state of an other Dirac operator: *the vacuum is polarized*. This polarization of the *dressed vacuum*, which takes the form of a local density of charge, is measurable in practice. Our main goal in this paper is to study a model for the polarized vacuum which was derived by Chaix and Iracane [5] from no-photon Quantum Electrodynamics .

It is natural to expect that the vacuum should be described by the projector $P^{\alpha\varphi}$ associated with the negative part of the spectrum of $D^{\alpha\varphi}$ (this choice is called the *Furry picture*). We shall see that this is only an approximation: we describe below a more exact model.

Mathematically speaking, we shall say that a *vacuum* is an orthogonal projector P with the additional requirement that $Q = P - P^0$ is in $\mathfrak{S}_2(\mathcal{H})$, the space of all Hilbert-Schmidt operators on $\mathcal{H}$. As explained in Appendix, this condition guarantees the existence of a dressed vacuum in the Fock space defined with respect to the splitting $\mathcal{H} = \mathcal{H}^0_- \oplus \mathcal{H}^0_+$, but we shall not give much more detail here.

Since the model takes the free case as reference, it can be seen using the formalism of Quantum Electrodynamics (further details are given in the Appendix) that the polarization of a dressed vacuum P can be described by the difference

$$Q = P - P^0$$

which is interpreted as the *one-body density matrix of the vacuum*. This means that the total Hamiltonian is now the formal operator

$$D_Q := D^{\alpha\varphi} + \alpha\rho_Q * \frac{1}{|\cdot|} - \alpha\frac{Q(x,y)}{|x-y|}. \tag{3}$$

The two terms $\alpha\rho_Q * \frac{1}{|\cdot|}$ and $\alpha\frac{Q(x,y)}{|x-y|}$ are called respectively the non-exchange and exchange potentials and they vanish when $P = P^0$. The function

$$\rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\left(Q(x,x)\right)$$

is the *charge density* of the vacuum P. Remark that since we only assume Q to be Hilbert-Schmidt, ρ_Q is not *a priori* a well-defined function, but an adequate framework will be given later.

Let us now explain how this P is chosen. According to Dirac's ideas, a "correct" P should be the projector associated with the negative part of the spectrum of the one-body Hamiltonian of the system. Therefore, it should be a solution of the *self-consistent equation*

$$\boxed{P = \chi_{(-\infty;0)}(D_Q) = \chi_{(-\infty;0)}\left(D^{\alpha\varphi} + \alpha\rho_Q * \frac{1}{|\cdot|} - \alpha\frac{Q(x,y)}{|x-y|}\right).} \tag{4}$$

Remark that if $\varphi = 0$ (no external potential), then P^0 is already a solution to this equation since $Q = 0$ in this particular case.

This equation can be interpreted as the Euler-Lagrange equation associated with the minimization of the Bogoliubov-Dirac-Fock (BDF) energy defined by Chaix and Iracane [5] (see also [7]). The study of this functional was our original motivation for solving (4). In this paper, we first give a rigorous meaning to formula (4) and then show the existence of a solution by a fixed-point argument. We then prove that our solution is a minimizer of the BDF energy.

Notice that the use of a fixed-point method to solve a self-consistent equation is very common in quantum chemistry and physics. The numerical algorithms used in practice are based on this idea. For a mathematical existence result using the Schauder fixed-point theorem, see the resolution of the Hartree equations in [34]. For the determination of projectors describing the vacuum, the fixed-point approach has been used for the first time by E.H. Lieb and H. Siedentop [22]. We use the Banach fixed-point theorem as in [22], but our model is different and the necessary estimates are much more delicate.

A model also inspired by [5] was studied by V. Bach, J.-M. Barbaroux, B. Helffer and H. Siedentop in [2] (see also [4]) . Although our model coincide with [2] when there is no external potential (i.e. $Z = 0$), it is very different in the presence of an external electrostatic field (i.e. $Z \neq 0$). Indeed, the authors of [2] have neglected the terms describing the polarization of the vacuum and, as this is explained in [5], the resulting energy is not bounded from below. Therefore a max-min procedure inspired by [24] was considered, leading to the solution $P = P^{\alpha\varphi}$. Since we keep the vacuum polarization terms, the BDF energy is bounded from below and we can define the polarized vacuum as the minimum of this energy. We find a P which solves (4) and is therefore different from $P^{\alpha\varphi}$.

When studying equation (4), a first problem occurs with the definition of the density ρ_Q. Let us explain this fact in the Furry picture, that is to say when P is chosen to be $P^{\alpha\varphi}$. Remark that $P^{\alpha\varphi}$ is the projector which is obtained after the first iteration of the fixed-point algorithm if we start at P^0.

It is known since the very beginning of QED [8, 18, 13, 31, 29] that the density $\rho^{\alpha\varphi}$ associated with $Q^{\alpha\varphi} = P^{\alpha\varphi} - P^0$ is *never well-defined*, since it diverges pointwise logarithmically. In physics literature [12, 28, 9, 10] (see also the books [20, 23, 32]), a procedure called *charge renormalization* aims at extracting the main information from $\rho^{\alpha\varphi}$ and a renormalized density $\rho^{\alpha\varphi}_{\mathrm{ren}}$ is used to replace the ill-defined density in the Hamiltonian

$$D^{\mathrm{ren}}_{Q^{\alpha\varphi}} = D^{\alpha\varphi} + \alpha\rho^{\alpha\varphi}_{\mathrm{ren}} * \frac{1}{|\cdot|} - \alpha\frac{Q(x,y)}{|x-y|}.$$

This procedure has been recently clarified by C. Hainzl and H. Siedentop in [16], where it is in addition shown that $D^{\rm ren}_{Q^{\alpha\varphi}}$ is then a well defined self-adjoint operator, under some reasonable assumption on φ. Some interesting features of $\rho^{\alpha\varphi}_{\rm ren}$, in the case of strong external fields, were obtained by Hainzl in [15]. We do not want to give a precise definition of $\rho^{\alpha\varphi}_{\rm ren}$ here and we refer the reader to [16, 15, 25].

For the same reason as for $\rho^{\alpha\varphi}$, it can be seen that if P is a solution to equation (4), then ρ_Q is necessarily logarithmically divergent. However our approach is different from [16] since we do not renormalize ρ_Q *a priori*: the interpretation of the solution as a minimizer of the BDF energy becomes unclear if a renormalization is used. Instead, we impose a momentum cut-off. In other words, from now on, we replace the ambiant space $\mathcal{H}$ by

$$\mathcal{H}_\Lambda := \left\{ f \in \mathcal{H},\ supp(\widehat{f}) \subset B(0,\Lambda) \right\}.$$

Since D^0 is a multiplication operator in Fourier space, $\mathcal{H}_\Lambda$ is invariant under P^0 and we keep the notation P^0 to avoid the introduction of a restricted operator.

As we shall see it later on, our results will be valid under a condition of the form $\alpha\sqrt{\ln\Lambda} \leq C$ for some constant $C \gtrsim 0.33$. If α has the physical value $1/137$, this leads to an extremely large Λ, which corresponds to scales that are far beyond the reach of experimental and theoretical physics at the present time.

We would like to emphasize that in QED calculations (see, e.g., [20, Equation (7.18)]) a momentum cut-off is necessary. It appears in the *charge renormalization* which consists of a replacement of the *bare* charge e by $e^2_{\rm eff} \simeq e^2(1 - \frac{2\alpha}{3\pi}\ln\Lambda)$. This charge renormalization is the physical explanation for the renormalization of $\rho^{\alpha\varphi}$ mentioned above.

The paper is organized as follows. In the next section, we define the Bogoliubov-Dirac-Fock model and state our main results. For the sake of clarity, we have brought all the proofs together in Sections 3 and 4. In the Appendix, we explain how the BDF energy can be deduced from no-photon QED.

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2 Model and main results

In this section, we study the Bogoliubov-Dirac-Fock model introduced in [5, 7]. Our system of notation is similar to [2], with the difference that we keep all the terms describing the vacuum polarization. As explained in [5], although these terms are negligible in most practical atomic computations, they are essential if one wants to deal with an energy which is *bounded from below* and *intrinsic*. By intrinsic, we mean that it does not depend on the choice of a particular normal ordering of the second-quantized Hamiltonian (see the Appendix for details). Remark also that the vacuum polarization terms play an essential role within the treatment of muonic atoms [14].

2.1 Supertrace-class operators

In order to define the BDF-functional properly, we introduce the concept of supertrace-class operators, in the spirit of [30, Section 5.7]. In this section only, we work in an abstract Hilbert space $\mathcal{H}$.

Definition 1. *Let P be a projector such that P and $1-P$ have infinite rank, and $A \in \mathfrak{S}_2(\mathcal{H})$. We shall say that A is* supertrace-class with respect to P *if and only if $A_{++} := (1-P)A(1-P)$ and $A_{--} := PAP$ are trace-class. Then we define*

$$\mathrm{str}_P(A) := \mathrm{tr}(A_{++}) + \mathrm{tr}(A_{--}).$$

We denote by $\mathfrak{S}_1^P(\mathcal{H})$ the set of all Hilbert-Schmidt operators which are supertrace-class with respect to P.

Remark that if A is a trace-class operator, then $A \in \mathfrak{S}_1^P(\mathcal{H})$ and $\mathrm{tr}(A) = \mathrm{str}_P(A)$ for any projector P. We want to mention the following result, which will be useful in the proofs of our main theorems, and which is proved in Section 3.

Theorem 1. *Let P and P' be two projectors such that $P - P' \in \mathfrak{S}_2(\mathcal{H})$. Then A is supertrace-class with respect to P if and only if it is supertrace-class with respect to P', and in this case $\mathrm{str}_P(A) = \mathrm{str}_{P'}(A)$.*

2.2 The Bogoliubov-Dirac-Fock model

The Bogoliubov-Dirac-Fock energy is defined by

$$\mathcal{E}(\Gamma) = \mathrm{str}_{P^0}(D^0\Gamma) - \alpha \int \rho_\Gamma \varphi + \frac{\alpha}{2} \iint \frac{\rho_\Gamma(x)\rho_\Gamma(y)}{|x-y|} dx\, dy - \frac{\alpha}{2} \iint \frac{|\Gamma(x,y)|^2}{|x-y|} dx\, dy \tag{5}$$

on the set

$$\mathcal{B}_\Lambda := \left\{ \Gamma \in \mathfrak{S}_1^{P^0}(\mathcal{H}_\Lambda),\ -P^0 \leq \Gamma \leq 1 - P^0,\ \rho_\Gamma \in \mathcal{C} \right\}$$

with

$$\mathcal{C} = \left\{ \rho \in L^2(\mathbb{R}^3),\ \int_{\mathbb{R}^3} \frac{|\widehat{\rho}(k)|^2}{|k|^2}\, dk < \infty \right\}, \qquad \|\rho\|_{\mathcal{C}}^2 := \int_{\mathbb{R}^3} \frac{1+|k|^2}{|k|^2} |\widehat{\rho}(k)|^2\, dk.$$

In (5), ρ_Γ is the well-defined diagonal of $\Gamma \in \mathfrak{S}_2(\mathcal{H}_\Lambda)$

$$\rho_\Gamma(x) = \mathrm{Tr}_{\mathbb{C}^4}\left(\Gamma(x,x)\right) = \frac{1}{(2\pi)^3} \iint_{|p|,|q| \leq \Lambda} \mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{\Gamma}(p,q)\right) e^{ix(p-q)} dp\, dq \tag{6}$$

so that

$$\widehat{\rho_\Gamma}(k) = \frac{1}{(2\pi)^{3/2}} \int_{|p| \leq \Lambda} \mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{\Gamma}(p+k/2, p-k/2)\right) dp$$

showing that $\widehat{\rho_\Gamma} \in L^1$, and so $\rho_\Gamma \in \mathcal{C}_0^0$. Notice that (6) shows that the function $\Gamma \in \mathfrak{S}_2(\mathcal{H}_\Lambda) \mapsto \rho_\Gamma \in \mathcal{C}_0^0 \cap L^2(\mathbb{R}^3)$ is continuous.

In the next subsection, we prove that $\mathcal{E}$ is well-defined and bounded from below on $\mathcal{B}_\Lambda$. We then show the existence of a minimizer, which can be interpreted as a stable polarized vacuum in the BDF approximation.

To this end, let us first explain how this energy is used in [5]. In the BDF setting, a state of the system is a pair (P, γ) where

- P is a projector such that $Q = P - P^0 \in \mathfrak{S}_2(\mathcal{H}_\Lambda)$, representing the dressed vacuum,
- $\gamma \in \mathfrak{S}_1(\mathcal{H}_\Lambda)$ is the density matrix of a BDF-state built with electrons and positrons defined by P. This means that

  $$\gamma = \gamma_+ - \gamma_-$$

  where γ_+ and γ_- are projectors of finite rank with $\mathrm{Ran}(\gamma_+) \subset (1-P)\mathcal{H}_\Lambda$ and $\mathrm{Ran}(\gamma_-) \subset P\mathcal{H}_\Lambda$. It therefore satisfies $-P \leq \gamma \leq 1 - P$.

Details are given in Appendix for the interested reader. The density matrix γ corresponds to Slater determinants involving electrons and positrons defined by means of the vacuum P. The energy of such a state (P,γ) is then given by

$$\mathcal{E}^{\rm BDF}(P,\gamma)=\mathcal{E}(Q+\gamma) \tag{7}$$

where we recall that $Q=P-P^0$. Remark that the real physical object is not really the pair (P,γ), but the sum $\Gamma=Q+\gamma=P-P^0+\gamma$. It fulfills $-P^0\leq\Gamma\leq 1-P^0$. Therefore the set $\mathcal{B}_\Lambda$, on which $\mathcal{E}$ is defined, is seen to be the convex hull of the BDF states taking the special form $P-P^0+\gamma$. For such models, it is a very common idea to extend the functional to the convex hull of the states under consideration (see for instance the notion of quasi-free states defined in [3] and used in [2]). To explain why $\mathcal{B}_\Lambda\subset\mathfrak{S}_1^{P^0}(\mathcal{H}_\Lambda)$, we now state the following

Lemma 1. *Let P be a projector on $\mathcal{H}_\Lambda$, such that $Q=P-P^0$ is a Hilbert-Schmidt operator. Then Q is supertrace-class with respect to P^0. Moreover, $\mathrm{str}_{P^0}(Q)$ is an integer which satisfies*

$$\forall n\geq 1,\ \mathrm{str}_{P^0}(Q)=\mathrm{tr}(Q^{2n+1}).$$

Proof – We have $Q^2=P-PP^0-P^0P+P^0=(1-P^0)Q(1-P^0)-P^0QP^0$. This implies that $(1-P^0)Q(1-P^0)$ and $-P^0QP^0$ are non-negative trace-class operators.

We now use the proof of [1, Theorem 4.1]. Since $Q\in\mathfrak{S}_2$, we infer $Q^3\in\mathfrak{S}_1$ and so (P,P^0) is a Fredholm pair, in the language of [1]. Therefore, $\mathrm{tr}(Q^3)$ is an integer and satisfies $\mathrm{tr}(Q^3)=\mathrm{tr}(Q^{2n+1})$ for all $n\geq 1$. Now we have

$$(P-P^0)^3=(P-P^0)^2P-(P-P^0)^2P^0=P(P-P^0)P+P^0(P-P^0)P^0$$

Applying this result to $1-P$ and $1-P^0$, we find

$$(P-P^0)^3=(1-P)(P-P^0)(1-P)+(1-P^0)(P-P^0)(1-P^0).$$

Summing up this two identities, we obtain by Theorem 1

$$2\,\mathrm{tr}(Q^3)=\mathrm{str}_P(Q)+\mathrm{str}_{P^0}(Q)=2\,\mathrm{str}_{P^0}(Q)\quad\square$$

Remark: Since $\mathrm{str}_{P^0}(Q)$ is an integer, it can be interpreted as the charge of the dressed vacuum P (see [15] for results in this direction).

In Chaix-Iracane [5], formula (4.8), the expression $\mathcal{E}(Q+\gamma)$ is expanded to get

$$\begin{aligned}\mathcal{E}^{\rm BDF}(P,\gamma) &= \mathrm{tr}\left(\left(D^{\alpha\varphi}+\alpha\rho_Q*\frac{1}{|\cdot|}-\alpha\frac{Q(x,y)}{|x-y|}\right)\gamma\right)\\ &\qquad+\frac{\alpha}{2}\iint\frac{\rho(x)\rho(y)}{|x-y|}dx\,dy-\frac{\alpha}{2}\iint\frac{|\gamma(x,y)|^2}{|x-y|}dx\,dy+\mathcal{E}(Q)\\ &= \mathrm{tr}\,(D_Q\gamma)+\frac{\alpha}{2}\iint\frac{\rho(x)\rho(y)}{|x-y|}dx\,dy-\frac{\alpha}{2}\iint\frac{|\gamma(x,y)|^2}{|x-y|}dx\,dy+\mathcal{E}(Q),\end{aligned} \tag{8}$$

since $\gamma\in\mathfrak{S}_1(\mathcal{H}_\Lambda)$ which implies $\int_{\mathbb{R}^3}\left(\rho_Q*\frac{1}{|\cdot|}-\varphi\right)\rho=\mathrm{tr}\left[\left(\rho_Q*\frac{1}{|\cdot|}-\varphi\right)\gamma\right]$.

In [2, Formula (21)], the polarization potentials appearing in D_Q and the energy of the vacuum $\mathcal{E}(Q)$ were neglected by the authors who used the following functional

$$\mathcal{E}_P^{[2]}(\gamma)=\mathrm{tr}\,(D^{\alpha\varphi}\gamma)+\frac{\alpha}{2}\iint\frac{\rho(x)\rho(y)}{|x-y|}dx\,dy-\frac{\alpha}{2}\iint\frac{|\gamma(x,y)|^2}{|x-y|}dx\,dy,$$

with the constraint $-P\leq\gamma\leq 1-P$. This energy is easily seen to be non intrinsic and unbounded from below: $\inf_P\inf_{-P\leq\gamma\leq 1-P}\mathcal{E}_P^{[2]}(\gamma)=-\infty$ (see the properties of the Dirac-Fock functional defined in [11]). Therefore, a procedure which takes the form $\sup_P\inf_{-P\leq\gamma\leq 1-P}\mathcal{E}_P^{[2]}(\gamma)$ inspired by [24] was considered in [2], leading to the solution $P=P^{\alpha\varphi}$. In fact, as explained in [5], the vacuum polarization potentials and the energy of the vacuum $\mathcal{E}(Q)$ are unavoidable if one wants to deal with a bounded-below and intrinsic energy.

2.3 Study of the BDF energy

We are now able to state the following result (recall that $\varphi = Zn * \frac{1}{|\cdot|}$).

Theorem 2. *Let be $n \in \mathcal{C} \cap L^1(\mathbb{R}^3)$ and $Z \geq 0$.*

1. *$\mathcal{E}$ is well-defined on*
$$\mathcal{A}_\Lambda := \Big\{ \Gamma \in \mathfrak{S}_1^{P^0}(\mathcal{H}_\Lambda),\ \rho_\Gamma \in \mathcal{C} \Big\} \supset \mathcal{B}_\Lambda.$$
2. *If $0 \leq \alpha \leq \frac{4}{\pi}$, then $\mathcal{E}$ is bounded from below on $\mathcal{B}_\Lambda$, independently of Λ.*
3. *If $0 \leq \alpha \leq \frac{4}{\pi}$ and $Z = 0$, then $\mathcal{E}$ is non-negative on $\mathcal{B}_\Lambda$ [2], 0 being the unique minimizer.*

Without external potential, the non-negativity of the functional $\mathcal{E}$ was first proved by Chaix, Iracane, and Lions [6] and later, with improvement in the parameter range, stated by Bach, Barbaroux, Helffer, and Siedentop [2]. This result is optimal in the sense that the functional becomes unbounded from below when $Z = 0$: $\inf_{\Gamma \in \mathcal{B}_\Lambda} \mathcal{E}(\Gamma) = -\infty$ if $\alpha > 4/\pi$ as shown by Hundertmark, Röhrl, and Siedentop [19].

Proof of Theorem 2 – Let us first show that $\mathcal{E}$ is well defined on $\mathcal{A}_\Lambda$. If $\Gamma \in \mathfrak{S}_1^{P^0}(\mathcal{H}_\Lambda)$, then we have $P^0 D^0 \Gamma P^0 = D^0 P^0 \Gamma P^0 = D^0 \Gamma_{++} \in \mathfrak{S}_1(\mathcal{H}_\Lambda)$ since P^0 commutes with D^0 and $|D^0| \leq \sqrt{1+\Lambda^2}$. With a similar argument for $1-P^0$, we obtain that $D^0\Gamma \in \mathfrak{S}_1^{P^0}(\mathcal{H}_\Lambda)$. Therefore, $\mathrm{str}_{P^0}(D^0\Gamma)$ is well-defined and

$$\mathrm{str}_{P^0}(D^0\Gamma) = \mathrm{tr}(D^0\Gamma_{++}) + \mathrm{tr}(D^0\Gamma_{--}) = \mathrm{tr}(|D^0|\Gamma_{++}) - \mathrm{tr}(|D^0|\Gamma_{--}). \tag{9}$$

On the other hand we have by Hardy's inequality

$$\iint \frac{|\Gamma(x,y)|^2}{|x-y|} dx\, dy \leq \frac{\pi}{2} \mathrm{tr}(|D^0|\Gamma^2)$$

showing that this last term is well-defined since $|D^0|$ is bounded on $\mathcal{H}_\Lambda$ and $\Gamma \in \mathfrak{S}_2(\mathcal{H}_\Lambda)$. Finally, let us introduce $D(f,g) := \iint \frac{f(x)g(y)}{|x-y|} dx\, dy$ which defines a scalar product on $\mathcal{C}$. We have

$$\int \rho_\Gamma \varphi = D(\rho_\Gamma, Zn) \quad \text{and} \quad \iint \frac{\rho_\Gamma(x)\rho_\Gamma(y)}{|x-y|} dx\, dy = D(\rho_\Gamma, \rho_\Gamma)$$

which show that the terms in ρ_Γ are well-defined as soon as n and ρ_Γ belong to $\mathcal{C}$.

Now, if $\Gamma \in \mathcal{A}_\Lambda$ fulfills the additional property $-P^0 \leq \Gamma \leq 1 - P^0$, then it is easily shown that $\Gamma_{++} := (1-P^0)\Gamma(1-P^0) \geq 0$ and $\Gamma_{--} := P^0\Gamma P^0 \leq 0$, and thus $\mathrm{str}_{P^0}(D^0\Gamma) \geq 0$, by (9). On the other hand, following an argument of [2], we derive from $0 \leq \Gamma + P^0 \leq 1$ that $\Gamma^2 + P^0\Gamma + \Gamma P^0 \leq \Gamma$ or equivalently $\Gamma^2 \leq \Gamma_{++} - \Gamma_{--}$. Therefore

$$\iint \frac{|\Gamma(x,y)|^2}{|x-y|} dx\, dy \leq \frac{\pi}{2} \mathrm{tr}(|D^0|(\Gamma_{++} - \Gamma_{--})) = \frac{\pi}{2} \mathrm{str}_{P^0}(D^0\Gamma).$$

If we now simply remark that

$$-\alpha \int \rho_\Gamma \varphi + \frac{\alpha}{2} \iint \frac{\rho_\Gamma(x)\rho_\Gamma(y)}{|x-y|} dx\, dy = \frac{\alpha}{2} \Big(D(\rho_\Gamma, \rho_\Gamma) - 2D(\rho_\Gamma, Zn) \Big) \geq -\frac{\alpha Z^2}{2} D(n,n),$$

we finally obtain

$$\mathcal{E}(\Gamma) \geq \Big(1 - \frac{\alpha\pi}{4}\Big) \mathrm{str}_{P^0}(D^0\Gamma) - \frac{\alpha Z^2}{2} D(n,n) \geq -\frac{\alpha Z^2}{2} D(n,n)$$

when $\alpha \leq 4/\pi$, which easily ends the proof. □

Even if it is more convenient to study the functional $\mathcal{E}$ on the convex hull $\mathcal{B}_\Lambda$, we are interested in minimizers which belong to the BDF class. For the study of the vacuum, this leads to the following definition

Definition 2. *We say that a projector P is a* BDF-stable vacuum *if and only if $P - P^0$ is a minimizer of $\mathcal{E}$ on $\mathcal{B}_\Lambda$.*

Theorem 2 implies that P^0 is a BDF-stable vacuum when there is no external potential [5, 2], which corresponds to Dirac's ideas. But if we consider a non-vanishing external potential $\varphi = Zn * \frac{1}{|\cdot|}$, then P^0 obviously cannot be BDF-stable, since it is easy to create a state $-P^0 \leq \gamma \leq 1 - P^0$ such that $\mathcal{E}(\gamma) < 0 = \mathcal{E}(0)$. This means that the vacuum is necessarily polarized.

To state the following result, we introduce the notation

$$\mathcal{P}_\Lambda = \left\{ P \text{ projector},\ P - P^0 \in \mathcal{A}_\Lambda \right\}.$$

Theorem 3 (BDF-Stability). *Let be $P \in \mathcal{P}_\Lambda$, $n \in \mathcal{C} \cap L^1(\mathbb{R}^3)$ and $Z \geq 0$. We assume that there exists a positive constant d such that*

$$d|D_Q| \geq |D^0| \quad \textit{with} \quad \alpha d \frac{\pi}{4} \leq 1, \tag{10}$$

where D_Q is defined in (3)*. Then, the following assertions are equivalent*

1. *P fulfills the equation*

$$P = \chi_{(-\infty;0)}(D_Q) = \chi_{(-\infty;0)} \left(D^{\alpha\varphi} + \alpha\rho_Q * \frac{1}{|\cdot|} - \alpha \frac{Q(x,y)}{|x-y|} \right). \tag{11}$$

2. *P is BDF-stable, i.e. $P - P^0$ is a minimizer of $\mathcal{E}$ on $\mathcal{B}_\Lambda$.*

The main ideas of the proof, which is given in Section 3, are taken from [2], with additional difficulties coming from the fact that we do not consider trace-class operators. Remark that it is easily seen from (11) that $P^{\alpha\varphi}$ is not a BDF-stable vacuum.

2.4 Existence of a BDF-stable vacuum

We may now state our main Theorem.

Theorem 4 (Existence of a BDF-stable vacuum). *Let be $2 - \sqrt{2} \leq b < 1$, $Z \geq 0$ and $n \in \mathcal{C} \cap L^1(\mathbb{R}^3)$ such that $n \geq 0$ and $\int_{\mathbb{R}^3} n = 1$. Then for all Λ, there exists an $\alpha_b(\Lambda) > 0$ such that for all α which satisfies*

$$4\sqrt{\pi}\alpha Z \|n\|_{\mathcal{C}} \leq b \quad \textit{and} \quad \alpha \leq \alpha_b(\Lambda)$$

where

$$\alpha_b(\Lambda) \sim_{\Lambda\to\infty} \frac{C(1-b)}{\sqrt{\log \Lambda}},$$

there exists a unique stable vacuum P in some ball $B(P^0, R_0(\alpha,\Lambda)) \subset \mathcal{P}_\Lambda$ containing $P^{\alpha\varphi}$, which is a solution of

$$P = \chi_{(-\infty;0)} \left(D^0 + \alpha(\rho_Q - Zn) * \frac{1}{|\cdot|} + \alpha \frac{Q(x,y)}{|x-y|} \right)$$

with $Q = P - P^0$.

Remarks: A precise definition of the constant C appearing in this result is given in the proof, but we do not know an explicit formula. However, we have obtained numerically the bound $C \geq 0.798$.

$\mathcal{P}_\Lambda$ is naturally equipped with the metric

$$d(P_1, P_2) = \|P_1 - P_2\|_{\mathfrak{S}_2(\mathcal{H}_\Lambda)}$$

which is weaker than the one we use in the proof (and which defines the ball in Theorem 4).

3 Proof of Theorem 3

In this section, we prove Theorem 3. To this end, we first need to prove Theorem 1.

3.1 Proof of Theorem 1

Let be P and P' two projectors such that $P' - P \in \mathfrak{S}_2(\mathcal{H})$, and a Hilbert-Schmidt operator A which is supertrace-class with respect to P. This means that PAP and $(1-P)A(1-P)$ are trace-class.

Let us first show that $P'AP'$ is trace-class. To this end, we write

$$\begin{aligned} P'AP' &= (P'-P+P)A(P'-P+P) \\ &= (P'-P)A(P'-P) + (P'-P)AP + PA(P'-P) + PAP. \end{aligned} \tag{12}$$

This shows that $P'AP'$ is trace-class since the last term is in $\mathfrak{S}_1$ by assumption, $P'-P$ and A are in $\mathfrak{S}_2$, and P is bounded. The same computation shows that $(1-P')A(1-P')$ is trace-class.

We now compute

$$\begin{aligned} \mathrm{tr}[P'AP'] &= \mathrm{tr}[(P'-P)A(P'-P)] + \mathrm{tr}[(P'-P)AP] + \mathrm{tr}[PA(P'-P)] + \mathrm{tr}[PAP] \\ &= \mathrm{tr}[A\left((P'-P)(P'-P) + P(P'-P) + (P'-P)P\right)] + \mathrm{tr}[PAP] \\ &= \mathrm{tr}[A(P'-P)] + \mathrm{tr}[PAP], \end{aligned}$$

where we have used the formula $\mathrm{tr}(AB) = \mathrm{tr}(BA)$, valid for $A, B \in \mathfrak{S}_2$. The same computation gives

$$\mathrm{tr}[P'_+AP'_+] = \mathrm{tr}[A(P'_+ - P_+)] + \mathrm{tr}[P_+AP_+] = -\mathrm{tr}[A(P'-P)] + \mathrm{tr}[P_+AP_+],$$

where we have used the notation $P_+ = 1-P$ and $P'_+ = 1-P'$. Summing this two results, we obtain the formula $\mathrm{str}_P[A] = \mathrm{str}_{P'}[A]$. □

3.2 Preliminaries

To prove Theorem 3, we need the following

Lemma 2. *Assume that $\varphi = \rho * \frac{1}{|\cdot|}$ for some $\rho \in \mathcal{C}$. Then*

$$\|\nabla\varphi\|_{H^1} = 4\pi\|\rho\|_{\mathcal{C}}, \qquad \|\varphi\|_{L^\infty} \leq C_\infty 4\pi\|\rho\|_{\mathcal{C}}, \qquad \|\varphi\|_{L^6} \leq C_6 4\pi\|\rho\|_{\mathcal{C}}$$

where $C_\infty := \frac{1}{2\pi^{1/2}}$ and C_6 is the Sobolev constant for the inequality $\|u\|_{L^6(\mathbb{R}^3)} \leq C_6 \|\nabla u\|_{L^2(\mathbb{R}^3)}$.

Proof – We have

$$\int_{\mathbb{R}^3} \frac{1+|k|^2}{|k|^2} |\widehat{\rho}(k)|^2 \, dk = \frac{1}{(4\pi)^2} \int_{\mathbb{R}^3} |k|^2(1+|k|^2)|\widehat{\varphi}(k)|^2 \, dk,$$

and so

$$\|\varphi\|_{L^\infty} \leq \frac{1}{(2\pi)^{3/2}} \|\hat{\varphi}\|_{L^1} \leq \frac{1}{(2\pi)^{3/2}} \left(\int_{\mathbb{R}^3} \frac{dk}{|k|^2(1+|k|^2)} \right)^{1/2} 4\pi\|\rho\|_{\mathcal{C}}.$$

The rest is easily obtained by the Sobolev inequalities. □

Lemma 3. *Let P be a projector such that $P - P^0 \in \mathcal{A}_\Lambda$. Then D_Q is bounded.*

Proof – Due to the cut-off in Fourier space, D^0 is bounded on $\mathcal{H}_\Lambda$. On the other hand, if $\varphi = \rho * \frac{1}{|\cdot|}$ for some $\rho \in \mathcal{C}$, then $\varphi \in L^\infty$ by Lemma 2 and so this is also a bounded operator. Let us now denote $R(x,y) = \frac{Q(x,y)}{|x-y|}$. We then have

$$|Rf(x)|^2 = \left| \int_{\mathbb{R}^3} \frac{Q(x,y) f(y)}{|x-y|}\, dy \right|^2 \leq \left(\int_{\mathbb{R}^3} \frac{|Q(x,y)|^2}{|x-y|}\, dy \right) \times \left(\int_{\mathbb{R}^3} \frac{|f(y)|^2}{|x-y|}\, dy \right)$$

and since, by a Hardy-type inequality,

$$\int_{\mathbb{R}^3} \frac{|f(y)|^2}{|x-y|}\, dy \leq \frac{\pi}{2} \langle f, |D^0| f \rangle$$

$$\iint_{\mathbb{R}^6} \frac{|Q(x,y)|^2}{|x-y|}\, dx\, dy \leq \frac{\pi}{2} \operatorname{tr}(|D^0|\, Q^2) \tag{13}$$

this shows that $R \leq C\, |D^0|^{1/2}$ and so R is bounded. □

Lemma 4. *Let be P a projector such that $P - P^0 \in \mathcal{A}_\Lambda$. Then $D_Q\Gamma \in \mathfrak{S}_1^{P_0}(\mathcal{H}_\Lambda)$ for all $\Gamma \in \mathcal{A}_\Lambda$ and we have*

$$\operatorname{str}_{P^0}(D^0\Gamma) + \alpha \int_{\mathbb{R}^3} \rho_\Gamma \left((\rho_Q - Zn) * \frac{1}{|\cdot|} \right) + \alpha \operatorname{tr} \left(\frac{Q(x,y)}{|x-y|} \Gamma \right) = \operatorname{str}_{P^0}(D_Q\Gamma).$$

Proof – Remark that $R\Gamma = \frac{Q(x,y)}{|x-y|}\Gamma$ is trace-class, since $\frac{Q(x,y)}{|x-y|^{1/2}}$ and $\frac{\Gamma(x,y)}{|x-y|^{1/2}}$ are in $\mathfrak{S}_2$ by (13). Let us now define $D = D^{-\alpha(\rho_Q - Zn) * \frac{1}{|\cdot|}} = D^0 + \alpha(\rho_Q - Zn) * \frac{1}{|\cdot|}$ and $P' = \chi_{(-\infty;0)}(D)$. By the result of Klaus-Scharf [21] (see also [17] and the proof of Theorem 4), it is known that $P' - P^0 \in \mathfrak{S}_2(\mathcal{H}_\Lambda)$. Thus $P'D\Gamma P' = DP'\Gamma P' \in \mathfrak{S}_1(\mathcal{H}_\Lambda)$ since $\Gamma \in \mathfrak{S}_1^{P_0} = \mathfrak{S}_1^{P'}$ by Theorem 1, and D is bounded by the proof of Lemma 3. Therefore, $D_Q\Gamma = D\Gamma + R\Gamma$ is in $\mathfrak{S}_1^{P_0}$.

To show the expected equality, we show

$$\operatorname{str}_{P^0}(D^0\Gamma) + \alpha \int_{\mathbb{R}^3} \rho_\Gamma \varphi'_Q = \operatorname{str}_{P^0}(D\Gamma) \tag{14}$$

where $\varphi'_Q = \rho'_Q * \frac{1}{|\cdot|}$, $\rho'_Q = \rho_Q - Zn \in \mathcal{C}$. This will end the proof since the other term is trace-class. The general idea of the proof is to approximate Γ by a trace-class operator for which this equality is true, and to pass to the limit. However, the behaviour of the associated density in the space $\mathcal{C}$ is not obvious and to overcome this difficulty, we shall also approximate the density ρ'_Q to obtain a potential in $L^2(\mathbb{R}^3)$. We thus start by choosing a sequence ρ_j which converges as $j \to +\infty$ to ρ'_Q in $\mathcal{C}$, such that $\varphi_j = \rho_j * \frac{1}{|\cdot|}$ is in $L^2(\mathbb{R}^3)$. We can choose for instance $\widehat{\rho_j}(k) = \widehat{\rho'_Q}(k)\chi(|k| \geq 1/j)$. We now show

$$\operatorname{str}_{P^0}(D^0\Gamma) + \alpha \int_{\mathbb{R}^3} \rho_\Gamma \varphi_j = \operatorname{str}_{P^0}(D_j\Gamma) \tag{15}$$

for all $\Gamma \in \mathcal{A}_\Lambda$, and where $D_j = D^0 - \alpha\varphi_j$. To this end, we may find a sequence Γ^n_{+-} of finite rank operator which converges to $\Gamma_{+-} = (1 - P^0)\Gamma P^0$ in $\mathfrak{S}_2$. Then

$$\Gamma^n := \begin{pmatrix} \Gamma_{++} & \Gamma^n_{+-} \\ (\Gamma^n_{+-})^* & \Gamma_{--} \end{pmatrix}$$

converges to Γ in $\mathfrak{S}_2$. Since $\Gamma^n \in \mathfrak{S}_1$ for all $n \geq 0$, we have

$$\operatorname{str}_{P^0}(D^0\Gamma^n) + \alpha \int_{\mathbb{R}^3} \rho_{\Gamma^n} \varphi_j = \operatorname{str}_{P^0}(D_j\Gamma^n). \tag{16}$$

By (6), the function $Q \in \mathfrak{S}_2(\mathcal{H}_\Lambda) \mapsto \rho_Q \in L^2(\mathbb{R}^3)$ is continuous. Therefore, $\rho_{\Gamma^n} \to \rho_\Gamma$ in $L^2(\mathbb{R}^3)$. Since $\varphi_j \in L^2(\mathbb{R}^3)$, we may now pass to the limit in (16) and obtain

$$\lim_{n\to\infty} \left(\mathrm{str}_{P^0}(D^0\Gamma^n) + \alpha \int_{\mathbb{R}^3} \rho_{\Gamma^n}\varphi_j \right) = \mathrm{str}_{P^0}(D^0\Gamma) + \alpha \int_{\mathbb{R}^3} \rho_\Gamma \varphi_j,$$

where we have used that

$$\mathrm{str}_{P^0}(D^0\Gamma^n) = \mathrm{tr}(D^0\Gamma^n_{++}) + \mathrm{tr}(D^0\Gamma^n_{--}) = \mathrm{tr}(D^0\Gamma_{++}) + \mathrm{tr}(D^0\Gamma_{--}) = \mathrm{str}_{P^0}(D^0\Gamma).$$

Let us now pass to the limit in the right hand side. Indeed, we can write, by Theorem 1,

$$\mathrm{str}_{P^0}(D_j\Gamma^n) = \mathrm{str}_{P'_j}(D_j\Gamma^n) = \mathrm{tr}(D_jP'_j\Gamma^nP'_j) + \mathrm{tr}(D_j(1-P'_j)\Gamma^n(1-P'_j))$$

where $P'_j = \chi_{(-\infty;0)}(D_j)$ and since $P'_j - P^0 \in \mathfrak{S}_2$ by [21]. Now, using (12), it is easily seen that $P'_j\Gamma^nP'_j \to P'_j\Gamma P'_j$ and $(1-P'_j)\Gamma^n(1-P'_j) \to (1-P'_j)\Gamma(1-P'_j)$ in $\mathfrak{S}_1$ as $n \to \infty$, since this terms can be expanded as a sum of trace-class operators and products of at least two Hilbert-Schmidt operators converging strongly in $\mathfrak{S}_2$. Since D_j is bounded by the proof of Lemma 3, we obtain that $\mathrm{str}_{P'_j}(D_j\Gamma^n) \to_{n\to\infty} \mathrm{str}_{P'_j}(D_j\Gamma) = \mathrm{str}_{P^0}(D_j\Gamma)$ by Theorem 1.

As a conclusion, we have proved (15) for all $\Gamma \in \mathcal{A}_\Lambda$. To finish the proof, it remains to pass to the limit as $j \to +\infty$. Since

$$\int_{\mathbb{R}^3} \rho_\Gamma \varphi_j = D(\rho_\Gamma, \rho_j)$$

and $\rho_\Gamma \in \mathcal{C}$ (recall that $\Gamma \in \mathcal{A}_\Lambda$), $\rho_j \to \rho'_Q$ strongly in $\mathcal{C}$ as $j \to \infty$, we may pass to the limit in the left hand side of (15). To pass to the limit in the right hand side, we use again the fact that

$$\mathrm{str}_{P^0}(D_j\Gamma) = \mathrm{str}_{P'_j}(D_j\Gamma) = \mathrm{tr}(D_jP'_j\Gamma P'_j) + \mathrm{tr}(D_j(1-P'_j)\Gamma(1-P'_j)).$$

By the results of Klaus-Scharf [21] (see also the proof of Theorem 4), it is known that $P'_j - P' \to 0$ in $\mathfrak{S}_2$, since $\rho_j \to \rho'_Q$ in $\mathcal{C}$. Using again (12), it is then easily seen that $P'_j\Gamma P'_j \to P'\Gamma P'$ and $(1-P'_j)\Gamma(1-P'_j) \to (1-P')\Gamma(1-P')$ in $\mathfrak{S}_1$ as $j \to \infty$. Since $D_j \to D$ in $\mathfrak{S}_\infty$ by Lemma 3, we may thus pass to the limit and obtain the desired equality (14). □

3.3 Proof of Theorem 3

We are now able to prove Theorem 3.

We start by proving 1) ⇒ 2). We thus consider a projector P that satisfies the assumption of the Theorem, and is also a solution to the equation $P = \chi_{(-\infty;0)}(D_Q)$. We fix some $\Gamma \in \mathcal{B}_\Lambda$ and show that $\mathcal{E}(\Gamma) \geq \mathcal{E}(Q)$. To this end, we write $\mathcal{E}(\Gamma) = \mathcal{E}(Q+\Gamma')$ where $\Gamma' = \Gamma - Q = \Gamma + P^0 - P$. By assumption, Γ fulfills $-P^0 \leq \Gamma \leq 1 - P^0$, and so Γ' fulfills $-P \leq \Gamma' \leq 1 - P$. Using Lemma 4, we may expand $\mathcal{E}(Q+\Gamma')$ and obtain

$$\mathcal{E}(Q+\Gamma') = \mathrm{str}_{P^0}\left(D_Q\Gamma'\right) + \frac{\alpha}{2}\iint \frac{\rho_{\Gamma'}(x)\rho_{\Gamma'}(y)}{|x-y|}dx\,dy - \frac{\alpha}{2}\iint \frac{|\Gamma'(x,y)|^2}{|x-y|}dx\,dy + \mathcal{E}(Q).$$

It is thus sufficient to prove that

$$\mathrm{str}_{P^0}\left(D_Q\Gamma'\right) + \frac{\alpha}{2}\iint \frac{\rho_{\Gamma'}(x)\rho_{\Gamma'}(y)}{|x-y|}dx\,dy - \frac{\alpha}{2}\iint \frac{|\Gamma'(x,y)|^2}{|x-y|}dx\,dy \geq 0.$$

Indeed we now essentially follow the proof of Theorem 2: we have

$$\iint \frac{\rho_{\Gamma'}(x)\rho_{\Gamma'}(y)}{|x-y|}dx\,dy \geq 0$$

and

$$\iint \frac{|\Gamma'(x,y)|^2}{|x-y|}dx\,dy \leq \frac{\pi}{2}\operatorname{tr}(|D^0|(\Gamma')^2) \leq \frac{\pi d}{2}\operatorname{tr}(|D_Q|(\Gamma')^2)$$

since by assumption $|D^0| \leq d|D_Q|$. From $-P \leq \Gamma' \leq 1-P$, we obtain as before $(\Gamma')^2 \leq P\Gamma'P - (1-P)\Gamma'(1-P)$. We thus have

$$\iint \frac{|\Gamma'(x,y)|^2}{|x-y|}dx\,dy \leq \frac{\pi d}{2}\operatorname{tr}\left[|D_Q|(P\Gamma'P-(1-P)\Gamma'(1-P))\right] = \frac{\pi d}{2}\operatorname{str}_P(D_Q\Gamma')$$

since P commutes with D_Q. Using Theorem 1 and the fact that $P - P^0 \in \mathfrak{S}_2$, we deduce that $\operatorname{str}_{P^0}(D_Q\Gamma') = \operatorname{str}_P(D_Q\Gamma') \geq 0$ and

$$\operatorname{str}_{P^0}\left(D_Q\Gamma'\right) + \frac{\alpha}{2}\iint \frac{\rho_{\Gamma'}(x)\rho_{\Gamma'}(y)}{|x-y|}dx\,dy - \frac{\alpha}{2}\iint \frac{|\Gamma'(x,y)|^2}{|x-y|}dx\,dy \geq \left(1-\alpha d\frac{\pi}{4}\right)\operatorname{str}_P(D_Q\Gamma') \geq 0$$

when $\alpha d\frac{\pi}{4} \leq 1$, which ends the proof of this first part.

We now show 2) $\Rightarrow$ 1). Let be P which satisfies the assumption of the Theorem, and such that $Q = P - P^0$ is a minimizer of $\mathcal{E}$ in $\mathcal{B}_\Lambda$. We therefore have for all $\gamma \in \mathfrak{S}_1 \cap \mathcal{A}_\Lambda$ such that $-P \leq \gamma \leq 1-P$

$$\mathcal{E}(Q+\gamma) \geq \mathcal{E}(Q)$$

or equivalently

$$\mathcal{E}'(\gamma) := \operatorname{tr}(D_Q\gamma) + \frac{\alpha}{2}\iint \frac{\rho_\gamma(x)\rho_\gamma(y)}{|x-y|}dx\,dy - \frac{\alpha}{2}\iint \frac{|\gamma(x,y)|^2}{|x-y|}dx\,dy \geq 0. \tag{17}$$

We now follow the proof of Theorem 4 by Bach *et al.* [2]. Their proof is done with D_Q replaced by $D^{\alpha\varphi}$ but they also mention that it can be extended to a more general case, provided $0 \notin \sigma(D_Q)$ and P, $1-P$ leave the domain of D_Q invariant, which is the case here. Let us however explain the general ideas of this proof for the reader's convenience.

If P does not commute with $\chi_{(-\infty;0)}(D_Q)$, then there exist two normalized vectors $f \in (1-P)\mathcal{H}_\Lambda$ and $g \in P\mathcal{H}_\Lambda$ such that the real part of $\langle f, D_Q g\rangle$ is not 0. We now let

$$\gamma_\epsilon = \epsilon^2\left(|f\rangle\langle f| - |g\rangle\langle g|\right) + \epsilon\sqrt{1-\epsilon^2}\left(|f\rangle\langle g| + |g\rangle\langle f|\right)$$

which is a trace-class operator satisfying $-P \leq \gamma \leq 1-P$. Computing now the energy (17) of γ_ϵ yields

$$\mathcal{E}'(\gamma_\epsilon) = 2\epsilon\,\Re\langle f, D_Q g\rangle + O(\epsilon^2)$$

which contradicts (17) since this can be made negative for ϵ small enough. This implies that P commutes with D_Q, and so it commutes with all spectral projections of D_Q, and namely with $P' = \chi_{(-\infty;0)}(D_Q)$ and $1-P'$.

We now show that $P = P' = \chi_{(-\infty;0)}(D_Q)$. Suppose that there exists a $u \in (1-P)\mathcal{H}_\Lambda \cap P'\mathcal{H}_\Lambda$. We then let $\gamma_0 = |u\rangle\langle u|$. The corresponding energy is then

$$\mathcal{E}'(\gamma_0) = \langle u, D_Q u\rangle < 0,$$

since the exchange and non-exchange terms cancel. This contradicts (17). Since we may show with the same argument that $P\mathcal{H}_\Lambda \cap (P'\mathcal{H}_\Lambda)^c = \emptyset$, we obtain that $P = P' = \chi_{(-\infty;0)}(D_Q)$. □

4 Proof of Theorem 4

In this section, we prove Theorem 4 by using a Banach fixed-point method.

4.1 Preliminaries

We start by defining the norms and spaces that will be used to apply this well-known result. In fact, the main challenge concerning the fixed-point argument consisted in finding suitable Banach spaces.

Norms and spaces

We choose the following norms

$$\|Q\|_{\mathcal{Q}} := \left(\iint E(p-q)^2 E(p+q) |\widehat{Q}(p,q)|^2 \, dp \, dq \right)^{1/2},$$

$$\|R\|_{\mathcal{R}} := \left(\iint \frac{E(p-q)^2}{E(p+q)} |\widehat{R}(p,q)|^2 \, dp \, dq \right)^{1/2},$$

$$\|\rho\|_{\mathcal{C}} := \left(\int \frac{E(k)^2}{|k|^2} |\widehat{\rho}(k)|^2 \, dk \right)^{1/2},$$

$$\|\varphi\|_{\mathcal{Y}} := \left(\int |k|^2 E(k)^2 |\widehat{\varphi}(k)|^2 \, dk \right)^{1/2},$$

where

$$E(k) = \sqrt{1+|k|^2}$$

and denote by $\mathcal{Q}$, $\mathcal{R}$, $\mathcal{C}$ and $\mathcal{Y}$ the associated Hilbert spaces. The dual space $\mathcal{C}'$ of $\mathcal{C}$ will be also useful and we introduce

$$\|\zeta\|_{\mathcal{C}'} := \int \frac{|k|^2}{E(k)^2} |\hat{\zeta}(k)|^2 \, dk.$$

In the following, it will be easier to use the norm $\|R\|_{\mathcal{R}}$ where $R = \frac{Q(x,y)}{|x-y|}$ in our estimates and a relation with $\|Q\|_{\mathcal{Q}}$ will then be needed. To this end, we first need the following Lemma, which will be useful throughout the rest of the proof.

Lemma 5. *For all ξ and η in $\mathbb{R}^3$, we have*

$$\forall s \geq 0, \;\; E(\xi)^s \leq 2^{\delta(s)} \left(E(\xi-\eta)^s + E(\eta)^s \right) \tag{18}$$

$$\forall s \in \mathbb{R}, \;\; E(\xi)^s \leq 2^{|s|} E(\xi-\eta)^s E(\eta)^{|s|}, \tag{19}$$

with

$$\delta(s) = \begin{cases} s & \text{if} \quad 0 \leq s < 1 \\ s-1 & \text{if} \quad s \geq 1 \end{cases}.$$

Proof – We have $E(\xi) = \|(1,\xi)\| \leq \|(1,\xi-\eta)\| + \|(0,\eta)\| \leq \|(1,\xi-\eta)\| + \|(1,\eta)\|$, proving (18) when $s = 1$. Now, for $s \geq 1$, the result follows from the convexity of $x \mapsto x^s$ on $[1;+\infty)$, using $(a/2 + b/2)^s \leq a^s/2 + b^s/2$. When $s \in [0;1)$, we simply write $(a+b)^s = (a+b)^{s+1}/(a+b) \leq 2^s a^s a/(a+b) + 2^s b^s b/(a+b) \leq 2^s(a^s + b^s)$, ending the proof of (18). On the other hand, the Peetre inequality (19), is easily obtained by reduction to the case $s = 1$. □

Remark: A trivial consequence of (18) is the following inequality

$$\frac{1}{E(p)+E(q)} \leq \min\left(\frac{1}{E(p+q)}, \frac{1}{E(p-q)} \right). \tag{20}$$

Now we can give a connection between $\|R\|_{\mathcal{R}}$ and $\|Q\|_{\mathcal{Q}}$ when $R = \frac{Q(x,y)}{|x-y|}$ (we also recall the easy relation between $\|\rho\|_{\mathcal{C}}$ and $\|\varphi\|_{\mathcal{Y}}$ when $\varphi = \rho * \frac{1}{|\cdot|}$).

Lemma 6. *If $\rho \in \mathcal{C}$ and $Q \in \mathcal{Q}$, then we have $\varphi = \rho * \frac{1}{|\cdot|} \in \mathcal{Y}$ and $R(x,y) = \frac{Q(x,y)}{|x-y|} \in \mathcal{R}$ and more precisely*

$$\begin{aligned} \|\varphi\|_{\mathcal{Y}} &= 4\pi \|\rho\|_{\mathcal{C}}, \\ \|R\|_{\mathcal{R}} &\leq C_R \|Q\|_{\mathcal{Q}}, \\ \left\| R \cdot |D_0|^{-1/2} \right\|_{\mathfrak{S}_2} &\leq 2\|R\|_{\mathcal{R}}, \end{aligned} \tag{21}$$

with

$$C_R := \frac{1}{2\pi^2} \inf_{\theta \in (0;2)} \sup_{x \in \mathbb{R}^3} \left(E(2x)^\theta \int_{\mathbb{R}^3} \frac{du}{E(2u)^{1+\theta} |u-x|^2} \right). \tag{22}$$

Proof of Lemma 6 – We have

$$\widehat{R}(p,q) = \frac{1}{2\pi^2} \int_{\mathbb{R}^3} \frac{\widehat{Q}(p-l, q-l)}{|l|^2} \, dl$$

so we obtain, for some fixed $\theta \in (0;2)$

$$\begin{aligned} \|R\|_{\mathcal{R}}^2 &= \iint \frac{E(p-q)^2}{E(p+q)} |\widehat{R}(p,q)|^2 \, dp \, dq \\ &= 8 \iint \frac{E(2v)^2}{E(2u)} |\widehat{R}(u+v, u-v)|^2 \, du \, dv \\ &= \frac{8}{(2\pi^2)^2} \iiiint \frac{E(2v)^2}{E(2u)} \frac{\widehat{Q}(l+v, l-v) \cdot \widehat{Q}(l'+v, l'-v)}{|l-u|^2 |l'-u|^2} \, du \, dv \, dl \, dl' \\ &= \frac{8}{(2\pi^2)^2} \iint du \, dv \frac{E(2v)^2}{E(2u)} \iint \frac{E(2l)^{\frac{1+\theta}{2}} \widehat{Q}(l+v, l-v) \, E(2l')^{\frac{1+\theta}{2}} \widehat{Q}(l'+v, l'-v)}{E(2l')^{\frac{1+\theta}{2}} |l-u| \, |l'-u| \, E(2l)^{\frac{1+\theta}{2}} |l-u| \, |l'-u|} dl \, dl' \\ &\leq \frac{8}{(2\pi^2)^2} \iiiint \frac{E(2v)^2}{E(2u)} \frac{E(2l)^{1+\theta}}{E(2l')^{1+\theta}} \frac{|\widehat{Q}(l+v, l-v)|^2}{|l-u|^2 |l'-u|^2} \, du \, dv \, dl \, dl' \\ &\leq 8 \iint E(2v)^2 E(2l) |\widehat{Q}(l+v, l-v)|^2 K_\theta(l) \, dv \, dl \end{aligned}$$

where

$$K_\theta(l) := \frac{E(2l)^\theta}{(2\pi^2)^2} \iint \frac{1}{E(2u) \cdot E(2l')^{1+\theta} |l-u|^2 |l'-u|^2} \, du \, dl'.$$

Now, let us introduce

$$C_\theta := \sup_{x \in \mathbb{R}^3} \left(E(2x)^\theta \int_{\mathbb{R}^3} \frac{du}{E(2u)^{1+\theta} |u-x|^2} \right).$$

Remark that

$$\int_{\mathbb{R}^3} \frac{du}{E(2u)^{1+\theta} |u-x|^2} \leq \frac{1}{2^{1+\theta} |x|^\theta} \int_{\mathbb{R}^3} \frac{du}{|u|^{1+\theta} |u - e_x|^2}$$

where $e_x := x/|x|$, showing that $C_\theta < \infty$ when $\theta \in (0;2)$. Now we have

$$\begin{aligned} K_\theta(l) &= \frac{E(2l)^\theta}{(2\pi^2)^2} \int du \frac{1}{E(2u)^{1+\theta} |l-u|^2} \left(E(2u)^\theta \int \frac{1}{E(2l')^{1+\theta} |l'-u|^2} dl' \right) \\ &\leq \frac{E(2l)^\theta}{(2\pi^2)^2} \int du \frac{1}{E(2u)^{1+\theta} |l-u|^2} \times C_\theta \leq \left(\frac{C_\theta}{2\pi^2} \right)^2 \end{aligned}$$

and so

$$\|R\|_{\mathcal{R}}^2 \leq 8\left(\frac{C_\theta}{2\pi^2}\right)^2 \iint E(2v)^2 E(2l)|\widehat{Q}(l+v,l-v)|^2\,dv\,dl \leq \left(\frac{C_\theta}{2\pi^2}\right)^2 \|Q\|_{\mathcal{Q}}^2$$

which ends the proof of (21).

Finally, we remark that we have

$$\left\|R\cdot|D_0|^{-1/2}\right\|_{\mathfrak{S}_2}^2 = \iint \frac{|\widehat{R}(p,q)|^2}{E(p)}\,dp\,dq \leq 2\iint \frac{|\widehat{R}(p,q)|^2}{E(2p)}\,dp\,dq$$
$$\leq 4\iint \frac{E(p-q)|\widehat{R}(p,q)|^2}{E(p+q)}\,dp\,dq \leq 4\|R\|_{\mathcal{R}}^2$$

by Lemma 5 □

An estimate from below for D_Q

We now state a Lemma in which we give a lower estimate for the operator

$$D_{Q,\rho} := D^{\alpha\varphi} + \alpha\rho * \frac{1}{|r|} - \alpha\frac{Q(x,y)}{|x-y|}$$

by D^0, in terms of the spaces introduced above.

For our result, we are interested in $D_Q = D_{Q,\rho_Q}$ but this definition with a different ρ will be useful in the following.

Lemma 7. *Assume that $(Q,\rho) \in \mathcal{Q}\times\mathcal{C}$ are such that*

$$\alpha\left(2\sqrt{\pi}\|\rho - Zn\|_{\mathcal{C}} + 2C_R\|Q\|_{\mathcal{Q}}\right) < 1. \tag{23}$$

Then $D_{Q,\rho}$ is a bounded operator which satisfies

$$|D_{Q,\rho}| \geq \left(1 - \alpha\left(2\sqrt{\pi}\|\rho - Zn\|_{\mathcal{C}} + 2C_R\|Q\|_{\mathcal{Q}}\right)\right)|D^0|. \tag{24}$$

Proof – We have, with $\varphi' = (\rho - Zn) * \frac{1}{|\cdot|}$,

$$\left\|\varphi' u\right\|_{L^2} \leq \left\|\varphi'\right\|_{L^\infty}\|u\|_{L^2} \leq 2\pi^{1/2}\|\rho - Zn\|_{\mathcal{C}}\,\||D_0|\cdot u\|_{L^2}$$

by Lemma 2, and

$$\|Ru\|_{L^2} = \left\|R|D_0|^{-1/2}|D_0|^{1/2}u\right\|_{L^2} \leq \left\|R|D_0|^{-1/2}\right\|_{\mathfrak{S}_2}\left\||D_0|^{1/2}u\right\|_{L^2} \leq 2C_R\|Q\|_{\mathcal{Q}}\,\||D_0|\cdot u\|_{L^2}$$

by Lemma 6. This shows that $|\varphi' - R| \leq (2\pi^{1/2}\|\rho_Q - Zn\|_{\mathcal{C}} + 2C_R\|Q\|_{\mathcal{Q}})|D^0|$, the square root being monotone. This proves that $D_{Q,\rho}$ is bounded since D_0 is bounded on $\mathcal{H}_\Lambda$, and gives the expected inequality. □

Remark that Lemma 7 will be useful when we shall apply Theorem 3 (see the condition (10) in the statement). It also implies $0 \notin \sigma(D_{Q,\rho})$, a fact that will be used to compute the projection $\chi_{(-\infty;0)}(D_{Q,\rho})$.

Expansion by Cauchy's formula

We want to solve the equation

$$Q = \chi_{(-\infty;0)}\left(D^0 + \alpha(\rho_Q - Zn) * \frac{1}{|r|} - \alpha\frac{Q(x,y)}{|x-y|}\right) - \chi_{(-\infty;0)}(D^0) := F_1(Q).$$

If $\alpha\,(2\sqrt{\pi}\|\rho_Q - Zn\|_{\mathcal{C}} + 2C_R\|Q\|_{\mathcal{Q}}) < 1$, then $0 \notin \sigma(D_Q)$ by Lemma 7. We may thus use the method of [16] and expand F_1 by Cauchy's formula

$$F_1(Q) = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\eta \left(\frac{1}{D_Q + i\eta} - \frac{1}{D^0 + i\eta}\right) = \sum_{n=1}^{\infty} \alpha^n Q_n$$

where

$$Q_n = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\eta \frac{1}{D^0 + i\eta}\left((R_Q - \varphi'_Q)\frac{1}{D^0 + i\eta}\right)^n$$

$$\rho'_Q = \rho_Q - Zn, \quad \varphi'_Q = \rho'_Q * \frac{1}{|r|}, \quad R_Q(x,y) = \frac{Q(x,y)}{|x-y|}.$$

We shall write

$$Q_n = \sum_{k,l/\ k+l=n} Q_{k,l}$$

$$Q_{k,l} = \frac{(-1)^{l+1}}{2\pi} \sum_{I\cup J=\{1,\dots,n\},\ |I|=k,\ |J|=l} \int_{-\infty}^{+\infty} d\eta \frac{1}{D^0 + i\eta}\prod_{j=1}^{n}\left(R_j \frac{1}{D^0 + i\eta}\right)$$

where $R_j = R_Q$ if $j \in I$ and $R_j = \varphi'_Q$ if $j \in J$ ($Q_{k,l}$ is the sum of all the terms containing k R_Q's and l φ'_Q's). We also denote $\rho_{k,l} := \rho_{Q_{k,l}}$.

Hence our equation can be written

$$\begin{cases} Q = \displaystyle\sum_{n=1}^{\infty} \alpha^n Q_n(Q, \rho_Q) \\ \rho_Q = \displaystyle\sum_{n=1}^{\infty} \alpha^n \rho_n(Q, \rho_Q), \end{cases} \tag{25}$$

where we recall that Q_n and ρ_n depend on both Q and ρ_Q. In order to have a better condition on α and Λ, we shall now change the second equation for the density, by taking into account the special form of the first order term ρ_1. To this end, we need to compute this term explicitely.

The first order density

Recall that

$$Q_{0,1} = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\eta \frac{1}{D^0 + i\eta}\varphi'_Q \frac{1}{D^0 + i\eta}$$

so that

$$\widehat{Q_{0,1}}(p,q) = (2\pi)^{-5/2}\int_{-\infty}^{+\infty} d\eta \frac{1}{\boldsymbol{\alpha}\cdot p + \beta + i\eta}\widehat{\varphi'_Q}(p-q)\frac{1}{\boldsymbol{\alpha}\cdot q + \beta + i\eta}.$$

We now introduce

$$\begin{aligned} M(p,q) &:= \frac{1}{\pi}\int_{-\infty}^{+\infty} d\eta \frac{1}{\boldsymbol{\alpha}\cdot p + \beta + i\eta}\cdot\frac{1}{\boldsymbol{\alpha}\cdot q + \beta + i\eta} \\ &= \frac{1}{\pi}\int_{-\infty}^{+\infty} d\eta \frac{\boldsymbol{\alpha}\cdot p + \beta - i\eta}{p^2 + 1 + \eta^2}\cdot\frac{\boldsymbol{\alpha}\cdot q + \beta - i\eta}{q^2 + 1 + \eta^2} \\ &= \frac{1}{E(p) + E(q)}\left(\frac{(\boldsymbol{\alpha}\cdot p + \beta)}{E(p)}\frac{(\boldsymbol{\alpha}\cdot q + \beta)}{E(q)} - 1\right). \end{aligned} \tag{26}$$

Hence

$$\widehat{Q_{0,1}}(p,q) = \frac{1}{2^{5/2}\pi^{3/2}}\widehat{\varphi'_Q}(p-q)M(p,q).$$

This enables us to compute

$$\begin{aligned}
\widehat{\rho_{0,1}}(k) &= \frac{1}{(2\pi)^{3/2}}\int_{|l|\leq\Lambda} \mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q_{0,1}}(l+k/2,l-k/2)\right)dl \\
&= \frac{1}{16\pi^3}\widehat{\varphi'_Q}(k)\int_{|l|\leq\Lambda} \mathrm{Tr}_{\mathbb{C}^4}\left(M(l+k/2,l-k/2)\right)dl \\
&= -\frac{1}{4\pi^2}\widehat{\varphi'_Q}(k)|k|^2 B'_\Lambda(k) = -\frac{1}{\pi}\widehat{\rho'_Q}(k)B'_\Lambda(k) \\
&= \frac{1}{\pi}(Z\widehat{n}(k) - \widehat{\rho_Q}(k))B'_\Lambda(k) \qquad (27)
\end{aligned}$$

where

$$B'_\Lambda(k) = -\frac{1}{\pi|k|^2}\int_{|l|\leq\Lambda} \frac{(l+k/2)\cdot(l-k/2)+1-E(l+k/2)E(l-k/2)}{E(l+k/2)E(l-k/2)(E(l+k/2)+E(l-k/2))}dl.$$

This function is computed in [26]

$$B'_\Lambda(k) = \int_0^{\frac{\Lambda}{E(\Lambda)}} \frac{z^2-z^4/3}{1-z^2}\frac{dz}{1+|k|^2(1-z^2)/4}$$

and so for instance

$$B'_\Lambda(k) \leq B'_\Lambda(0) = \int_0^{\frac{\Lambda}{E(\Lambda)}} \frac{z^2-z^4/3}{1-z^2}\,dz = \frac{2}{3}\log(\Lambda) - \frac{5}{9} + \frac{2}{3}\log 2 + O(1/\Lambda^2).$$

In the following, we shall use the notation $B_\Lambda := \frac{B'_\Lambda(0)}{\pi} \sim_{\Lambda\to\infty} \frac{2}{3\pi}\log(\Lambda)$.

Equation

We are now able to introduce the function on which we shall apply the fixed-point theorem. According to what we said above, the equation in ρ_Q can be written

$$\rho_Q = \sum_{n=1}^{\infty} \alpha^n \rho_n(Q,\rho_Q) \qquad (28)$$

or equivalently (we forget the dependence in Q and ρ_Q for simplicity)

$$\widehat{\rho_Q}(k) = \frac{\alpha B'_\Lambda(k)}{\pi}(Z\widehat{n}(k) - \widehat{\rho_Q}(k)) + \alpha\widehat{\rho_{1,0}}(k) + \sum_{n=2}^{\infty}\alpha^n\widehat{\rho_n}(k)$$

and

$$\widehat{\rho_Q}(k) = \frac{\alpha B'_\Lambda(k)}{\pi+\alpha B'_\Lambda(k)}Z\widehat{n}(k) + \frac{\pi}{\pi+\alpha B'_\Lambda(k)}\left(\alpha\widehat{\rho_{1,0}}(k) + \sum_{n=2}^{\infty}\alpha^n\widehat{\rho_n}(k)\right), \qquad (29)$$

which is the equation that we want to solve for the density.

Since the equations in Q and ρ_Q are now different, we have to introduce the following space:

$$\mathcal{X} = \mathcal{Q}\times\mathcal{C}$$

consisting of all the pairs (Q,ρ) such that $Q\in\mathcal{Q}$ and $\rho\in\mathcal{C}$. Notice that in this space, ρ can be different from ρ_Q. However, we shall find a solution of the equations in this space, which satisfies $\rho=\rho_Q$. We also introduce on $\mathcal{X}$ the norm

$$\|(Q,\rho)\| = C_R\sqrt{2}\|Q\|_{\mathcal{Q}} + 2\sqrt{\pi}\|\rho\|_{\mathcal{C}},$$

where we recall that C_R is defined in Lemma 6.

We now introduce the function $F : \mathcal{X} \to \mathcal{X}$ defined by

$$F(Q,\rho) = \Big(F_Q(Q,\rho)\ ,\ F_\rho(Q,\rho) \Big)$$

where

$$F_Q(Q,\rho) = \chi_{(-\infty;0)}(D_{Q,\rho}) - P^0 = \sum_{n=1}^{\infty} \alpha^n Q_n(Q,\rho) \tag{30}$$

$$\widehat{F_\rho(Q,\rho)} = \frac{\alpha B'_\Lambda}{\pi + \alpha B'_\Lambda} Z\widehat{n} + \frac{\pi}{\pi + \alpha B'_\Lambda} \left(\alpha \widehat{\rho_{1,0}}(Q,\rho) + \sum_{n=2}^{\infty} \alpha^n \widehat{\rho_n}(Q,\rho) \right) \tag{31}$$

where $Q_n(Q,\rho)$ and $\rho_n(Q,\rho)$ are defined in (25) (replace ρ_Q by ρ). Remark that $\rho_n = \rho_{Q_n}$ for all $n \geq 2$. In the proof of Theorem 4, we solve the fixed-point equation in $\mathcal{X}$

$$F(Q,\rho) = (Q,\rho).$$

4.2 Proof of Theorem 4

To prove our main Theorem, we need the following estimates

Proposition 8. *Assume that $(Q,\rho) \in \mathcal{X}$ is such that $0 \notin \sigma(D_{Q,\rho})$. Then we have*

$$\|F(Q,\rho)\| \leq \kappa_1(\Lambda)\alpha \,\|(Q,\rho)\| + \left(\frac{\alpha B_\Lambda}{1+\alpha B_\Lambda} + \alpha\kappa_1(\Lambda) \right) 2\sqrt{\pi} Z \|n\|_{\mathcal{C}} + \sum_{n=2}^{+\infty} \kappa_n \Big[\alpha(\|(Q,\rho)\| + 2\sqrt{\pi} Z \|n\|_{\mathcal{C}}) \Big]^n \tag{32}$$

$$\big\| F'(Q,\rho) \big\| \leq \kappa_1(\Lambda)\alpha + \alpha \sum_{n=2}^{+\infty} n\kappa_n \Big[\alpha(\|(Q,\rho)\| + 2\sqrt{\pi} Z \|n\|_{\mathcal{C}}) \Big]^{n-1} \tag{33}$$

where

$$\kappa_1(\Lambda) = \max\left(\frac{C_R\sqrt{2}}{\sqrt{\pi}} \sqrt{\log\Lambda}\,,\ \sqrt{2}C_R + \frac{\sqrt{\log\Lambda}}{2^{3/2}\sqrt{\pi}} \right) \sim_{\Lambda\to\infty} \frac{C_R\sqrt{2}}{\sqrt{\pi}} \sqrt{\log\Lambda}$$

and $(\kappa_n)_{n\geq 2}$ is a sequence of positive numbers independent of Λ and which satisfies $\kappa_n \sim_{n\to\infty} K\sqrt{n}$ for some constant K.

To prove this proposition, we have to do some tedious estimates that we postpone until the end of the proof of Theorem 4.

We are now able to prove Theorem 4

Let us introduce the function $f(x) = \sum_{n=2}^{\infty} \kappa_n x^n$, which is a power serie with a radius of convergence equal to 1. The estimates (32) and (33) can be written

$$\begin{aligned} \|F(Q,\rho)\| &\leq \kappa_1(\Lambda)\alpha \,\|(Q,\rho)\| + \left(\frac{\alpha B_\Lambda}{1+\alpha B_\Lambda} + \alpha\kappa_1(\Lambda) \right) 2\sqrt{\pi} Z \|n\|_{\mathcal{C}} + f\big(\alpha \,\|(Q,\rho)\| + 2\sqrt{\pi}\alpha Z \|n\|_{\mathcal{C}} \big) \\ \big\| F'(Q,\rho) \big\| &\leq \kappa_1(\Lambda)\alpha + \alpha f'\big(\alpha \,\|(Q,\rho)\| + 2\sqrt{\pi}\alpha Z \|n\|_{\mathcal{C}} \big). \end{aligned} \tag{34}$$

To apply Banach fixed-point theorem, we now have to find a ball $B(0,R) \subset \mathcal{X}$ which is invariant under the function F and on which F is a contraction. Let $R > 0$ be some fixed radius. We have

$$\sup_{(Q,\rho)\in B(0,R)} \big\| F'(Q,\rho) \big\| \leq \kappa_1(\Lambda)\alpha + \alpha f'\big(\alpha R + 2\sqrt{\pi}\alpha Z \|n\|_{\mathcal{C}} \big) := \mu.$$

Moreover, we also have

$$\|F(Q,\rho)\| \leq \|F(Q,\rho) - F(0,0)\| + \|F(0,0)\| \leq \mu \|(Q,\rho)\| + \|F(0,0)\|.$$

Therefore a condition for the ball $B(0,R)$ to be invariant under the action of F is $\|F(0,0)\| \leq (1-\mu)R$. Additionally due to Lemma 7 we assume $\alpha\sqrt{2}R < 1$ as well as

$$\frac{\alpha\pi}{4(1-\alpha\sqrt{2}R)} \leq 1,$$

due to Theorem 3 and Lemma 7 which is equivalent to

$$\alpha \leq \frac{1}{\pi/4 + R\sqrt{2}}.$$

As a conclusion, if (α, R) fulfills

$$\begin{cases} \left(\dfrac{\alpha B_\Lambda}{1+\alpha B_\Lambda} + \kappa_1(\Lambda)\right) 2\sqrt{\pi}Z\|n\|_{\mathcal{C}} + f(2\sqrt{\pi}Z\|n\|_{\mathcal{C}}) + \kappa_1(\Lambda)\alpha R + \alpha R f'(\alpha R + 2\sqrt{\pi}Z\|n\|_{\mathcal{C}}) \leq R \\ \alpha \leq \dfrac{1}{\pi/4 + R\sqrt{2}}, \end{cases} \tag{35}$$

then we are able to apply the Banach Fixed-Point Theorem on $B(0,R)$. Remark that these inequalities also contain the conditions $\mu < 1$ and $\alpha\sqrt{2}R < 1$. Notice also that if (α, R) is a solution to (35), then (α', R) is a solution to (35) for all $\alpha' \leq \alpha$, since the function which appears on the left of (35) is increasing in α.

Now, if we assume that $4\sqrt{\pi}\alpha Z\|n\|_{\mathcal{C}} \leq b$, we obtain that if (α, R) fulfills

$$\begin{cases} \dfrac{b}{2\alpha} + \kappa_1(\Lambda)b/2 + f(b/2) + \kappa_1(\Lambda)\alpha R + \alpha R f'(\alpha R + b/2) \leq R \\ \alpha \leq \dfrac{1}{\pi/4 + R\sqrt{2}}, \end{cases} \tag{36}$$

then it also fulfills (35), f being increasing. Remark that we have used the estimate

$$\frac{\alpha B_\Lambda}{1+\alpha B_\Lambda} 2\sqrt{\pi}Z\|n\|_{\mathcal{C}} \leq \frac{b}{2\alpha}.$$

The first inequation of (36) is simpler when it is written in terms of the variables α and $x := \alpha R$. It becomes

$$\frac{b}{2\alpha} + \kappa_1(\Lambda)b/2 + f(b/2) + \kappa_1(\Lambda)x + xf'(x + b/2) \leq \frac{x}{\alpha} \tag{37}$$

which implies $b/2 \leq x$. Since necessarily $x < 1 - b/2$ (recall that f is defined on $[0;1)$), we see that we need $b < 1$. Now, let us call $a_\Lambda(x)$ the solution of (37) where the $\leq$ is replaced by $=$, i.e.

$$a_\Lambda(x) = \frac{x - b/2}{\kappa_1(\Lambda)b/2 + f(b/2) + \kappa_1(\Lambda)x + xf'(x + b/2)}, \tag{38}$$

a smooth function on $[b/2; 1-b/2)$. Since $a_\Lambda(b/2) = \lim_{x\to 1-b/2} a_\Lambda(x) = 0$, we deduce that a_Λ attains its maximum on $(b/2; 1-b/2)$ and we may denote by x_Λ the largest $x \in (b/2; 1-b/2)$ such that

$$a_\Lambda(x_\Lambda) = A_b(\Lambda) := \max_{x\in(b/2;1-b/2)} a_\Lambda(x). \tag{39}$$

We now define $R_\Lambda := x_\Lambda / A_\Lambda$ and

$$\alpha_b(\Lambda) := \min\left(A_b(\Lambda), \frac{1}{\pi/4 + R_\Lambda\sqrt{2}}\right).$$

As a conclusion, for all $0 \leq \alpha \leq \alpha_b(\Lambda)$, there exists some $R_0 = R_0(\alpha, \Lambda, b)$ such that (α, R_0) is a solution of (35). This means that F is a contraction on $B(0, R_0)$, on which we can apply Banach Theorem. This gives a unique solution to the equation $F(Q, \rho) = (Q, \rho)$ in $B(0, R_0) \subset \mathcal{X}$.

Let us now show that P is indeed a solution to (4). In fact ρ is a solution to (29) and so it is a solution to (28). On the other hand, we have $Q = \chi_{(-\infty;0)}(D_{Q,\rho}) - P^0$, and so equation (28) means exactly that $\rho = \rho_Q$. Hence, P is a solution to $P = \chi_{(-\infty;0)}(D_Q)$. Thanks to the proof, we know that P satisfies the assumptions of Theorem 3, and so P is a BDF-stable vacuum.

To end the proof, let us study the behaviour of $A_b(\Lambda)$ as $\Lambda \to \infty$. Differentiating (38) with respect to x, we arrive at

$$\kappa_1(\Lambda)b + f(b) + \frac{bf'(x_\Lambda + b/2)}{2} = (x_\Lambda - b/2)x_\Lambda f''(x_\Lambda + b/2). \tag{40}$$

Since $\kappa_1(\Lambda) \to \infty$ as $\Lambda \to \infty$, we deduce that $x_\Lambda + b/2 \to 1$, or equivalently $x_\Lambda \to 1 - b/2$. If we now use the fact that $f'(y) = o\big(f''(y)\big)$ as $y \to 1^-$, we finally obtain $f''(x_\Lambda + b/2) \sim_{\Lambda\to\infty} \frac{b\kappa_1(\Lambda)}{(1-b)(1-b/2)}$ and $f'(x_\Lambda + b/2) = o\big(\kappa_1(\Lambda)\big)$. By (38), this implies

$$A_\Lambda \sim_{\Lambda\to\infty} \frac{1-b}{\kappa_1(\Lambda)}.$$

Remark also that $R_\Lambda = x_\Lambda/A_\Lambda \sim \frac{1-b/2}{1-b}\kappa_1(\Lambda)$, which ends the proof since when $2 - \sqrt{2} \leq b$,

$$\alpha_b(\Lambda) \sim_{\Lambda\to\infty} \frac{\min\left(1-b, \frac{1-b}{\sqrt{2}(1-b/2)}\right)}{\kappa_1(\Lambda)} = \frac{1-b}{\kappa_1(\Lambda)} \sim_{\Lambda\to\infty} \frac{\sqrt{\pi}(1-b)}{C_R\sqrt{2}\sqrt{\log\Lambda}} = \frac{C(1-b)}{\sqrt{\log\Lambda}}$$

with $C = \frac{\sqrt{\pi}}{C_R\sqrt{2}}$. □

4.3 Proof of Proposition 8: estimates

In this section, we prove the claimed estimates of Proposition 8.

Remark first that we have

$$\frac{\alpha B'_\Lambda(k)}{\pi + \alpha B'_\Lambda(k)} \leq \frac{\alpha B'_\Lambda(0)}{\pi + \alpha B'_\Lambda(0)} = \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} \quad \text{and} \quad \frac{\pi}{\pi + \alpha B'_\Lambda(k)} \leq 1$$

for all $k \in \mathbb{R}^3$. Therefore, to estimate the norm $\|F_\rho(Q, \rho)\|_{\mathcal{C}}$, it suffices to estimate the norms of $\rho_{1,0}(Q, \rho)$ and $\rho_n(Q, \rho)$, due to (31).

For $(Q, \rho) \in \mathcal{X}$, we introduce the notation $R = \frac{Q(x,y)}{|x-y|} \in \mathcal{R}$, $\rho' = \rho - Zn$ and $\varphi' = (\rho - Zn) * \frac{1}{|\cdot|}$.

We then remark that

$$\|F(Q, \rho)\| \leq \frac{\alpha B_\Lambda}{1 + \alpha B_\Lambda} 2\sqrt{\pi}Z\|n\|_{\mathcal{C}} + \alpha \left\|(Q_1, \rho_{1,0})\right\| + \sum_{n\geq 2} \alpha^n \left\|(Q_n, \rho_n)\right\|$$

and estimate each term separately. A similar argument can be done for $F'(Q, \rho)$.

4.3.1 First order terms

Lemma 9. *We have the following estimates:*

$$\|Q_{0,1}\|_{\mathcal{Q}} \leq \frac{(\log\Lambda)^{1/2}}{2\pi}\|\varphi'\|_{\mathcal{Y}} = 2(\log\Lambda)^{1/2}\|\rho'\|_{\mathcal{C}},$$

$$\|Q_{1,0}\|_{\mathcal{Q}} \leq \|R_Q\|_{\mathcal{R}} \leq C_R\|Q\|_{\mathcal{Q}}, \qquad \|\rho_{1,0}\|_{\mathcal{C}} \leq \frac{C_R(\log\Lambda)^{1/2}}{4\pi}\|Q\|_{\mathcal{Q}}.$$

Therefore

$$\|(Q_1,\rho_{1,0})\| \le \kappa_1(\Lambda)\,\|(Q,\rho')\| \le \kappa_1(\Lambda)\,\|(Q,\rho)\| + \kappa_1(\Lambda)2\sqrt{\pi}Z\|n\|_{\mathcal{C}},$$

where

$$\kappa_1(\Lambda) = \max\left(\frac{C_R\sqrt{2}}{\sqrt{\pi}}\sqrt{\log\Lambda}\,,\ \sqrt{2}C_R + \frac{\sqrt{\log\Lambda}}{2^{3/2}\sqrt{\pi}}\right).$$

Proof – Recall that

$$\widehat{Q_{0,1}}(p,q) = \frac{1}{2^{5/2}\pi^{3/2}}\widehat{\varphi'}(p-q)M(p,q), \tag{41}$$

where the matrix $M(p,q)$ is defined in (26), and whose properties are summarized in the following

Lemma 10. *Let $\Lambda^+(p) = \frac{\boldsymbol{\alpha}\cdot p+\beta+E(p)}{2E(p)}$ and $\Lambda^-(p) = \frac{-(\boldsymbol{\alpha}\cdot p+\beta)+E(p)}{2E(p)}$ be the projections matrices in $\mathbb{C}^4$ onto the eigenspaces of D^0 in Fourier space. We then have*

$$\mathrm{Tr}_{\mathbb{C}^4}\left(M(p,q)\right) = -4\frac{1}{E(p)+E(q)}\mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^+(p)\Lambda^-(q)\right)$$

$$|M(p,q)|^2 = \mathrm{Tr}_{\mathbb{C}^4}\left(M(p,q)M(p,q)^*\right) = 8\frac{1}{(E(p)+E(q))^2}\mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^+(p)\Lambda^-(q)\right)$$

$$\mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^+(p)\Lambda^-(q)\right) = \mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^-(p)\Lambda^+(q)\right) = 1 - \frac{p\cdot q+1}{E(p)E(q)}.$$

Moreover, we have

$$\forall p,q\in\mathbb{R}^3,\quad \mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^+(p)\Lambda^-(q)\right) \le \min\left(\frac{|p-q|^2}{2E((p+q)/2)^2}\,,\,\frac{1}{2}\right). \tag{42}$$

Proof of Lemma 10 – We only prove (42). We have $\mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^+(p)\Lambda^-(q)\right) \le |\Lambda^+(p)|\,|\Lambda^-(q)| = 1/2$, so when $t := \frac{|p-q|^2}{4E((p+q)/2)^2} \ge 1/2$, there is nothing to prove. Now we have

$$\begin{aligned} 1 - \frac{p\cdot q+1}{E(p)E(q)} &= 1 - \frac{l^2-k^2+1}{E(l+k)E(l-k)} \text{ with } l = \frac{p+q}{2},\ k = \frac{p-q}{2} \\ &= 1 - \frac{1-t}{\sqrt{(1+t)^2-4zt}} \end{aligned}$$

where $t = |k|^2/E(l)^2$ and $z = \frac{(l\cdot k)^2}{|k|^2(1+l^2)} \in [0;1)$. When $t\in[0;1/2)$ and $z\in[0;1)$, the expression above is decreasing in z and so we obtain

$$1 - \frac{p\cdot q+1}{E(p)E(q)} \le 1 - \frac{1-t}{\sqrt{(1+t)^2}} = \frac{2t}{1+t} \le 2t$$

which ends the proof. □

• Let us now treat $Q_{0,1}$. From (41), we obtain

$$|\widehat{Q_{0,1}}(p,q)|^2 = \frac{1}{2^5\pi^3}|\widehat{\varphi'}|^2(p-q)|M(p,q)|^2,$$

and so

$$\begin{aligned} &\iint E(p-q)^2E(p+q)|\widehat{Q_{0,1}}(p,q)|^2dp\,dq \\ &\qquad = \frac{1}{2^5\pi^3}\iint dk\,du E(k)^2E(2u)|\widehat{\varphi'}|^2(k)\chi(|u|\le\Lambda)|M(u+k/2,u-k/2)|^2 \\ &\qquad\qquad \le \frac{4}{2^5\pi^3}\left(\int dk|k|^2E(k)^2|\widehat{\varphi'}|^2(k)\right)\left(\int_{|u|\le\Lambda}\frac{1}{E(2u)E(u)^2}\right) \end{aligned}$$

by Lemma 10. Now we have

$$\int_{|u|\leq\Lambda}\frac{du}{E(2u)E(u)^2}=4\pi\left(\frac{1}{2}\mathrm{argsh}(2\Lambda)+\frac{1}{\sqrt{3}}\mathrm{argth}\left(\frac{\sqrt{3}\Lambda}{\sqrt{1+4\sqrt{\Lambda}}}\right)\right)\leq 2\pi\log\Lambda \qquad (43)$$

for $\Lambda\geq 3$. So we obtain

$$\|Q_{0,1}\|_{\mathcal{Q}}\leq\frac{(\log\Lambda)^{1/2}}{2\pi}\|\varphi'\|_{\mathcal{Y}}=2(\log\Lambda)^{1/2}\|\rho'\|_{\mathcal{C}}.$$

• $\rho_{1,0}$ and $Q_{1,0}$.

We have

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

so that

$$\begin{aligned}\widehat{Q_{1,0}}(p,q) &= -(2\pi)^{-1}\int_{-\infty}^{+\infty}d\eta\frac{1}{\boldsymbol{\alpha}\cdot p+\beta+i\eta}\widehat{R}(p,q)\frac{1}{\boldsymbol{\alpha}\cdot q+\beta+i\eta}\\ &= -\frac{1}{2}\frac{1}{E(p)+E(q)}\left(\frac{(\boldsymbol{\alpha}\cdot p+\beta)}{E(p)}\widehat{R}(p,q)\frac{(\boldsymbol{\alpha}\cdot q+\beta)}{E(q)}-\widehat{R}(p,q)\right)\end{aligned}$$

and

$$|\widehat{Q_{1,0}}(p,q)|^2\leq\frac{1}{(E(p)+E(q))^2}|\widehat{R}(p,q)|^2\leq\frac{1}{E(p+q)^2}|\widehat{R}(p,q)|^2,$$

showing that

$$\|Q_{1,0}\|_{\mathcal{Q}}\leq\|R\|_{\mathcal{R}}\leq C_R\|Q\|_{\mathcal{Q}}.$$

Now, we have

$$\begin{aligned}\widehat{\rho_{1,0}}(k) &= \frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q_{1,0}}\left(l+\frac{k}{2},l-\frac{k}{2}\right)\right)dl\\ &= -\frac{1}{2^{5/2}\pi^{3/2}}\int_{\mathbb{R}^3}\mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{R}\left(l+\frac{k}{2},l-\frac{k}{2}\right)M\left(l+\frac{k}{2},l-\frac{k}{2}\right)\right)\chi(|l|\leq\Lambda)dl,\end{aligned}$$

so we obtain

$$|\widehat{\rho_{1,0}}(k)|\leq\frac{1}{2^{5/2}\pi^{3/2}}\left(\int_{\mathbb{R}^3}E(2l)^{-1}|\widehat{R}(l+k/2,l-k/2)|^2\,dl\right)^{1/2}\left(\int_{\mathbb{R}^3}E(2l)|M(l+k/2,l-k/2)|^2\,dl\right)^{1/2}$$

and finally

$$\int\frac{E(k)^2}{|k|^2}|\widehat{\rho_{1,0}}(k)|^2\,dk\leq\frac{1}{2^5\pi^3}\|R\|_{\mathcal{R}}^2\int_{|l|\leq\Lambda}\frac{1}{E(2l)E(l)^2}\,dl\leq\frac{\log\Lambda}{2^4\pi^2}\|R\|_{\mathcal{R}}^2$$

by (43) which implies

$$\|\rho_{1,0}\|_{\mathcal{C}}\leq\frac{C_R(\log\Lambda)^{1/2}}{4\pi}\|Q\|_{\mathcal{Q}}.\quad\square$$

4.3.2 Second order terms

To simplify the presentation, we introduce the following notation:

$$S_{p,q} := (4\pi)(2\pi)^{-3/p}\left(\int_{\mathbb{R}^3}\frac{du}{E(u)^q}\right)^{\frac{1}{p}}, \qquad S_p := S_{p,p}, \qquad K_p := \frac{1}{2\pi}\int_{-\infty}^{+\infty}\frac{d\eta}{E(\eta)^p}.$$

Let us recall the following inequality [27, Theorem 4.1]

$$\|f(x)g(-i\nabla)\|_{\mathfrak{S}_p} \leq (2\pi)^{-3/p}\,\|f\|_{L^p(\mathbb{R}^3)}\,\|g\|_{L^p(\mathbb{R}^3)}\,, \tag{44}$$

which implies

$$\left\|\frac{1}{|D_0|^a}f\right\|_{\mathfrak{S}_p} \leq \frac{S_{p,ap}}{4\pi}\,\|f\|_{L^p(\mathbb{R}^3)}\,.$$

On the other hand, we shall often use the following trick

$$\begin{aligned}(E(p)^2+\eta^2)(E(q)^2+\eta^2) &= (E(p)E(q))^2 + (E(p)^2+E(q)^2)\eta^2 + \eta^4\\ &\geq \frac{1}{4}E(p+q)^2 + \frac{1}{2}E(p+q)^2\eta^2\\ &\geq \frac{1}{4}E(p+q)^2E(\eta)^2\end{aligned}$$

by Lemma 5. This implies

$$\frac{1}{\sqrt{E(p)^2+\eta^2}\sqrt{E(q)^2+\eta^2}} \leq \frac{2}{E(p+q)E(\eta)}. \tag{45}$$

Recall now that we have $Q_2 = Q_{2,0} + Q_{1,1} + Q_{0,2}$ with

$$\begin{aligned}Q_{2,0} &= -\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\eta\frac{1}{D^0+i\eta}R\frac{1}{D^0+i\eta}R\frac{1}{D^0+i\eta}\\ Q_{1,1} &= \frac{1}{2\pi}\int_{-\infty}^{+\infty}d\eta\frac{1}{D^0+i\eta}R\frac{1}{D^0+i\eta}\varphi'\frac{1}{D^0+i\eta} + \frac{1}{2\pi}\int_{-\infty}^{+\infty}d\eta\frac{1}{D^0+i\eta}\varphi'\frac{1}{D^0+i\eta}R\frac{1}{D^0+i\eta}\\ Q_{0,2} &= -\frac{1}{2\pi}\int_{-\infty}^{+\infty}d\eta\frac{1}{D^0+i\eta}\varphi'\frac{1}{D^0+i\eta}\varphi'\frac{1}{D^0+i\eta}.\end{aligned}$$

We shall now treat each term separately.

Lemma 11. *We have $\rho_{0,2}=0$ and the following estimates:*

$$\|Q_{2,0}\|_{\mathcal{Q}} \leq 2^{5/2}K_{3/2}(C_R)^2\|Q\|_{\mathcal{Q}}^2, \qquad \|Q_{1,1}\|_{\mathcal{Q}} \leq 4S_6C_6K_{3/2}C_R\|Q\|_{\mathcal{Q}}\|\rho'\|_{\mathcal{C}},$$

$$\|Q_{0,2}\|_{\mathcal{Q}} \leq 2\sqrt{10}S_{6,5}C_MC_6\|\rho'\|_{\mathcal{C}}^2,$$

$$\|\rho_{2,0}\|_{\mathcal{C}} \leq \frac{S_6C_6(C_R)^2}{\pi}\|Q\|_{\mathcal{Q}}^2, \qquad \|\rho_{1,1}\|_{\mathcal{C}} \leq 4\frac{S_{6,5}C_MC_6C_R}{\pi}\|\rho'\|_{\mathcal{C}}\|Q\|_{\mathcal{Q}},$$

and so

$$\|(Q_2,\rho_2)\| \leq \kappa_2\left\|(Q,\rho')\right\|^2,$$

with

$$\kappa_2 = C_{Q_2}C_R\sqrt{2} + 2\sqrt{\pi}C_{\rho_2},$$

$$C_{Q_2} = \max\left(2^{3/2}K_{3/2}\,,\,\frac{S_6C_6K_{3/2}}{\sqrt{2\pi}}\,,\,\frac{\sqrt{5}S_{6,5}C_MC_6}{\pi\sqrt{2}}\right), \qquad C_{\rho_2} = \max\left(\frac{S_6C_6}{2\pi}\,,\,\frac{S_{6,5}C_MC_6}{\pi^{3/2}\sqrt{2}}\right).$$

Proof – **Step 1 : Estimates on the exchange term Q_2.**

- $Q_{2,0}$. To estimate $Q_{2,0}$, we write

$$|\widehat{Q_{2,0}}(p,q)| \leq \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\eta \int_{\mathbb{R}^3} dp_1 \frac{|\widehat{R}(p,p_1)|}{\sqrt{E(p)^2+\eta^2}}\frac{|\widehat{R}(p_1,q)|}{\sqrt{E(p_1)^2+\eta^2}}\frac{1}{\sqrt{E(q)^2+\eta^2}}$$

and so by (45)

$$|\widehat{Q_{2,0}}(p,q)| \leq \frac{2^{3/2}}{2\pi}\int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^{3/2}E(p+q)^{1/2}}\int_{\mathbb{R}^3}\frac{|\widehat{R}(p,p_1)|}{E(p+p_1)^{1/2}}\frac{|\widehat{R}(p_1,q)|}{E(p_1+q)^{1/2}}\,dp_1$$

which implies

$$E(p-q)E(p+q)^{1/2}|\widehat{Q_{2,0}}(p,q)| \leq 2^{5/2}K_{3/2}\int_{\mathbb{R}^3}\frac{E(p-p_1)|\widehat{R}(p,p_1)|}{E(p+p_1)^{1/2}}\frac{E(p_1-q)|\widehat{R}(p_1,q)|}{E(p_1+q)^{1/2}}\,dp_1$$

and finally

$$\|Q_{2,0}\|_{\mathcal{Q}} \leq 2^{5/2}K_{3/2}\|R\|_{\mathcal{R}}^2 \leq 2^{5/2}K_{3/2}(C_R)^2\|Q\|_{\mathcal{Q}}^2.$$

- $Q_{1,1}$. We treat for instance

$$Q'_{1,1} := \frac{1}{(2\pi)^{5/2}}\int_{-\infty}^{+\infty} d\eta \frac{1}{D^0+i\eta}R\frac{1}{D^0+i\eta}\varphi'\frac{1}{D^0+i\eta}$$

and use the same method to obtain

$$\begin{aligned}E(p-q)E(p+q)^{1/2}|\widehat{Q'_{1,1}}(p,q)| \leq \frac{4}{(2\pi)^{5/2}}\int_{-\infty}^{+\infty}\frac{d\eta}{E(\eta)}\times \\ \times\int_{\mathbb{R}^3}\frac{E(p-p_1)}{E(p+p_1)^{1/2}}|\widehat{R}(p,p_1)|\frac{E(p_1-q)}{(E(p_1)^2+\eta^2)^{1/4}(E(q)^2+\eta^2)^{1/4}}|\widehat{\varphi'}(p_1-q)|\,dp_1.\end{aligned}$$

This means that

$$\|Q'_{1,1}\|_{\mathcal{Q}} \leq \frac{4}{2\pi}\int_{-\infty}^{+\infty}\frac{d\eta}{E(\eta)}\left\|R'\frac{1}{(|D_0|^2+\eta^2)^{1/4}}f\frac{1}{(|D_0|^2+\eta^2)^{1/4}}\right\|_{\mathfrak{S}_2}$$

where we have introduced R' and f defined by

$$\widehat{R'}(p,q) := \frac{E(p-q)}{E(p+q)^{1/2}}|\widehat{R}(p,q)|, \quad \widehat{f}(k) := E(k)|\widehat{\varphi'}(k)|.$$

But now

$$\begin{aligned}\left\|R'\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}f\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}\right\|_{\mathfrak{S}_2} &\leq \|R'\|_{\mathfrak{S}_2}\left\|\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}f\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}\right\|_{\mathfrak{S}_\infty} \\ &\leq \|R\|_{\mathcal{R}}\left\|\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}f\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}\right\|_{\mathfrak{S}_6}.\end{aligned}$$

If we now use inequality (44), we obtain

$$\begin{aligned}\left\|\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}f\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}\right\|_{\mathfrak{S}_6} &\leq \left\|\frac{1}{(|D_0|^2+\eta^2)^{\frac14}}|f|^{1/2}\right\|_{\mathfrak{S}_{12}}^2 \\ &\leq (2\pi)^{-1/2}\left(\int_{\mathbb{R}^3}\frac{du}{1+|u|^2+\eta^2)^3}\right)^{1/6}\|f\|_{L^6} \\ &= \frac{S_6}{4\pi E(\eta)^{1/2}}\|f\|_{L^6}.\end{aligned}$$

Finally since

$$\|f\|_{L^6} \leq C_6 \|\nabla f\|_{L^2} = C_6 \|\varphi'\|_{\mathcal{Y}}, \tag{46}$$

and $\|\varphi'\|_{\mathcal{Y}} = (4\pi)\|\rho'\|_{\mathcal{C}}$, we obtain

$$\|Q'_{1,1}\|_{\mathcal{Q}} \leq \frac{4S_6C_6}{2\pi} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^{3/2}} \|R\|_{\mathcal{R}} \|\rho'\|_{\mathcal{C}}$$

and

$$\|Q_{1,1}\|_{\mathcal{Q}} \leq 8S_6C_6K_{3/2}C_R\|Q\|_{\mathcal{Q}}\|\rho'\|_{\mathcal{C}}.$$

• $Q_{0,2}$. Unfortunately, the method used above cannot be applied to $Q_{0,2}$. In this case, we have to calculate this term explicitely. We can write

$$Q_{0,2} = \sum_{\epsilon_1,\epsilon_2,\epsilon_3 \in \{\pm\}} Q_{0,2}^{\epsilon_1\epsilon_2\epsilon_3}$$

where for instance (by a residuum formula)

$$\widehat{Q_{0,2}^{+++}}(p,q) = \widehat{Q_{0,2}^{---}}(p,q) = 0,$$

$$\widehat{Q_{0,2}^{+--}}(p,q) = (2\pi)^{-3} \int_{\mathbb{R}^3} dp_1 \frac{\Lambda^+(p)\widehat{\varphi'}(p-p_1)\Lambda^-(p_1)\widehat{\varphi'}(p_1-q)\Lambda^-(q)}{(E(p)+E(q))(E(p)+E(p_1))},$$

$$\widehat{Q_{0,2}^{+-+}}(p,q) = (2\pi)^{-3} \int_{\mathbb{R}^3} dp_1 \frac{\Lambda^+(p)\widehat{\varphi'}(p-p_1)\Lambda^-(p_1)\widehat{\varphi'}(p_1-q)\Lambda^+(q)}{(E(p)+E(p_1))(E(q)+E(p_1))},$$

and similar formulas for the other $Q_{0,2}^{\epsilon_1\epsilon_2\epsilon_3}$. We now treat for instance $\widehat{Q_{0,2}^{+--}}$. Using (20), we may obtain

$$E(p-q)E(p+q)^{1/2}|\widehat{Q_{0,2}^{+--}}| \leq 2(2\pi)^{-3} \int_{\mathbb{R}^3} dp_1 \frac{E(p-p_1)}{E(p+p_1)^{2/3}} \times \\ \times \left|\Lambda^+(p)\widehat{\varphi'}(p-p_1)\Lambda^-(p_1)\right| \times \frac{E(p_1-q)|\widehat{\varphi'}(p_1-q)|}{E(p_1)^{1/3}E(q)^{1/2}} dp_1.$$

So, we may write

$$\|Q_{0,2}^{+--}\|_{\mathcal{Q}} \leq 2 \left\| M_f \frac{1}{|D_0|^{1/3}} f \frac{1}{|D_0|^{1/2}} \right\|_{\mathfrak{S}_2} \leq 2 \|M_f\|_{\mathfrak{S}_2} \left\| \frac{1}{|D_0|^{1/3}} f \frac{1}{|D_0|^{1/2}} \right\|_{\mathfrak{S}_\infty},$$

where

$$\widehat{M_f}(p,q) := (2\pi)^{-3/2} \frac{\widehat{f}(p-q)\,|\Lambda^+(p)\Lambda^-(q)|}{E(p+q)^{2/3}}. \tag{47}$$

Lemma 12. *When M_f is defined by formula* (47)*, then*

$$\|M_f\|_{\mathfrak{S}_2} \leq \frac{C_M}{4\pi} \left(\int_{\mathbb{R}^3} |k|^2 |\widehat{f}(k)|^2 dk \right)^{1/2}$$

where $C_M := 2\left(\int_0^\infty \frac{t^2\,dt}{E(2t)^{4/3}E(t)^2}\right)^{1/2} \simeq 2.1589.$

Proof – We have $|\Lambda^+(p)\Lambda^-(q)|^2 = \mathrm{Tr}_{\mathbb{C}^4}\left(\Lambda^+(p)\Lambda^-(q)\right)$ and so, by (42),

$$\begin{aligned}\iint dp\,dq|\widehat{M_f}(p,q)|^2 &\leq (2\pi)^{-3}\iint dp\,dq\frac{|p-q|^2|\widehat{f}(p-q)|^2}{2E((p+q)/2)^2E(p+q)^{4/3}}\\ &\leq (2\pi)^{-3}\int dk|k|^2|\widehat{f}(k)|^2\int\frac{du}{2E(2u)^{4/3}E(u)^2}\\ &\leq (2\pi)^{-2}\left(\int dk|k|^2|\widehat{f}(k)|^2\right)\int_0^\infty\frac{t^2\,dt}{E(2t)^{4/3}E(t)^2}.\quad\square\end{aligned}$$

Finally, since by (46)

$$\left\|\frac{1}{|D_0|^{1/3}}f\frac{1}{|D_0|^{1/2}}\right\|_{\mathfrak{S}_\infty}\leq\left\|\frac{1}{|D_0|^{1/3}}f\frac{1}{|D_0|^{1/2}}\right\|_{\mathfrak{S}_6}\leq\frac{S_{6,5}}{4\pi}\left\|f\right\|_{L^6},$$

we obtain

$$\|Q_{0,2}^{+--}\|_{\mathcal{Q}}\leq 2S_{6,5}C_MC_6\|\rho'\|_{\mathcal{C}}^2.$$

This result is immediatly extended to the others terms and since we can prove

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

we arrive at

$$\|Q_{0,2}\|_{\mathcal{Q}}\leq 2\sqrt{10}S_{6,5}C_MC_6\|\rho'\|_{\mathcal{C}}^2.$$

Step 2 : Estimates on the density ρ_2. Let us now treat the density ρ_2. The general idea of the proof is to estimate $\langle\rho_2,\zeta\rangle$ in terms of the norm $\|\zeta\|_{\mathcal{C}'}$ by using

$$|\langle\rho,\zeta\rangle|=|\mathrm{Tr}\left(Q\zeta\right)|=\left|\mathrm{Tr}\left(\widehat{Q\zeta}\right)\right|=\left|\int_{\mathbb{R}^3}\mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q\zeta}\right)(p,p)\,dp\right|\leq\int_{\mathbb{R}^3}|\widehat{Q\zeta}(p,p)|dp.$$

This can be done if we know that $Q\zeta\in\mathfrak{S}_1$. But we have

$$\|Q\zeta\|_{\mathfrak{S}_1}=\left\|Q|D_0|^2\frac{1}{|D_0|^2}\zeta\right\|_{\mathfrak{S}_1}\leq\left\|Q|D_0|^2\right\|_{\mathfrak{S}_2}\left\|\frac{1}{|D_0|^2}\zeta\right\|_{\mathfrak{S}_2}\leq E(\Lambda)^2\left\|Q\right\|_{\mathfrak{S}_2}\frac{S_{2,4}}{4\pi}\left\|\zeta\right\|_{L^2},$$

showing that $Q\zeta\in\mathfrak{S}_1$ when $\zeta\in L^2$. So, in what follows, we shall assume that $\zeta\in\mathcal{C}'\cap L^2$ and prove a bound depending only on $\|\zeta\|_{\mathcal{C}'}$. By the density of $\mathcal{C}'\cap L^2$ in $\mathcal{C}'$, this will give us a bound on $\|\rho\|_{\mathcal{C}}$.

Let us remark first that $\rho_{0,2}$ vanishes. Indeed we have

$$\widehat{\rho_{0,2}}(k)=\frac{1}{(2\pi)^{3/2}}\int_{|p|\leq\Lambda}\mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q_{0,2}}(p+k/2,p-k/2)\right)dp$$

and

$$\begin{aligned}\mathrm{Tr}_{\mathbb{C}^4}\left(\widehat{Q_{0,2}}(p,q)\right)&=\frac{1}{(2\pi)^4}\int_{-\infty}^{+\infty}d\eta\int_{\mathbb{R}^3}dp_1\mathrm{Tr}_{\mathbb{C}^4}\left(\frac{1}{D_0(p)+i\eta}\widehat{\varphi'}(p-p_1)\times\right.\\ &\qquad\left.\times\frac{1}{D_0(p_1)+i\eta}\widehat{\varphi'}(p_1-q)\frac{1}{D_0(q)+i\eta}\right)\\ &=\frac{1}{(2\pi)^4}\int_{-\infty}^{+\infty}d\eta\int_{\mathbb{R}^3}dp_1\frac{\widehat{\varphi'}(p-p_1)\widehat{\varphi'}(p_1-q)}{\sqrt{E(p)^2+\eta^2}\sqrt{E(p_1)^2+\eta^2}\sqrt{E(q)^2+\eta^2}}\times\\ &\qquad\times\mathrm{Tr}_{\mathbb{C}^4}\Big[(D_0(p)-i\eta))(D_0(p_1)-i\eta)(D_0(q)-i\eta)\Big].\end{aligned}$$

Now the terms linear in the Dirac matrices are traceless and the remaining terms are odd in η and vanish after integration. This can be easily generalized to $\rho_{0,2k}$ for all k, and is known as *Furry's Theorem* in the physics litterature.

• $\rho_{2,0}$. We use here a method similar to what we have done above. We estimate for some $\zeta \in \mathcal{C}' \cap L^2$ and $Q_\zeta := Q_{2,0}\zeta$

$$\begin{aligned}
|\widehat{Q_\zeta}(p,p)| &\leq (2\pi)^{-5/2} \int_{-\infty}^{+\infty} d\eta \iint \frac{|\widehat{R}(p,p_1)|\,|\widehat{R}(p_1,p_2)|\,|\widehat{\zeta}(p_2-p)|\,dp_1\,dp_2}{\sqrt{E(p)^2+\eta^2}\sqrt{E(p_1)^2+\eta^2}\sqrt{E(p_2)^2+\eta^2}}, \\
&\leq 4(2\pi)^{-5/2} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)} \iint dp_1\,dp_2 \frac{E(p-p_1)|\widehat{R}(p,p_1)|\,E(p_1-p_2)|\widehat{R}(p_1,p_2)|}{E(p+p_1)^{1/2}E(p_1+p_2)^{1/2}} \times \\
&\qquad \times \frac{|\widehat{\zeta}(p_2-p)|}{E(p_2-p)(E(p)^2+\eta^2)^{1/4}(E(p_2)^2+\eta^2)^{1/4}}, \\
&\leq 4(2\pi)^{-5/2} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)} \iint dp_1\,dp_2 \frac{R'(p,p_1)R'(p_1,p_2)\widehat{\zeta'}(p_2-p)}{(E(p)^2+\eta^2)^{1/4}(E(p_2)^2+\eta^2)^{1/4}}
\end{aligned}$$

where $\widehat{R'}(p,q) = \frac{E(p-q)|\widehat{R}(p,q)|}{E(p+q)^{1/2}}$ and $\widehat{\zeta'}(k) = E(k)^{-1}\widehat{\zeta}(k)$. This means that

$$\begin{aligned}
|\langle \rho_{2,0}, \zeta\rangle| &\leq \frac{4}{2\pi} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)} \left\| R'R' \frac{1}{(|D_0|^2+\eta^2)^{1/4}} \zeta' \frac{1}{(|D_0|^2+\eta^2)^{1/4}} \right\|_{\mathfrak{S}_1} \\
&\leq \frac{4S_6}{(2\pi)(4\pi)} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^{3/2}} \left\|R'\right\|_{\mathfrak{S}_2}^2 \left\|\zeta'\right\|_{L^6} \leq \frac{S_6 C_6 (C_R)^2 K_{3/2}}{\pi} \|Q\|_{\mathcal{Q}}^2 \|\zeta\|_{\mathcal{C}'}
\end{aligned}$$

by (46), showing that

$$\|\rho_{2,0}\|_{\mathcal{C}} \leq \frac{S_6 C_6 (C_R)^2}{\pi} K_{3/2} \|Q\|_{\mathcal{Q}}^2.$$

• $\rho_{1,1}$. Unfortunately, as for $Q_{0,2}$, we have to calculate $\rho_{1,1}$ explicitely. Let us start for instance with $\rho_{1,1}^{+--}$, the density associated with one of the two terms of $Q_{1,1}$

$$(2\pi)^{-3/2} \int_{\mathbb{R}^3} dp_1 \frac{\Lambda^+(p)\widehat{R}(p-p_1)\Lambda^-(p_1)\widehat{\varphi'}(p_1-q)\Lambda^-(q)}{(E(p)+E(q))(E(p)+E(p_1))}.$$

We use the same method as above and estimate for some $\zeta \in \mathcal{C}' \cap L^2$ the term

$$\widehat{Q_\zeta}(p,p) = (2\pi)^{-3} \iint dp_1\,dp_2 \frac{\Lambda^+(p)\widehat{R}(p,p_1)\Lambda^-(p_1)\widehat{\varphi'}(p_1-p_2)\Lambda^-(p_2)}{(E(p)+E(p_2))(E(p)+E(p_1))} \widehat{\zeta}(p_2-p),$$

by

$$\begin{aligned}
|\widehat{Q_\zeta}(p,p)| &\leq (2\pi)^{-3} \iint \frac{|\Lambda^+(p)\widehat{R}(p,p_1)\Lambda^-(p_1)|}{E(p+p_1)^{1/2}} \frac{|\widehat{\varphi'}(p_1-p_2)|}{E(p_1)^{1/2}E(p_2)^{1/3}} \times \\
&\qquad \times \frac{|\widehat{\zeta}(p_2-p)| \times |\Lambda^-(p_2)\Lambda^+(p)|}{E(p+p_2)^{2/3}} dp_1\,dp_2, \\
&\leq 2(2\pi)^{-3/2} \iint \frac{E(p-p_1)|\Lambda^+(p)\widehat{R}(p,p_1)\Lambda^-(p_1)|}{E(p+p_1)^{1/2}} \times \\
&\qquad \times \frac{\widehat{f}(p_1-p_2)}{E(p_1)^{1/2}E(p_2)^{1/3}} \widehat{M_{\zeta'}}(p_2,p) dp_1\,dp_2,
\end{aligned}$$

with $\widehat{f}(k) := E(k)|\widehat{\varphi'}(k)|$ and $\widehat{\zeta'}(k) := |\widehat{\zeta}(k)|/E(k)$. Now

$$|\widehat{Q_\zeta}(p,p)| \leq 2(2\pi)^{-3/2} \iint \widehat{R_1}(p,p_1) \frac{\widehat{f}(p_1-p_2)}{E(p_1)^{1/2}E(p_2)^{1/3}} \widehat{M_{\zeta'}}(p_2,p)\, dp_1\, dp_2$$

with

$$\widehat{R_1}(p,p_1) := \frac{E(p-p_1)|\Lambda^+(p)\widehat{R}(p,p_1)\Lambda^-(p_1)|}{E(p+p_1)^{1/2}}.$$

We thus have

$$\begin{aligned}
|\langle \rho_{1,1}^{+--}, \zeta\rangle| &\leq 2\left\| R_1 \frac{1}{|D_0|^{1/2}} f \frac{1}{|D_0|^{1/3}} M_{\zeta'} \right\|_{\mathfrak{S}^1} \\
&\leq 2\|\Lambda^+ R \Lambda^-\|_{\mathcal{R}} \left\|M_{\zeta'}\right\|_{\mathfrak{S}_2} \left\| \frac{1}{|D_0|^{1/2}} f \frac{1}{|D_0|^{1/3}} \right\|_{\mathfrak{S}_\infty} \\
&\leq 2\|\Lambda^+ R \Lambda^-\|_{\mathcal{R}} \left\|M_{\zeta'}\right\|_{\mathfrak{S}_2} \left\| \frac{1}{|D_0|^{1/2}} f \frac{1}{|D_0|^{1/3}} \right\|_{\mathfrak{S}_6} \\
&\leq \frac{S_{6,5} C_M C_6}{2\pi} \|\Lambda^+ R \Lambda^-\|_{\mathcal{R}} \|\zeta\|_{\mathcal{C}'} \|\rho'\|_{\mathcal{C}},
\end{aligned}$$

and finally

$$\|\rho_{1,1}^{+--}\|_{\mathcal{C}} \leq \frac{S_{6,5} C_M C_6}{2\pi} \|\Lambda^+ R \Lambda^-\|_{\mathcal{R}} \|\rho'\|_{\mathcal{C}}.$$

We now treat $\rho_{1,1}^{+-+}$ and estimate

$$\widehat{Q_\zeta}(p,p) = (2\pi)^{-3} \iint dp_1\, dp_2 \frac{\Lambda^+(p)\widehat{R}(p,p_1)\Lambda^-(p_1)\widehat{\varphi'}(p_1-p_2)\Lambda^+(p_2)}{(E(p)+E(p_1))(E(p_1)+E(p_2))} \widehat{\zeta}(p_2-p),$$

by

$$\begin{aligned}
|\widehat{Q_\zeta}(p,p)| \leq 2(2\pi)^{-3} \iint \frac{E(p-p_1)|\Lambda^+(p)\widehat{R}(p,p_1)\Lambda^-(p_1)|}{E(p+p_1)^{1/2}} \times \\
\times \frac{\widehat{f}(p_1-p_2)|\Lambda^-(p_1)\Lambda^+(p_2)|}{E(p_1+p_2)^{2/3}} \frac{\widehat{\zeta'}(p_2-p)}{E(p_2)^{5/6}} dp_1\, dp_2.
\end{aligned}$$

Using the same argument as above, we arrive at

$$\|\rho_{1,1}^{+-+}\|_{\mathcal{C}} \leq \frac{S_{6,5} C_M C_6}{2\pi} \|\Lambda^+ R \Lambda^-\|_{\mathcal{R}} \|\rho'\|_{\mathcal{C}}.$$

To treat $\rho_{1,1}^{++-}$, we remark that

$$\begin{aligned}
\frac{1}{(E(p)+E(p_2))(E(p_1)+E(p_2))} \leq \frac{1}{(E(p)+E(p_1))(E(p_1)+E(p_2))} \\
+ \frac{1}{(E(p)+E(p_1))(E(p)+E(p_2))}
\end{aligned}$$

and use the same estimates as above to get

$$\|\rho_{1,1}^{++-}\|_{\mathcal{C}} \leq \frac{S_{6,5} C_M C_6}{\pi} \|\Lambda^+ R \Lambda^-\|_{\mathcal{R}} \|\rho'\|_{\mathcal{C}}.$$

Finally, since $\sum_{\epsilon_1,\epsilon_2\in\{\pm\}} \|\Lambda^{\epsilon_1} R \Lambda^{\epsilon_2}\|_{\mathcal{R}}^2 = \|R\|_{\mathcal{R}}^2$, we end up with

$$\|\rho_{1,1}\|_{\mathcal{C}} \leq 2\frac{S_{6,5} C_M C_6}{\pi} \|\rho'\|_{\mathcal{C}} \left(\sum_{\epsilon_1,\epsilon_2\in\{\pm\}} \|\Lambda^{\epsilon_1} R \Lambda^{\epsilon_2}\|_{\mathcal{R}} \right) \leq 4\frac{S_{6,5} C_M C_6 C_R}{\pi} \|\rho'\|_{\mathcal{C}} \|Q\|_{\mathcal{Q}}.$$

4.3.3 The general n^{th} order case

Now that we have explained how the proof works for the second order, let us estimate the general n^{th} order term.

Lemma 13. *We have the following estimates*

$$\forall n \geq 3, \qquad \|Q_n\|_{\mathcal{Q}} \leq nK_{\frac{n}{2}} C_Q \left\|(Q,\rho')\right\|^n, \quad \textit{with} \quad C_Q = \sqrt{2}\left(\frac{S_6 C_6}{2\sqrt{\pi}}\right)^3,$$

$$\forall n \geq 5, \qquad \|\rho_n\|_{\mathcal{C}} \leq nK_{\frac{n+1}{2}} C_\rho \left\|(Q,\rho')\right\|^n, \quad \textit{with} \quad C_\rho = \frac{S_6 C_6}{4\pi}\left(\frac{S_6 C_6}{2\sqrt{\pi}}\right)^5,$$

$$\|\rho_4\|_{\mathcal{C}} \leq C_{\rho_4} \left\|(Q,\rho')\right\|^4, \quad \textit{with} \quad C_{\rho_4} := \frac{K_2 S_6 C_6}{\pi}\left(\frac{S_6 C_6}{2\sqrt{\pi}}\right)^2.$$

Therefore,

$$\forall n \geq 4, \qquad \|(Q_n,\rho_n)\| \leq \kappa_n \left\|(Q,\rho')\right\|^n$$

with

$$\kappa_4 = 4C_R K_2 C_Q \sqrt{2} + 2\sqrt{\pi} C_{\rho_4}, \qquad \kappa_n = nC_R K_{\frac{n}{2}} C_Q \sqrt{2} + 2nK_{\frac{n+1}{2}} C_\rho \sqrt{\pi}.$$

Remark that it can be proved that $K_n \sim_{n\to\infty} \frac{C}{\sqrt{n}}$, which gives the claimed behaviour for κ_n as $n \to \infty$.

Proof – **Step 1 : Estimates on the exchange term Q_n.**

- *$Q_{k,l}$ with $k \geq 1$ and $k + l = n \geq 3$.* Recall that

$$Q_{k,l} = \frac{(-1)^{l+1}}{2\pi} \sum_{I\cup J=\{1,\dots,n\},\ |I|=k,\ |J|=l} \int_{-\infty}^{+\infty} d\eta \frac{1}{D^0 + i\eta} \prod_{j=1}^{n} \left(R_j \frac{1}{D^0 + i\eta}\right),$$

where $R_j = R$ if $j \in I$ and $R_j = \varphi'$ if $j \in J$. For the sake of simplicity, we treat only

$$Q'_{k,l} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} d\eta \frac{1}{D^0 + i\eta} \left(R \frac{1}{D^0 + i\eta}\right)^k \left(\varphi' \frac{1}{D^0 + i\eta}\right)^l.$$

We have

$$\begin{aligned}
|\widehat{Q'_{k,l}}(p,q)| \leq \frac{1}{(2\pi)^{1+\frac{3l}{2}}} \int_{-\infty}^{+\infty} d\eta \int\cdots\int \frac{1}{(E(p)^2+\eta^2)^{1/2}} |\widehat{R}(p,p_1)| \times \\
\times \frac{1}{(E(p_1)^2+\eta^2)^{1/4}} \prod_{j=1}^{k-1} \left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}} |\widehat{R}(p_j,p_{j+1})| \frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}}\right) \times \\
\times \prod_{j=k}^{n-2} \left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}} |\widehat{\varphi'}(p_j - p_{j+1})| \frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}}\right) \times \\
\times \frac{1}{(E(p_{n-1})^2+\eta^2)^{1/4}} |\widehat{\varphi'}(p_{n-1} - q)| \frac{1}{(E(q)^2+\eta^2)^{1/2}} \, dp_1 \cdots dp_{n-1}
\end{aligned}$$

so by (45),

$$\begin{aligned}
E(p-q)E(p+q)^{1/2} |\widehat{Q'_{k,l}}(p,q)| \leq \frac{2^{\frac{k+1}{2}} E(p-q)}{(2\pi)^{1+\frac{3l}{2}}} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^{\frac{k+1}{2}}} \int\cdots\int \frac{|\widehat{R}(p,p_1)|}{E(p+p_1)^{1/2}} \times \\
\times \prod_{j=1}^{k-1} \frac{|\widehat{R}(p_j,p_{j+1})|}{E(p_j+p_{j+1})^{1/2}} \prod_{j=k}^{n-2} \left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}} |\widehat{\varphi'}(p_j - p_{j+1})| \frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}}\right) \times \\
\times \frac{1}{(E(p_{n-1})^2+\eta^2)^{1/4}} |\widehat{\varphi'}(p_{n-1} - q)| \frac{1}{(E(q)^2+\eta^2)^{1/4}} \, dp_1 \cdots dp_{n-1}.
\end{aligned}$$

Now if we use the easy generalization of (18),

$$E(p-q) \leq E(p-p_1) + E(p_1-p_2) + \cdots + E(p_{n-2}-p_{n-1}) + E(p_{n-1}-q),$$

we obtain by a similar argument as before

$$\|Q'_{k,l}\|_{\mathcal{Q}} \leq \frac{2^{\frac{k+1}{2}}}{2\pi} \left[k(C_R)^k (4\pi C_\infty)^l \left(\int_{-\infty}^{\infty} \frac{d\eta}{E(\eta)^{l+\frac{k+1}{2}}} \right) \right.$$
$$\left. + l(C_R)^k (4\pi C_\infty)^{l-1} S_6 C_6 \left(\int_{-\infty}^{\infty} \frac{d\eta}{E(\eta)^{l+\frac{k}{2}}} \right) \right] \|Q\|_{\mathcal{Q}}^k \|\rho'\|_{\mathcal{C}}^l.$$

To obtain this result, we have estimated each term containing a φ' by using

$$\left\| \frac{1}{(|D_0|^2 + E(\eta)^2)^{1/4}} \varphi' \frac{1}{(|D_0|^2 + E(\eta)^2)^{1/4}} \right\|_{\mathfrak{S}_\infty} \leq \frac{1}{E(\eta)} \|\varphi'\|_{L^\infty} \leq \frac{C_\infty}{E(\eta)} \|\varphi'\|_{\mathcal{Y}}$$

and when $E(p_j - p_{j+1})$ appears in front of a $\widehat{\varphi'}(p_j - p_{j+1})$ (i.e. when $j \geq k$), by using

$$\left\| \frac{1}{(|D_0|^2 + E(\eta)^2)^{1/4}} f \frac{1}{(|D_0|^2 + E(\eta)^2)^{1/4}} \right\|_{\mathfrak{S}_\infty}$$
$$\leq \left\| \frac{1}{(|D_0|^2 + E(\eta)^2)^{1/4}} f \frac{1}{(|D_0|^2 + E(\eta)^2)^{1/4}} \right\|_{\mathfrak{S}_6} \leq \frac{S_6}{E(\eta)^{1/2} 4\pi} \|f\|_{L^6}.$$

So we have

$$\begin{aligned} \|Q'_{k,l}\|_{\mathcal{Q}} &\leq 2^{\frac{k+1}{2}} \left[k(C_R)^k (4\pi C_\infty)^l K_{l+\frac{k+1}{2}} + l(C_R)^k (4\pi C_\infty)^{l-1} S_6 C_6 K_{l+\frac{k}{2}} \right] \|Q\|_{\mathcal{Q}}^k \|\rho'\|_{\mathcal{C}}^l \\ &\leq 2^{\frac{k+1}{2}} n (C_R)^k (4\pi C_\infty)^l K_{l+\frac{k}{2}} \max\left(1, \frac{S_6 C_6}{4\pi C_\infty}\right) \|Q\|_{\mathcal{Q}}^k \|\rho'\|_{\mathcal{C}}^l \end{aligned}$$

which implies

$$\|Q_{k,l}\|_{\mathcal{Q}} \leq \tbinom{n}{k} 2^{\frac{k+1}{2}} n (C_R)^k (4\pi C_\infty)^l K_{l+\frac{k}{2}} \max\left(1, \frac{S_6 C_6}{4\pi C_\infty}\right) \|Q\|_{\mathcal{Q}}^k \|\rho'\|_{\mathcal{C}}^l.$$

- $Q_{0,n}$ *with* $n \geq 3$. Recall that

$$Q_{0,n} = \frac{(-1)^{n+1}}{2\pi} \int_{-\infty}^{+\infty} d\eta \frac{1}{D^0 + i\eta} \left(\varphi' \frac{1}{D^0 + i\eta} \right)^n$$

so that

$$E(p-q)E(p+q)^{1/2} |\widehat{Q_{0,n}}(p,q)| \leq \frac{E(p-q)}{(2\pi)^{1+\frac{3n}{2}}} \int_{-\infty}^{+\infty} \frac{d\eta}{E(\eta)^{\frac{1}{2}}} \int \cdots \int dp_1 \cdots dp_{n-1} \times$$
$$\times \frac{|\widehat{\varphi'}(p-p_1)|}{(E(p)^2+\eta^2)^{1/4}(E(p_1)^2+\eta^2)^{1/4}} \prod_{j=1}^{n-2} \left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}} |\widehat{\varphi'}(p_j - p_{j+1})| \frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}} \right) \times$$
$$\times \frac{1}{(E(p_{n-1})^2+\eta^2)^{1/4}} |\widehat{\varphi'}(p_{n-1}-q)| \frac{1}{(E(q)^2+\eta^2)^{1/4}}.$$

We now use (46) to bound for some f_1, f_2 and f_3

$$\left\| \prod_{j=1}^{3} \left(\frac{1}{(|D_0|^2+\eta^2)^{1/4}} f_j \frac{1}{(|D_0|^2+\eta^2)^{1/4}} \right) \right\|_{\mathfrak{S}^2} \leq \frac{(S_6)^3}{E(\eta)^{3/2}(4\pi)^3} \prod_{j=1}^{3} \|f_j\|_{L^6} \tag{48}$$

to obtain

$$\|Q_{0,n}\|_{\mathcal{Q}} \leq n\frac{\sqrt{2}}{2\pi}\left(\int_{-\infty}^{\infty}\frac{d\eta}{E(\eta)^{2+(n-3)}}\right)(S_6C_6)^3(4\pi C_\infty)^{n-3}\|\rho'\|_{\mathcal{C}}^n$$

or

$$\|Q_{0,n}\|_{\mathcal{Q}} \leq nK_{n-1}\sqrt{2}(S_6C_6)^3(4\pi C_\infty)^{n-3}\|\rho'\|_{\mathcal{C}}^n.$$

Finally, we can write for instance (recall that $C_\infty = 1/(2\sqrt{\pi})$)

$$\|Q_n\|_{\mathcal{Q}} \leq nK_{n/2}C_Q\left(C_R\sqrt{2}\|Q\|_{\mathcal{Q}} + 2\sqrt{\pi}\|\rho'\|_{\mathcal{C}}\right)^n \tag{49}$$

where

$$C_Q = \sqrt{2}\max\left(1, \frac{S_6C_6}{4\pi C_\infty}, \left(\frac{S_6C_6}{4\pi C_\infty}\right)^3\right) = \sqrt{2}\frac{(S_6C_6)^3}{8\pi^{3/2}},$$

and since $K_{n/2} \geq K_{n-1}$ when $n \geq 2$.

Step 2 : Estimates on the density ρ_n.

• *$\rho_{k,l}$ with $k \geq 2$ and $n \geq 3$.* As before we treat for instance the density $\rho'_{k,l}$ of the $Q'_{k,l}$ where the k R's are on the left and the l φ''s are on the right. For some fixed $\zeta \in \mathcal{C}' \cap L^2$, we introduce $Q_\zeta := Q'_{k,l}\zeta$. We thus estimate

$$\begin{aligned}
|\widehat{Q_\zeta}(p,p)| \leq \frac{1}{(2\pi)^{1+\frac{3(l+1)}{2}}}\int_{-\infty}^{+\infty}d\eta\int\cdots\int\frac{1}{(E(p)^2+\eta^2)^{1/4}}|\widehat{R}(p,p_1)|\times \\
\times\frac{1}{(E(p_1)^2+\eta^2)^{1/4}}\prod_{j=1}^{k-1}\left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}}|\widehat{R}(p_j,p_{j+1})|\frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}}\right)\times \\
\times\prod_{j=k}^{n-1}\left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}}|\widehat{\varphi'}(p_j-p_{j+1})|\frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}}\right)\times \\
\times\frac{1}{(E(p_n)^2+\eta^2)^{1/4}}|\widehat{\zeta}(p_n-p)|\frac{1}{(E(p)^2+\eta^2)^{1/4}}\,dp_1\cdots dp_n.
\end{aligned}$$

We now use as before

$$|\widehat{\zeta}(p_n-p)| \leq \frac{|\widehat{\zeta}(p_n-p)|}{E(p_n-p)}\big(E(p-p_1)+E(p_1-p_2)+\cdots+E(p_{n-1}-p_n)\big)$$

to obtain

$$|\langle\rho'_{k,l},\zeta\rangle| \leq n\frac{2^{k/2}S_6C_6}{4\pi}(C_R)^k(4\pi C_\infty)^l\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\eta}{E(\eta)^{l+\frac{k+1}{2}}}\right)\|Q\|_{\mathcal{Q}}^k\|\rho'\|_{\mathcal{C}}^l\|\zeta\|_{\mathcal{C}'}$$

and so

$$\|\rho_{k,l}\|_{\mathcal{C}} \leq n\binom{n}{k}\frac{S_6C_6}{4\pi}(C_R\sqrt{2})^k(4\pi C_\infty)^l K_{l+\frac{k+1}{2}}\|Q\|_{\mathcal{Q}}^k\|\rho'\|_{\mathcal{C}}^l.$$

• *$\rho_{1,l}$ with $l \geq 2$.* We may treat for instance with the same notation as before

$$\begin{aligned}
|\widehat{Q_\zeta}(p,p)| \leq \frac{1}{(2\pi)^{1+\frac{3n}{2}}}\int_{-\infty}^{+\infty}d\eta\int\cdots\int\frac{1}{(E(p)^2+\eta^2)^{1/4}}|\widehat{R}(p,p_1)|\times \\
\times\frac{1}{(E(p_1)^2+\eta^2)^{1/4}}\prod_{j=1}^{n-1}\left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}}|\widehat{\varphi'}(p_j-p_{j+1})|\frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}}\right)\times \\
\times\frac{1}{(E(p_n)^2+\eta^2)^{1/4}}|\widehat{\zeta}(p_n-p)|\frac{1}{(E(p)^2+\eta^2)^{1/4}}\,dp_1\cdots dp_n.
\end{aligned}$$

We now use (48) and obtain

$$|\langle \rho'_{1,l}, \zeta\rangle| \le n\frac{2^{1/2}(S_6C_6)^3}{4\pi} C_R(4\pi C_\infty)^{l-2}\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\eta}{E(\eta)^{l-2+\frac{4}{2}}}\right)\|Q\|_{\mathcal{Q}}\|\rho'\|_{\mathcal{C}}^l\|\zeta\|_{\mathcal{C}'}$$

and so

$$\|\rho_{1,l}\|_{\mathcal{C}} \le n\binom{n}{n-1}\frac{2^{1/2}(S_6C_6)^3K_l}{4\pi} C_R(4\pi C_\infty)^{l-2}\|Q\|_{\mathcal{Q}}\|\rho'\|_{\mathcal{C}}^l.$$

- $\rho_{0,l}$ *with* $l \ge 5$. We want to estimate

$$\begin{aligned}|\widehat{Q_\zeta}(p,p)| \le \frac{1}{(2\pi)^{1+\frac{3(n+1)}{2}}}\int_{-\infty}^{+\infty}d\eta\int\cdots\int\frac{1}{(E(p)^2+\eta^2)^{1/4}}|\widehat{\varphi'}(p-p_1)|\times\\ \times\frac{1}{(E(p_1)^2+\eta^2)^{1/4}}\prod_{j=1}^{n-1}\left(\frac{1}{(E(p_j)^2+\eta^2)^{1/4}}|\widehat{\varphi'}(p_j-p_{j+1})|\frac{1}{(E(p_{j+1})^2+\eta^2)^{1/4}}\right)\times\\ \times\frac{1}{(E(p_n)^2+\eta^2)^{1/4}}|\widehat{\zeta}(p_n-p)|\frac{1}{(E(p)^2+\eta^2)^{1/4}}\,dp_1\cdots dp_n.\end{aligned}$$

Since there are at least 6 functions, we may use (48) twice and obtain

$$|\langle \rho'_{0,l}, \zeta\rangle| \le n\frac{(S_6C_6)^6}{4\pi}(4\pi C_\infty)^{l-5}\left(\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{d\eta}{E(\eta)^{l-2}}\right)\|\rho'\|_{\mathcal{C}}^n\|\zeta\|_{\mathcal{C}'}$$

and so

$$\|\rho_{0,l}\|_{\mathcal{C}} \le n\frac{(S_6C_6)^6}{4\pi}(4\pi C_\infty)^{l-5}K_{l-2}\|\rho'\|_{\mathcal{C}}^n.$$

Now since $K_{n-2} \le K_{(n+1)/2}$ when $n \ge 5$, we obtain

$$\|\rho_n\|_{\mathcal{C}} \le nK_{\frac{n+1}{2}}C_\rho\left(C_R\sqrt{2}\|Q\|_{\mathcal{Q}} + 2\sqrt{\pi}\|\rho'\|_{\mathcal{C}}\right)^n \tag{50}$$

with

$$C_\rho := \frac{S_6C_6}{4\pi}\max\left(1, \left(\frac{C_6S_6}{2\sqrt{\pi}}\right)^2, \left(\frac{C_6S_6}{2\sqrt{\pi}}\right)^5\right) = \frac{S_6C_6}{4\pi}\left(\frac{C_6S_6}{2\sqrt{\pi}}\right)^5.$$

For ρ_4, we notice that $\rho_{0,4} = 0$ for the same reason as $\rho_{0,2}$, and that $K_2 \ge K_{5/2}$. Therefore we obtain

$$\|\rho_4\|_{\mathcal{C}} \le C_{\rho_4}\left(C_R\sqrt{2}\|Q\|_{\mathcal{Q}} + 2\sqrt{\pi}\|\rho'\|_{\mathcal{C}}\right)^4 \tag{51}$$

with

$$C_{\rho_4} := \frac{4K_2S_6C_6}{4\pi}\max\left(1, \left(\frac{C_6S_6}{2\sqrt{\pi}}\right)^2\right) = \frac{S_6C_6K_2}{\pi}\left(\frac{C_6S_6}{2\sqrt{\pi}}\right)^2. \quad \square$$

4.3.4 The third order density ρ_3

Lemma 14. *We have*

$$\|\rho_3\|_{\mathcal{C}} \le C_{\rho_3}\left(C_R\sqrt{2}\|Q\|_{\mathcal{Q}} + 2\sqrt{\pi}\|\rho'\|_{\mathcal{C}}\right)^3$$

and therefore

$$\|(Q_3, \rho_3)\| \le \kappa_3\left\|(Q, \rho')\right\|^3$$

with

$$\kappa_3 = 3C_RK_{3/2}C_Q\sqrt{2} + 2\sqrt{\pi}C_{\rho_3}, \qquad C_{\rho_3} = \frac{15C_MS_6(S_{6,4})^2(C_6)^4}{\pi(4\pi C_\infty)^3}.$$

Proof – Notice that thanks to the previous proof, we already have some estimates on $\rho_{3,0}$, $\rho_{2,1}$ and $\rho_{1,2}$. It remains to study $\rho_{0,3}$. As before and as in [16], we have to compute $\rho_{0,3}$ explicitely by a residuum formula. We thus write

$$\rho_{0,3} = \sum_{\epsilon_1,\dots,\epsilon_4\in\{\pm\}} \rho_{0,3}^{\epsilon_1\epsilon_2\epsilon_3\epsilon_4}$$

with an obvious definition.

• Let us treat first $\rho_{0,3}^{+---}$. We thus fix some $\zeta \in \mathcal{C}' \cap L^2$ and estimate the term

$$\widehat{Q_\zeta}(p,p) = (2\pi)^{-6} \iiint dp_1\, dp_2\, dp_3 \frac{\Lambda^+(p)\widehat{\varphi'}(p-p_1)\Lambda^-(p_1)}{E(p)+E(p_1)} \times \\ \times \frac{\widehat{\varphi'}(p_1-p_2)\Lambda^-(p_2)\widehat{\varphi'}(p_2-p_3)\Lambda^-(p_3)}{(E(p)+E(p_2))(E(p)+E(p_3))}\widehat{\zeta}(p_3-p),$$

by

$$|\widehat{Q_\zeta}(p,p)| \leq (2\pi)^{-6} \iiint dp_1\, dp_2\, dp_3 \frac{\left|\Lambda^+(p)\widehat{\varphi'}(p-p_1)\Lambda^-(p_1)\right|}{E(p+p_1)^{2/3}} \times \\ \times \frac{\left|\widehat{\varphi'}(p_1-p_2)\right|\left|\widehat{\varphi'}(p_2-p_3)\right|}{E(p_1)^{1/3}E(p_2)E(p)}\left|\widehat{\zeta}(p_3-p)\right|.$$

So if we follow the method used above, we obtain

$$\|\rho_{0,3}^{+---}\|_{\mathcal{C}} \leq \frac{3C_M S_6 (S_{6,4})^2 (C_6)^4}{4\pi}\|\rho'\|_{\mathcal{C}}^3.$$

Now, it is easily seen that $\rho_{0,3}^{-+++}$, $\rho_{0,3}^{--+-}$, $\rho_{0,3}^{++--}$, $\rho_{0,3}^{-+--}$, $\rho_{0,3}^{+-++}$, $\rho_{0,3}^{--+-}$ and $\rho_{0,3}^{++-+}$ can be treated by exactly the same method.

• Let us now treat for instance $\rho_{0,3}^{++--}$. Thanks to the residuum formula, we have to study

$$\widehat{Q_\zeta}(p,p) = (2\pi)^{-6} \iiint dp_1\, dp_2\, dp_3 \Lambda^+(p)\widehat{\varphi'}(p-p_1)\Lambda^+(p_1)\widehat{\varphi'}(p_1-p_2)\Lambda^-(p_2) \\ \widehat{\varphi'}(p_2-p_3)\Lambda^-(p_3)\widehat{\zeta}(p_3-p) \times \left(\frac{1}{(E(p)+E(p_2))(E(p_1)+E(p_2))(E(p_1)+E(p_3))} + \right. \\ \left. \frac{1}{(E(p)+E(p_2))(E(p)+E(p_3))(E(p_1)+E(p_3))} \right).$$

If we now use the same method as above for each of the two terms of this sum, we arrive at

$$\|\rho_{0,3}^{++--}\|_{\mathcal{C}} \leq 2\frac{3C_M S_6 (S_{6,4})^2 (C_6)^4}{4\pi}\|\rho'\|_{\mathcal{C}}^3.$$

This is easily generalized to the study of $\rho_{0,3}^{--++}$, $\rho_{0,3}^{+-+-}$, $\rho_{0,3}^{-+-+}$, $\rho_{0,3}^{+--+}$ and $\rho_{0,3}^{-++-}$.

Summing now all these terms, we obtain

$$\|\rho_{0,3}\|_{\mathcal{C}} \leq 20\frac{3C_M S_6 (S_{6,4})^2 (C_6)^4}{4\pi}\|\rho'\|_{\mathcal{C}}^3 = \frac{15C_M S_6 (S_{6,4})^2 (C_6)^4}{\pi}\|\rho'\|_{\mathcal{C}}^3$$

and

$$\|\rho_3\|_{\mathcal{C}} \leq C_{\rho_3}\left(C_R\sqrt{2}\|Q\|_{\mathcal{Q}} + 2\sqrt{\pi}\|\rho'\|_{\mathcal{C}}\right)^3, \tag{52}$$

with

$$C_{\rho_3} = 3\frac{S_6 C_6}{4\pi}\max\left(K_{3+1/2}\,,\, K_3\,,\, K_2\left(\frac{S_6C_6}{4\pi C_\infty}\right)^2, \frac{20C_M(S_{6,4})^2(C_6)^3}{(4\pi C_\infty)^3}\right) = \frac{15C_M S_6(S_{6,4})^2(C_6)^4}{\pi(4\pi C_\infty)^3}. \quad \square$$

Appendix: Derivation of the BDF energy

In this section, we recall some basics about the second-quantization in no-photon QED and explain how the energy $\mathcal{E}^{\mathrm{BDF}}$ is derived from this theory, as a mean-field approximation. We mainly follow the method of Chaix-Iracane [5, 7], but with the notation of [30, 2, 17]. See also [16] for more details concerning the polarization of the vacuum.

Since this derivation is somewhat formal, we may work in $\mathcal{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$. To simplify the presentation, we introduce $P_-^0 := P^0$ and $P_+^0 := 1 - P^0$.

Free particles, Fock space, free vacuum

We first introduce $\mathcal{F}_+^{(1)} := P_+^0\mathcal{H}$ and $\mathcal{F}_-^{(1)} := CP_-^0\mathcal{H}$ which are called respectively the free electron and the free positron state subspace. C is the charge-conjugation operator defined by $C\psi = i\beta\alpha_2\overline{\psi}$. We define $\mathcal{F}_+^{(0)} = \mathcal{F}_-^{(0)} = \mathbb{C}$ and $\mathcal{F}_+^{(n)} = \bigwedge_{k=1}^n \mathcal{F}_+^{(1)}$, $\mathcal{F}_-^{(m)} = \bigwedge_{k=1}^m \mathcal{F}_-^{(1)}$ for $n, m \geq 1$. The space of n free electrons and m free positrons is then defined by $\mathcal{F}^{(n,m)} = \mathcal{F}_+^{(n)} \otimes \mathcal{F}_-^{(m)}$ and the associated Fock space is

$$\mathcal{F} := \bigoplus_{n,m=0}^{\infty} \mathcal{F}^{(n,m)}. \tag{53}$$

For any $f \in \mathcal{H}$, we define the free electron annihilation and creation operators $a_0(f)$ and $a_0^*(f)$. The free electron annihilation operator $a_0(f)$ fulfills $a_0(f)(\mathcal{F}^{(n,m)}) \subset \mathcal{F}^{(n-1,m)}$ for $n \geq 1$ and is defined on $\mathcal{F}^{(n,m)}$ by

$$a_0(f)(\psi)(x_1, ..., x_{n-1}; y_1, ..., y_m) = \sqrt{n+1} \int_{\mathbb{R}^3} \overline{P_+^0(f)} \cdot \psi(x, x_1, ..., x_{n-1}; y_1, ..., y_m)\, dx,$$

and $a_0(f)(\mathcal{F}^{(0,m)}) = 0$. The free electron creation operator $a_0^*(f)$ fulfills $a_0^*(f)(\mathcal{F}^{(n,m)}) \subset \mathcal{F}^{(n+1,m)}$ for $n \geq 0$ and is defined on tensor products of $\mathcal{F}^{(n,m)}$ by

$$a_0^*(f)(\psi_+ \otimes \psi_-) = \Big(P_+^0(f) \wedge \psi_+\Big) \otimes \psi_-$$

when $\psi_+ \in \mathcal{F}_+^{(n)}$ and $\psi_+ \in \mathcal{F}_-^{(m)}$, or more explicitely for $\psi \in \mathcal{F}^{(n,m)}$

$$a_0^*(f)(\psi)(x_1, ..., x_{n+1}; y_1, ..., y_m) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j+1} P_+^0(f)(x_j) \psi(x_1, ..., x_{j-1}, x_{j+1}, ..., x_n; y_1, ..., y_m).$$

Correspondingly, the free positron annihilation and creation operators $b_0(f)$ and $b_0^*(f)$ are defined by

$$b_0(f)(\psi)(x_1, ..., x_n; y_1, ..., y_{m-1}) = (-1)^n \sqrt{m+1} \int_{\mathbb{R}^3} \overline{CP_-^0(f)} \cdot \psi(x_1, ..., x_n; y, y_1, ..., y_{m-1})\, dx,$$

$$b_0(f)(\mathcal{F}^{(n,0)}) = 0, \qquad b_0^*(f)(\psi_+ \otimes \psi_-) = (-1)^n \psi_+ \otimes \Big(CP_-^0(f) \wedge \psi_-\Big)$$

when $\psi_+ \in \mathcal{F}_+^{(n)}$ and $\psi_+ \in \mathcal{F}_-^{(m)}$. As before, $b_0(f)(\mathcal{F}^{(n,m)}) \subset \mathcal{F}^{(n,m-1)}$ and $b_0^*(f)(\mathcal{F}^{(n,m)}) \subset \mathcal{F}^{(n,m+1)}$. Remark that a_0 and b_0^* are anti-linear, while a_0^* and b_0 are linear. They fulfill the Canonical Anti-commutation Relations

$$\begin{aligned}\{a_0(f), a_0(g)\} = \{a_0^*(f), a_0^*(g)\} = \{a_0(f), b_0(g)\} \\ = \{a_0^*(f), b_0^*(g)\} = \{a_0^*(f), b_0(g)\} = \{a_0(f), b_0^*(g)\} = 0,\end{aligned} \tag{54}$$

$$\{a_0(f), a_0^*(g)\} = \langle f, P_+^0 g\rangle, \qquad \{b_0^*(f), b_0(g)\} = \langle f, P_-^0 g\rangle, \tag{55}$$

where $\langle \cdot, \cdot \rangle$ denotes the usual scalar product of $L^2(\mathbb{R}^3, \mathbb{C}^4)$.

For the *free vacuum state* Ω_0, a unit vector spanning $\mathcal{F}^{(0,0)} = \mathbb{C}$, we obtain

$$a_0(f)\Omega_0 = 0 \text{ and } b_0(f)\Omega_0 = 0, \tag{56}$$

a property that caracterizes uniquely Ω_0 up to a phase factor.

Let us now define the *field operator* $\Psi(f)$ on the Fock space $\mathcal{F}$ by

$$\Psi(f) = a_0(f) + b_0^*(f).$$

In terms of $\Psi(f)$, the CAR become

$$\{\Psi(f), \Psi(g)\} = \{\Psi^*(f), \Psi^*(g)\} = 0, \qquad \{\Psi(f), \Psi^*(g)\} = \langle f, g\rangle 1,$$

for all $(f, g) \in \mathcal{H}^2$.

Remark that we have by definition

$$\Psi(P_+^0 f) = a_0(f), \qquad \Psi^*(P_-^0 f) = b_0(f) \tag{57}$$

and $\Psi(P_+^0 f)\Omega_0 = \Psi^*(P_-^0 f)\Omega_0 = 0$, which also caracterizes the free vacuum Ω_0 up to a phase factor.

Dressed particles and vacuum

In this description, the free electrons and positrons are defined with respect to the projector P^0, or equivalently the spitting $\mathcal{H} = \mathcal{H}_-^0 \oplus \mathcal{H}_+^0$. We want now to change this definition and introduce the *dressed electrons and positrons*. To this end, we fix a new projector P on $\mathcal{H}$, use again the notation $P_- := P$ and $P_+ := 1 - P$, and introduce the dressed particle annihilation operators

$$a_P(f) := \Psi(P_+ f), \qquad b_P(f) := \Psi^*(P_- f), \tag{58}$$

by using (57). Similar formula can be given for the dressed particle creation operators a_P^* and b_P^*. These dressed operators satisfy the same anti-commutation relations as for the free operators (54) (55). We also introduce the dressed electrons and positrons state subspaces

$$\mathcal{H}_+^P = (1 - P)\mathcal{H}, \qquad \mathcal{H}_-^P = P\mathcal{H}.$$

Now, the main question is to know if there exists a *dressed vacuum* Ω_P in the Fock space $\mathcal{F}$. This state has to be a solution to the analogue of (56)

$$a_P(f)\Omega_P = 0 \text{ and } b_P(f)\Omega_P = 0 \tag{59}$$

for all $f \in \mathcal{H}$. The answer is given by the celebrated Shale-Stinespring Theorem (see Thaller's book [30, Theorem 10.6])

Theorem 5 (Shale-Stinespring Theorem). *There exists a dressed vacuum Ω_P in the Fock space $\mathcal{F}$ satisfying* (59) *if and only if $P - P^0$ is a Hilbert-Schmidt operator. In this case, Ω_P is unique up to a phase factor.*

This result explains why we assumed in the previous section that $P - P^0 \in \mathfrak{S}_2(\mathcal{H}_\Lambda)$.

Second-quantized Hamiltonian

In the physics literature, the creation and annihilation operators are defined differently. For instance, instead of $a_0^*(f)$ which creates an electron in the state $P_+^0 f$, the operator $a_0^*(x)$ which creates an electron at x is formally used, where $a_0^*(x) = \sum_{i=1}^\infty a_0^*(f_i) f_i(x)$, $(f_i)_{i\geq 1}$ being an orthonormal basis of $\mathcal{H}_+^0$. The operators $a_P(x)$ and $b_P(x)$ are defined similarly.

We shall now use this formalism and follow mainly [16]. Formally, the CAR (54, 55) are equivalent to

$$\{a_0(x), a_0(y)\} = \{a_0^*(x), a_0^*(y)\} = \{a_0(x), b_0(y)\} \\ = \{a_0^*(x), b_0^*(y)\} = \{a_0^*(x), b_0(y)\} = \{a_0(x), b_0^*(y)\} = 0, \quad (60)$$

$$\{a_0(x), a_0^*(y)\} = [1 - P^0](x, y),\ \{b_0^*(x), b_0(y)\} = P^0(x, y) \quad (61)$$

where $[1 - P^0](x, y)$, $P^0(x, y)$ are the integral kernels of the projectors $1 - P$ and P.

We now start with writing down the formal unregularized no-photon Hamiltonian

$$\mathbb{H}_{\rm ur} = \int dx\, \Psi^*(x) D^{\alpha\varphi} \Psi(x) + \frac{\alpha}{2} \int dx \int dy \frac{\Psi^*(x)\Psi(x)\Psi^*(y)\Psi(y)}{|\mathbf{x} - \mathbf{y}|}, \quad (62)$$

which acts on the Fock space $\mathcal{F}$. As explained for instance in [30, 17], the free vacuum may not belong to the domain of this formally defined operator. Therefore, the formal energy of the free vacuum is substracted from (62) by a procedure which is called "normal ordering", denoted by double dots $: - :_{P^0}$. In each product of annihilation and creation operators, the a_0^* and b_0^* are moved to the left as if they anticommute with the a_0 and b_0. For instance

$$: \Psi^*(x)\Psi(y) :_{P^0} = a_0^*(x)a_0(y) + a_0^*(y)b_0(x) + b_0(x)a_0(y) - b_0^*(y)b_0(x) = \Psi^*(x)\Psi(y) - P^0(x, y). \quad (63)$$

As a first step we thus regularize $\mathbb{H}_{\rm ur}$ as done in Chaix and Iracane [5, Sections 3.5 and 4.1], namely we normal order with respect to the free Projector P^0,

$$\mathbb{H} = \int dx\ : \Psi^*(x) D^{\alpha\varphi} \Psi(x) :_{P^0} + \frac{\alpha}{2} \int dx \int dy \frac{: \Psi^*(x)\Psi(x)\Psi^*(y)\Psi(y) :_{P^0}}{|\mathbf{x} - \mathbf{y}|}. \quad (64)$$

This kind of regularization appears implicitly in any QED textbook. It corresponds to the subtraction of the energy of the free Dirac sea, and the interaction energy with the free Dirac sea, which is usually referred to as mass renormalization. In fact in [16, Section 3] these subtractions were justified by the first two guiding principles (denoted as **W1** and **W2**) formulated and justified by Weisskopf [33].

The definition of the normal ordering depends on the annihilation and creation operators and it thus depends on the projector P which is used. Now we want to express $\mathbb{H}$ in terms of $: - :_P$ for some P. Using (63) we obtain the reordering relations

$$: \Psi^*(x)\Psi(y) :_{P^0} = : \Psi^*(x)\Psi(y) :_P + Q(x, y), \quad (65)$$

where $Q = P - P^0$, and

$$: \Psi^*(x)\Psi(x)\Psi^*(y)\Psi(y) :_{P^0} = : \Psi^*(x)\Psi(x)\Psi^*(y)\Psi(y) :_P + 2 : \Psi^*(x)\Psi(x) :_P \mathrm{Tr}_{\mathbb{C}^4}(Q(y, y)) \\ - 2 : \Psi^*(x)\Psi(y) :_P Q(x, y) + \mathrm{Tr}_{\mathbb{C}^4}(Q(x, x))\mathrm{Tr}_{\mathbb{C}^4}(Q(y, y)) - |Q(x, y)|^2.$$

Therefore we can rewrite $\mathbb{H}$ with respect to an arbitrary dressed vacuum P,

$$\mathbb{H} = \int : \Psi^*(x) D^{\alpha\varphi} \Psi(x) :_P dx + \frac{\alpha}{2} \iint \frac{: \Psi^*(x)\Psi(x)\Psi^*(y)\Psi(y) :_P}{|x - y|} dx\, dy \\ + \alpha \iint \frac{: \Psi^*(x)\Psi(x) :_P \mathrm{Tr}_{\mathbb{C}^4}(Q(y, y))}{|x - y|} dx\, dy - \alpha \iint \frac{: \Psi^*(x)\Psi(y) :_P Q(x, y)}{|x - y|} dx\, dy \\ + \mathrm{Tr}(D^\varphi Q) + \frac{\alpha}{2} \iint \frac{\mathrm{Tr}_{\mathbb{C}^4}(Q(x, x))\mathrm{Tr}_{\mathbb{C}^4}(Q(y, y))}{|x - y|} dx\, dy - \frac{\alpha}{2} \iint \frac{|Q(x, y)|^2}{|x - y|} dx\, dy. \quad (66)$$

The last line represents the energy of the dressed vacuum P measured with respect to P^0, whereas in the second line the vacuum polarization potentials appear.

Restriction to Bogoliubov-Dirac-Fock states

A general strategy would now be to fix a charge q and to look at the expectation value of the operator $\mathbb{H}$ in an electron-positron state ψ with total charge q (electrons and positrons are defined with respect to P) and then minimizing over all admissible states ψ and over P.

For a slight simplification, we will follow [5] and restrict ourselves to Bogoliubov-Dirac-Fock type states. In this approximation method, a dressed vacuum P is first chosen such that $P - P^0 \in \mathfrak{S}_2(\mathcal{H})$. Then a BDF state is simply a Slater determinant made with n electrons and m positrons defined with respect to the dressed vacuum P ($n, m \geq 0$ are not fixed in this theory). This is a state of $\mathcal{F}$ which takes the form

$$\psi = a_P^*(f_1) \cdots a_P^*(f_n)\, b_P^*(g_1) \cdots b_P^*(g_m)\, \Omega_P,$$

where $(f_1, ..., f_n) \in (\mathcal{H}_+^P)^n$ and $(g_1, ..., g_m) \in (\mathcal{H}_-^P)^m$ are such that $\langle f_i, f_j \rangle = \delta_{ij}$, $\langle g_i, g_j \rangle = \delta_{ij}$, and Ω_P is the dressed vacuum in $\mathcal{F}$ obtained by Theorem 5. The *one-body density matrix* of such a state is the operator γ_ψ defined by its kernel

$$\gamma_\psi(x,y) = \sum_{i=1}^n f_i(x)\overline{f_i(y)}^T - \sum_{j=1}^m g_j(x)\overline{g_j(y)}^T$$

often written as

$$\gamma_\psi = \sum_{i=1}^n |f_i\rangle\langle f_i| - \sum_{j=1}^m |g_j\rangle\langle g_j|,$$

and it satisfies

$$-P \leq \gamma_\psi \leq 1 - P.$$

The associated *density of charge* is the function $\rho_\psi(x) = \mathrm{Tr}_{\mathbb{C}^4}(\gamma(x,x))$ or

$$\rho_\psi(x) = \sum_{i=1}^n |f_i(x)|^2 - \sum_{j=1}^m |g_j(x)|^2.$$

The energy $\langle\psi|\mathbb{H}|\psi\rangle$ of such a BDF-state $\psi \in \mathcal{F}$ is easily computed with formula (66). As usually in this type of approximation, it only depends on the one-body density matrix γ_ψ (and its spin-summed diagonal ρ_ψ) and it is shown to be (see [2] for details and [5, Formula 4.8])

$$\begin{aligned}
\mathcal{E}^{\mathrm{BDF}}(P, \gamma_\psi) &:= \langle\psi|\mathbb{H}|\psi\rangle = \mathrm{tr}\left(\left(D^{\alpha\varphi} + \alpha\rho_Q * \frac{1}{|\cdot|} - \alpha\frac{Q(x,y)}{|x-y|}\right)\gamma_\psi\right) \\
&\quad + \frac{\alpha}{2}\iint \frac{\rho_\psi(x)\rho_\psi(y)}{|x-y|}dx\,dy - \frac{\alpha}{2}\iint \frac{|\gamma_\psi(x,y)|^2}{|x-y|}dx\,dy + \mathcal{E}(Q) \\
&= \mathcal{E}(Q + \gamma_\psi).
\end{aligned}$$

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