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Abstract

We study the Bogoliubov-Dirac-Fock model which is a mean-field approximation of QED. It allows to consider relativistic electrons interacting with the Dirac sea. We study the system of two electrons in the vacuum: it has been shown in a previous paper [21] that an electron alone can bind due to the vacuum polarisation, under some technical assumptions. Here we prove the absence of binding for the system of two electrons:the response of the vacuum is not sufficient to counterbalance the repulsion of the electrons.

1 Introduction and main results

The Dirac operator

The theory of relativistic quantum mechanics is based on the Dirac operator D_0, that describes the kinetic energy of a relativistic electron. To simplify formulae, we take relativistic units $\hbar = c = 4\pi\varepsilon_0 = 1$ and set the bare particle mass equal to 1.

In this case, the Dirac operator is defined by [24]: $D^0 = -i\boldsymbol{\alpha}\cdot\nabla + \beta$ where $\beta, \alpha_j \in \mathcal{M}_4(\mathbf{C})$ are the Dirac matrices:

$$\beta = \begin{pmatrix} \mathrm{Id}_2 & 0 \\ 0 & -\mathrm{Id}_2 \end{pmatrix}, \qquad \alpha_j = \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix}, j = 1, 2, 3 \tag{1a}$$

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

It acts on the Hilbert space $\mathfrak{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$. Its spectrum is not bounded from below: $\sigma(D_0) = (-\infty, -1] \cup [1, +\infty)$, which implies the existence of states with arbitrarily small negative energy. Dirac postulated that all the negative energy states are already occupied by "virtual" electrons forming the so-called Dirac sea: by Pauli principle a real electron can only have positive energy.

According to this interpretation, the vacuum, filled by the Dirac sea, is a polarizable medium that reacts to the presence of an electromagnetic field.

BDF model

In this paper we study the Bogoliubov-Dirac-Fock (BDF) model which is a no-photon, mean-field approximation of Quantum Electrodynamics (QED) which was introduced by Chaix and Iracane [3]. It enables us to consider a system of relativistic electrons interacting with the vacuum in the presence of an electrostatic field. This paper is a

continuation of previous works by Hainzl, Gravejat, Lewin, Séré, Siedentop [10, 7, 8, 9, 6] and Sok [21, 20].

The derivation of the BDF model from QED is explained in [3] and [7, Appendix]: we refer the reader to these papers for full details.

In QED, an electronic system is described by a state in the fermionic Fock space $\mathcal{F}_{el}$ [24, Chapter 10] on which (formally) acts the Hamiltonian $\mathbb{H}_{\rm QED}$ [7, Appendix]. The mean-field approximation consists to restricting the study to Hartree-Fock type states, called BDF states. They are fully characterized by their one-body density matrix (1pdm) which are orthogonal projectors of $\mathfrak{H}$.

For instance, the projector $P_-^0 := \chi_{(-\infty,0)}(D_0)$ is the 1pdm of the vacuum state $\Omega_0 \in \mathcal{F}_{el}$: it must be thought of as the infiniter Slater determinant $f_1 \wedge f_2 \wedge \cdots$ where $(f_i)_{i\geq 1}$ is an orthonormal basis (BON) of $\mathrm{Ran}(P_-^0)$. A projector P defines a BDF state *iff* $P - P_-^0$ is Hilbert-Schmidt (*i.e.* its integral kernel is square integrable).

We take P_-^0 as a reference state and define a renormalized Hamiltonian $:\mathbb{H}_{\rm QED}:$ by a procedure of normal ordering relative to P_-^0 [3, 7]. The energy $\langle \Omega_P\,, :\mathbb{H}_{\rm QED}: \Omega_P\rangle$ of a state Ω_P, turns out to be a function of the reduced density matrix (r1pdm) $Q := P - P_-^0$. Formally this function is

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

where $\alpha > 0$ is the fine structure constant, ν is the external density of charge, $\rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big)$ is the density of Q, with $Q(x,y)$ the integral kernel of Q, and:

$$D(\nu,\nu) = \|\nu\|^2_{\mathcal{C}} := 4\pi \int_{\mathbb{R}^3} \frac{|\widehat{\nu}(k)|^2}{|k|^2} dk \text{ and } \|Q\|^2_{\rm Ex} := \iint\limits_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|Q(x,y)|^2}{|x-y|} dxdy. \tag{3}$$

The hat in $\widehat{\nu}$ denotes the Fourier transform and $D(\nu,\nu) < +\infty$ is the Coulomb energy of ν: it coincides with $\iint \frac{\nu(x)^*\nu(y)}{|x-y|}dxdy$ whenever this integral makes sense. We also write

$$\mathcal{C} := \Big\{\nu \in \mathcal{S}'(\mathbb{R}^3),\ \widehat{\nu} \text{ measurable and } \int \frac{|\widehat{\nu}(k)|^2}{|k|^2}dk < +\infty\Big\}. \tag{4}$$

In (2) we recognize the kinetic energy, the interaction energy with ν, the direct term $\frac{\alpha}{2}D(\rho_Q,\rho_Q)$ and the exchange term $-\frac{\alpha}{2}\|Q\|^2_{\rm Ex}$. *A priori* this formula makes sense only when Q and D_0Q are trace-class and the variational problem is ill-defined.

An ultraviolet cut-off $\Lambda > 0$ is necessary. Following [6], we replace D_0 by

$$\mathbf{D} := D_0\big(1 - \frac{\Delta}{\Lambda^2}\big) \text{ with domain } H^{3/2}(\mathbf{R}^3,\mathbf{C}^4),$$

and only consider states Q such that $\mathrm{Tr}\big(|\mathbf{D}|\,|Q|^2\big) < +\infty$.

By adapting (2), we get a well-defined energy $\mathcal{E}^{\nu}_{\rm BDF}$ (defined in the next section).

Remark 1. We use the terms Direct space and Fourier space: a function that depends on position variables (such as a wave function $\psi(x)$ or a 1pdm $Q(x,y)$) is in Direct space, while its Fourier transform that depends on momentum variables is in Fourier space (such as $\widehat{\psi}(p)$ or $\widehat{Q}(p,q)$).

Remark 2. Other choices of cut-off are possible. This one, the *smooth* cut-off, is convenient for the study of functions in Direct space. In [7, 8, 9] Hainzl *et al.* have chosen the *sharp* cut-off, replacing $L^2(\mathbb{R}^3,\mathbb{C}^4)$ by its subspace $\mathfrak{H}_\Lambda$ made of square-integrable functions whose Fourier transform vanishes outside the ball $B_{\mathbb{R}^3}(0,\Lambda)$.

Remark 3. We still have $\chi_{(-\infty,0)}(\mathbf{D}) = P_-^0$. We also write $P_+^0 := \chi_{(-\infty,0)}(D^0) = \mathrm{Id} - P_-^0$ the projector on its positive spectral subspace.

Notation 1. For an operator Q, we define R_Q by its integral kernel:

$$R_Q(x,y) := \frac{Q(x,y)}{|x-y|},\ x,y \in \mathbb{R}^3\times\mathbb{R}^3,\ x \neq y. \tag{5}$$

Moreover for any $\rho \in \mathcal{C}$ we write

$$v_\rho := \rho * \tfrac{1}{|\cdot|}. \tag{6}$$

For a r1pdm $Q = P - P^0_-$, the charge of the system is given by its so-called P^0_--trace $\mathrm{Tr}_{P^0_-}(Q)$, defined by

$$\mathrm{Tr}_{P^0_-}(Q) := \mathrm{Tr}\big(P^0_- Q P^0_-\big) + \mathrm{Tr}\big(P^0_+ Q P^0_+\big). \tag{7}$$

It coincides with the usual trace for trace-class operators and is well-defined for r1pdm because of their structure. Indeed as a difference of orthogonal projectors Q satisfies:

$$P^0_+(P-P^0_-)P^0_+ - P^0_-(P-P^0_-)P^0_- = (P-P^0_-)^2. \tag{8}$$

A minimizer for $\mathcal{E}^\nu_{\mathrm{BDF}}$ among states with charge $M \in \mathbb{N}$ is interpreted as a ground state of the system with M electrons in the presence of ν. For $q \in \mathbb{R}$, the infimum of the BDF energy on the charge sector $\mathcal{Q}_\Lambda(q) := \{Q : \ \mathrm{Tr}_{P^0_-}(Q) = q\}$ is written $E^\nu(q)$.

A sufficient condition for the existence of a minimizer for $E^\nu(q)$ is the validity of binding inequalities at level q [9, Theorem 1]. This result is stated for the *sharp* cut-off, however it is possible to adapt its proof to get this Theorem:

Theorem 1. *Let $0 \leq \alpha < \frac{4}{\pi}$, $\Lambda > 0$, $\nu \in \mathcal{C}$ and $q \in \mathbb{R}$. Then the following assertions are equivalent:*

1. *the binding inequalities hold: $\forall\, k \in \mathbb{R}\backslash\{0\},\ E^\nu(q) < E^\nu(q-k) + E^0(k)$,*
2. *each minimizing sequence $(Q_n)_{n\geq 1}$ for $E^\nu(q)$ is precompact in $\mathcal{Q}_\Lambda(q)$ and converges, up to a subsequence, to a minimizer for $E^\nu(q)$. If $\nu = 0$, this result holds up to translation.*

If q is an integer, then we can only consider $k \in \mathbb{Z}\backslash\{0\}$ in the first assertion.

Checking binding inequalities is a difficult task. Hainzl *et al.* checked them in some cases with non-vanishing ν [9, Theorems 2 and 3]. [9, Theorem 3] states that for $\nu \in L^1(\mathbb{R}^3, \mathbb{R}_+) \cap \mathcal{C}$, there exists a minimizer for $E^\nu(M)$ provided that $M - 1 < \int \nu$ under technical assumptions on α, Λ.

In [21], the existence of a ground state for $E^0(1)$ is proved, still under technical assumptions on α, Λ. It is remarkable that an electron can bind alone without any external potential: this is due to the vacuum polarisation. The electron creates a hole in the Dirac sea that allows it to bind. This effect causes a charge screening: from far away the charge of the electron appears smaller as it is surrounded by the hole.

Let Q be a minimizer for $E^0(1)$, then its density ρ_Q is integrable [20], and we have the *charge renormalisation formula*:

$$\int \rho_Q = 1 \times Z_3 \approx 1 \times \frac{1}{1 + \frac{2}{3\pi}\alpha \log(\Lambda)} \neq 1. \tag{9}$$

Here Z_3 is the *renormalisation constant*. This inadequacy is possible because the minimizer is *not* trace-class (hence the mere fact that ρ_Q is integrable is non-trivial).

We emphasize that these results were proved with the *sharp* cut-off, but the proofs can be adapted in the present case.

Our purpose in this paper is to study the variational problem $E^0(2)$, that is two electrons in the vacuum. We recall that an electron does not see its own field, but in the case of two electrons any electron feel the field induced by the other resulting to a repulsive force. If the vacuum polarisation is not strong enough to counterbalance this repulsion, then there is no minimizer for $E^0(2)$. This constitutes our main Theorem.

Theorem 2. *There exist α_0, Λ_0, L_0 such that if $\alpha \leq \alpha_0$, $\Lambda \geq \Lambda_0$ and $\alpha \log(\Lambda) \leq L_0$, then there is no minimizer for $E^0(2)$.*

Remark 4. This result is proved in the case of the *smooth* cut-off, and we expect it to be true for the *sharp* one but we were unable to show it.

We prove it *ad absurdum*. Let us give the main ideas.

Along this paper we suppose that there exists a minimizer Q for $E^0(2)$. Such a minimizer satisfies a self-consistent equation [9, Proposition 1], [6] and can be decomposed as follows:

$$Q = |\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + \gamma, \tag{10}$$

where the ψ_j's are eigenvectors of the so-called mean-field operator:

$$D_Q := \mathbf{D} + \alpha\big(v_{\rho_Q} - R_Q\big), \tag{11}$$

where for a density $\rho \in \mathcal{C}$ and an operator Q, we define

$$R_Q(x,y) := \frac{Q(x,y)}{|x-y|},\ x,y \in \mathbb{R}^3 \text{ and } v_\rho := \rho * \tfrac{1}{|\cdot|}. \tag{12}$$

For short we will also write

$$B_Q := v_{\rho_Q} - R_Q. \tag{13}$$

By studying $E^0(2) \leq 2E^0(1)$, we get *a priori* information on the ψ_j's. In particular we show that the subspace $\mathrm{Span}(\psi_1,\psi_2)$ splits as follows

$$\mathrm{Span}(\psi_1,\psi_2) = \mathbb{C}h_1 \overset{\perp}{\oplus} \mathbb{C}h_2,\ \|h_j\|_{L^2} = 1,$$

where h_1 and h_2 are essentially two bump functions which are some distance R_g away from each other. The operator γ is also localised around each h_j such that the energy $\mathcal{E}^0_{\mathrm{BDF}}(Q)$ can be written

$$\mathcal{E}^0_{\mathrm{BDF}}(Q) = 2E^0(1) + \theta_{12},$$

where $\theta_{12} > 0$ in our range of parameters (α,Λ).

Roughly speaking the BDF energy should be the sum of the BDF energy of these two parts plus the interaction energy. This interaction energy is too big to ensure $E^0(2)$ is attained.

Remark 5. Throughout this paper, we work in the regime where α and Λ satisfy these conditions: $\alpha \leq \alpha_0, \alpha\log(\Lambda) := L \leq L_0$ and $\Lambda \geq \Lambda_0 > 0$ for small constants $\alpha_0, L_0, \Lambda_0^{-1}$. K is some constant independent of those numbers while $K(\lambda)$ means a constant depending on the quantity λ. Symbols $o(\cdot)$,$\mathcal{O}(\cdot)$ and $\Theta(\cdot)$ are to be understood in this regime.

The paper is organised as follows. In the next section we properly define our model and give *a priori* estimates about $E^0(2)$ and its hypothetical minimizer in Lemma 1. This Lemma is proved in Section 5.

Then in Section 3, we study the Pekar-Tomasevitch functional to exploit these results (Propositions 3, 4 and 5). These Propositions are proved in Appendix B.

Section 4 is devoted to introduce important tools of the proof: the Cauchy expansion (part 4.1) and useful inequalities (part 4.3). We recall in part 4.2 the form of the density of a minimizer.

Section 6 is dedicated to prove Theorem 2. We show how the energy is distributed in Direct space (Proposition 6). This enables us to prove Theorem 2 (part 6.3). To this end we first study the localisation of the "real" electrons' wave functions (Lemma 7, proved in Appendix C). We then show how this enables us to get localisation of the energy of a minimizer (Lemma 8, proved in this Section but using Appendix D). For the sake of clarity we explain in Remark 16 how Appendix D is used to prove Lemma 8.

We have postponed the most technical proofs in the appendices. In Appendix A, we prove Proposition 1 and Lemma 6. This last Lemma shows estimates on a minimizer by bootstrap arguments. Maybe the most difficult results lie in Appendices C and D, dedicated to prove localisation estimates in Direct space.

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2 Presentation of the model

Remark 6 (Fourier transform). In this paper, the Fourier transform is defined on $L^1(\mathbb{R}^3)$ by the formula:

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

Notation 2 (Splitting w.r.t. $P^0_\pm$). For an operator Q and $e_1, e_2 \in \{+,-\}$ we write $Q^{e_1\, e_2} := P^0_{e_1} Q P^0_{e_2}$.

Notation 3 (Schatten classes). We recall that for $1 \leq p \leq \infty$, the set of compact operators whose singular values form a sequence in ℓ^p is denoted by $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ [19, 19]. The case $p = 2$ (resp. $p = 1$) corresponds to Hilbert-Schmidt operators (resp. trace-class operators).

Those Banach spaces satisfy Hölder-type inequalities [18]. We also recall the Kato-Seiler-Simon inequalities [19]:

$$\forall\, 2 \leq p \leq \infty,\ \forall\, f, g \in\ L^p(\mathbb{R}^3),\ \|f(x) g(-i\nabla)\|_{\mathfrak{S}_p} \leq (2\pi)^{-3/p} \|f\|_{L^p} \|g\|_{L^p}. \tag{14}$$

Furthermore we write $\mathcal{B}(\mathfrak{H}_\Lambda)$, the set of bounded linear endomorphisms on $\mathfrak{H}_\Lambda$.

Notation 4 (On D_0 and $\mathbf{D}$). We write $\mathbf{s}_p$ for $\frac{\widehat{D_0}(p)}{\sqrt{1+|p|^2}}$ the action of $\mathrm{sign}(D_0)$ in the Fourier space. The function $\sqrt{1+|p|^2}$ is also written $E(p)$ and $\overline{E}_p := \sqrt{1+|p|^1}(1 + |p|^2/\Lambda^2)$.

Throughout this paper

$$\varepsilon[\Lambda] = \varepsilon_\Lambda := \frac{1}{\log(\Lambda)} \text{ and } a[\Lambda] := \frac{1+\varepsilon[\Lambda]}{2}. \tag{15}$$

We have

$$|D_0|^{1+\varepsilon_\Lambda} \leq E(\Lambda)^\varepsilon |\mathbf{D}| \leq (1+e)|\mathbf{D}|,\ \Lambda \geq e = \exp(1). \tag{16}$$

2.1 The BDF energy

Let ν be an external charge density in $\mathcal{C}$ and $\alpha, \Lambda > 0$ be given. We want to extend (2): the result is the BDF energy (24) below.

Following [6] we define the set:

$$\mathcal{Q}_{\mathrm{Kin}} := \left\{ Q \in \mathfrak{S}_2, |\mathbf{D}|^{1/2} Q, Q|\mathbf{D}|^{1/2} \in \mathfrak{S}_2, |\mathbf{D}|^{1/2} Q^{++} |\mathbf{D}|^{1/2}, |\mathbf{D}|^{1/2} Q^{--} |\mathbf{D}|^{1/2} \in \mathfrak{S}_1 \right\}. \tag{17}$$

The kinetic energy functional is defined on $\mathcal{Q}_{\mathrm{Kin}}$ by the following formula

$$\mathrm{Tr}_{P^0_-}(\mathbf{D}Q) := \mathrm{Tr}(|\mathbf{D}|^{1/2}(Q^{++} - Q^{--})|\mathbf{D}|^{1/2}). \tag{18}$$

It coincides with $\mathrm{Tr}(\mathbf{D}Q)$ when $\mathbf{D}Q$ is trace-class. We will work in the subset of this space defined by:

$$\mathcal{K} := \{ Q \in \mathcal{Q}_{\mathrm{Kin}},\ -P^0_- \leq Q \leq P^0_+ \} \subset \left\{ Q \in \mathcal{Q}_{\mathrm{Kin}},\ Q^* = Q \right\}, \tag{19}$$

the closed convex hull (under that norm) of the difference of two orthogonal projectors: $P - P^0_-$.

We also define $\mathbf{Q}_1$ the Hilbert space of $Q(x,y) \in L^2(\mathbf{R}^3 \times \mathbf{R}^3, \mathbf{C}^4)$ such that

$$\|Q\|^2_{\mathbf{Q}_1} := \iint (\overline{E}_p + \overline{E}_q) |\widehat{Q}(p,q)|^2 dp dq < +\infty. \tag{20}$$

The definition of the density ρ_Q must coincide with the usual one when Q is (locally) trace-class and ρ_Q must be of finite Coulomb norm: $\|\rho_Q\|_{\mathcal{C}} < +\infty$. For Q in $\mathfrak{S}_1^{P^0_-}$, ρ_Q is defined by duality:

$$\forall\ V \in \mathcal{C}',\ QV \in \mathfrak{S}_1^{P^0_-} \text{ and } \mathrm{Tr}_{P^0_-}(QV) = \langle V\, ,\, \rho_Q \rangle_{\mathcal{C}' \times \mathcal{C}}. \tag{21}$$

We have the following proposition (proved in Appendix A).

Proposition 1. *The map $Q \in \mathfrak{S}_1^{P_-^0} \mapsto \rho_Q \in \mathcal{C}$ is continuous and:*

$$\begin{aligned} \|\rho_Q\|_{\mathcal{C}} \quad &\lesssim \||D_0|^{a[\Lambda]} Q^{++} |D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1} + \||D_0|^{a[\Lambda]} Q^{--} |D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1} \\ &\quad + \sqrt{\log(\Lambda)} \||D_0|^{a[\Lambda]} Q\|_{\mathfrak{S}_2}. \end{aligned} \tag{22}$$

Thanks to Kato's inequality (60), the exchange term is well-defined [1]

$$\begin{aligned} \frac{2}{\pi} \iint \frac{|Q(x,y)|^2}{|x-y|} dxdy \quad &\leq \mathrm{Tr}(|D_0| Q^2) = \mathrm{Tr}\{|D_0|^{1/2} Q^2 |D_0|^{1/2}\} \\ \text{and for } Q \in \mathcal{K}: \quad &\leq \mathrm{Tr}\{|D_0|^{1/2} (Q^{++} - Q^{--}) |D_0|^{1/2}\} \leq \mathrm{Tr}_{P_-^0}(\mathbf{D}Q), \end{aligned} \tag{23}$$

The BDF energy is defined as follows:

$$\mathcal{E}^{\nu}_{\mathrm{BDF}}(Q) := \mathrm{Tr}_{P_-^0}(\mathbf{D}Q) - \alpha D(\nu, \rho_Q) + \frac{\alpha}{2}\Big(D(\rho_Q, \rho_Q) - \iint \frac{|Q(x,y)|^2}{|x-y|} dxdy \Big), \ Q \in \mathcal{K}. \tag{24}$$

Any charge sector $\mathcal{Q}(q) := \{Q \in \mathcal{K}, \ \mathrm{Tr}_{P_-^0}(Q) = q\}$ leads to a variational problem

$$E^{\nu}_{\mathrm{BDF}}(q) := \inf_{Q \in \mathcal{Q}(q)} \mathcal{E}_{\mathrm{BDF}}(Q). \tag{25}$$

By Lieb's variational principle [9, Proposition 3], a minimizer Q for $E^{\nu}(M)$ with $M \in \mathbb{Z}$ is necessarily a difference of two projectors $P - P_-^0$.

2.2 Form of a minimizer

To simplify, from this point we assume that $\nu = 0$. For an integer $M \in \mathbb{N}$, let Q be a ground state for $E^0(M)$, then necessarily $Q = \overline{P} - P_-^0$, where $\overline{P}$ is an orthogonal projector.

The study of the first and second derivative gives more information: we have $\big[D_Q, \overline{P}\big] = 0$, and [9, Proposition 1]

$$\overline{P} = \chi_{(-\infty,\mu]}\big(D_Q\big), \ 0 < \mu < 1, \tag{26}$$

where we recall the mean-field operator is defined in (11). We decompose Q with respect to the positive and negative spectrum:

$$N := \chi_{(0,\mu]}(D_Q) \text{ and } \boldsymbol{\pi}_{\mathrm{vac}} = \gamma + P_-^0 := \chi_{(-\infty,0)}(D_Q), \tag{27}$$

where $\boldsymbol{\pi}_{\mathrm{vac}}$ (resp. n) is interpreted as the polarized vacuum (resp. as the real electrons). If αM is small enough, then we can show that $\mathrm{Tr}_{P_-^0}(\gamma) = 0$ and thus N has rank M [9, 20]. We will recall the proof below.

In the present case, a minimizer for $E^0(2)$ can be written as in (26)-(27). For small enough α, we have

$$N = |\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2|, \ D_Q \psi_j = \mu_j \psi_j, \ 0 < \mu_2 \leq \mu_1 = \mu < 1, \ j \in \{1,2\}. \tag{28}$$

These equations constitutes the starting point of our proof: they enable us to get estimates on the Sobolev norms of the ψ_j's. More precisely we will prove Lemma 1.

Before stating it, let us recall the Pekar-Tomasevitch functional:

$$\mathcal{E}_{\mathrm{PT}}(\psi) := \|\nabla\psi\|_{L^2}^2 - \iint \frac{|\psi(x)|^2 |\psi(y)|^2}{|x-y|} dxdy, \ \forall \psi \in H^1.$$

It describes the energy of a single electron in its own hole. In the case of M electrons, the energy is [5]:

$$\forall\, 0 \leq \Gamma \leq 1, \ \mathrm{Tr}\,\Gamma = M, \ \mathcal{E}^{U}_{\mathrm{PT}}(\Gamma) := \mathrm{Tr}\big(-\Delta\big) - \|\rho_\Gamma\|_{\mathcal{C}}^2 + U\Big(\|\rho_\Gamma\|_{\mathcal{C}}^2 - \|\Gamma\|_{\mathrm{Ex}}^2\Big), \tag{29}$$

where $U > 0$ is some number. By scaling we can assume $U = 1$ but $-\|\rho_\Gamma\|_{\mathcal{C}}^2$ has to be replaced by U^{-1}: this last number measures the strength of the polarisation.

In this paper, a specific value $U = U_0(\alpha, \Lambda)$ is considered: $U_0^{-1} = 1 - Z_3(\alpha, \Lambda)$ where Z_3 is the renormalisation constant that we have mentionned in the introduction. Its precise expression is given below (57).

We write $E_{\rm PT}^U(M)$ the infimum of the Pekar-Tomasevitch energy on the set $\{0 \leq \Gamma \leq 1,\ {\rm Tr}\,\Gamma = M\}$, with $U = U_0$.

Remark 7. We assume that $U_0 > 2U_{\rm c}$, where $U_{\rm c}$ is the critical value above which, there is no minimizer for $E_{\rm PT}^U(M)$ for any integer $M \geq 2$. This important result is proved in [5].

For unitary wave functions $\phi_1 \perp \phi_2$, we also write

$$\mathcal{E}_{\rm PT}^U(\phi_1 \wedge \phi_2) := \mathcal{E}_{\rm PT}^U\Big(\sum_{j=1}^2 |\phi_j\rangle\langle\phi_j|\Big).$$

Lemma 1. *In the regime of Remark 5, let $Q = N + \gamma$ be a minimizer for $E^0(2)$, decomposed as in* (26)-(28).

Let c be $\big\{\alpha(1 - Z_3(\alpha, \Lambda))\big\}^{-1}$ where Z_3 is defined in (57). *We write $\underline{\psi_j}$ the scaling of ψ_j by c:*

$$\underline{\psi_j}(x) := c^{3/2}\psi_j(cx),\ x \in \mathbb{R}^3,$$

Then we have the following:

$$\left\{\begin{array}{rcl} E_{BDF}^0(1) &=& 1 + \frac{1}{2c^2}E_{PT}(1) + \mathcal{O}(\alpha c^{-2}), \\ E_{BDF}^0(2) = \mathcal{E}_{BDF}^0(Q) &=& 2 + \frac{1}{2c^2}\mathcal{E}_{PT,U_0}(\underline{\psi_1} \wedge \underline{\psi_2}) + \mathcal{O}(\alpha c^{-2}). \end{array}\right. \tag{30}$$

We split each ψ_j into an upper spinor φ_j and a lower one χ_j, both in $L^2(\mathbb{R}^3, \mathbb{C}^2)$. We write $n_j = |\psi_j|^2$ (resp $\underline{n_j} = |\underline{\psi_j}|^2$) and $n = n_1 + n_2$ (resp $\underline{n} = \underline{n_1} + \underline{n_2}$). Then we have

$$\mu_j = 1 + \frac{\|\nabla\underline{\varphi_j}\|_{L^2}^2}{2c^2} - \frac{1}{c^2}D(\underline{n_j}, \underline{n}) + \mathcal{O}(\alpha c^{-2}), \tag{31}$$

in particular:

$$(1 - \mu_j)c^2 \gtrsim 1. \tag{32}$$

Estimate (32) follows from (47)-(48). This quantitative error $\mathcal{O}(\alpha c^{-2})$ gives *a priori* information about the $\underline{\psi_j}$'s thanks to [15, 5] (see the next Section).

Notation 5. Throughout this paper, we will use the following notations.

$$\begin{array}{rcl|rcl} N_j &=& |\psi_j\rangle\langle\psi_j| & N &=& N_1 + N_2, \\ n_j &=& |\psi_j|^2 & n &=& n_1 + n_2, \\ \gamma' = Q &=& = \gamma + N, & \rho'_\gamma &=& \rho_\gamma + n. \end{array} \tag{33}$$

When we add an underline $\underline{N_j}$ etc. we mean the scaled object by $c = (\alpha(1 - Z_3))^{-1}$. Writing

$$O_c : \phi(x) \in L^2 \mapsto c^{3/2}\phi(cx),$$

we have $\underline{\psi_j} = O_c\psi_j$, $\underline{N_j} := O_cN_jO_c^{-1}$, $\underline{\gamma} = O_c\gamma O_c^{-1}$.

3 The Pekar-Tomasevitch functional

3.1 Decoupling of almost minimizers for $E_{\rm PT}^{U_0}(2)$

Thanks to [15], one knows that there exists but one minimizer for $E_{\rm PT}(1)$ up to a phase and to translation in $L^2(\mathbb{R}^3, \mathbb{C})$. This minimizer can be chosen positive radially symmetric and decreasing. It is also smooth and with exponential falloff. As $\int \big||\nabla|\phi|\big|^2 \leq \int |\nabla\phi|^2$ [16], there holds the same in $L^2(\mathbb{R}^3, \mathbb{C}^4)$. The set of minimizers is a manifold $\mathscr{P} \simeq \mathbb{S}^7 \times \mathbb{R}^3$ where $\mathbb{S}^7$ is the unit sphere of $\mathbb{C}^4$. There also holds coercivity inequality [11]:

Proposition 2. *Let $\phi \in H^1$ with $\|\phi\|_{L^2} = 1$ and let $\overline{\phi} \in \mathscr{P}$ such that:*
$\|\phi - \overline{\phi}\|_{H^1} = \inf_{f \in \mathscr{P}} \|\phi - f\|_{H^1}$*, then there exists $\kappa > 0$ such that (at least in a neighborhood of $\mathscr{P}$):*

$$\mathcal{E}_{PT}(\phi) - E_{PT}(1) \geq \kappa \|\phi - \overline{\phi}\|_{H^1}^2.$$

Notation 6. We write $\mathscr{P}_0 \subset \mathscr{P}$ the submanifold of $\mathscr{P}$ made of minimizers with center $0 \in \mathbb{R}^3$: it is isomorphic to $\mathbb{S}^7$.

We are interested in $E^U_{\mathrm{PT}}(2)$, with $U = U_0 > 2U_{\mathrm{c}}$, where U_{c} is the critical value above which there is no mminimizers for $E_{\mathrm{PT}}(2)$ [5]: in particular $E_{\mathrm{PT}}(2) = 2E_{\mathrm{PT}}(1)$ (the proof of [5] also applies for spinor-valued functions). If we *choose* $U_0 > 2\mathrm{U}_c$:

$$\forall \Psi \in L^2_a(\mathbb{R}^3 \times \mathbb{R}^3),\ \|\Psi\|_{L^2} = 1 :\ \mathcal{E}_{\mathrm{PT}}(\Psi) - 2E_{\mathrm{PT}}(1) \geq \frac{U_0}{2}(D(\rho_\Psi, \rho_\Psi) - \mathrm{Tr}(\gamma_\Psi R[\gamma_\psi])) \tag{34}$$

where we recall ρ_Ψ is the density of Ψ and γ_Ψ is its one-body density matrix.

There holds Lieb's variational principle: $E^U_{\mathrm{PT}}(2)$ is also the infimum of $\mathcal{E}^U_{\mathrm{PT}}$ over Slater determinant $h_1 \wedge h_2$ with $h_j \in H^1$ and $\langle h_j\,,\, h_k \rangle = \delta_{jk}$.

Let us consider such a state $\Psi = h_1 \wedge h_2$. The plane $\mathrm{Span}(h_1, h_2)$ can be defined with other orthonormal families: $\mathbf{U}(2)$ acts on the set $\mathrm{S}[\Psi]$ of those families:

$$\left(\begin{pmatrix} a & c \\ b & d \end{pmatrix}, \begin{pmatrix} h_1 \\ h_2 \end{pmatrix}\right) \in \mathbf{U}(2) \times \mathrm{S}[\Psi] \mapsto \begin{pmatrix} ah_1 + bh_2 \\ ch_1 + dh_2 \end{pmatrix} \in \mathrm{S}[\Psi], \tag{35}$$

The first vector is written $(\mathbf{m} \cdot \mathbf{h})_1$ and the second is written $(\mathbf{m} \cdot \mathbf{h})_2$.

Characteristic length For $\Psi = h_1 \wedge h_2$ we define the inverse d_Ψ of the *characteristic length* $R_{12}(\Psi)$:

$$d_\Psi := \inf_{\mathbf{m} \in \mathbf{SU}(2)} D(|(\mathbf{m} \cdot \mathbf{h})_1|^2, |(\mathbf{m} \cdot \mathbf{h})_2|^2) = R_{12}(\Psi)^{-1}. \tag{36}$$

Let $\phi_0 \in \mathscr{P}_0$ be the radially symmetric and positive function (with $\phi_0(x)$ parallel to $(1\ \ 0\ \ 0\ \ 0)^*$ for instance). Let $\phi_{\mathbf{x}_0} = \tau_{\mathbf{x}_0}\phi_0$ be its translation by $\mathbf{x}_0 \in \mathbb{R}^3$. We have:

$$\forall x_0,\ |\mathbf{x}_0| \geq 1 :\ |\mathbf{x}_0| \times D(|\phi_0|^2, |\phi_{\mathbf{x}_0}|^2) \leq \sup_{|\mathbf{z}| \geq 1} |\mathbf{z}| \sqrt{\iint \frac{|\phi_0(x)|^2 |\phi_{\mathbf{z}}(y)|^2}{|x-y|^2} dxdy} := \mathrm{Y}_0 < +\infty. \tag{37}$$

Geometric length For a Slater determinant $\Psi = h_1 \wedge h_2$ where h_1 and h_2 satisfy $D(|h_1|^2, |h_2|^2) = d_\Psi$, we define the *geometric length* R_g as follows.

Let $\phi_{(j)} \in \mathscr{P}$ be the closest function of $\mathscr{P}$ to h_j in H^1. Each $\phi_{(j)}$ is radial with respect to some vector $z_j \in \mathbb{R}^3$, we set $\mathrm{R}_g(\Psi) := |z_1 - z_2|$ (or the smallest of such $|z_1 - z_2|$): it should be seen as the *interparticle distance*.

Remark 8. The geometric length R_g does not appear in the energy and $R_{12} = d_\Psi^{-1}$ may be much smaller.

Proposition 3. *There exist $a_0 > 0$ and $b = b(a_0) > 0$ such that*

$$\forall \Psi = h_1 \wedge h_2 :\ \Delta_2\mathcal{E} = \mathcal{E}^U_{PT}(\Psi) - 2E_{PT}(1) < a_0 \ \Rightarrow\ \frac{\Delta_2\mathcal{E}}{d_\Psi} \geq b. \tag{38}$$

Proposition 4. *There exist $a_0' > 0$ and $b' > 0$ such that:*

$$\forall \Psi = h_1 \wedge h_2 :\ \Delta_2\mathcal{E} < a_0' \ \Rightarrow \iint \frac{|\Psi(x,y)|^2}{|x-y|} dxdy \geq \frac{b'}{R_g}. \tag{39}$$

More precisely:

For any $0 < \lambda$ let B_j^λ be $B(z_j, \lambda R_g)$ and $\mathcal{B}^\lambda := B_1^\lambda \times B_2^\lambda \cup B_2^\lambda \cup B_1^\lambda$. Then there exist $a_\lambda > 0, k_\lambda > 0$ such that

$$\forall \Psi = h_1 \wedge h_2 :\ \Delta_2\mathcal{E} < a_\lambda \ \Rightarrow \iint_{(x,y) \in \mathcal{B}^\lambda} \frac{|\Psi(x,y)|^2}{|x-y|} dxdy \geq \frac{k_\lambda}{R_g} \tag{40}$$

Remark 9. It is not possible to replace R_g^{-1} by d_Ψ.

To prove Proposition 4, we need to compare $R_{12}(\Psi)$ and R_g.

3.2 On the relation between $R_{12}(\Psi)$ and $\mathbf{R}_g$

Let us consider an almost minimizer for $E^U_{\mathrm{PT}}(2)$:

$$\Psi = h_1 \wedge h_2,\ \mathcal{E}^U_{\mathrm{PT}}(2) - E^U_{\mathrm{PT}}(2) \lesssim a_0 \ll 1, U \text{ big enough.} \tag{41}$$

We suppose that $D(|h_1|^2, |h_2|^2) = d_\Psi$ and write ϕ_j the closest function to h_j in $\mathscr{P}$. We write $\delta_j = h_j - \phi_j$. By Propositions 2 and 3 we have:

$$d_\Psi = \tfrac{1}{R_{12}} \quad \lesssim \varepsilon_0 \quad \text{and} \quad \|\delta_1\|^2_{H^1} + \|\delta_2\|^2_{H^1} \lesssim a_0.$$

We will here compare R_{12} and R_g (defined as $|z_1 - z_2|$ where z_j is the center of ϕ_j).

As $\phi_j(\cdot - z_j)$ is radial and smooth then:

$$0 < \inf_{x\in\mathbb{R}^3} \frac{(|\phi_j|^2 * \frac{1}{|\cdot|})(x)}{\big((|\phi_j|^2 * \frac{1}{|\cdot|^2})(x)\big)^{1/2}} \leq \sup_{x\in\mathbb{R}^3} \frac{(|\phi_j|^2 * \frac{1}{|\cdot|})(x)}{\big((|\phi_j|^2 * \frac{1}{|\cdot|^2})(x)\big)^{1/2}} < +\infty. \tag{42}$$

By Newton's Theorem [16], writing $|\phi_0|^2 = |\phi_j(\cdot - z_j)|^2$ we have:

$$\forall\, x \in \mathbb{R}^3,\ (|\phi_0|^2 * \tfrac{1}{|\cdot|})(x) = \frac{1}{|x|}\int_{|y|\leq|x|} |\phi_0(y)|dy + \int_{|y|\geq|x|} \frac{|\phi_0(y)|^2}{|y|}dy \leq \frac{1}{|x|}. \tag{43}$$

As a consequence, for sufficiently small a_0:

$$|D(\mathfrak{Re}(\delta_1^*\phi_1), |\delta_2|^2)| \quad \lesssim \|\delta_1\|_{L^2} D(|\phi_1|^2, |\delta_2|^2), \quad |D(\mathfrak{Re}(\delta_1^*\phi_1), |\phi_2|^2)| \quad \lesssim \tfrac{\|\delta_1\|_{L^2}}{\mathrm{R}_g}, \tag{44}$$

where we used Cauchy-Schwarz inequality:

$$\int_x |\delta_1(x)^*\phi_1(x)| \tfrac{dx}{|x-y|} \leq \|\delta_1\|_{L^2}\{\int_x |\phi_1(x)|^2 \tfrac{dx}{|x-y|^2}\}^{1/2}.$$

Thus there holds the following.

Proposition 5. *Let Ψ be as in (41). We write $\|\delta\| = \sum_j \|\delta_j\|$: there exists $\kappa > 0$ such that for sufficiently small $a_0 > 0$:*

$$\begin{aligned} &d_\Psi \geq (1 - \kappa\sqrt{a_0})\big(D(|\phi_1|^2, |\phi_2|^2) + D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2)\big) + D(|\delta_1|^2, |\delta_2|^2), \\ &\iint \tfrac{|h_1(x)|^2|h_2(y)|^2}{|x-y|^2}dxdy \lesssim \frac{1}{R_g^2} + \frac{\|\delta\|_{L^2}\|\delta\|_{H^1}}{R_g} + \|\delta\|^2_{L^2}\|\delta\|_{H^1}, \end{aligned} \tag{45}$$

Remark 10. In particular $R_{12} = \mathcal{O}(\mathrm{R}_g)$. Moreover for sufficiently small a_0, we have

$$\Delta_1\mathcal{E} := \sum_j \big(\mathcal{E}_{\mathrm{PT}}(h_j) - E_{\mathrm{PT}}(1)\big) = \Theta(\|\delta\|^2_{H^1}).$$

With the help of Proposition 3, we get the following estimates:

$$\iint \frac{|h_1(x)|^2|h_2(y)|^2}{|x-y|^2}dxdy \lesssim a_0^3. \tag{46}$$

3.3 On the decomposition of $\underline{\psi_1} \wedge \underline{\psi_2}$

In our problem, we consider a couple (a_0, b) described in Lemma 3, and we *choose* (α, Λ) such that $U_0 \geq (2+1)U_{\mathrm{c}}$.

We consider $\underline{\Psi} = \underline{\psi_1} \wedge \underline{\psi_2}$ of Lemma 1. We have: $\mathcal{E}^U_{\mathrm{PT}}(\underline{\psi_1} \wedge \underline{\psi_2}) \lesssim \alpha$ and $d_\Psi \lesssim \alpha$.

This result and the estimate of Remark 10 lead to the following Lemma.

Lemma 2. *For $(k,k') = (1,2)$ or $(2,1)$ and $\psi_k(x) = c^{-3/2}\underline{\psi_k}(x/c)$, we have*

$$\| |\psi_{k'}|^2 * \tfrac{1}{|\cdot|} \times \psi_k - (\psi^*_{k'}\psi_k) * \tfrac{1}{|\cdot|} \times \psi_{k'} \|^2_{L^2} \lesssim \frac{1}{c^2} \iint \frac{|h_1(x)|^2 |h_2(y)|^2}{|x-y|^2} dxdy \lesssim \frac{\alpha^3}{c^2}.$$

Proof: Indeed the quantity in the l.h.s. of (2) corresponds to the squared L^2-norm of $(\rho_\Psi * \frac{1}{|\cdot|}\psi_k - R[\gamma_\Psi]\psi_k)$ where $\Psi := \psi_1 \wedge \psi_2$. Then we decompose ψ_k with respect to an orthonormal family (h_1, h_2) with $h_1 \wedge h_2 = \Psi$ and $D(|h_1|^2, |h_2|^2) = d_\Psi$. □

We recall that ψ_1 and ψ_2 are eigenvectors of the mean-field operator with eigenvalues μ_1 and μ_2. In the case $\mu_1 \neq \mu_2$ we cannot choose $\underline{\psi_1} = h_1$ and $\underline{\psi_2} = h_2$.

From the estimation of the μ_j's (31) we may ask whether the quantity

$$F_{\mathcal{E}}(\underline{\psi_k}) := \mathcal{E}_{\mathrm{PT}}(\underline{\psi_k}) - D(|\underline{\psi_k}|^2, |\underline{\psi_{k'}}|^2) \tag{47}$$

is negative and away from 0 or not. As $h_k = \phi_k + \delta_k$ with $\phi_k \in \mathscr{P}$ and $\|\delta_k\|_{H^1} = \mathcal{O}(\sqrt{\Delta_2 \mathcal{E}})$ a simple computation shows that:

$$\forall (a,b) \in \mathbb{C}^2 \cap \mathbb{S}^3 : \; F_{\mathcal{E}}(ah_1 + bh_2) = \frac{3}{2} E_{\mathrm{PT}}(1) + \mathcal{O}((\Delta_2 \mathcal{E})^{1/4}). \tag{48}$$

4 Technical tools

4.1 The Cauchy expansion

In this part we use the functions $\mathbf{s}.$, $E(\cdot)$ and $\overline{E}.$ and numbers $\varepsilon_\lambda, a[\Lambda]$ defined in Notation 4. We recall Ineq. (16). The results stated here follow from [21, 20].

Let $\widetilde{\gamma}$ be the operator defined by:

$$\widetilde{\gamma} = \chi_{(-\infty,0)}(\mathbf{D} + \alpha(v_{\widetilde{\rho}} - R_{\widetilde{Q}})) - P^0_-, \; (\widetilde{Q}, \widetilde{\rho}) \in \mathbf{Q}_1 \times \mathcal{C}.$$

For instance we can take γ of (27). Provided that $\|\widetilde{Q}\|_{\mathrm{Kin}}, \|\widetilde{\rho}\|_{\mathcal{C}}$ are small enough, by Lemma 3 we have

$$|D + \alpha(v_{\widetilde{\rho}} - R_{\widetilde{Q}})| \geq |\mathbf{D}|\big(1 - \alpha(\|\rho_Q\|_{\mathcal{C}} + \|Q\|_{\mathrm{Ex}})\big) = |\mathbf{D}|(1 + o(1)).$$

As a result we can expand $\widetilde{g}$ in power of α, this is the Cauchy expansion [7]:

$$\left\{ \begin{array}{rcl} \widetilde{\gamma} & = & \displaystyle\sum_{j=1}^{+\infty} \alpha^j Q_j[\widetilde{Q}, \widetilde{\rho}], \\ Q_j[\widetilde{Q}, \widetilde{\rho}] & := & \displaystyle -\tfrac{1}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega}{\mathbf{D} + i\omega} \Big(\big(R_{\widetilde{Q}} - v[\widetilde{\rho}]\big) \frac{1}{\mathbf{D} + i\omega} \Big)^j. \end{array} \right. \tag{49}$$

We can further expand each Q_j into $\sum_{j=0}^{j} Q_{k,j-k}[\widetilde{Q}, \rho_{\widetilde{Q}}]$ where each $Q_{k,j-k}$ is polynomial in $R_{\widetilde{Q}}$ (resp. $v[\rho_{\widetilde{Q}}]$) of degree k (resp. $j-k$).

The respective densities of $Q_{k,j-k}$ and Q_j are written $\rho_{k,j-k}$ and ρ_j.

Convergence of the series (49) In [7, 6], Hainzl *et al.* proved that this series is well-defined and in [21, 20] the functions $(Q_{k,j-k}, \rho_{k,j-k})[\cdot,\cdot]$ are studied in several norms.

It is possible to adapt the proofs to show that these functions are multilinear continuous in $\mathbf{Q}_1 \times \mathcal{C}$ or more generally in the banach spaces $\mathcal{X}_w = \mathbf{Q}_w \times \mathfrak{C}_w$, defined by the following norms:

$$||Q||^2_{\mathbf{Q}_w} := \iint (\overline{E}_p + \overline{E}_q) w(p-q) |\widehat{Q}(p,q)|^2 dpdq \text{ and } \|\rho\|^2_{\mathfrak{C}_w} := \iint \frac{w(k)}{|k|^2} |\widehat{\rho}(k)|^2 dk, \quad (50)$$

where $\sqrt{w} : \mathbb{R}^3 \to [1, +\infty)$ is a weight function satisfying some sub-additive assumptions.

Furthermore the growth of the norms $\|(Q_{k,j-k}, \rho_{k,j-k})\|_{\mathcal{B}(\mathcal{X}_w)}$ is also polynomial: it follows that there exists some radius $A(\alpha, \Lambda, w)$ such that

$$(\widetilde{Q}, \widetilde{\rho}) \in B_{\mathcal{X}_w}(0, A) \mapsto \left(\widetilde{\gamma} := \sum_{j=1}^{+\infty} \alpha^j Q_j \left[\widetilde{Q}, \widetilde{\rho} \right], \rho_{\widetilde{\gamma}} \right) \in B_{\mathcal{X}_g}(0, A),$$

is well-defined and contractant.

The main ingredients of the proof are the following inequalities:

$$\begin{array}{rcl|rcl} \|P^0_{\pm} v_{\widetilde{\rho}} P^0_{\mp} \frac{1}{|D_0|^{a[\Lambda]}}\|_{\mathfrak{S}_2} & \lesssim & \sqrt{\log(\Lambda)} \|\widetilde{\rho}\|_{\mathcal{C}} & \|R_{\widetilde{Q}} \frac{1}{|\nabla|^{1/2}}\|_{\mathfrak{S}_2} & \lesssim & \|\widetilde{Q}\|_{\mathrm{Ex}}, \\ \|v_{\widetilde{\rho}} \frac{1}{|D_0|^{a[\Lambda]}}\|_{\mathfrak{S}_6} & \lesssim & \|\widetilde{\rho}\|_{\mathcal{C}} & \|v_{\widetilde{\rho}} \frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} & \lesssim & \|\widetilde{\rho}\|_{\mathcal{C}} \end{array} \quad (51)$$

In the l.h.s. the first estimate follows from a simple computation in Fourier space [7, 21], and the second one is an application of the KSS inequality (14).

In the r.h.s. the first is proved below (Lemma 3) and the last follows from an homogeneous Sobolev inequality (59). We will say no more about these results and refer the reader to the cited articles and to [22].

4.2 On the minimizers: equation and density

The results of this part are proved in [20].

Let $Q = \gamma + N$ be a minimizer for $E^0(M)$ with $M \in \{1, 2\}$. It satisfies Eq. (26)-(27) and rank $N = M$ for α sufficiently small. We recall:

$$\gamma = \chi_{(-\infty,0)}(D_Q) - P^0_-. \quad (52)$$

In [7, 21, 20], a fixed-point scheme is used to see γ as a fixed point of some function $F^{(1)}$ (with parameter N). This scheme enables us to get estimates on γ and N. By the Cauchy expansion, Eq. (52) is rewritten as follows:

$$\big(\mathrm{Id} - \alpha Q_{1,0}[\cdot]\big)\big[\gamma'\big] = N + \alpha Q_{0,1}\big[\rho'_\gamma\big] + \sum_{j=2}^{+\infty} \alpha^j Q_j\big[\gamma', \rho'_\gamma\big].$$

In [20], it is proved that the linear operator $\big(\mathrm{Id} - \alpha Q_{1,0}[\cdot]\big)$ is a continuous endomorphism for $\mathbf{Q}_g$ and $\mathfrak{S}_p$ $(1 \le p \le 2)$ provided that $\alpha \log(\Lambda) \le L_0$ is small enough.

Its inverse $\mathbf{T}$ is written and it has a uniform bound for all those Banach spaces.

This gives

$$\gamma = \alpha \mathbf{T}[Q_{1,0}(N)] + \alpha \mathbf{T}[Q_{0,1}(\rho'_\gamma)] + \sum_{j=2}^{+\infty} \alpha^j \mathbf{T}\big[Q_j[\gamma', \rho'_\gamma]\big]. \quad (53)$$

In [20], the density $\alpha\rho\big[Q_{0,1}(\rho'_\gamma)\big]$ is computed and we have:

$$\alpha\rho\big[Q_{0,1}(\rho'_\gamma)\big] = -\check{f}_\Lambda * \rho'_\gamma,$$

where $\check{f}_\Lambda \in L^1$ with norm $\|\check{f}_\lambda\|_{L^1} \lesssim L$.

Remark 11. For the *smooth* cut-off, the same proof applies for $|\cdot|^\ell \check{f}_\Lambda$. For any fixed integer ℓ, there exists $K(\ell) > 0$ such that, if $\alpha \leq K(\ell)$ then

$$\begin{array}{rcl} \| \, |\cdot|^\ell \check{f}_\Lambda \|_{L^1} & \leq & \Big\{ \displaystyle\int |x|^{2(1+\ell)} (1+|x|^2) |\check{f}_\Lambda(x)|^2 dx \int \frac{dx}{|x|^2(1+|x|^2)} \Big\}^{1/2}, \\ & \lesssim & \alpha. \end{array} \tag{54}$$

The same results hold for

$$\check{F}_\Lambda := \mathscr{F}^{-1}\Big(\frac{f_\Lambda}{1+f_\Lambda}\Big) = \sum_{j=1}^{+\infty} (-1)^{j+1} \check{f}_\Lambda^{*j} \tag{55}$$

provided that $\alpha \leq K'(\ell)$ with a smaller bound $K'(\ell) \leq K(\ell)$.

We write $\tau_j[\cdot] := \rho\big[\mathbf{T} Q_j[\cdot]\big]$ and $\tau_{k,j-k}[\cdot] := \rho\big[\mathbf{T} Q_{k,j-k}[\cdot]\big]$. There holds:

$$\begin{array}{rcl} \rho_\gamma & = & -\check{F}_\Lambda * n + (\delta_0 - \check{F}_\Lambda) * \big(\alpha \tau_{1,0}[N] + \displaystyle\sum_{j=2}^{+\infty} \alpha^j \tau_j[\gamma', \rho'_\gamma] \big), \\ & = & -\check{F}_\Lambda * n + (\delta_0 - \check{F}_\Lambda) * \big(\alpha \tau_{1,0}[N] + \alpha^2 \widetilde{\tau}_2[\gamma', \rho'_\gamma] \big). \end{array} \tag{56}$$

We have $\rho_\gamma \in L^1$ with $\int \rho_\gamma = -F_\Lambda(0) \times M$. The renormalisation constant Z_3 is

$$Z_3 := 1 - F_\Lambda(0) = \frac{1}{1+f_\Lambda(0)} \approx \frac{1}{1+\frac{2}{3\pi}\alpha \log(\Lambda)} \text{ and } U_0 := \frac{1}{F_\Lambda(0)}. \tag{57}$$

We also recall [20]

$$\forall \, k, k' \in B_{\mathbb{R}^3}(0,2) : \ |F_\Lambda(k) - F_\Lambda(k')| \lesssim \alpha |k - k'| \tag{58}$$

we will use below with $k' = 0$.

4.3 Some inequalities

– Let us recall some Sobolev inequalities in $\mathbb{R}^3$:

$$\|f\|_{L^6} \lesssim \|\nabla f\|_{L^2}, \quad \|f\|_{L^4} \lesssim \||\nabla|^{3/4} f\|_{L^2}, \quad \|f\|_{L^3} \lesssim \||\nabla|^{1/2} f\|_{L^2} \tag{59}$$

The last one gives $\|v_{\widetilde{\rho}} \frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} \lesssim \|\widetilde{\rho}\|_{\mathcal{C}}$ for $\widetilde{\rho} \in \mathcal{C}$.

– We also recall Kato's inequality and Hardy's inequality:

$$\left\{ \begin{array}{rcl} \displaystyle\int_{\mathbb{R}^3} \frac{|\phi(x)|^2}{|x|} dx & \leq & \frac{\pi}{2} \langle |\nabla| \phi \, , \, \phi \rangle, \\ \displaystyle\int_{\mathbb{R}^3} \frac{|\phi(x)|^2}{|x|^2} dx & \leq & 4 \langle (-\Delta) \phi \, , \, \phi \rangle. \end{array} \right. \tag{60}$$

– The following Lemma gives estimates about the operator R_Q.

Lemma 3. *Let $Q(x,y)$ be an operator of finite exchange term and ρ of finite Coulomb energy, then:*

$$\left\{ \begin{array}{rcl} \| \frac{1}{|\nabla|^{1/2}} R_Q \|_{\mathfrak{S}_2} & = \mathrm{Tr}(R_Q^* \frac{1}{|\nabla|} R_Q) \leq \big(\displaystyle\int \frac{dy}{|y|^2 |y - \mathbf{e}|^2} \big)^2 \mathrm{Tr}(Q^* R_Q), \\ \displaystyle\iint \frac{|Q(x,y)|^2}{|x-y|} dx dy & = \mathrm{Tr}(Q^* R_Q) \leq \frac{\pi}{2(2\pi)^3} \displaystyle\iint |u| |\widehat{Q}(u+k/2, u-k/2)|^2 du dk, \\ \|v_\rho \frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} & \lesssim \|\rho\|_{\mathcal{C}}. \end{array} \right.$$

In particular $\|(v_\rho - R_Q) f\|_{L^2} \lesssim (\|\rho\|_{\mathcal{C}} + \|Q\|_{\mathrm{Ex}}) \||\nabla|^{1/2} f\|_{L^2}$.

Proof: The proof for $\|\frac{1}{|\nabla|^{1/2}}R_Q\|_{\mathfrak{S}_2}$ is just an application of the Cauchy-Schwarz inequality once we remark that $|\nabla|^{-1}$ is the convolution by $\mathrm{Const}/|\cdot|^2$ [16]. For the last inequality we write $s=\frac{x+y}{2}$ and $t=x-y$ and $A(s,t):=Q(s+t/2,s-t/2)$ *a.e.* By Kato's inequality:

$$\begin{aligned}\iint\frac{|Q(x,y)|^2}{|x-y|}dxdy &= \iint\frac{|A(s,t)|^2}{|t|}dsdt\\ &\leq\frac{\pi}{2}\int ds\langle|\nabla|A(s,\cdot)\,,\,A(s,\cdot)\rangle\\ &\leq\frac{\pi}{2}\iint|u||\widehat{Q}(u+k/2,u-k/2)|dudk.\end{aligned}$$

Those inequalities are true at least for $Q(x,y)$ in the Schwartz class $\mathcal{S}(\mathbb{R}^3\times\mathbb{R}^3)$, we conclude by density. □

– To end this part we give estimates about $\mathbf{D}$.

We have

$$\mathrm{Id}-\mathbf{s}_p\mathbf{s}_q=\mathbf{s}_p(\mathbf{s}_p-\mathbf{s}_q)=(\mathbf{s}_p-\mathbf{s}_q)\mathbf{s}_q$$

and

$$|\mathrm{Id}-\mathbf{s}_p\mathbf{s}_q|\leq|\mathbf{s}_p-\mathbf{s}_q|=\Big|\frac{\widehat{D_0}(p)}{E(p)}-\frac{\widehat{D_0}(p)}{E(q)}+\frac{\widehat{D_0}(p)-\widehat{D_0}(q)}{E(q)}\Big|\leq\frac{2|p-q|}{\max(E(p),E(q))}.\quad(61)$$

Notation 7. The symbol $\mathbf{e}$ will always stand for any unitary vector in $\mathbb{R}^3$.

Remark 12. There holds (*cf* [16] for the expression of $(a^2-\Delta)^{-1}$):

$$\begin{aligned}\frac{1}{|D_0|}(x-y) &= \frac{2}{\pi}\int_0^{+\infty}\frac{d\omega}{|D_0|^2+\omega^2}(x-y)\\ &=\sqrt{\frac{2}{\pi}}\int_0^{+\infty}\frac{e^{-E_\omega|x-y|}}{|x-y|}d\omega\\ &=\mathrm{Cnst}\frac{\mathrm{K}_1(|x-y|)}{|x-y|}\end{aligned}$$

where K_1 is the modified Bessel function [25].

5 Proof of Proposition 1

5.1 *A priori* estimates on a minimizer for $E^0(2)$

This part is devoted to prove (63).

Let us say $\gamma'=\gamma+N$ is a minimizer for $E^0(2)$ written as in (26)-(27).

First we prove (28). There holds *a priori* estimates [20]:

$$\frac{1}{2}\mathrm{Tr}\big(\frac{-\Delta(1-\frac{\Delta}{\Lambda^2})}{|D_0|}(\gamma')^2\big)+\frac{\alpha}{2}\|\rho'_\gamma\|_{\mathcal{C}}^2\leq\mathcal{E}(\gamma')-2+\frac{\alpha}{2}\mathrm{Tr}(\gamma'R[\gamma'])\leq\frac{\alpha\pi}{4}\mathrm{Tr}(|\nabla|(\gamma')^2)$$

where we have used $|\mathbf{D}|-1\geq\frac{1}{2}\frac{-\Delta\left(1-\frac{\Delta}{\Lambda^2}\right)}{|D_0|}$. It follows that:

$$\mathrm{Tr}\big(\frac{-\Delta(1-\frac{\Delta}{\Lambda^2})}{|D_0|}(\gamma')^2\big)+\alpha\|\rho'_\gamma\|_{\mathcal{C}}^2\leq K\alpha.$$

As in [20], we can apply a fixed point scheme on (γ,ρ_γ) with the help of the self-consistent equation (in $\mathbf{Q}_1\times\mathcal{C}$ for instance). This gives:

$$\|\gamma\|_{\mathbf{Q}_1}\lesssim\sqrt{L\alpha}\|\rho'_\gamma\|_{\mathcal{C}}+\alpha\||\nabla|^{1/2}\gamma'\|_{\mathfrak{S}_2}\text{ and }\|\rho_\gamma\|_{\mathcal{C}}\lesssim L\|\rho'_\gamma\|_{\mathcal{C}}+\sqrt{L\alpha}\||\nabla|^{1/2}\gamma'\|_{\mathfrak{S}_2}.$$

Hence $|\mathrm{Tr}_0(\gamma)|\leq\|\gamma\|_{\mathfrak{S}_2}<1$ and $\mathrm{Tr}_0(\gamma)=0$ as shown in [7]. This proves $\mathrm{Tr}(N)=\mathrm{Tr}_0(N)=\mathrm{Tr}_0(\gamma')-\mathrm{Tr}_0(\gamma)=2$.

Let $(\psi_i)_{1\leq i\leq 2}$ be a basis of orthonormal eigenvectors of $\chi_{0,\mu}(D_{\gamma'})$ with eigenvalues $0<\mu_1\leq\mu_2<1$. We write $N_j:=|\psi_j\rangle\langle\psi_j|$ and $|n_j:=\psi_j|^2$. From the equation satisfied by ψ_j

$$(\mathbf{D}+\alpha(v[\rho_\gamma+n]-R[\gamma+N]))\psi_j=\mu_j\psi_j \tag{62}$$

we get the following.

Lemma 4. *Let γ' and $(\psi_j)_j$ be as above in the regime of Remark 5. Then there holds:*

$$\begin{cases} \frac{1}{(2\pi)^3}\displaystyle\int |p|^2\big(\Lambda^{-2}(2+\tfrac{|p|^2}{\Lambda^2})+(1+\tfrac{|p|^2}{\Lambda^2})\big)|\widehat{\psi_j}(p)|^2dp\leq\|\mathbf{D}\psi_j\|_{L^2}^2-1 \text{ and} \\ \|\mathbf{D}\psi_j\|_{L^2}^2-1\leq\alpha\|\rho_\gamma\|_{\mathfrak{C}}\|n_j\|_{\mathfrak{C}}+\alpha\|\gamma\|_{\mathfrak{S}_2}\|R[N_j]\|_{\mathfrak{S}_2}+\big(\alpha\|B_{\gamma'}\tfrac{1}{|\nabla|^{1/2}}\|_{\mathfrak{B}}\||\nabla|^{1/2}\psi_j\|_{L^2}\big)^2. \end{cases}$$

As a consequence we also have:

$$\mathrm{Tr}(-\Delta(1-\tfrac{\Delta}{\Lambda^2}+\tfrac{\Delta^2}{\Lambda^4})N)\lesssim c^{-2}. \tag{63}$$

It suffices to use the inequalities in the r.h.s. of (51) in Eq. (62).

Remark 13. Compared to the case of $E^0(1)$ there is an additional term $(v_n-R_N)\psi_j$ that has been neglected in $-2\alpha\mathfrak{Re}\langle B_N\psi_j\,,\,\psi_j\rangle$: this term is non-positive.

Notation 8. From now on, we write $v_{jk}=(\psi_j^*\psi_k)*\frac{1}{|\cdot|}$ and $v_j:=v_{jj}$ and define $a_{jk}:=\|v_k\psi_j-v_{kj}\psi_k\|_{L^2}$.

5.2 Proof of Lemma 1: estimate of $E^0(1)$

We compute the energy of a particular test function $Q_0'=Q_0+N_0$, defined as follows [21]. First, we take $\phi_{\mathrm{CP}}=\phi_1$ a minimizer for $E_{\mathrm{PT}}(1)$ in $L^2(\mathbb{R}^3,\mathbb{C})$ (*e.g.* real-valued and positive centered in 0, *cf* [15]). Then let ψ_1 be:

$$\psi_1:={}^t(\,\phi_1\;\;0\;\;0\;\;0\,)\in L^2(\mathbb{R}^3,\mathbb{C}^4). \tag{64}$$

Then, we define $\psi_{\frac{1}{c}}:=c^{-3/2}\psi_1(c^{-1}(\cdot))$ where $c^{-1}:=\alpha^2F_\Lambda(0)$ and

$$\begin{array}{lll|ll} \overline{N}_0 & :=|\psi_{\frac{1}{c}}\rangle\langle\psi_{\frac{1}{c}}|, & & Q_0+P_-^0=\Pi_0 & :=\chi_{-\infty,0}\big\{\mathbf{D}+\alpha\big((\rho_{Q_0}+\overline{n}_0)*\frac{1}{|\cdot|}-(R_{Q_0}+R_{\overline{N}_0})\big)\big\}, \\ \overline{n}_0 & :=|\psi_{\frac{1}{c}}|^2, & & \psi_0 & :=\frac{1}{\sqrt{1-\|\Pi_0\psi_{\frac{1}{c}}\|_{L^2}^2}}(\psi_{\frac{1}{c}}-\Pi_0\psi_{\frac{1}{c}}). \end{array}$$

We have used the fixed point scheme of Section 4.1 to define Q_0. We also write

$$\begin{array}{lll|ll} N_0 & :=|\psi_0\rangle\langle\psi_0|, & & Q_0' & :=Q_0+N_0, \\ B_0 & :=(\rho_{Q_0}+\overline{n}_0)*\frac{1}{|\cdot|}-\alpha(R_{Q_0}+R_{\overline{N}_0}), & & \mathbf{D}_{Q_0} & :=\mathbf{D}+\alpha B_0. \end{array}$$

The test function Q_0' is the difference between the orthogonal projections Π_0+N_0 and P_-^0. Following the same method as in [21], the following estimates hold.

$$\begin{array}{lll|ll} \|Q_0\|_{\mathbf{Q}_{w_2}} & \lesssim\alpha & & \|\overline{n}_0\|_{\mathfrak{C}_{w_2}} & \lesssim c^{-1/2} \\ \|Q_0\|_{\mathbf{Q}_{w_1}} & \lesssim c^{-1} & & \|\rho_{Q_0}\|_{\mathfrak{C}_{w_2}} & \lesssim Lc^{-1/2} \\ \|Q_0\|_{\mathfrak{S}_2} & \lesssim\alpha c^{-1/2} & & \|R_{\overline{N}_0}\|_{\mathfrak{S}_2} & \lesssim c^{-1} \end{array} \tag{65}$$

where $w_1(p-q)=E(p-q)$ and $w_2(p-q)=E(p-q)^2$.

As shown previously in [21, 20] there holds

$$\begin{aligned} \mathcal{E}_{\mathrm{BDF}}(Q_0')=\langle\mathbf{D}\psi_0\,,\,\psi_0\rangle-\tfrac{\alpha}{2}\mathrm{Tr}_0(B[Q_0]Q_0)-\tfrac{1}{2}(\mathrm{Tr}(|\mathbf{D}+\alpha B_0|Q_0^2)-\mathrm{Tr}(|\mathbf{D}|Q_0^2)) \\ +\tfrac{\alpha}{2}\big(D(\rho[Q_0]+n_0,\rho[Q_0]+n_0)-\mathrm{Tr}(Q_0'R[Q_0'])\big) \end{aligned} \tag{66}$$

Estimate of the density ρ_{Q_0} By Section 4.2, we write

$$\rho_{Q_0'} = (\delta_0 - \check{F}_\Lambda) * (\overline{n}_0 + \mathfrak{t}[\overline{N}_0] + \alpha^2\widetilde{\tau}_2), \tag{67}$$

$$= (\delta_0 - \check{F}_\Lambda) * \overline{n}_0 + \tau_{rem}. \tag{68}$$

We have

$$\|(\delta_0 - \check{F}_\Lambda) * \overline{n}_0 * \tfrac{1}{|\cdot|}\|_{L^\infty} \leq \frac{\pi}{2}(1 + \|\check{F}_\Lambda\|_{L^1})\langle|\nabla|\psi_{\frac{1}{c}}\,,\,\psi_{\frac{1}{c}}\rangle \lesssim \|\nabla\psi_{\frac{1}{c}}\|_{L^2} = \mathcal{O}(c^{-1}).$$

We use Ineq. (51) to estimate the norm $\|\tau_{rem}\|_{\mathcal{C}}$ of the remainder τ_{rem}.

The traces in (66) By Lemma 3, we can estimate $\big|\mathbf{D} + \alpha B_0\big| - \big|\mathbf{D}\big|$ and get the following [21].

Lemma 5. *There holds:*

$$\begin{aligned}|\delta\mathrm{Tr}| \;&:= \Big|\mathrm{Tr}\big\{|\mathbf{D} + \alpha B[Q_0']|\gamma_0^2 - |\mathbf{D}|Q_0^2\big\}\Big| \\ &\leq \{\|Q_0\|_{\mathcal{B}}^2 + \alpha(\|Q_0\|_{\mathrm{Kin}} + \|\tau_{rem}\|_{\mathcal{C}})\}\|Q_0\|_{\mathrm{Kin}}^2 + \alpha\{\|\tau_{rem}\|_{\mathcal{C}} + \|\nabla\psi_{\frac{1}{c}}\|_{L^2}\}\|Q_0\|_{\mathfrak{S}_2}^2 \\ &\lesssim \alpha c^{-3} + \alpha c^{-1} \times \alpha^2 c^{-1} \lesssim \alpha c^{-3}.\end{aligned} \tag{69}$$

$\langle\mathbf{D}\psi_0\,,\,\psi_0\rangle$ **in** (66) There holds $(1 - \Pi_0)\psi_{\frac{1}{c}} = -Q_0\psi_{\frac{1}{c}} + P_+^0\psi_{\frac{1}{c}}$. Then

$$\begin{aligned}\langle\mathbf{D}\psi_{\frac{1}{c}}\,,\,\psi_{\frac{1}{c}}\rangle \;&= \langle\mathbf{D}Q_0\psi_{\frac{1}{c}}\,,\,Q_0\psi_{\frac{1}{c}}\rangle - 2\mathfrak{Re}\langle P_+^0Q_0\psi_{\frac{1}{c}}\,,\,P_+^0\psi_{\frac{1}{c}}\rangle + \langle|\mathbf{D}|P_+^0\psi_{\frac{1}{c}}\,,\,\psi_{\frac{1}{c}}\rangle \\ \langle|\mathbf{D}|P_+^0\psi_{\frac{1}{c}}\,,\,\psi_{\frac{1}{c}}\rangle \;&= 1 + \tfrac{1}{2}\|\nabla\psi_{\frac{1}{c}}\|_{L^2}^2 + \mathcal{O}(c^{-4}).\end{aligned}$$

Then thanks to Lemma 3: $\||\mathbf{D}|^{1/2}Q_0\psi_{\frac{1}{c}}\|_{L^2} \leq \||\mathbf{D}|^{1/2}Q_0\frac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}}\||\nabla|^{1/2}\psi_{\frac{1}{c}}\|_{L^2}$ and

$$\||\mathbf{D}|^{1/2}Q_0\psi_{\frac{1}{c}}\|_{L^2} \lesssim \alpha c^{-1}.$$

As $Q_0 = \alpha Q_1[Q_0', \rho_{Q_0'}] + \alpha^2\widetilde{Q}_2[Q_0', \rho_{Q_0'}]$ and that $Q_1 = Q_1^{+-} + Q_1^{-+}$:

$$P_+^0Q_0\psi_{\frac{1}{c}} = \alpha Q_1^{+-}P_-^0\psi_{\frac{1}{c}} + \alpha^2 P^0 + \widetilde{Q}_2\psi_{\frac{1}{c}}.$$

Therefore:

$$\begin{aligned}\alpha^2\langle|\mathbf{D}|\widetilde{Q}_2\psi_{\frac{1}{c}}\,,\,P^0 + \psi_{\frac{1}{c}}\rangle \;&\leq \alpha^2\||\nabla|^{1/2}\psi_{\frac{1}{c}}\|_{L^2}^2\|\tfrac{|\mathbf{D}|}{|\nabla|^{1/2}}\widetilde{Q}_2\tfrac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}} \\ &\lesssim \alpha^2 c^{-1} \times c^{-1} = \mathcal{O}(\alpha^2 c^{-2}) \\ \alpha\langle|\mathbf{D}|Q_1^{+-}P_-^0\psi_{\frac{1}{c}}\,,\,P_+^0\psi_{\frac{1}{c}}\rangle \;&\leq \alpha\||\mathbf{D}|^{1/2}Q_1^{+-}\tfrac{1}{|\nabla|^{1/2}}\|_{\mathcal{B}}\||\nabla|^{1/2}P_-^0\psi_{\frac{1}{c}}\|_{L^2}\||\mathbf{D}|^{1/2}\psi_{\frac{1}{c}}\|_{L^2} \\ &\lesssim \alpha c^{-1/2} \times c^{-3/2} = \mathcal{O}(\alpha c^{-2}).\end{aligned}$$

Hence:

$$\langle\mathbf{D}(1 - \Pi_0)\psi_{\frac{1}{c}}\,,\,(1 - \Pi_0)\psi_{\frac{1}{c}}\rangle/(1 - \|\Pi_0\psi_{\frac{1}{c}}\|_{L^2}^2) = 1 + \frac{1}{2}\|\nabla\psi_{\frac{1}{c}}\|_{L^2}^2 + \mathcal{O}(\alpha c^{-2}). \tag{70}$$

The potential energy in (66) By the same methods we prove:

$$\begin{aligned}&\tfrac{\alpha}{2}\big(2D(\rho[Q_0], n_0) - D(\rho[Q_0], \overline{n}_0) - \mathfrak{Re}(2\mathrm{Tr}(Q_0R[N_0]) - \mathrm{Tr}(Q_0R[\overline{N}_0]))\big) \\ &\quad = -\tfrac{\alpha}{2}D(\check{F}_\Lambda * \overline{n}_0, \overline{n}_0) + \mathcal{O}(\alpha^2 c^{-3/2}).\end{aligned} \tag{71}$$

For instance by Cauchy-Schwarz inequality followed by Hardy inequality:

$$\big|D\big(\rho[Q_0], (P_+^0\psi_{\frac{1}{c}})^*(Q_0\psi_{\frac{1}{c}})\big)\big| \leq \|\rho[Q_0]\|_{\mathcal{C}} \times 4^{1/4}\|\nabla\psi_{\frac{1}{c}}\|_{L^2}^{1/2}\|Q_0\psi\|_{L^2} = \mathcal{O}(c^{-3}).$$

By Ineq. (58), there holds:

$$-\frac{\alpha}{2}D(\check{F}_\Lambda * \overline{n}_0, \overline{n}_0) = -\frac{1}{2c}D(\overline{n}_0, \overline{n}_0) + \mathcal{O}(\alpha^2 c^{-2} + c^{-1}\|\overline{n}_0\|_{L^2}^2) = \mathcal{O}(\alpha^2 c^{-2});$$

indeed: $\|\overline{n}_0\|_{L^2} = \|\psi_{\frac{1}{c}}\|_{L^4}^2 \lesssim \||\nabla|^{3/4}\psi_{\frac{1}{c}}\|_{L^2}^2$. As a consequence:

$$E^0_{\mathrm{BDF}}(1) \leq \mathcal{E}_{\mathrm{BDF}}(Q_0 + N_0) = 1 + \frac{\mathcal{E}_{\mathrm{PT}}(\phi_1)}{2c^2} + \mathcal{O}(\alpha c^{-2}). \tag{72}$$

We have proved the inequality the $\leq$ part. For the $\geq$ part, it suffices to take a *real* minimizer and with the same estimates as above and [21] we prove similar estimates.

That there exists a minimizer for $E^0(1)$ follows from Theorem 1, using the same method as in [21]. We have proved $E^0(1) < 1$, then by Lieb's variational principle we get that for any $0 < q < 1$, $E^0(q) > qE^0(1)$, hence the binding inequalities holds for $0 < q < 1$. For $q \in [0,1]^c$, binding inequalities hold for sufficiently small α. We refer to [21] for more details.

Similar estimates apply for $E^0(2)$, in particular we have $E^0(2) \leq 2E^0(1) \leq 2 + \frac{\mathcal{E}_{\mathrm{PT}}(\phi_1)}{2c^2} + \mathcal{O}(\alpha c^{-2})$.

5.3 Study of a minimizer γ' for $E^0(2)$

Bootstrap argument We write $x^2 := \mathrm{Tr}(-\Delta(1 - \frac{\Delta}{\Lambda^2} + \frac{\Delta^2}{\Lambda^4})N)$. By Lemma 4, we have $x^2 \lesssim c^{-2}$. This fact enables us to use the method of [4, 21].

We scale ψ_j by c: $\underline{\psi_j}(x) = c^{3/2}\psi_j(cx)$ and scale γ accordingly: $\underline{\gamma}(x,y) = c^3\gamma(cx, cy)$. Then writing $\mathcal{L}_A := (1 - \Delta/A^2)$, the wave function $\underline{\psi_j}$ satisfies:

$$(c^2\beta - ic\boldsymbol{\alpha}\cdot\nabla)\underline{\psi_j} + \alpha c\mathcal{L}_{c\Lambda}^{-1}(v[\rho[\underline{\gamma}] + \underline{n}] - R[\underline{g} + \underline{N}])\underline{\psi_j} = c^2\mu_j\mathcal{L}_{c\Lambda}^{-1}\underline{\psi_j}. \tag{73}$$

Splitting $\underline{\psi_j}$ between upper spinor $\underline{\varphi_j}$ and lower spinor $\underline{\chi_j}$ both in $L^2(\mathbb{R}^3, \mathbb{C}^2)$, this gives:

$$\|\underline{\chi_1}\|_{L^2} + \|\underline{\chi_2}\|_{L^2} \lesssim c^{-1}.$$

Going back to ψ_j one gets $\langle \mathbf{D}\psi_j\,,\,\psi_j\rangle = 1 + \mathcal{O}(c^{-2})$ and it shows that for $j = 1, 2$: $0 < (1 - \mu_j)c^2 \leq K$ thanks to the equation (28). As

$$0 \leq c^2(1 - \mathcal{L}_{c\Lambda}^{-1}) = \frac{-c^2\Delta}{c^2\Lambda^2 - \Delta} \leq \frac{-\Delta}{\Lambda^2}, \text{ then} \tag{74}$$

$$\begin{aligned} c^2(\mu_j\mathcal{L}_{c\Lambda} - 1)\underline{\varphi_j} &= c^2(\mu_j - 1)\underline{\varphi_j} + \tfrac{c^2\Delta}{c^2\Lambda^2 - \Delta}\underline{\varphi_j} \\ &= c^2(\mu_j - 1)\underline{\varphi_j} + \mathcal{O}_{L^2}\left(\tfrac{c}{\Lambda}\right) \end{aligned}$$

thanks to Lemma 1 ($\mathcal{O}_{L^2}$ means in L^2-norm). We can get another estimate: in the spirit of [21, 20] we can use bootstrap argument with the norms

$$||Q||_{\mathfrak{Q}_w}^2 = \iint E(p-q)^{2k}(E(p+q))|\widehat{Q}(p,q)|^2 dpdq \text{ and } \|\rho\|_{\mathfrak{C}_w}^2 = \int \frac{E(k)^2|\widehat{\rho}(k)|^2}{|k|^2}dk,$$

to get the following statement:

Lemma 6. *For any fixed $k \in \mathbb{N}^*$, there exists $\alpha_{(k)} > 0$ such that for $\alpha \leq \alpha_{(k)}$, ψ_j with $j = 0, 1, 2$ is in $H^{k/2}$ with norms $\mathcal{O}(1)$ and*

$$||\gamma_0||_{\mathfrak{Q}_w}, ||\gamma||_{\mathfrak{Q}_w}, \|\rho[\gamma]\|_{\mathfrak{C}_w}, \|\rho[\gamma_0]\|_{\mathfrak{C}_w} \lesssim 1.$$

It is supposed $\alpha\log(\Lambda) \leq L_0$. There also holds:

$$\|\Delta\psi\|_{L^2} \lesssim \min(c^{-1}(c^{-1} + \Lambda^{-1}), c^{-3/2}),\ \|\underline{\chi}\|_{L^2} \lesssim c^{-1} \text{ and } \|\nabla\underline{\chi}\|_{L^2} \lesssim c^{-1},$$

The estimation of $\mathcal{E}_{\mathrm{BDF}}(\gamma')$ is proven with the help of the estimate $\|\Delta\psi\|_{L^2} \lesssim c^{-3/2}$ as shown in the (technical) proof of Lemma 6 in Appendix A.2.

Remark 14. By Estimate (63) we can prove that n, γ, ρ_γ have estimates of the same kind of those stated in (65) [21, 20]: we have

$$\|n\|_{\mathcal{C}} \lesssim c^{-1/2},\ \|\rho_\gamma\|_{\mathcal{C}} \lesssim Lc^{-1/2},\ \|R_{N_j}\|_{\mathfrak{S}_2} \lesssim c^{-1}, \||\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2} \lesssim c^{-1}, \|\gamma\|_{\mathfrak{S}_2} \lesssim \alpha c^{-1/2}. \tag{75}$$

There also holds $\|n_j\|_{L^2} \lesssim c^{-3/2}$.

By Lemma 6, we get:

$$\|\rho_\gamma\|_{L^2} \lesssim Lc^{-3/2}.$$

Following [20] we can prove $\rho_\gamma \in L^1$ and $\|\rho_\gamma\|_{L^1} \lesssim L$.

Estimate on $c^2(1-\mu_j)$ Using estimates on $\nabla\varphi_j$ and $\nabla\chi_j$ (Lemma 6) together with Ineq. (58), we get the following estimate from (28):

$$\mu_j = 1 + \frac{\|\nabla\underline{\varphi_j}\|_{L^2}^2}{2c^2} - \frac{1}{c^2}D(\underline{n_j}, \underline{n}) + \mathcal{O}(\alpha c^{-2}). \tag{76}$$

With (47)-(48), we get:

$$(1-\mu_j)c^2 \leq -\tfrac{3}{2}E_{\mathrm{PT}}(1) + \mathcal{O}(\alpha^{1/4}) \gtrsim 1. \tag{77}$$

6 Localisation of minimizers in Direct space

6.1 Decay estimates on the $\underline{\psi_j}$'s

It is known $\underline{\psi_1} \wedge \underline{\psi_2}$ can be split into two almost minimizers of Choquard-Pekar energy h_1 and h_2: $h_1 \wedge h_2 = \underline{\psi_1} \wedge \underline{\psi_2}$. For $j \in \{1,2\}$, we write $\phi_j \in \mathscr{P}$ the closest Pekar minimizer to h_j and its center is written z_j. We write

$$\mathrm{R}_g := |z_1 - z_2|. \tag{78}$$

By Section 3, we have:

$$M^2(\underline{\psi_1} \wedge \underline{\psi_2}) := \iint \frac{|\underline{\psi_1} \wedge \underline{\psi_2}(x,y)|^2}{|x-y|}dxdy \gtrsim \frac{1}{\mathrm{R}_g}. \tag{79}$$

Our aim is to show decay estimates far away from z_1 and z_2. Up to translations, we assume the mean $z_m = \frac{z_1+z_2}{2}$ is 0.

Localisation functions Let $\xi_1 \geq 0$ be some *radial* Schwartz function in $\mathcal{S}(\mathbb{R}^3)$ satisfying

$$|x| \leq 1 \ \Rightarrow\ \xi_1(x) = 1 \text{ and } |x| \geq 2 \ \Rightarrow\ \xi_1(x) = 0.$$

We define $\xi_A(x) := \xi_1(\frac{x}{A})$ for any $A > 0$ and $\theta_A := \sqrt{1-\xi_A^2}$. For any $x \in \mathbb{R}^3$ we write

$$d(x) := \min\{|x-z_1|, |x-z_2|\}. \tag{80}$$

Let H be the plane $\{x :\ |x-z_1| = |x-z_2|\}$; the function $d(\cdot)$ is differentiable in $\mathbb{R}^3 \backslash \big(\{z_1, z_2\} \cup H\big)$. For any $A \gg \mathrm{R}_g$ and $0 < \lambda < 2$ we define

$$\boldsymbol{\eta}_{\mathrm{R}_g}^{\lambda}(x) := \big(1 - \xi_{\lambda \mathrm{R}_g}^2(x-z_1) - \xi_{\lambda\mathrm{R}_g}^2(x-z_2)\big)^{1/2}. \tag{81}$$

We define $\lambda_0 > 0$, defined by the formula

$$\lambda_0 \mathrm{R}_g = \tfrac{C_0}{L} \text{ where } C_0(L, \mathrm{R}_g) > 1 \text{ is chosen large.} \tag{82}$$

The function $\boldsymbol{\eta}_{\mathrm{R}_g}^{\lambda}$ can be seen as the dilation of $\boldsymbol{\eta}_1^{\lambda} := \sqrt{1 - \xi_\lambda^2(\cdot - e_1) - \xi_\lambda^2(\cdot - e_2)}$ by R_g where $e_j := \frac{z_j - z_m}{\mathrm{R}_g}$.

At last we define:

$$\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}(x) := \sqrt{1 - \xi_{c\lambda\mathrm{R}_g}^2(x - cz_1) - \xi_{c\lambda\mathrm{R}_g}^2(x-cz_2)}, \tag{83}$$

we use it in Section D.2.3.

Lemma 7. • *For each $\lambda_0 \leq \lambda < 2^{-1}$, there exists K_λ such that:*

$$\forall\, A>0,\ \int d(x)^2\xi_A^2(x)(\boldsymbol{\eta}_{R_g}^{\lambda}(x))^2\Big(\big||D_0|^{1/2}\underline{\psi_1}(x)\big|^2+\big||D_0|^{1/2}\underline{\psi_2}(x)\big|^2\Big)dx \quad \leq K_\lambda \tag{84}$$

Moreover we can choose $(K_\lambda)_\lambda$ to be nonincreasing and K_{λ_0} is (uniformly) bounded in the regime α, L, Λ^{-1} small.
• *For any $2\lambda_0 \leq \lambda < 2^{-1}$ the same holds for $d_{A,\lambda}^{(2)} := d(x)^2\xi_A\boldsymbol{\eta}_{cR_g}^{(\lambda)}$:*

$$\int d(x)^4\xi_A^2(x)(\boldsymbol{\eta}_{cR_g}^{(\lambda)})^2(x)\Big(\big||D_0|^{1/2}\underline{\psi_1}(x)\big|^2+\big||D_0|^{1/2}\underline{\psi_2}(x)\big|^2\Big)dx \leq K'_\lambda, \tag{85}$$

where $K'_\lambda > K_\lambda$ depends on λ, K_λ, ξ_1.
• *We can replace $|D_0|^{1/2}\underline{\psi_j}$ by $\underline{\psi_j}$ above.*

Remark 15. This is a weak estimate due to the presence of $\underline{v_k\psi_j} - \underline{v_{kj}\psi_k}$.

This proposition is proved in Appendix C.1.

6.2 Localisation operators

We want to prove that minimizers are localised in space around the centers z_1, z_2 of the electrons. To this end we use localisation operators of [9, 14] with respect to the functions $\xi_{c\lambda \mathrm{R}_g}$ and $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$ introduced in the previous Section (6.1).

By Lemma 7 we know that the wave functions $\underline{\psi_1}$ and $\underline{\psi_2}$ are localized near z_1 and z_2. By scaling, it follows that ψ_1 and ψ_2 are localized near cz_1 and cz_2. We consider:

$$\begin{aligned} &\xi_1^{(\lambda)}(x) := \xi_{c\lambda \mathrm{R}_g}(x-cz_1) \qquad \text{and} \quad \xi_2^{(\lambda)}(x) := \xi_{c\lambda \mathrm{R}_g}(x-cz_2),\\ &X_1^{(\lambda)} := (\xi_1^{(\lambda)})^{++} + (\xi_1^{(\lambda)})^{--} \quad \text{and} \quad X_2^{(\lambda)} := (\xi_2^{(\lambda)})^{++} + (\xi_2^{(\lambda)})^{--}, \end{aligned}$$

and localise γ':

$$\xi_1^{(\lambda)}\cdot[\gamma'] := X_1^{(\lambda)}(\gamma')X_1^{(\lambda)},\ \xi_2^{(\lambda)}\cdot[\gamma'] = X_2^{(\lambda)}(\gamma')X_2^{(\lambda)}.$$

We define the set

$$B_\lambda := \big\{B(cz_1, c\lambda \mathrm{R}_g)\times B(cz_2, c\lambda \mathrm{R}_g)\big\}\cup\big\{B(cz_2, c\lambda \mathrm{R}_g)\times B(cz_2, c\lambda \mathrm{R}_g)\big\} \subset \mathbb{R}^3\times\mathbb{R}^3. \tag{86}$$

Our aim in this section is to prove:

Proposition 6. *If γ' is a minimizer of $E^0(2)$ in the regime α, L, Λ^{-1} small then:*

$$\mathcal{E}^0_{BDF}(\gamma') = \mathcal{E}^0_{BDF}(\xi_1^{3^{-1}}\cdot[\gamma'])+\mathcal{E}^0_{BDF}(\xi_2^{3^{-1}}\cdot[\gamma'])+\frac{\alpha}{2}\iint\limits_{(x,y)\in B_{3^{-1}}}\frac{|\psi_1\wedge\psi_2(x,y)|^2}{|x-y|}dxdy+\mathcal{O}\Big(\frac{1}{c^2R_g}\Big). \tag{87}$$

Moreover:

$$\begin{cases} \mathrm{Tr}_0(\xi_j^{(\frac{1}{3})}\cdot[\gamma']) = 1+\varepsilon_j,\ \varepsilon_j = o(1), j=1,2,\\ \mathrm{Tr}_0(\xi_1^{(\frac{1}{3})}\cdot[\gamma']) + \mathrm{Tr}_0(\xi_2^{(\frac{1}{3})}\cdot[\gamma']) = 2+\mathcal{O}\Big(\frac{1}{c^2R_g}\Big). \end{cases} \tag{88}$$

Assuming this Proposition – proved in Subsection (6.5) – we can prove Theorem 2.

6.3 Proof of Theorem 2

By Proposition 4, for sufficiently small α, L, there holds:

$$\frac{\alpha}{2}\iint\limits_{(x,y)\in B_{3^{-1}}}\frac{|\psi_1\wedge\psi_2(x,y)|^2}{|x-y|}dxdy \geq \frac{L^{-1}}{c^2K_{\mathrm{g}}\mathrm{R}_g},$$

for some constant $K_{\rm g} > 1$ independent of α, Λ in the regime of Remark 5. This gives:

$$\mathcal{E}_{\rm BDF}(\gamma') \geq E^0_{\rm BDF}(1+\varepsilon_1) + E^0_{\rm BDF}(1+\varepsilon_2) + \frac{L^{-1}}{K_{\rm g} c^2 {\rm R}_g} + \mathcal{O}\Big(\frac{1}{c^2 {\rm R}_g}\Big).$$

We know that the function $E^0_{\rm BDF}(\cdot) : \mathbb{R} \mapsto \mathbb{R}$ is uniformly Lipschitz with constants 1 and this function is concave on each interval $[M, M+1]$ where $M \in \mathbf{Z}$ [9, Corollary 3 *mutatis mutandis*]. Furthermore we may assume $\varepsilon_1 = -\varepsilon_2 > 0$ up to an error $\mathcal{O}\Big(\frac{1}{c^2 {\rm R}_g}\Big)$. The case $\varepsilon_1, \varepsilon_2 < 0$ is easily excluded by concavity of $E^0_{\rm BDF}$ in $[0,1]$ because $E^0_{\rm BDF}(0) = 0$ and $2E^0_{\rm BDF}(1) \geq E^0_{\rm BDF}(2)$. Then:

$$\begin{aligned} E^0_{\rm BDF}(1+\varepsilon_1) + E^0_{\rm BDF}(1-\varepsilon_1) &\geq \varepsilon_1 E^0_{\rm BDF}(2) + (1-\varepsilon_1) E_{\rm BDF}(1) + (1-\varepsilon_1) E_{\rm BDF}(1) \\ &\geq \varepsilon_1 E^0_{\rm BDF}(2) + (1-\varepsilon_1)(2E^0_{\rm BDF}(1)) \geq (1-\varepsilon_1+\varepsilon_1) E^0_{\rm BDF}(2) = E^0_{\rm BDF}(2). \end{aligned}$$

Thus taking $F_\Lambda(0) = \Theta(\alpha \log(\Lambda))$ sufficiently small, the quantity L^{-1} is big enough to compensate the error term $\mathcal{O}\Big(\frac{1}{c^2 {\rm R}_g}\Big)$. We get the desired contradiction:

$$E^0_{\rm BDF}(2) = \mathcal{E}_{\rm BDF}(\gamma') \geq E^0_{\rm BDF}(2) + \frac{1}{c^2 {\rm R}_g K'_{\rm g}} > E^0_{\rm BDF}(2).$$

6.4 Localisation of the energy of the vacuum γ

Lemma 8. *For $\lambda_0 \leq \lambda < 2^{-1}$ big enough (*e.g. $\lambda = \frac{1}{12}, \frac{1}{6}, \frac{1}{3}$*) there holds:*

$$\|\boldsymbol{\eta}^{(\lambda)}_{cR_g} \rho_\gamma\|_{\mathcal{C}} \lesssim \frac{L}{\sqrt{c\lambda R_g}} \text{ and } \|\boldsymbol{\eta}^{(\lambda)}_{cR_g} |\mathbf{D}|^{1/2} \gamma\|_{\mathfrak{S}_2}, \|\boldsymbol{\eta}^{(\lambda)}_{cR_g} |D_0|^{1/2} \gamma\|_{\mathfrak{S}_2} \lesssim \frac{1}{c\sqrt{\lambda R_g}}. \quad (89)$$

This part comes after lots of technicalities: we put together results of Lemma 7, Propositions 7, 8, 9, Remark 18 and the known estimates of Remark 14. We refer the reader to Remark 16 for explanation.

Here we assume that L is small enough in such a way that $\lambda_0 {\rm R}_g = \mathcal{O}(L^{-1})$ is big enough. Lemma 8 gives that for all $\lambda_0 \leq \lambda < 2^{-1}$:

$$\|\boldsymbol{\eta}^{(\lambda)}_{c{\rm R}_g} \rho_\gamma\|_{\mathcal{C}} \leq \frac{\epsilon_1}{\sqrt{c\lambda {\rm R}_g}} + \epsilon_2 \|\boldsymbol{\eta}^{(\lambda/2)}_{c{\rm R}_g} \rho_\gamma\|_{\mathcal{C}}, \ \epsilon_1, \epsilon_2 = \mathcal{O}(L). \quad (90)$$

We recall that $\lambda_0 {\rm R}_g := \frac{C_0}{L}$ with $C_0(L, {\rm R}_g) > 1$ to be chosen. Up to taking a bigger C_0: $C_0 \leq \widetilde{C}_0 < 6C_0$ we assume $\lambda_0 = 2^{-J_0}, J_0 \in \mathbb{N}$. Taking $\ell_0 := c\frac{\widetilde{C}_0}{3L}$ as unity of length, we define the sequences $(u_m), (v_m), (w_m)$ by the formulae:

$$\begin{cases} u_0 = v_0 = w_0 = \|\boldsymbol{\eta}^{(\lambda_0)}_{c{\rm R}_g} \rho_\gamma\|_{\mathcal{C}}, \\ u_m := \|\boldsymbol{\eta}^{(2^m \lambda_0)}_{c{\rm R}_g} \rho_\gamma\|_{\mathcal{C}}, \ v_m = 2^{m/2} u_m, \\ w_{m+1} := \epsilon_1 \sqrt{\dfrac{2}{\ell_0}} + \epsilon_2 \sqrt{2} w_m \end{cases} \quad (91)$$

It is clear from (90) that $v_{m+1} \leq \epsilon_1 \sqrt{\frac{2}{\ell_0}} + \epsilon_2 \sqrt{2} v_m$. Thus we have:

$$\forall m \in \mathbb{N}^* : \ v_m \leq w_m = w_\infty + (2^{1/2} \epsilon_2)^m (w_0 - w_\infty)$$

where $w_\infty = \epsilon_1 (2/\ell_0)^{1/2} (1 - \epsilon_2 \sqrt{2})^{-1/2}$ is well defined provided $\epsilon_2 < 2^{-1/2}$. In particular:

$$\forall m \in \mathbb{N}^* : \ u_m \leq \frac{\epsilon_1 \sqrt{2}}{\sqrt{2^m \ell_0}} + \frac{(\sqrt{2}\epsilon_2)^m}{\sqrt{2^m}} \Big\{ \|\boldsymbol{\eta}^{(\lambda_0)}_{c{\rm R}_g} \rho_\gamma\|_{\mathcal{C}} - \frac{\epsilon_1 \sqrt{2}}{\sqrt{\ell_0}(1 - \epsilon_2 \sqrt{2})} \Big\}$$

It remains to evaluate at $m = J_0$: this gives $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(3^{-1})}\rho_\gamma\|_{\mathcal{C}}$. Similarly the case $m = J_0 - 1$ corresponds to 6^{-1} etc. By Hardy-Littlewood-Sobolev inequality [16, Theorem 4.3]:

$$\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda_0)}\rho_\gamma\|_{\mathcal{C}} \leq \||\rho_\gamma|\|_{\mathcal{C}} \lesssim \|\rho_\gamma\|_{L^{6/5}} \lesssim \|\rho_\gamma\|_{L^1}^{\frac{2}{3}}\|\rho_\gamma\|_{L^2}^{\frac{1}{3}} \lesssim Lc^{-1/2}.$$

For $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}$ it suffices to use this result, Proposition 8 with Lemma 7.

Remark 16. The following holds.

1. Lemma 7 states that each ψ_j is localized around its center cz_j,
2. we give in Remark 14 estimates on the norms of γ,N, ρ_γ and n. In particular the densities have the "correct behaviour" in L^1, L^2 and Coulomb norms. We call these estimates: "non-localized estimates".

The other cited results are used of as follows. We remark that $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)} = \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{\lambda}{2})}$.

Proposition 8 gives an estimate of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}$ and $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{\widetilde{a}}\gamma\|_{\mathfrak{S}_2}$ (where $\widetilde{a} \in \{2^{-1}, a[\Lambda]\}$) in terms of

$$\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}v[\rho'_\gamma]\|_{L^2}, \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\|_{\mathrm{Ex}}, \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}R_N\|_{\mathfrak{S}_2} \text{ and } \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}v[\rho'_\gamma]\|_{L^6},$$

and in terms of the non-localized estimates (with the "correct behaviour" with respect to $c\lambda\mathrm{R}_g$, that is as in (89)). Below, we shorten: non. loc. est. w. the c. b.

Proposition 9 gives an estimate of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\nabla v[\rho_\gamma]\|_{L^2}$ in terms of

$$\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2} \text{ and } \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\rho_\gamma\|_{\mathcal{C}} = \|\rho[\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{\lambda}{2})}]\|_{\mathcal{C}},$$

and in terms of the non. loc. est. w. the c. b.

Furthermore, it gives an estimate of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}v_{\rho_\gamma}\|_{L^6}$ in terms of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\nabla v_{\rho_\gamma}\|_{L^2}$ and of the non. loc. est. w. the c. b. The term $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\|_{\mathrm{Ex}}$ is controlled by $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}$ and by the non. loc. est. w. the c. b.

Thanks to Lemma 7, the term $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}R_N\|_{\mathrm{Ex}}$ (resp. $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}n\|_{\mathcal{C}}$) is proved to be of order $(c^2\lambda\mathrm{R}_g)^{-1}$ (resp. $(c\lambda\mathrm{R}_g)^{-1/2}$).

Finally Proposition 7 together with Remark 18 gives an estimate of $\|\rho[\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{\lambda}{2})}]\|_{\mathcal{C}}$ in terms of $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{\lambda}{2})}P_\pm^0\gamma\|_{\mathfrak{S}_2}$, $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}P_\pm^0\gamma\|_{\mathfrak{S}_2}$, and in terms of the non. loc. est. w. the c. b. The presence of $P_\pm^0$ is harmless as we can check from the proofs.

6.5 Proof of Proposition 6

We consider each term of the BDF energy and write $1 = (\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2 + (\xi_1^{(\frac{1}{3})})^2 + (\xi_2^{(\frac{1}{3})})^2$.

We use once again Lemma 7, Proposition 8 and Remark 14. We treat one after the other the case of N and γ. We write

$$(\xi^{(\lambda)})^2 := (\xi_1^{(\lambda)})^2 + (\xi_2^{(\lambda)})^2.$$

The function ζ refers to $\xi^{(\lambda)}$ or $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$.

6.5.1 Kinetic energy

Kinetic energy for γ :

$$\begin{aligned}
\mathrm{Tr}\big((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})|\mathbf{D}|^{1/2}\gamma^2|\mathbf{D}|^{1/2}\big) &\leq \|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}^2 \lesssim \tfrac{1}{c^2\mathrm{R}_g} \\
\mathrm{Tr}\big(\zeta^{\pm\mp}|\mathbf{D}|^{1/2}\gamma^2|\mathbf{D}|^{1/2}\big) &\leq \|\zeta^{\pm\mp}\|_{\mathcal{B}}\||\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2}^2 \lesssim \tfrac{1}{c^3\lambda\mathrm{R}_g}
\end{aligned}$$

Kinetic energy for N : We recall the following equalities: $\mathbf{D}\psi_j = \mu_j - \alpha B\psi_j$ and $(v_n - R_N)\psi_1 = v_2\psi_1 - v_{21}\psi_2 = \mathcal{O}_{L^2}(\alpha^{3/2}c^{-1})$. Thus, we have:

$$\begin{aligned}\langle \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\mathbf{D}\psi_j\,,\,\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\rangle &= \langle \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}(\mu_j-\alpha B)\psi_j\,,\,\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\rangle\\ |\langle \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\mathbf{D}\psi_j\,,\,\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\rangle| &\leq (1+\alpha\|v[\rho'_\gamma]\|_{L^\infty})\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\|_{L^2}^2 + \alpha\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_j\|_{L^2}(\|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})R_\gamma\psi_j\|_{L^2}\\ &\quad +\alpha\|v_{kj}\|_{L^\infty}\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}\psi_k\|_{L^2}) \lesssim \tfrac{1}{\mathrm{R}_g^4} + \tfrac{\alpha\|\gamma\|_{\mathrm{Ex}}}{c\mathrm{R}_g^3} = o(c^{-2}\mathrm{R}_g^{-1}).\end{aligned}$$

We write :

$$(\xi^{(\frac{1}{3})})^2 = (P_+^0+P_-^0)(\xi^{(\frac{1}{3})})(P_+^0+P_-^0)(\xi^{(\frac{1}{3})})(P_+^0+P_-^0),$$

we have to show that $\langle \xi^{\varepsilon_1\varepsilon_2}\xi^{\varepsilon_2\varepsilon_3}\mathbf{D}\psi_j\,,\,\psi_j\rangle$ is $\mathcal{O}(c^{-2}\mathrm{R}_g^{-1})$ whenever $\varepsilon_1\neq\varepsilon_2$ or $\varepsilon_2\neq\varepsilon_3$.

We recall that $\|P_-^0\psi_j\|_{L^2}$ and $\alpha\|B\psi_j\|_{L^2}$ are $\mathcal{O}(c^{-1})$.

The operator $(\xi^{(\frac{1}{3})})^{+-}(\xi^{(\frac{1}{3})})^{-+}$ is $\mathcal{O}(c^{-2}\mathrm{R}_g^{-2})$ in $\|\cdot\|_{\mathcal{B}}$-norm. Except for the corresponding term, we have $\varepsilon_1 = -$ or $\varepsilon_3 = -$, leading to an upper bound:

$$\mathcal{O}\big(\|(\xi^{(\frac{1}{3})})^{+-}\|_{\mathcal{B}}(\|P_-^0\psi_j\|_{L^2}+\alpha\|B\psi_j\|_{L^2})\big) = \mathcal{O}\Big(\frac{1}{c^2\mathrm{R}_g}\Big).$$

Similar estimates lead to (88). The estimates $\varepsilon_1,\varepsilon_2 = o(1)$ follow from the fact that $n = |\underline{\psi_1}|^2 + |\underline{\psi_2}|^2 = |h_1|^2 + |h_2|^2$, where the h_j's satisfy $h_1\wedge h_2 = \underline{\psi_1}\wedge\underline{\psi_2} = \underline{\Psi}$ and

$$D\big(|h_1|^2,|h_2|^2\big) = d_{\underline{\Psi}}.$$

In fact, this $o(1)$ is an $\mathcal{O}(\alpha + e^{-K\mathrm{R}_g})$.

6.5.2 Direct term

On the outside: $\boldsymbol{\eta}_{c\mathbf{R}_g}^{(\lambda)}$. By Lemma 7 and Kato's inequality (Appendix A):

$$\|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2 n\|_{\mathcal{C}} \lesssim \frac{1}{c^{1/2}\lambda^2\mathrm{R}_g^2}.$$

On the inside: $\xi^{(\frac{1}{3})}$. We remark the following:

$$\begin{aligned}(\xi^{(\frac{1}{3})})^2 &= (\xi^{(\frac{1}{3})})^2\big((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{12})})^2 + (\xi^{(\frac{1}{12})})^2\big) = (\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{12})})^2 - (\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{12})})^2(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2 + (\xi^{(\frac{1}{12})})^2(\xi^{(\frac{1}{3})})^2\\ &= (\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{12})})^2 - (\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2 + (\xi^{(\frac{1}{12})})^2.\end{aligned} \tag{92}$$

Thus:

$$\begin{aligned}\Big|D\big((\xi^{(\frac{1}{3})})^2\rho_\gamma,(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2\rho'_\gamma\big)\Big| &\leq \|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2\rho_\gamma\|_{\mathcal{C}}(\|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2\rho_\gamma\|_{\mathcal{C}} + \|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{12})})^2\rho'_\gamma\|_{\mathcal{C}})\\ &\quad +|D((\xi^{(\frac{1}{12})})^2\rho_\gamma,(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2\rho'_\gamma)| \lesssim \frac{\|\rho_\gamma\|_{L^1}\|\rho'_\gamma\|_{L^1}}{c\mathrm{R}_g} + o\big(\tfrac{L}{c\mathrm{R}_g}\big).\end{aligned}$$

We treat $D\big((\xi_1^{(\frac{1}{3})})^2\rho_\gamma,(\xi_1^{(\frac{1}{3})})^2\rho'_\gamma\big)$ in a similar way: it is $\mathcal{O}\big(\frac{L}{c\mathrm{R}_g}\big)$. We have proved so far:

$$\begin{aligned}D(\rho'_\gamma,\rho'_\gamma) &= D((\xi_1^{(\frac{1}{3})})^2\rho'_\gamma,(\xi_1^{(\frac{1}{3})})^2\rho'_\gamma) + D((\xi_2^{(\frac{1}{3})})^2\rho'_\gamma,(\xi_2^{(\frac{1}{3})})^2\rho'_\gamma)\\ &\quad +2D((\xi_1^{(\frac{1}{3})})^2 n,(\xi_2^{(\frac{1}{3})})^2 n) + \mathcal{O}\big(\frac{L}{c\mathrm{R}_g}\big).\end{aligned}$$

In appendix D we prove the following Lemma.

Lemma 9. *For $j=1,2$, we have:*

$$D\big((\xi_1^{(\frac{1}{3})})^2\rho'_\gamma,(\xi_1^{(\frac{1}{3})})^2\rho'_\gamma\big) = D\Big(\rho\Big[\xi_j^{(\frac{1}{3})}\cdot[\gamma']\Big],\rho\Big[\xi_j^{(\frac{1}{3})}\cdot[\gamma']\Big]\Big) + \mathcal{O}\big(\frac{L}{cR_g}\big).$$

6.5.3 Exchange term

By Lemma 7 and Kato's inequality (60):

$$\mathrm{Tr}\Big((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2 N R_N\Big) \lesssim \sum_j \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\psi_j\|_{L^2}^2 \mathrm{Tr}\big(|\nabla|N\big) \lesssim \frac{1}{c(\lambda \mathrm{R}_g)^2} = o\big(\frac{\alpha}{\lambda^2 c R_g}\big).$$

With the same trick used before, we have:

$$\iint \frac{|\gamma'(x,y)|^2}{|x-y|}dxdy = \iint ((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}(x))^2 + (\xi^{\frac{1}{3}}(x))^2)\frac{|\gamma'(x,y)|^2}{|x-y|}((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})}(y))^2 + (\xi^{\frac{1}{3}}(y))^2)dxdy.$$

We use Kato's inequality as usual to get:

$$\begin{aligned}\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma'\|_{\mathrm{Ex}} \lesssim \||D_0|^{1/2}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma'\|_{\mathfrak{S}_2} &\leq \|[|D_0|^{1/2}, \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}]\tfrac{1}{|D_0|^{1/2}}\|_{\mathcal{B}}\||D_0|^{1/2}\gamma'\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma'\|_{\mathfrak{S}_2},\\ &\lesssim \frac{1}{c\sqrt{\lambda \mathrm{R}_g}}.\end{aligned}$$

Using trick (92), we get

$$\begin{aligned}\iint \frac{|\gamma'(x,y)|^2}{|x-y|}dxdy \quad &= \|\xi_1^{\frac{1}{3}}\gamma'\|_{\mathrm{Ex}}^2 + \|\xi_2^{\frac{1}{3}}\gamma'\|_{\mathrm{Ex}}^2 + 2\iint (\xi_1^{\frac{1}{3}}(x))^2\frac{|\gamma'(x,y)|^2}{|x-y|}(\xi_2^{\frac{1}{3}}(y))^2 dxdy\\ &+\mathcal{O}\Big(\frac{\|\gamma\|_{\mathfrak{S}_2}^2}{c\mathrm{R}_g} + \mathrm{Tr}\Big((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{3})})^2 N R_N\Big) + \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\frac{1}{12})}\gamma'\|_{\mathrm{Ex}}^2\Big).\end{aligned}$$

Now let us show that for $j = 1, 2$:

$$\|\xi_j^{\frac{1}{3}}\gamma'\|_{\mathrm{Ex}}^2 = \|\xi_j^{\frac{1}{3}}\cdot[\gamma']\|_{\mathrm{Ex}}^2 + \mathcal{O}\big(\frac{1}{(c\mathrm{R}_g)^2}\big). \tag{93}$$

It suffices to use Kato's inequality and Eq. (94), we have:

$$\begin{aligned}\||D_0|^{1/2}\xi^{+-}Q\|_{\mathfrak{S}_2} \quad &\leq \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega \Big\|\frac{|D_0|^{1/2}}{D_0+i\omega}\boldsymbol{\alpha}\cdot\nabla\xi\frac{1}{D_0+i\omega}Q\Big\|_{\mathfrak{S}_2}\\ &\lesssim \|\nabla(\xi_{c\lambda \mathrm{R}_g})\|_{L^\infty}\|Q\|_{\mathfrak{S}_2}\int_{-\infty}^{+\infty}\frac{d\omega}{E(\omega)^{3/2}} \lesssim \frac{\|Q\|_{\mathfrak{S}_2}}{c\lambda \mathrm{R}_g}.\end{aligned}$$

A Estimates

A.1 $[V, P_-^0]$ and proof of Proposition 1

For any smooth complex valued function V, there holds [6]:

$$[V, P_-^0] = -\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{D_0+i\eta}\boldsymbol{\alpha}\cdot\nabla V\frac{d\eta}{D_0+i\eta}. \tag{94}$$

Thanks to the KSS inequality as shown in [2], provided smoothness of V ($\nabla V \in L^p$) then this operator is $\mathfrak{S}_p(L^2(\mathfrak{R}^3, \mathfrak{C}^4))$ for $p > 3$.

The integral kernel of its Fourier transform [7] is:

$$\mathscr{F}\big([V, P_-^0]; p, q\big) = \frac{i}{2(2\pi)^{3/2}}\frac{1}{E(p)+E(q)}(\alpha_j\widehat{\partial_j V}(p-q) - \mathbf{s}_p\alpha_j\widehat{\partial_j V}(p-q)\mathbf{s}_q). \tag{95}$$

We prove Proposition 1 by duality, following [6]. Let V be in $\mathcal{S}(\mathbb{R}^3)$, $Q \in \mathfrak{S}_1^{P^0}$ (we recall that $2a[\Lambda] = 1 + \frac{1}{\log(\Lambda)}$), then

$$\begin{aligned}\mathrm{Tr}_0(QV) \quad &= \mathrm{Tr}(P_+^0 Q(P_+^0 + P_-^0)VP_+^0) + \mathrm{Tr}(P_-^0 Q(P_+^0 + P_-^0)VP_-^0).\end{aligned}$$

The operator $Q^{+-}|D_0|^{a[\Lambda]}\frac{1}{|D_0|^{a[\Lambda]}}[P_-^0, V]$ is in $\mathfrak{S}_1$: indeed thanks to (95) we have

$$\iint \frac{|\widehat{V}(p-q)|^2|p-q|^2 dpdq}{E(p)^{1+\frac{1}{\log(\Lambda)}}(E(p)+E(q))} \lesssim \log(\Lambda)\|\nabla V\|_{L^2}^2$$

showing $\|\frac{1}{|D_0|^{a[\Lambda]}}[P_-^0,V]\|_{\mathfrak{S}_2}\lesssim\sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}$. This also treats the case $Q^{-+}V^{+-}\in\mathfrak{S}_1$. Then we have $Q^{++}V^{++}=Q^{++}|D_0|^{a[\Lambda]}\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\in\mathfrak{S}_1$.

Indeed $|D_0|^{a[\Lambda]}Q^{++}|D_0|^{a[\Lambda]}\in\mathfrak{S}_1$ and $\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\in\mathfrak{S}_6$ with norm $\mathcal{O}((\log(\Lambda))^{1/6}\|\nabla V\|_{L^2})$. Then $\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\frac{1}{|D_0|^{a[\Lambda]}}\in\mathfrak{S}_6$ with norm $\mathcal{O}(\|\nabla V\|_{L^2})$. So:

$$\begin{aligned}\mathrm{Tr}(Q^{++}V^{++}) &= \mathrm{Tr}\big(\frac{|D_0|^{a[\Lambda]}}{|D_0|^{a[\Lambda]}}Q^{++}\frac{|D_0|^{a[\Lambda]}}{|D_0|^{a[\Lambda]}}V^{++}\big)\\ &= \mathrm{Tr}\big(\{|D_0|^{a[\Lambda]}Q^{++}|D_0|^{a[\Lambda]}\}\{\tfrac{1}{|D_0|^{a[\Lambda]}}\}V^{++}\tfrac{1}{|D_0|^{a[\Lambda]}}\big)\\ &= \mathcal{O}\big(\||D_0|^{a[\Lambda]}Q^{++}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1}\|\nabla V\|_{L^2}\big).\end{aligned}$$

The same holds for $Q^{--}V^{--}$. This ends the proof.

Remark 17. In Appendix D we do analogous estimates but with an additional localisation operator.

We adapt [2, Lemma 5]:

Lemma 10. *Let p be in $(3,+\infty]$ and V a smooth function with $\nabla V\in L^p$. Then for any $0<a<1$:*

$$[|D_0|^a,V]\tfrac{1}{|D_0|^a}\in\mathfrak{S}_p. \tag{96}$$

To prove it we use [17, p. 87]

$$\forall\, x>0,\ 0<a<1:\ x^a=\frac{\sin(a\pi)}{\pi}\int_0^{+\infty}\frac{ds}{s^{1-a}}\frac{x}{x+s}. \tag{97}$$

A.2 Proof of Lemma 6

Proof: Let us explain the bootstrap argument.

– We show that $\mathrm{Tr}((-\Delta)^{a+1}N)\lesssim 1$. As a consequence:

$$\begin{aligned}\||\nabla|^a n_j\|_{L^2} &\le \textstyle\sum_{\ell=0}^a K(\ell,a)\||\nabla|^\ell\mathscr{F}^{-1}(|\widehat{\psi}_j|)\|_{L^4}\||\nabla|^{a-\ell}\mathscr{F}^{-1}(|\widehat{\psi}_j)|\|_{L^4}\\ &\lesssim \textstyle\sum_{\ell=0}^a K(\ell,a)\||\nabla|^{\ell+3/4}\mathscr{F}^{-1}(|\widehat{\psi}_j|)\|_{L^2}\||\nabla|^{a-\ell+3/4}\mathscr{F}^{-1}(|\widehat{\psi}_j|)\|_{L^2}\\ &\lesssim K(a).\end{aligned}$$

– As shown in [20], (γ',ρ'_γ) is the fixed point of some function $F^{(1)}$ in a ball of $\widetilde{\mathcal{X}}_a$:

$$\widetilde{\mathcal{X}}_a=\{(Q,\rho)\in\mathfrak{S}_2\times\mathcal{S}':\iint E(p-q)^{2a}E(p+q)|\widehat{Q}(p,q)|^2<+\infty\text{ and }\int\frac{E(k)^a}{|k|^2}|\widehat{\rho}(k)|^2<+\infty\}.$$

– We multiply by $|D_0|^{(a+3)/2}$ the equation $D_0\psi_j=\mathcal{L}_\Lambda^{-1}(\mu_j\psi_j-\alpha B_{\gamma'}\psi_j)$ and we show that $\mathrm{Tr}((-\Delta)^{a+2}N)\lesssim 1$. We have to deal with $[|D_0|^{(a+3)/2},v]\psi_j$ and $[|D_0|^{(a+3)/2},R]\psi_j$: it suffices to compute in Fourier space and to use Taylor's formula on the function $E(\cdot)^{(a+3)/2}$.

Proof of the estimates Here as $\mathrm{Tr}(-\Delta N)\lesssim 1$, the fixed point method can be applied on $\widetilde{\mathcal{X}}_{a=1}$. Indeed $\|n\|_{L^2}\lesssim\||\nabla|^{3/2}\sqrt{n}\|_{L^2}\lesssim 1$. We get that

$$\iint|p-q|E(p+q)|\widehat{\gamma}(p,q)|^2dpdq\lesssim 1.$$

Let us show the assumption on the H^2-norm of ψ_j.

There holds $f(-i\nabla)\mathbf{D}\psi_j=f(-i\nabla)(\mu_j-\alpha B[\gamma])\psi_j$ for any $f\ge 0$. Taking the L^2-norm we have to deal with $[f(-i\nabla),R_{\gamma'}]$ and $[f(-i\nabla),v[\rho(\gamma')]]$. For $f(-i\nabla)=|\nabla|^{1/2}$ there holds

$$\begin{aligned}\|[|\nabla|^{1/2},v_\rho]\psi\|_{L^2}^2 &\lesssim\iint\frac{|\widehat{\rho}(p-q)|^2}{|p-q|^2}\frac{dpdq}{|q|^2E(q)^2}\int dqE(q)^2|q||\widehat{\psi}(q)|^2\\ \|[|\nabla|^{1/2},R_Q]\psi\|_{L^2}^2 &\lesssim\iint|p-q||\widehat{Q}(p,q)|^2dpdq\,\||\nabla|^{1/2}\psi\|_{L^2}^2\\ |\nabla|^{1/2}D_0\psi &=\mu\tfrac{|\nabla|^{1/2}}{\mathcal{L}_\Lambda}\psi-\alpha\tfrac{|\nabla|^{1/2}}{\mathcal{L}_\Lambda}B\psi=\mathcal{O}_{L^2}(1)\text{ a priori}\\ |\nabla|^{1/2}B\psi &=[|\nabla|^{1/2},B]\psi+B\tfrac{1}{|\nabla|^{1/2}}|\nabla|\psi\text{ and:}\end{aligned}$$

$\langle|\nabla|(1-\Delta)\psi_1\,,\,\psi_1\rangle - \langle|\nabla|\psi_1\,,\,\psi_1\rangle \lesssim \alpha c^{-1}\|v_2\psi_1 - v_{21}\psi_2\|_{L^2} + c^{-3} + \alpha^2 c^{-2} = \mathcal{O}(c^{-3} + \alpha c^{-1} a_{12})$.

We get $\mathrm{Tr}(|D_0|^3 N) \lesssim 1$ and by the fixed-point Theorem:

$$\|\gamma\|_{\mathbf{Q}}^2 = \iint E(p-q)^2 E(p+q) |\widehat{\gamma}(p,q)|^2 dpdq \lesssim 1.$$

Notation 9. The star in $\|\cdot\|_{\mathbf{Q}}^*$ means that we replace $E(p-q)^2 E(p+q)$ by $|p-q|^2|p+q|$.

Using the methods of [7, 21] we have:

$$\begin{cases} \|\gamma\|_{\mathbf{Q}}^* & \lesssim c^{-1/2}\|\rho'_\gamma\|_{L^2} + \alpha(\|\gamma'\|_{\mathbf{Q}}^*) + \alpha(\|\rho'_\gamma\|_{L^2} + \|\gamma'\|_{\mathbf{Q}}^*) \sum_{k=1}^{+\infty} \sqrt{k} (\alpha K(\|\rho'_\gamma\|_{\mathcal{C}} + \|\gamma'\|_{\mathbf{Q}_1}))^k, \\ \|[\nabla, \gamma]\|_{\mathfrak{S}_2} & \lesssim \alpha(\|\rho'_\gamma\|_{L^2} + \|N\|_{\mathbf{Q}}^*) + \alpha(\|\rho'_\gamma\|_{L^2} + \|\gamma'\|_{\mathbf{Q}}^*) \sum_{k=1}^{+\infty} \sqrt{k} (\alpha K(\|\rho'_\gamma\|_{\mathcal{C}} + \|\gamma'\|_{\mathbf{Q}_1}))^k, \\ \|\rho_\gamma\|_{L^2} & \lesssim L\|n\|_{L^2} + c^{-1/2}\|\gamma'\|_{\mathbf{Q}}^* + \alpha(\|\rho'_\gamma\|_{L^2} + \|\gamma'\|_{\mathbf{Q}}^*) \sum_{k=1}^{+\infty} \sqrt{k} (\alpha K(\|\rho'_\gamma\|_{\mathcal{C}} + \|\gamma'\|_{\mathbf{Q}_1}))^k. \end{cases}$$

Therefore

$\|\gamma'\|_{\mathbf{Q}}^* = \mathcal{O}(c^{-2})$, $\|[\nabla, \gamma]\|_{\mathfrak{S}_2} = \mathcal{O}(\alpha c^{-3/2})$ and $\|\rho_\gamma\|_{L^2} = \mathcal{O}(Lc^{-3/2} + c^{-2} + c^{-1}(\sqrt{\alpha a_{12}}))$.

For $f(-i\nabla) = \partial_k$ with $k = 1, 2, 3$ we have:

$$\begin{aligned} \partial_k R_Q \psi &= [\partial_k, R[Q]]\psi + R_Q \partial_k \psi \text{ and } \partial_k v\psi = (\partial_k v)\psi + v(\partial_k \psi) \\ \|[\partial_k, R_Q]\psi\|_{L^2} &= \|R([\partial_k, Q])\psi\|_{L^2} \leq \|[\partial_k, Q]\|_{\mathfrak{S}_2} \|\nabla\psi\|_{L^2} \text{ and } \|R_Q \partial_k \psi\|_{L^2} \leq \|Q\|_{\mathfrak{S}_2} \|\Delta\psi\|_{L^2} \\ \|v_\rho(\partial_k\psi)\|_{L^2} &\leq \|v_\rho\|_{L^6} \|\partial_k\psi\|_{L^3} \lesssim \|\rho\|_{\mathcal{C}} \||\nabla|^{3/2}\psi\|_{L^2} \leq \|\rho\|_{\mathcal{C}} \sqrt{\|\nabla\psi\|_{L^2} \|\Delta\psi\|_{L^2}} \\ \|(\partial_k v_\rho)\psi\|_{L^2}^2 &\lesssim \iint \frac{|\widehat{\rho}(k)|^2}{|k|^2} \frac{dkdq}{|q|^2(1+|q|^2)} [\|\nabla\psi\|_{L^2}^2 + \|\Delta\psi\|_{L^2}^2] \end{aligned}$$

$$\begin{aligned} \sum_{k=1}^{3} (\|\partial_k \mathbf{D}\psi\|_{L^2}^2) - \|\nabla\psi\|_{L^2}^2 &\leq (\mu^2 - 1)\|\nabla\psi\|_{L^2}^2 + 6\alpha\mu \|\nabla\psi\|_{L^2} \|B[\gamma']\psi\|_{L^2} + \alpha^2 \|\nabla B[\gamma']\psi\|_{L^2}^2 \\ \mathrm{Tr}(\Delta^2(1 - \tfrac{\Delta}{\Lambda^2} + \tfrac{\Delta^2}{\Lambda^4})N) &\lesssim \alpha a_{12} c^{-1} + c^{-3}. \end{aligned}$$

This gives $\|\Delta\psi_j\|_{L^2}^2 \lesssim \alpha c^{-2}$ and in particular:

$$\|c^2(1 - \mathcal{L}_{c\Lambda}^{-1})\underline{\psi_j}\|_{L^2} = \mathcal{O}\big(\frac{\sqrt{\alpha} c}{\Lambda^2}\big).$$

As a consequence we have:

$$\|\nabla \underline{\chi_j}\|_{L^2} = \|i\boldsymbol{\sigma} \cdot \nabla \underline{\chi_j}\|_{L^2} = \mathcal{O}(c^{-1}). \tag{98}$$

□

Thanks to those estimates, we get:

$$\mathcal{E}_{\mathrm{BDF}}(\gamma + N) = 2 + \frac{\mathcal{E}_{\mathrm{PT}}(\underline{\psi_1} \wedge \underline{\psi_2})}{2c^2} + \mathcal{O}(\alpha^2 c^{-3/2} + c^{-3}). \tag{99}$$

We recall that $1 - \mathcal{L}_\Lambda^{-1} = \frac{-\Delta}{\Lambda^2 - \Delta}$.

Thanks to Section B there holds

$$D(\underline{n}_1, \underline{n}_2) - D(\underline{\psi_1}^* \underline{\psi_2}, \underline{\psi_1}^* \underline{\psi_2}) \lesssim c^{-1} \text{ and } a_{12} \lesssim \alpha^{3/2} c^{-1}.$$

From this point we get better estimate on $\|\Delta\psi\|_{L^2}^2 \lesssim c^{-3}$ but this is still unsatisfactory. Let us be more precise about $\mu = \langle(\mathbf{D}+\alpha B)\psi\,,\,\psi\rangle$ and χ:

$$\begin{aligned}
(1+\mu_1)\chi_1 &= -i\sigma\cdot\nabla\phi_1 - \tfrac{\mu\Delta}{\Lambda^2-\Delta}\chi_1 + \tfrac{\alpha}{\mathcal{L}_\Lambda}(v_{\rho_\gamma}\chi_1 + (v_2\chi_1 - v_{21}\chi_2) - (R_\gamma\psi_1)_\downarrow)\\
&= \tfrac{1}{1+\mu}(-i\sigma\cdot\nabla\phi_1 + X_1^{(r)}) = \frac{-i\sigma\cdot\nabla}{2}\phi_1 + \mathcal{O}_{L^2}(c^{-2}/\Lambda + c^{-2})\\
\langle\mathbf{D}\psi\,,\,\psi\rangle &= \langle D_0\psi\,,\,\psi\rangle - \langle\tfrac{\Delta}{\Lambda^2}\beta\psi\,,\,\psi\rangle + \langle\tfrac{\Delta}{\Lambda^2} - i\boldsymbol{\alpha}\cdot\nabla\psi\,,\,\psi\rangle\\
&= 1 - 2\|\chi\|_{L^2}^2 + 2\mathfrak{Re}\langle -i\sigma\cdot\nabla\varphi\,,\,\chi\rangle + \mathcal{O}\big(\tfrac{\|\nabla\psi\|_{L^2}^2}{\Lambda^2} + \|\Delta\varphi\|_{L^2}\tfrac{\|\nabla\chi\|_{L^2}}{\Lambda^2}\big)\\
&= 1 + \tfrac{2}{1+\mu}\big(1-\tfrac{1}{1+\mu}\big)\|\nabla\varphi\|_{L^2}^2 + \mathfrak{Re}\tfrac{2}{1+\mu}\big(1-\tfrac{2}{1+\mu}\big)\mathfrak{Re}\langle -i\sigma\cdot\nabla\varphi\,,\,X^{(r)}\rangle + \mathcal{O}\big(\tfrac{1+\|\Delta\varphi\|_{L^2}}{c^2\Lambda^2}\big)\\
&= 1 + \tfrac{1}{2}\|\nabla\varphi\|_{L^2}^2 + \mathcal{O}(c^{-4} + c^{-2}\Lambda^{-2}(1+\|\Delta\varphi\|_{L^2})).
\end{aligned}$$

Then:

$$\begin{aligned}
\|\mathcal{L}_\Lambda^{-1}\psi\|_{L^2}^2 &= 1 + \mathcal{O}(c^{-2}\Lambda^{-2} + \|\Delta\psi\|_{L^2}^2/\Lambda^4)\\
\|\nabla\mathcal{L}_\Lambda^{-1}\psi\|_{L^2}^2 &= \|\nabla\psi\|_{L^2}^2 + \mathcal{O}(\|\Delta\psi\|_{L^2}/(c\Lambda^2) + \|\Delta\psi\|_{L^2}^2/\Lambda^2)\\
-2\alpha\mu\mathfrak{Re}\langle\tfrac{1-\Delta}{\mathcal{L}_\Lambda}B\psi\,,\,\psi\rangle &= -2\alpha\mu\langle B\psi\,,\,\psi\rangle + \mathcal{O}(\alpha\|B\psi\|_{L^2}\|\Delta\psi\|_{L^2}/\Lambda^2)\\
\|-i\boldsymbol{\alpha}\nabla B\psi\|_{L^2} &\lesssim \|[\nabla,B]\psi\|_{L^2} + \|B\nabla\psi\|_{L^2} = \mathcal{O}(c^{-3/2} + \|\Delta\psi\|_{L^2}^{1/2}c^{-1} + \|\Delta\psi\|_{L^2}c^{-1/2}).
\end{aligned}$$

and thus:

$$\begin{aligned}
\langle(1-\Delta)\psi\,,\,(1-\Delta)\psi\rangle &= \mu^2\langle\tfrac{1-\Delta}{\mathcal{L}_\Lambda^2}\psi\,,\,\psi\rangle - 2\alpha\mu\mathfrak{Re}\langle\tfrac{1-\Delta}{\mathcal{L}_\Lambda}B\psi\,,\,\psi\rangle + \|\tfrac{D_0}{\mathcal{L}_\Lambda}B\psi\|_{L^2}^2\\
&= 1 + 2(\mu - 1 - \alpha\langle B\psi\,,\,\psi\rangle) + \|\nabla\psi\|_{L^2}^2\\
&\quad + \mathcal{O}(c^{-2}(c^{-2}+\Lambda^{-2}) + \tfrac{\|\Delta\psi\|_{L^2}}{c^2\Lambda^2} + \|\Delta\psi\|_{L^2}^2(\Lambda^{-2} + \alpha^2c^{-1})).
\end{aligned}$$

From (62) and the expression of $D_0\psi_j$, we have $\|\nabla\psi_j\|_{L^2}^2 = -2\alpha\mathfrak{Re}\langle B\psi_j\,,\,\psi_j\rangle$. We conclude $\|\Delta\psi\|_{L^2}^2 \lesssim c^{-2}(c^{-2}+\Lambda^{-2})$ and

$$\|\Delta\psi\|_{L^2}^2 \lesssim \min\big(c^{-3}, c^{-2}(c^{-2}+\Lambda^{-2}\big).$$

B Proofs of Section 3

B.1 Proof of Proposition 3

Reductio ad absurdum.

We assume this is false and take a non-increasing sequence $(a_j)_{j\geq 0}$ tending to 0 such that there exists Ψ_j that does not satisfy (38) with $\mathrm{b} = a_j$: $\Delta_2\mathcal{E} < a_j$ and $\frac{\Delta_2\mathcal{E}}{d_\Psi} < a_j$. In particular $(\Psi_j)_j$ is a minimizing sequence for $E_{\mathrm{PT}}(2)$. By geometrical methods [12] we see that Ψ_j can be decomposed in two pieces of mass one, each piece tending to a minimizer for $E_{\mathrm{PT}}(1)$. Indeed it is clear that $(\mathrm{Tr}(-\Delta\gamma_{\Psi_j}))_j$ is bounded and that there is no vanishing for $(\rho_{\Psi_j})_{j\geq 0}$. If we follow a bubble [13] of ρ_{Ψ_j} (one of the biggest) let us show its mass is 1 at the limit.
By scaling, for any $0<\lambda<1$ we have $E_{\mathrm{PT}}(\lambda) \geq \lambda^3 E_{\mathrm{PT}}(1)$, where $E_{\mathrm{PT}}(\lambda)$ is defined as the infimum of $\mathcal{E}_{\mathrm{PT}}$ over non-negative one-body density matrix whose trace is λ.

Up to following a bubble and extracting a subsequence there holds with $\Psi_j = h_{1,j}\wedge h_{2,j}$:

$$|h_{1,j}\wedge h_{2,j}\rangle\langle h_{1,j}\wedge h_{2,j}| \rightharpoonup_g G_{00}\oplus G_{11}\oplus G_{22},\ \sum_{j=0}^{2}\mathrm{Tr}(G_{jj}) = 1 \text{ and } \mathrm{Tr}(G_{00}) < 1.$$

We recall that each G_{jj} is a density matrix in $(L^2)^{\wedge(j)}$. Following [12, part 5]: $G_{jj} = \mathrm{Tr}(G_{jj})\widetilde{G}_{jj}$

$$\begin{aligned}
\liminf_{j\to+\infty}\mathcal{E}_{\mathrm{PT}}^U(\Psi_j) &= E_{\mathrm{PT}}^U(2) \geq \sum_{j=0}^{2}(\mathcal{E}_{\mathrm{PT}}^U(G_{jj}) + \mathrm{Tr}(G_{jj})E_{\mathrm{PT}}^U(2-j))\\
&\geq \sum_{j=0}^{2}\mathrm{Tr}(G_{jj})(\mathcal{E}_{\mathrm{PT}}^U(\widetilde{G}_{jj}) + E_{\mathrm{PT}}^U(2-j)) \geq E_{\mathrm{PT}}^U(2).
\end{aligned}$$

As not all particles are lost (we follow a bubble) either $G_{11} \neq 0$ or $G_{22} \neq 0$. In the case $G_{2,2} \neq 0$, [5] enables us to say $\mathcal{E}^U_{\rm PT}(\widetilde{G}_{22}) > E_{\rm PT}(2)$. So $G_{22} = 0$ and $G_{11} \neq 0$. Thanks to [15] and Lieb's variational principle (we may assume $G_{11} = \mathrm{Tr}(G_{11})|\phi\rangle\langle\phi|$) there holds

$$\mathcal{E}_{\rm PT}(G_{11}) \geq (\mathrm{Tr}(G_{11}))^3 E_{\rm PT}(1),$$

then necessarily $\mathrm{Tr}(G_{11}) = 1$.

As a consequence there is exactly two bubbles in $(\rho_{\Psi_j})_j$, there exist a decomposition $\Psi_j = \underline{h_{1,j}} \wedge \underline{h_{2,j}}$ and a sequence $(z_{1,j}; z_{2,j})_j$ of $(\mathbb{R}^3)^2$ such that (up to extraction)

1. $\langle \underline{h_{k,j}}, \underline{h_{\ell,j}} \rangle = \delta_{k\ell}$ and $|z_{1,j} - z_{2,j}| \underset{j\to\infty}{\to} +\infty$,
2. $\underline{h_{k,j}}(\cdot - z_{k,j}) \overset{H^1}{\underset{j\to\infty}{\to}} \phi_{j,\infty}$ where $\phi_{j,\infty} \in \mathscr{P}$ is radial.

Then it suffices to compute: $\mathcal{E}^U_{\rm PT}(\Psi_j)$ with this decomposition:

$$\begin{aligned}\mathcal{E}^U_{\rm PT}(\Psi_j) &= \mathcal{E}^U_{\rm PT}(\underline{h_{1,j}}) + \mathcal{E}^U_{\rm PT}(\underline{h_{2,j}}) - D(|\underline{h_{1,j}}|^2, |\underline{h_{2,j}}|^2) + \tfrac{U}{2} \iint |\underline{h_{1,j}} \wedge \underline{h_{2,j}}(x,y)|^2 \frac{dxdy}{|x-y|} \\ &= \mathcal{E}_1 + \mathcal{E}_2 + \tfrac{U}{2} W_{12} - \underline{D_{12}} \geq \tfrac{U}{4} W_{12} + 2E_{\rm PT}(1).\end{aligned}$$

The last equality holds because we have $U > 2\mathrm{U}_c$. Let us write

$$\Delta_1\mathcal{E} := \mathcal{E}_{\rm PT}(\underline{h_{1,j}}) + \mathcal{E}_{\rm PT}(\underline{h_{2,j}}) - 2E_{\rm PT}(1).$$

Then:

$$-a_j < \Delta_1\mathcal{E} - \underline{D_{12}} < a_j \text{ and } \Delta_1\mathcal{E} \geq \kappa \sum_{k=1}^{2} \|\underline{h_{k,j}} - \phi_{k,j}\|^2_{H^1}$$

where $\phi_{k,j} \in \mathscr{P}$ is the closest function to $\underline{h_{k,j}}$ in H^1 (Proposition 2). We may assume that $\underline{D_{12}} = d_{\Psi_j}$ because minimizing this quantity corresponds to minimizing $\Delta_1\mathcal{E}$. In particular:

$$|\Delta_1\mathcal{E} - \underline{D_{12}}| < a_j = \underset{j\to+\infty}{o}(\underline{D_{12}}) \;\Rightarrow\; \Delta_1\mathcal{E} \underset{j\to+\infty}{\sim} \underline{D_{12}} \gg a_j.$$

Indeed, let us say that $\underline{D_{12}} > d_{\Psi_j}$, then $(\underline{f_{k,j}}(\cdot - z_k))_j$ still converges to $\phi_{j,\infty}$, in particular $(\Delta_1\mathcal{E})_j$ converges to 0. But if $(\underline{f'_{1,j}}, \underline{f'_{2,j}})_j$ is a decomposition with $\underline{D'_{12}} = d_{\Psi_j}$, then $\Delta'_1\mathcal{E} \leq \Delta_1\mathcal{E}$ and

$$\mathrm{dist}(\underline{f'_{k,j}}, \mathscr{P}) \underset{j\to+\infty}{\to} 0.$$

From now we will drop the subscript j for convenience and suppose $\underline{D_{12}} = d_{\Psi_j}$.

Notation 10. We introduce $\underline{h_k} = (\underline{h_k} - \phi_k) + \phi_k = \delta_k - \phi_k$ in $|\underline{h_k}|^2$ and in $\underline{h_1}^* \underline{h_2}$. We use the convention

$$\|\delta\|_{L^2} := \|\delta_1\|_{L^2} + \|\delta_2\|_{L^2},\ \|\delta\|_{H^1} := \|\delta_1\|_{H^1} + \|\delta_2\|_{H^1}.$$

We recall that an element of $\mathscr{P}$ has an exponential falloff with respect to its center. For some constant $\overline{\varepsilon} > 0$, there holds:

$$\begin{aligned}|\underline{h_k}|^2 &= |\delta_k|^2 + |\phi_k|^2 + 2\mathfrak{Re}(\delta_k^*\phi_k) \\ \underline{h_1}^* \underline{h_2}^* &= \delta_1^*\delta_2 + \phi_1^*\phi_2 + \delta_1^*\phi_2 + \phi_1^*\delta_2 \\ \|\underline{h_1}^* \underline{h_2}\|^2_{\mathcal{C}} &= \|\delta_1^*\phi_2\|^2_{\mathcal{C}} + \|\phi_1^*\delta_2\|^2_{\mathcal{C}} + \mathcal{O}\big((\|\delta_1\|_{L^2}\|\delta_2\|_{L^2})(\mathrm{R}_g^{-1} + \|\delta\|_{L^2}(1 + \|\nabla\delta\|_{L^2}) + e^{-\overline{\varepsilon}\mathrm{R}_g})\big) \\ \underline{D_{12}} &= D(|\phi_1|^2, |\phi_2|^2) + D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2) \\ &\quad + \mathcal{O}\big(\tfrac{\|\delta\|_{L^2}}{\mathrm{R}_g} + \|\delta_1\|_{L^2}\|\delta_2\|_{L^2}(\|\delta\|_{L^2}(1 + \|\nabla\delta\|_{L^2}) + e^{-\overline{\varepsilon}\mathrm{R}_g})\big)\end{aligned}$$

$$\text{Thus:}\quad a_j U^{-1} \gtrsim \underline{D_{12}} - \|\underline{h_1}^* \underline{h_2}\|^2_{\mathcal{C}} \gtrsim \frac{1}{\mathrm{R}_g} + \underset{j\to+\infty}{\mathcal{O}}(\|\delta\|^3_{L^2})$$

$$\text{and}\quad \tfrac{1}{\mathrm{R}_g} = \underset{j\to+\infty}{\mathcal{O}}(a_j U^{-1} + \|\delta\|^3_{L^2}).$$

As $j \to +\infty$, thanks to the coercivity inequality (2) there holds

$$\underline{D_{12}} \sim \Delta_1 \mathcal{E} = \Theta(\|\delta_1\|_{H^1}^2 + \|\delta_2\|_{H^1}^2) \text{ and } \frac{1}{\mathrm{R}_g} = \underset{j\to+\infty}{o}(\underline{D_{12}}).$$

Studying more precisely $M^2(\underline{h_1} \wedge \underline{h_2}) := \iint |\underline{h_1} \wedge \underline{h_2}(x,y)|^2 \frac{dxdy}{|x-y|}$:

$$\begin{aligned} M^2(\underline{h_1} \wedge \underline{h_2}) &= M^2(\delta_1 \wedge \phi_2) + M^2(\phi_1 \wedge \delta_2) + \underset{j\to+\infty}{\mathcal{O}}(\mathrm{R}_g^{-1} + \|\delta\|_{L^2}^3) = \underset{j\to+\infty}{o}(\underline{D_{12}}) \\ \underline{D_{12}} &= D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2) + \underset{j\to+\infty}{o}(\underline{D_{12}}) \gtrsim \|\delta_1\|_{H^1}^2 + \|\delta_2\|_{H^1}^2. \end{aligned} \tag{100}$$

We can easily exclude the case $\delta_1, \delta_2 = 0$ for then it is clear $M^2(\phi_1 \wedge \phi_2) \gtrsim D(|\phi_1|^2, |\phi_2|^2)$ thanks to $\langle \phi_1 \, , \, \phi_2 \rangle = 0$. Say then that $\|\delta_1\|_{H^1} \geq \|\delta_2\|_{H^1}$: $\delta_1 \neq 0$. The case $\delta_2 = 0$ and $\delta_1 \neq 0$ is an easy adaptation of what follows, we treat it later. As there holds

$$|\phi_2|^2 * \tfrac{1}{|\cdot|}(x) \leq \tfrac{1}{|x - z_2|}$$

where z_2 is the center of ϕ_2, Estimate (100) is true only if there lies a mass of δ_1 near z_2: the quantity $\|\delta_1^* \phi_2\|_{\mathcal{C}}^2$ must compensate $D(|\delta_1|^2, |\phi_2|^2)$. Eventually the same phenomena occurs for δ_2 around z_1 the center of ϕ_1. Up to extraction:

$$\frac{\delta_k(\cdot - z_k)}{\|\delta_k\|_{H^1}} \rightharpoonup_{H^1} \ell_k,$$

and $(\ell_1, \ell_2) \neq (0,0)$. Indeed up to contraction there is convergence in L^2_{loc} and if $\ell_k = 0$ then for all $r > 0$ and $(i_1, i_2) \in \big\{(1,2),(2,1)\big\}$

$$\limsup_{j\to+\infty} \int \frac{|\delta_{i_1}(x)|^2}{\|\delta_{i_1}\|_{H^1}^2} |\phi_{i_2}|^2 * \frac{1}{|\cdot|}(x)dx \leq \frac{1}{r} + \limsup_{j\to+\infty} \int_{|x - z_{i_2}| \leq r} \frac{|\delta_{i_1}(x)|^2}{\|\delta_{i_1}\|_{H^1}^2} |\phi_2|^2 * \frac{1}{|\cdot|}(x)dx = \frac{1}{r},$$

this would contradict (100). Then as we have:

$$\lim_{j\to+\infty} M^2\big(\frac{\delta_1}{\|\delta_1\|_{H^1}} \wedge \phi_2\big) = \lim_{j\to+\infty} \frac{1}{\underline{D_{12}}} M^2\big(\delta_1 \wedge \phi_2\big) = 0,$$

then necessarily $\ell_1 = \varepsilon_1 \phi_{2,\infty}$ with $|\varepsilon_1| \leq 1$. Furthermore, either $\|\delta_2\|_{H^1} = \underset{j\to+\infty}{o}(\|\delta_1\|_{H^1})$ or $\|\delta_2\|_{H^1} = \underset{j\to+\infty}{\Theta}(\|\delta_1\|_{H^1})$.

– In the first case then $\|\delta_2\|_{H^1}^2 = \underset{j\to+\infty}{o}(\underline{D_{12}})$ and $\ell_1 \neq 0$. We get a contradiction by computing:

$$\begin{aligned} 0 = \int \underline{h_1}^* \underline{h_2} &= \int \phi_1^* \phi_2 + \int \delta_1^* \phi_2 + \int \phi_1^* \delta_2 + \int \delta_1^* \delta_2 \\ &= \underset{j\to+\infty}{\mathcal{O}}(e^{-\overline{\varepsilon}\mathrm{R}_g}) + \int \delta_1^* \phi_2 + \underset{j\to+\infty}{\mathcal{O}}(\|\delta_2\|_{L^2}(1 + \|\delta_1\|_{L^2})) \\ &= \int \delta_1^* \phi_2 + \underset{j\to+\infty}{o}(\|\delta_1\|_{H^1}). \end{aligned}$$

– In the second case we also get $\lim_{j\to+\infty} \|\delta_2\|_{H^1}^{-2} M^2(\delta_2 \wedge \phi_1)$ and $\ell_2 = \varepsilon_2 \phi_{1,\infty}$, $|\varepsilon_2| \leq 1$. Writing for $k \neq k'$: $\underline{h_k} = \phi_k + \varepsilon_k \|\delta_k\|_{H^1} \phi_{k'} + h_k^{(r)}$, up to extraction the following holds:

$$\begin{aligned} 0 = \int \underline{h_1}^* \underline{h_2} &= \underset{j\to+\infty}{\mathcal{O}}(e^{-\overline{\varepsilon}\mathrm{R}_g}) + \varepsilon_1^* \|\delta_1\|_{H^1} + \varepsilon_2 \|\delta_2\|_{H^1} + \int (h_1^{(r)})^* \underline{h_2} + \int \underline{h_1}^* h_2^{(r)} \\ \int (h_1^{(r)})^* \underline{h_2} &= \int (h_1^{(r)})^* \phi_2 + \int (h_1^{(r)})^* (\varepsilon_1 \|\delta_1\|_{H^1} \phi_1) + \int (h_1^{(r)})^* h_2^{(r)} \\ &= \underset{j\to+\infty}{o}(\|\delta_1\|_{H^1}) + \underset{j\to+\infty}{\mathcal{O}}(\|\delta_1\|_{H^1}^2) + \underset{j\to+\infty}{\mathcal{O}}(\|\delta_1\|_{H^1} \|\delta_2\|_{H^1}). \end{aligned}$$

The $\underset{j\to+\infty}{o}(\|\delta_1\|_{H^1})$ comes from the L^2_{loc}-convergence to 0 of $\frac{h_1^{(r)}(\cdot - z_2)}{\|\delta_1\|_{H^1}}$ and the uniform shape of the $\phi_2(\cdot - z_2)$'s. In particular:

$$\varepsilon_1^* \|\delta_2\|_{H^1} = -\varepsilon_2 \|\delta_1\|_{H^1} + \underset{j\to+\infty}{o}(\|\delta\|_{H^1}).$$

Writing $\varepsilon_1\|\delta_1\|_{H^1} = a$ and $\varepsilon_2\|\delta_2\|_{H^2} = b = -a^* + (\delta a)$:

$$\left\{\begin{array}{ll|ll} \underline{h_1} & = \phi_1 + a\phi_2 + h_1^{(r)} & h_1^{(r)} & = \delta_1 - a\phi_2 \\ \underline{h_2} & = \phi_2 - a^*\phi_1 + (\delta a)\phi_1 + h_2^{(r)} & h_2^{(r)} & = \delta_2 - b\phi_2. \end{array}\right.$$

We apply $\begin{pmatrix} \sqrt{1-|a|^2} & a^* \\ -a & \sqrt{1-|a|^2} \end{pmatrix}$ with $\sqrt{1-|a|^2} =: s$

$$\begin{pmatrix} \underline{g_1} \\ \underline{g_2} \end{pmatrix} = \begin{pmatrix} \phi_1(s+|a|^2 - a(\delta a)) + \phi_2(a(s-1)) + sh_1^{(r)} - ah_2^{(r)} \\ \phi_2(s+|a|^2) + \phi_1(a^*(1-s) + (\delta a)s) + sh_2^{(r)} + a^*h_1^{(r)} \end{pmatrix},$$

replacing $s = 1 - \frac{|a|^2}{2} + \underset{j\to+\infty}{\mathcal{O}}(|a|^4)$ and neglecting the term $\mathcal{O}_{H^1}(|a|^3)$:

$$\begin{pmatrix} \underline{g_1} \\ \underline{g_2} \end{pmatrix} = \begin{pmatrix} \phi_1(1 + \frac{|a|^2}{2} - a(\delta a)) + h_1^{(r)} - ah_2^{(r)} + \mathcal{O}_{H^1}(|a|^3) \\ (1+\frac{|a|^2}{2})\phi_2 + \phi_1((\delta a)(1-\frac{|a|^2}{2})) + h_2^{(r)} + a^*h_1^{(r)} + \mathcal{O}_{H^1}(|a|^3) \end{pmatrix}.$$

By $L^2_{\rm loc}$-convergence, it is clear that $D(|\phi_k|^2, |h_{k'}^{(r)}|^2) = \underset{j\to+\infty}{o}(\|\delta_{k'}\|_{H^1}^2)$ for (k,k') equal to $(1,2)$ or $(2,1)$. Using $\delta a = \underset{j\to+\infty}{o}(\|\delta\|_{H^1})$, at last we have:

$$D(|\underline{g_1}|^2, |\underline{g}_2|^2) \lesssim D(|\phi_1|^2, |\phi_2|^2) + \underset{j\to+\infty}{o}(\|\delta\|_{H^1}^2) = \underset{j\to+\infty}{o}(\|\delta\|_{H^1}^2) = \underset{j\to+\infty}{o}(\underline{D_{12}} = d_\Psi),$$

which gives the desired contradiction.
– Let us treat at last the case $\delta_1 \neq 0$ and $\delta_2 = 0$. Then as before:

$$D(|\underline{h_1}|^2, |\phi_2|^2) \quad = D(|\delta_1|^2, |\phi_2|^2) + \mathcal{O}\big(\tfrac{1+\|\delta_1\|_{L^2}}{\mathrm{R}_g}\big) = D(|\delta_1|^2, |\phi_2|^2) + \underset{j\to+\infty}{o}(\underline{D_{12}}).$$

Then necessarily there lies some mass of δ_1 near z_2 and:

$$\frac{\delta_1(\cdot - z_2)}{\|\delta_1\|_{H^1}} \rightharpoonup_{H^1} \ell_1 \neq 0.$$

As before necessarily: $\ell_1 = \varepsilon_1\phi_{2,\infty}$ with $0 < |\varepsilon_1| \leq 1$. But this contradicts:

$$0 = \int \underline{h_1}^*\phi_2 = \int \delta_1^*\phi_2 + \int \phi_1^*\phi_2 = \int \delta_1^*\phi_2 + \underset{j\to+\infty}{\mathcal{O}}(e^{-\overline{\varepsilon}\mathrm{R}_g}).$$

B.2 Proof of Proposition 4

The proof is similar to that of Proposition 3: by contradiction we assume the existence of $(a_j)_j$ decreasing to 0 together with $(\Psi_j = h_1 \wedge h_2)$ with $\mathcal{E}^U_{\rm PT}(\Psi_j) < a_j$ and $M^2(\Psi_j) < a_j R_{{\rm g};j}$. We re-use the same notations of the previous Subsection.

Thanks to Proposition 5 we know that d_{Ψ_j} is bounded from below by

$$(1 - \kappa\sqrt{a_0'})\big\{D(|\phi_1|^2, |\phi_2|^2) + D(|\delta_1|^2, |\phi_2|^2) + D(|\phi_1|^2, |\delta_2|^2)\big\} + D(|\delta_1|^2, |\delta_2|^2)$$

As $(h_{k;j}(\cdot - z_{k;j}))_j$ tends to $\phi_{k,\infty} \in \mathscr{P}$ in H^1 for $k = 1, 2$, then for any $A > 0$:

$$\lim_{j\to+\infty} \int_{B(z_{k,j},A)} |h_{k,j}(x)|^2 dx = \int_{B(z_{k,j},A)} |\phi_{k,\infty}(x)|^2 dx.$$

For any $2^{-1/2} < \lambda < 1$ let $A_\lambda > 0$ be the number such that the last integral with $A = A_\lambda$ is equal to λ. We have:

$$\iint\limits_{|x-y|<\mathrm{R}_g+2A_\lambda} \frac{|h_1 \wedge h_2(x,y)|^2}{|x-y|} dxdy \geq \frac{2}{\mathrm{R}_g + 2A_\lambda} \iint\limits_{|x-y|<\mathrm{R}_g+2A_\lambda} |h_1(x)|^2|h_2(y)|^2 dxdy$$
$$- \frac{2}{\mathrm{R}_g + 2A_\lambda} \int dx h_1^* h_2(x) \int\limits_{y\in B(x,\mathrm{R}_g+2A_\lambda)} h_2^* h_1(y) dy$$

$$\liminf_{j\to+\infty} \iint\limits_{|x-y|<\mathrm{R}_g+2A_\lambda} \frac{|h_1 \wedge h_2(x,y)|^2}{|x-y|} dxdy \geq \tfrac{2}{\mathrm{R}_g+2A_\lambda}(\lambda^2 - 2^{-1}).$$

We used the following trick: if $\int h_1^* h_2 = 0$ where $\|h_k\|_{L^2} = 1$, then for any Borelian set B:

$$\Big| \int_B h_1^* h_2 \Big| \leq \frac{1}{2}.$$

The more precise result has the same proof: in the limit there holds similar inequality: for sufficiently small $a > 0$, $\lambda \mathrm{R}_g > A_\varepsilon$ where

$$\int_{|x| \leq A_\varepsilon} |\phi(x)|^2 dx = \varepsilon, \ \varepsilon > 2^{-1/2}, \ \phi \in \mathscr{P}_0.$$

We conclude with the same argument.

C Localisation in Direct space: the $\underline{\psi_j}$'s

C.1 Proof of Lemma 7

Notation 11. For convenience here we write $V \cdot \underline{\varphi_k} := \underline{v'_\gamma \varphi_k} - R_{\underline{N}} \underline{\varphi_k}$ (and a similar expression for $\underline{\chi_k}$). The function $r_k := R_\gamma \underline{\psi_k}$ is split into its upper part $r_{k,\uparrow} := (R_\gamma \underline{\psi_k})_\uparrow$ and its lower part $r_{k,\downarrow}$ both in $L^2(\mathbb{R}^3, \mathbb{C}^2)$.

Moreover we write:

$$P_k(-\Delta) := c^2(1 - \mu_k^2 \mathcal{L}_{c\Lambda}^{-2}) - \Delta \text{ and } y_c := \mathcal{L}_{c\Lambda}^{-1} = \frac{c^2\Lambda^2}{c^2\Lambda^2 - \Delta}.$$

The operator $P_k(-\Delta)$ can be rewritten as follows: with $a_k := c^2(1 - \mu_k)$ and $b := c\Lambda$ then

$$\begin{aligned} c^2(1 - \mu_k y_c^2) - \Delta &= a_k(1 + \mu_k) - \Delta \Big[1 + \tfrac{\mu_k c^2 - a_k}{c^2\Lambda^2} \tfrac{b^2}{b^2 - \Delta} + \tfrac{\mu_k^2}{\Lambda^2} \Big(\tfrac{b^2}{b^2 - \Delta^2} \Big)^2 \Big] \\ &= (a_k(1 + \mu_k) - \Delta) \Big\{ 1 + \big(1 - \tfrac{a_k(1+\mu_k)}{a_k(1+\mu_k) - \Delta} \big) \Big[\tfrac{\mu_k c^2 - a_k}{c^2\Lambda^2} \tfrac{b^2}{b^2 - \Delta} + \tfrac{\mu_k^2}{\Lambda^2} \Big(\tfrac{b^2}{b^2 - \Delta^2} \Big)^2 \Big] \Big\} \end{aligned} \tag{101}$$

Proof We remark that $\underline{n}(x) = |h_1(x)|^2 + |h_2(x)|^2 = |\underline{\psi_1}(x)|^2 + |\underline{\psi_2}(y)|^2$.

Thanks to (47)-(48), there holds:

$$(\mathbf{D} + \alpha B)\psi_k = (1 + \tfrac{3E_{\mathrm{PT}(1)}}{2c^2} + \mathcal{O}(\alpha^{1/4} c^{-2}))\psi_k. \tag{102}$$

Up to applying some $\mathbf{m} \in \mathbf{SU}(2)$ to $\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$, we consider $\underline{\psi_k} = h_k$ with the following:

$$(c^2\beta - ic\boldsymbol{\alpha} \cdot \nabla h_k) + \alpha c y_c (V \cdot h_k - R_{\underline{\gamma}} h_k) = (c^2 - \tfrac{3E_{\mathrm{PT}}(1)}{2}) y_c h_k + \mathcal{O}(\alpha^{1/4} y_c h)$$

We write $a = -\frac{3E_{\mathrm{PT}}(1)}{2}$ and the additional term $\mathcal{O}(\alpha^{1/4} y_c h) = \delta_k h$.

– We now rewrite (73) once again: by substitution, we get:

$$\begin{cases} \underline{\varphi_k} &= \alpha c y_c \dfrac{1 + \mu_k y_c}{P_k(-\Delta)} (V \cdot \underline{\varphi_k} - r_{k,\uparrow}) + \dfrac{\alpha y_c}{P_k(-\Delta)} i\sigma \cdot \nabla \big[V \cdot \underline{\chi_k} - r_{k,\downarrow} \big] \\ \underline{\chi_k} &= \alpha \dfrac{y_c}{P_k(-\Delta)} i\sigma \cdot \nabla (V \cdot \underline{\varphi_k} - r_{k,\uparrow}) + \alpha y_c \dfrac{c^2(1 - \mu_k y_c)}{c P_k(-\Delta)} \big[V \cdot \underline{\chi_k} - r_{k,\downarrow} \big] \end{cases} \tag{103}$$

There holds similar equation for h_k but with additional terms $\frac{1}{\alpha c}(\delta_k h)_\uparrow$ with $-r_{k,\uparrow}$ and $\frac{1}{\alpha c}(\delta_k h)_\downarrow$ with $-r_{k,\downarrow}$.

There holds:

$$\alpha c(1 - \mu_k y_c) = \alpha c(1 - \mu_k) + \alpha c \mu_k (1 - y_c).$$

For any $A \geq \Gamma(\mathrm{R}_g)\mathrm{R}_g$, we multiply each term by $|D_0|^{1/2}$ and then by $d_{A,\lambda}(\cdot)$ defined by $d(\cdot)\xi_A(\cdot)\boldsymbol{\eta}^\lambda_{\mathrm{R}_g}$.

We take the L^2-norm, let us show estimates *independent* of A (but depending on ξ_1):

$$\|d_{A,\lambda}|D_0|^{1/2}\underline{\psi_k}\|_{L^2} \leq K_\lambda + \varepsilon_{(\lambda)}\|E^{1/2}_{A,\lambda}|D_0|^{1/2}\underline{\psi_k}\|_{L^2}, \text{ with } \varepsilon_{(\lambda)} < 1.$$

This will end the proof, the family $(K_\lambda)_\lambda$ depending on $(\varepsilon_{(\lambda)})_\lambda$ and the latter being nonincreasing in $\lambda \in (\lambda_0, 2^{-1})$.

We prove the estimation of $\|d^{(2)}_{A,\lambda}|D_0|^{1/2}\underline{\psi_j}\|_{L^2}$ with $j = 1, 2$ by the same method: we need finiteness of $\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g}|D_0|^{1/2}\underline{\psi_k}\|_{L^2}$ with $k = 1, 2$ and of $\||x-y|\gamma\|_{\mathfrak{S}_2}$. We refer to Appendix C for more details.

– In Appendix C, we show:

$$|d_{A,\lambda}(x) - d_{A,\lambda}(y)| \lesssim |x-y|. \tag{104}$$

Let us first multiply (103) by $|D_0|^{1/2}$: let $\mathcal{F}_{j,k} := \frac{|D_0|^{1/2}\partial_j}{P_k(-\Delta)}$ and $\mathcal{F}_{0,k} := \frac{|D_0|^{1/2}}{P_k(-\Delta)}$. It is clear that they are bounded (convolution) operators, we show in Appendix C that

$$\||\cdot|\mathcal{F}_{j,k}\|_{L^1} \lesssim 1,\ j \in \{1,2,3\},\ k \in \{1,2\}. \tag{105}$$

The function associated to y_c is a Yukawa potential Y_c [16, Section 6.23]:

$$Y_c(x-y) = \sqrt{\frac{\pi}{2}}\frac{(c\Lambda)^2 e^{-c\Lambda|x-y|}}{|x-y|},$$

in particular $\||\cdot|Y_c\|_{L^1} \lesssim \frac{1}{c\Lambda}$. The idea is to take first the commutator $[d_{A,\lambda}, \mathcal{F}_{j,k}]$ and $[d_{A,\lambda}, y_c]$. Then we study $d_{A,\lambda}v\underline{\varpi_k}$ ($\varpi_k \in \{\varphi_k, \chi_k\}$) and $d_{A,\lambda}r_{\uparrow/\downarrow}$.

Estimate of $\alpha c\|V\cdot\underline{\varphi_k}\|_{L^2}, \alpha c\|V\cdot\underline{\chi_k}\|_{L^2}$ We use the same method for both cases. We recall the following:

$$v_{\underline{\gamma}} = \big(-\underline{\check{F}_\Lambda} * \underline{n} + (\delta_0 - \underline{\check{F}_\Lambda}) * (\mathfrak{t}_{\underline{N}} - \alpha^2\underline{\widetilde{\tau_2}})\big) * \frac{1}{|\cdot|} = -\underline{\check{F}_\Lambda} * \underline{n} * \frac{1}{|\cdot|} + \underline{\rho_{rem}} * \frac{1}{|\cdot|}.$$

By (58):

$$\begin{aligned}\big|\alpha c\underline{\check{F}_\Lambda} * \underline{n} * \tfrac{1}{|\cdot|}\big|(x) &\leq \underline{n} * \tfrac{1}{|\cdot|}(x) + \alpha c\big|(\underline{\check{F}_\Lambda} - F_\Lambda(0)\delta_0) * v_{\underline{n}}(x)\big| \\ &\leq \underline{n} * \tfrac{1}{|\cdot|}(x) + \mathcal{O}\big(\tfrac{1}{\sqrt{c}}\big).\end{aligned}$$

We used $\|f\|_{L^\infty} \lesssim \|\widehat{f}\|_{L^1}$, split the integral in Fourier space at level $2c$ and used Cauchy-Schwarz inequality. By Appendix A.2 and Proposition 5:

$$\begin{aligned}\big|\alpha c\underline{\rho_{rem}} * \tfrac{1}{|\cdot|}\big|(x) &\lesssim \alpha c(c^{1/2}\|\rho_{rem}\|_{\mathcal{C}} + c^{3/2}\|\rho_{rem}\|_{L^2}) \\ &\lesssim \alpha c^{3/2}(\alpha c^{-1} + \alpha^2 c^{-1}) + \alpha c^{5/2}(c^{-2} + c^{-1}(\alpha(a_{12}+a_{21}))^{1/2}) \\ &\lesssim \tfrac{\alpha}{\sqrt{\log(\Lambda)}} + \tfrac{1}{\sqrt{\log(\Lambda)}} + \tfrac{\alpha^{5/4}}{\sqrt{\log(\Lambda)}} \lesssim \tfrac{1}{\sqrt{\log(\Lambda)}}.\end{aligned}$$

We recall $a_{jk} = \|v_k\psi_k - v_{kj}\psi_k\|_{L^2}$ and by Proposition 5 we know it is $\mathcal{O}(c^{-1}\alpha^{3/2})$. We decompose each $\underline{\psi_j}$ in sum of h_1, h_2: $\underline{\psi_k} = c_{k1}h_1 + c_{k2}h_2$. Then:

$$\begin{aligned}v_{\underline{\gamma}}\underline{\psi_k} &= v_{\underline{\gamma}}(c_{k1}h_1 + c_{k2}h_2) \\ (v_{\underline{n}} - R_{\underline{N}})\underline{\psi_k} &= c_{k1}(v_{|h_2|^2}h_1 - v_{h_2^*h_1}h_2) + c_{k2}(v_{|h_1|^2}h_2 - v_{h_1^*h_2}h_1).\end{aligned}$$

We write $h_k = \delta_k + \phi_k$ where $\phi_k \in \mathscr{P}$: as in Section B $\|\delta_k\|^2_{H^1} \lesssim \alpha$. By fast decay of the ϕ_k's: $(|\phi_k|^2 * \frac{1}{|\cdot|}(x))^2 = \Theta(|\phi_k|^2 * \frac{1}{|\cdot|^2}(x))$ and for $|x| \gtrsim 1$ this is $\mathcal{O}(\frac{1}{|x-z_k|^2})$.

In particular for $|x| > \lambda\mathrm{R}_g$

$$v\big[|h_k|^2\big](x) \lesssim \frac{1 + \|\delta_k\|_{L^2}}{|x-z_k|} + \langle|\nabla|\delta_k\,,\,\delta_k\rangle \lesssim \frac{1}{\lambda\mathrm{R}_g} + \alpha,$$

we choose $C_0 > 1$ such that $\frac{\alpha c}{\lambda\mathrm{R}_g} < 1 - \varepsilon_0$ where $0 < \varepsilon_0 < 1$ is fixed (for instance 2^{-1}).

By Cauchy-Schwarz inequality we have $v\big[h_1^*h_2\big](x), v\big[h_2^*h_1\big](x) = \mathcal{O}(\|\delta\|_{L^2})$. It follows that

$$\alpha c\|d_{A,\lambda}V\cdot\underline{\varphi_k}\|_{L^2} \lesssim \varepsilon'_{(\lambda)}\|d_{A,\lambda}\underline{\varphi_k}\|_{L^2}, \text{ with } 0 < \varepsilon'_{(\lambda)} < 1.$$

Estimate of $\alpha c d_{A,\lambda} R_{\underline{\gamma\psi_k}}$

$$\begin{aligned}
|[d_{A,\lambda}, R_{\underline{\gamma}}](x,y)| &\lesssim |\underline{\gamma}(x,y)| \text{ so:}\\
\alpha c \|[d_{A,\lambda}, R_{\underline{\gamma]\psi_k}}\|_{L^2} &\lesssim \alpha c \|\underline{\gamma}\|_{\mathfrak{S}_2} \|\underline{\psi_k}\|_{L^2} \lesssim \alpha^2 c^{1/2} = \mathcal{O}(\tfrac{\alpha}{\sqrt{\log(\Lambda)}}).\\
\|R_{\underline{\gamma}} d_{A,\lambda} \underline{\psi_k}\|_{L^2}^2 &\lesssim \mathrm{Tr}(\gamma R_{\underline{\gamma}}) \langle |\nabla| d_{A,\lambda} \underline{\psi_k},\, d_{A,\lambda} \underline{\psi_k}\rangle\\
&\lesssim c^{-1} \||D_0|^{1/2} d_{A,\lambda} \underline{\psi_k}\|_{L^2}^2.
\end{aligned}$$

By Lemma (10), $[|D_0|^{1/2}, d_{A,\lambda}]|D_0|^{-1/2}$ is a bounded operator (with norm $\mathcal{O}(\|\nabla d_{A,\lambda}\|_{L^\infty})$) and at last we get:

$$\alpha c \|d_{A,\lambda} R_{\underline{\gamma\psi_k}}\|_{L^2} \lesssim \alpha c^{1/2}(1 + \|d_{A,\lambda}|D_0|^{1/2} \underline{\psi_k}\|_{L^2}) \text{ and } \alpha c^{1/2} = \mathcal{O}\big(\frac{1}{\sqrt{\log(\Lambda)}}\big).$$

We know deal with the case of $d^{(2)}_{A,\lambda} R_{\underline{\gamma\psi_k}}$, using (108), proved below.

The aim is to prove:

$$\begin{aligned}
\|d^{(2)}_{A,\lambda} R_{\underline{\gamma\psi_k}}\|_{L^2} \lesssim \||x-y|\underline{\gamma}\|_{\mathfrak{S}_2} + \|\underline{\gamma}\|_{\mathfrak{S}_2} \|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g} \underline{\psi_k}\|_{L^2}\\
+ c^{1/2} \|\gamma\|_{\mathrm{Ex}} (\|\underline{\psi_k}\|_{L^2} + \|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g} \underline{\psi_k}\|_{L^2}).
\end{aligned} \tag{106}$$

First of all we use Taylor's formula (108) to get:

$$\|[d^{(2)}_{1,\lambda}, R_{\underline{\gamma]\psi_k}}\|_{L^2} \lesssim \||x-y|\underline{\gamma}\|_{\mathfrak{S}_2} + \|\underline{\gamma}\|_{\mathfrak{S}_2} \|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g} \underline{\psi_k}\|_{L^2}.$$

Let us prove at the end $\||x-y|\underline{\gamma}\|_{\mathfrak{S}_2} = c^{-1}\||x-y|\gamma\|_{\mathfrak{S}_2} \lesssim \alpha c^{-1}$.

There remains $\|R_{\underline{\gamma} d^{(2)}_{A,\lambda} \underline{\psi_k}}\|_{L^2} \lesssim \||D_0|^{1/2} d^{(2)}_{A,\lambda} \underline{\psi_k}\|_{L^2}$.

We commute: using (97), there holds

$$\begin{aligned}
[|D_0|^{1/2}, d^{(2)}_{A,\lambda}] &= \frac{1}{2^{-1/2}\pi} \int_0^{+\infty} \frac{s^{1/4} ds}{1-\Delta+s} [-\Delta, d^{(2)}] \frac{1}{1-\Delta+s},\\
[-\Delta, d^{(2)}] &= (-\Delta d^{(2)}) - 2\sum_{j=1}^{3} (\partial_j d^{(2)}) \partial_j.
\end{aligned}$$

First $\|\Delta d^{(2)}\|_{L^\infty} \lesssim 1$. Then thanks to (108):

$$\begin{aligned}
\|(\partial_j d^{(2)}) \tfrac{\partial_j}{1-\Delta+s} \underline{\psi_k}\|_{L^2} &\lesssim \|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g} \tfrac{\partial_j}{1-\Delta+s} \underline{\psi_k}\|_{L^2}\\
&\lesssim \||x-y| \mathscr{F}^{-1}(\tfrac{p_j}{1+s+|p|^2})\|_{L^1} \|\underline{\psi_k}\|_{L^2} + \tfrac{\|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g} \underline{\psi_k}\|_{L^2}}{1+s}\\
&\lesssim \frac{1}{1+s} (\|\underline{\psi_k}\|_{L^2} + \|d(\cdot)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g} \underline{\psi_k}\|_{L^2}).
\end{aligned}$$

To end this section we prove $\||x-y|\gamma\|_{\mathfrak{S}_2}, \||x-y||\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2} \lesssim \alpha$. This is almost trivial: for each $j \in \{1,2,3\}$ we consider $(x_j - y_j)\gamma(x,y)$ and use the Cauchy expansion of γ. For each $Q_{0,k}$, $k \in [\![1,5]\!]$, we replace at least one $P^0_\varepsilon v'_\gamma P^0_{-\varepsilon}$ as in (94) ([6]) and write:

$$x_j - y_j = x_j - \ell^{(1)}_j + \ell^{(1)}_j - \ell^{(2)}_j + \cdots + \ell^{(n)}_j - y_j.$$

For each convolution operator $\frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}(x-y)$, $\frac{P^0_\varepsilon}{\mathbf{D}+i\eta}(x-y)$, $\frac{1}{D_0+i\omega}(x-y)$, multiplying by $(x_j - y_j)$ corresponds to take the derivative ∂_j in Fourier space enabling us to take KSS inequalities (14) under the integral sign. Indeed we have:

$$\begin{aligned}
&|\partial_j \overline{E}_p^{1/2}| \lesssim \overline{E}_p^{1/6}, && |\partial_j \tfrac{1}{\overline{E}_{(p)}+i\eta}| \lesssim \tfrac{1}{|\overline{E}_p+i\eta|^{1+3^{-1}}},\\
&|\partial_j \tfrac{1}{E(p)+i\omega}| \lesssim \tfrac{1}{E(\omega_2)+|p|^2}, && |\partial_j P^0_\varepsilon(p)| \lesssim \tfrac{1}{E(p)}.
\end{aligned}$$

Then operators of type $\rho * \frac{1}{|\cdot|}$ or $\alpha_k \partial_k (\rho * \frac{1}{|\cdot|})$ remains unchanged while operators of type $(x_j - y_j) R_Q(x,y)$ are trivially Hilbert-Schmidt. This end the proof ; the biggest term comes from $Q_{1,0}((x_j - y_j)\gamma'(x,y))$.

C.2 Proof of (104) and variation for $d^{(2)}_{A,\lambda}$

1. We recall that ξ_1 is a *radial* smooth function with $\xi_1(x) = 1$ for $|x| \leq 1$ and $\xi_1(x) = 0$ for $|x| \geq 2$. We study $d_{A,\lambda} := d(\cdot)\xi_A(\cdot)\boldsymbol{\eta}^{\lambda}_{\mathrm{R}_g}(\cdot)$.
First remark to be done: $H = \{x : |x - z_1| = |x - z_2|\}$ splits the space into two half-spaces E_1 (set of points closest to z_1) and E_2. Let s_H be the orthogonal symmetry with respect to H: $s_H(z_1) = z_2$. If $x \in E_1$ and $y \in E_2$, then

$$|d(x) - d(y)| = \big||x - z_1| - |s_H(y) - z_1|\big| \leq |x - s_H(y)| \leq |x - y|.$$

Moreover $d_{A,\lambda}(y) = d_{A,\lambda}(s_H(y))$ and

$$\big|d_{A,\lambda}(x) - d_{A,\lambda}(y)\big| = \big|d_{A,\lambda}(x) - d_{A,\lambda}(s_H(y))\big|.$$

So we may assume that $d(x) = |x - z_1|$ and $d(y) = |y - z_1|$, and in this case we can write:

$$d_{A,\lambda}(x) = F_\lambda(d(x))\xi_A(x) := d(x)\sqrt{1 - \xi_{\lambda \mathrm{R}_g^2(d(x))}}G_A(|x - z_m|)$$

the same holds for y. We will write $F_\lambda(\cdot)$ for $x \mapsto F_\lambda(d(x))$ for convenience. There holds

$$\nabla d_{A,\lambda}(x) = \big(\nabla F_\lambda(x)\big)\xi_A(x) + F_\lambda(x)(\frac{\nabla\xi_1(x/A)}{A}),$$

and as we have chosen $A \gg \mathrm{R}_g$ we may assume that if $\nabla\xi_A(x) \neq 0$, then $|x - z_m| = \Theta(d(x))$. By simple computation:

$$|\nabla d_{A,\lambda}(x)| \quad \lesssim \big(1 + \|| \cdot |\nabla\xi_1\|_{L^\infty} + \|| \cdot |\nabla\boldsymbol{\eta}^{\lambda}_1\|_{L^\infty}\big). \tag{107}$$

2. For $x, y \in E_\varepsilon$, $\varepsilon = 1, 2$ (say E_1) and $A \gg \mathrm{R}_g$, there holds:

$$\begin{aligned} d^{(2)}_{A,\lambda}(x) - d^{(2)}_{A,\lambda}(y) &= |x - z_1|^2\xi_A(x)\boldsymbol{\eta}^{(\lambda)}_{\mathrm{cR}_g}(x) - |y - z_1|^2\xi_A(y)\boldsymbol{\eta}^{(\lambda)}_{\mathrm{cR}_g}(y) \\ &= |y - z_1|^2\big(\tfrac{\boldsymbol{\eta}^{(\lambda)}_{\mathrm{cR}_g}(y)}{A}\nabla\xi_1(\tfrac{y}{A}) + \tfrac{\xi_A(y)}{c\lambda\mathrm{R}_g}\nabla(\boldsymbol{\eta}^1_1)(\tfrac{y}{c\lambda\mathrm{R}_g})\big)\cdot(x - y) \\ &\qquad + \xi_A(y)\boldsymbol{\eta}^{(\lambda)}_{\mathrm{cR}_g}(y)\langle y - z_1\,,\, x - y\rangle + |y - z_1|^2 + \mathcal{O}\big(|x - y|^2\big) \\ &= \mathcal{O}\big(d(y)\boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}(y)|x - y| + |x - y|^2\big). \end{aligned} \tag{108}$$

Above we used $\nabla\boldsymbol{\eta}^{(\lambda)}_{\mathrm{cR}_g} = \boldsymbol{\eta}^{(\lambda/2)}_{\mathrm{cR}_g}\nabla\boldsymbol{\eta}^{(\lambda)}_{\mathrm{cR}_g}$ and the $\mathcal{O}(\cdot)$ depends on $\xi_1, \boldsymbol{\eta}^1_1$. This estimate enables us to consider commutators with $\frac{|D_0|^{1/2}\sigma\cdot\nabla}{P_k(-\Delta)}$ and $y_c := \frac{(c\Lambda)^2}{(c\Lambda)^2 - \Delta}$, as shown in the next section.

C.3 Proof of (105) and variation for $d^{(2)}_{A,\lambda}$

1. For any borelian function $\mathcal{F}$:

$$\int_{\mathbb{R}^3} |x||\mathcal{F}(x)|dx \leq \Big\{\int |x|^4 E(x)^2|\mathcal{F}(x)|^2dx \int \frac{dx}{|x|^2E(x)^2}\Big\}^{1/2}.$$

To prove $|\cdot|\mathcal{F} \in L^1$ it suffices to check all integrals on the right side converge: in Fourier space, we have to prove:

$$\|\Delta\widehat{\mathcal{F}}\|^2_{L^2} + \|\nabla\Delta\widehat{\mathcal{F}}\|^2_{L^2} < +\infty.$$

Applying this method for $\mathcal{F}_{j,k}(x - y) := \frac{|D_0|^{1/2}\partial_j}{P_k(-\Delta)}(x - y)$:

$$\widehat{\mathcal{F}_{j,k}}(p) = \frac{E(p)^{1/2}p_j}{a_k + |p|^2}\Big\{1 + \frac{\mu_k^2|p|^2}{\Lambda^2(a_k + |p|^2)}\frac{2b^4 + b^2|p|^2}{(b^2 + |p|^2)^2}\Big\}^{-1}$$

where we recall $b = c\Lambda$, $a_k = c^2(1 - \mu_k)$. From this expression, it is easy to see that for $\ell = 1, 2, 3$ and $m = 1, 2$ we have

$$\|\partial^m_\ell\mathcal{F}_{j,k}\|^2_{L^2} \lesssim 1.$$

The constant depends on a_k but for sufficiently small α, L, Λ^{-1} then $a_k > \varepsilon_0 > 0$.
2. By the same method we can show that:

$$\int_{\mathbb{R}^3} |x|^2 |\mathcal{F}(x)| dx \leq \Big\{ \int |x|^6 E(x)^2 |\mathcal{F}(x)|^2 dx \int \frac{dx}{|x|^2 E(x)^2} \Big\}^{1/2},$$

enabling us to treat $d^{(2)}_{A,\lambda}$.

D Localisation in Direct space: γ

We recall we explain in Remark 16 how we use the technical results proved here: Propositions 7, 8 and 9.

D.1 Estimates on the localised density

Let $Q \in \mathcal{K}$ and $0 \leq \zeta \leq 1$ a smooth function (*e.g.* $\xi_{\lambda \mathrm{R}_g}$ or $\boldsymbol{\eta}^{\lambda}_{\mathrm{R}_g}$). Our aim is to give a semi-quantitative estimate of the localisation of the function $\zeta^2 \rho_Q = \rho_{\zeta Q \zeta}$ around the support of ζ.

Proposition 7. *Let Q and ζ be as above, then we have:*

$$\|\zeta^2 \rho_Q - \rho[\zeta^{++} Q \zeta^{++} + \zeta^{--} Q \zeta^{--}]\|_{\mathcal{C}} \leq F_{est}[\Lambda, \zeta, Q], \tag{109}$$

with

$$\begin{aligned} F_{est}[\Lambda, \zeta, Q] &= (\sqrt{\log(\Lambda)} \|\nabla \zeta\|_{L^3} + \|\nabla \zeta\|_{L^\infty})(\|\zeta P^0_{\pm} |D_0|^{a[\Lambda]} Q\|_{\mathfrak{S}_2} + \|\nabla \zeta\|_{L^\infty} \|Q\|_{\mathfrak{S}_2}) \\ &+ \|\nabla \zeta\|^2_{L^6} \||D_0|^{a[\Lambda]} Q\|_{\mathfrak{S}_2} + \sqrt{\log(\Lambda)} (\|\zeta Q^{\pm\mp} |D_0|^{a[\Lambda]} \zeta\|_{\mathfrak{S}_2} + \|\zeta Q^{\pm\mp}\|_{\mathfrak{S}_2} \|\nabla \zeta\|_{L^\infty}) \\ &+ \sqrt{\log(\Lambda)} \|\nabla \zeta\|_{L^\infty} (\|\nabla \zeta\|_{L^\infty} \|Q^{\pm\pm}\|_{\mathfrak{S}_1} + \|\zeta |D_0|^{a[\Lambda]} Q^{\pm\pm}\|_{\mathfrak{S}_1}) \\ &+ (\log(\Lambda))^{1/6} \|\nabla \zeta\|^2_{L^\infty} \||D_0|^{a[\Lambda]} Q^{\pm\pm}\|_{\mathfrak{S}_1}. \end{aligned} \tag{110}$$

Moreover there holds for $\varepsilon = \pm$:

$$\begin{aligned} \|\rho[\zeta^{\varepsilon\varepsilon} Q \zeta^{\varepsilon\varepsilon}]\|_{\mathcal{C}} &\leq \|[\zeta^{\varepsilon\varepsilon}, |D_0|^{a[\Lambda]}]\|_{\mathcal{B}} \|Q^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1} + \|\zeta^{\varepsilon\varepsilon} Q^{\varepsilon\varepsilon} |D_0|^{a[\Lambda]} \zeta^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1} \\ &\lesssim \|\nabla \zeta\|_{L^\infty} \|Q^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1} + \|\zeta^{\varepsilon\varepsilon} Q^{\varepsilon\varepsilon} |D_0|^{a[\Lambda]} \zeta^{\varepsilon\varepsilon}\|_{\mathfrak{S}_1}. \end{aligned} \tag{111}$$

Remark 18. 1. In the case $Q = \Pi - P^0_-$ with $\Pi^* = \Pi^2 = \Pi$ then (*cf* [7]):
$Q^2 = Q^{++} - Q^{--} \geq Q^{++}$. As shown in [20] we can consider an orthonormal family of eigenvectors of Q^2 that split into those in $\mathrm{Ran}(P^0_+)$ and those in $\mathrm{Ran}(P^0_-)$. It is then clear that:

$$\begin{aligned} \|\zeta^{++} Q^{++} |D_0|^{a[\Lambda]} \zeta^{++}\|_{\mathfrak{S}_1} &\leq \|\zeta Q^{++} |D_0|^{a[\Lambda]} \zeta\|_{\mathfrak{S}_1} \\ &\leq \|\zeta |D_0|^{a[\Lambda]} Q\|_{\mathfrak{S}_2} \|\zeta Q\|_{\mathfrak{S}_2} \end{aligned}$$

2. There is also an analogous estimate if we choose two different functions ζ_1, ζ_2, that is with $\zeta_1 \zeta_2 \rho(Q) = \rho(\zeta_1 Q \zeta_2)$. The same proof shows also localisation estimates, but we have to "polarize" the inequalities just like for a quadratic form and its associated bilinear form.

Proof: We prove it by duality. Let V be some Schwartz function: we study $\mathrm{Tr}_0(\zeta Q \zeta V)$. By symmetry we just treat $(\zeta Q \zeta V)^{++}$. There holds:

$$\begin{aligned} P^0_+ \zeta Q \zeta V P^0_+ &= P^0_+ \zeta (P^0_+ + P^0_-) Q (P^0_+ + P^0_-) \zeta (P^0_+ + P^0_-) V P^0_+ \\ &= \zeta^{++} Q^{++} \zeta^{++} V^{++} + \zeta^{++} Q^{++} \zeta^{+-} V^{-+} + \zeta^{++} Q^{+-} \zeta^{-+} V^{++} + \zeta^{++} Q^{+-} \zeta^{--} V^{-+} \\ &+ \zeta^{+-} Q^{-+} \zeta^{++} V^{++} + \zeta^{+-} Q^{-+} \zeta^{+-} V^{-+} + \zeta^{+-} Q^{--} \zeta^{-+} V^{++} + \zeta^{+-} Q^{--} \zeta^{--} V^{-+}. \end{aligned}$$

We first show those operators are trace-class and then prove (109).

Remark 19. We recall that by Sobolev inequality: $\|V\|_{L^6} \lesssim \|\nabla V\|_{L^2}$.
Moreover $\||D_0|^{-a[\Lambda]}V\|_{\mathfrak{S}_2} \lesssim \sqrt{\log(\Lambda)}\|V\|_{L^2}$.
As shown in Appendix A:

$$\zeta^{-+} = \frac{i}{2\pi}\int_{-\infty}^{+\infty} \frac{1}{D_0+i\eta}\boldsymbol{\alpha}\cdot\nabla\zeta\frac{P_+^0 d\eta}{D_0+i\eta}. \tag{112}$$

It can be rewritten as:

$$\zeta^{-+} = \frac{i}{2}\int_0^{+\infty} e^{-s|D_0|}P_-^0\boldsymbol{\alpha}\cdot\nabla\zeta P_+^0 e^{-s|D_0|}ds, \tag{113}$$

by writing $\frac{1}{E(p)+E(q)} = \int_0^{+\infty} e^{-s(E(p)+E(q))}$ in the kernel of its Fourier transform *cf* Appendix A.

$\zeta^{++}Q\zeta^{++}V^{++}$**:**

$$\zeta^{++}Q\zeta^{++}V^{++} = \zeta^{++}(Q^{++}\zeta^{++}|D_0|^{a[\Lambda]})\frac{1}{|D_0|^{a[\Lambda]}}V^{++}$$

and $(Q^{++}\zeta^{++}|D_0|^{a[\Lambda]}) \in \mathfrak{S}_1$, $\frac{1}{|D_0|^{a[\Lambda]}}V^{++} \in \mathfrak{S}_6$ with norm $\mathcal{O}((\log(\Lambda))^{1/6}\|\nabla V\|_{L^2})$ by the KSS inequality (14). We write

$$\begin{aligned}\|\zeta Q^{++}\zeta^{++}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1} &\leq \|\zeta Q^{++}\|_{\mathfrak{S}_1}\|[\zeta^{++},|D_0|^{a[\Lambda]}]\|_{\mathcal{B}} + \|\zeta Q^{++}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_1}\\ &\lesssim \|\zeta Q^{++}\|_{\mathfrak{S}_1}\|\nabla\zeta\|_{L^\infty} + \|\zeta Q^{++}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_1}.\end{aligned}$$

In general whenever there is Q^{++} or Q^{--} we can easily estimate.

$$\begin{aligned}|\mathrm{Tr}(\zeta^{++}Q^{++}\zeta^{+-}V^{-+})| &= |\mathrm{Tr}(V^{-+}\tfrac{1}{|D_0|^{a[\Lambda]}}|D_0|^{a[\Lambda]}\zeta^{++}Q^{++}\zeta^{+-})|\\ &\lesssim \sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}\|\nabla\zeta\|_{L^\infty}(\|\nabla\zeta\|_{L^\infty}\|Q^{++}\|_{\mathfrak{S}_1} + \|\zeta|D_0|^{a[\Lambda]}Q^{++}\|_{\mathfrak{S}_1}),\\ |\mathrm{Tr}(\zeta^{+-}Q^{--}\zeta^{-+}V^{++})| &\leq \|\tfrac{1}{|D_0|^{a[\Lambda]}}V\|_{\mathfrak{S}_6}\|\zeta^{+-}\|_{\mathcal{B}}\|Q^{--}\zeta^{-+}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1}\\ &\lesssim (\log(\Lambda))^{1/6}\|\nabla V\|_{L^2}\|\nabla\zeta\|_{L^\infty}^2\|Q^{--}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_1},\\ |\mathrm{Tr}(\zeta^{+-}Q^{--}\zeta^{--}V^{-+})| &\lesssim \sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}\|\nabla\zeta\|_{L^\infty}(\|\nabla\zeta\|_{L^\infty}\|Q^{--}\|_{\mathfrak{S}_1} + \|\zeta|D_0|^{a[\Lambda]}Q^{--}\|_{\mathfrak{S}_1}).\end{aligned}$$

The term $\zeta^{+-}Q^{-+}\zeta^{+-}V^{-+}$:

$$\begin{aligned}\|\zeta^{+-}Q^{-+}\zeta^{+-}V^{-+}\|_{\mathfrak{S}_1} &\leq \|\zeta^{-+}\|_{\mathfrak{S}_6}\|Q^{+-}|D_0|^{a[\Lambda]}\|_{\mathfrak{S}_2}\|\tfrac{1}{|D_0|^{a[\Lambda]}}\zeta^{-+}V^{++}\|_{\mathfrak{S}_3}\\ \|\tfrac{1}{|D_0|^{a[\Lambda]}}\zeta^{-+}V^{++}\|_{\mathfrak{S}_3} &\lesssim \sum_{j=1}^3\frac{1}{2\pi}\int_{-\infty}^{+\infty}\|\tfrac{1}{|D_0|^{a[\Lambda]}(D_0+i\eta)}\partial_j\zeta\tfrac{P_+^0}{D_0+i\eta}V\|_{\mathfrak{S}_3}d\eta\\ &\lesssim \sum_{j=1}^3\|\partial_j\zeta\|_{L^6}\|V\|_{L^6}\|\tfrac{1}{E(\cdot)^{5/8}}\|_{L^6}^2\int_{-\infty}^{+\infty}\frac{d\eta}{E(\eta)^{5/4}},\\ \|\zeta^{-+}\|_{\mathfrak{S}_6} &\lesssim \|\nabla\zeta\|_{L^6}.\end{aligned}$$

The term $\zeta^{++}Q^{+-}\zeta^{--}V^{-+}$:

$$|\mathrm{Tr}(\zeta^{++}Q^{+-}\zeta^{--}V^{-+})| \lesssim \sqrt{\log(\Lambda)}\|\nabla V\|_{L^2}(\|\zeta Q^{+-}|D_0|^{a[\Lambda]}\zeta\|_{\mathfrak{S}_2} + \|\zeta Q^{+-}\|_{\mathfrak{S}_2}\|\nabla\zeta\|_{L^\infty}).$$

The terms $\zeta^{+-}Q^{-+}\zeta^{++}V^{++}$ and $\zeta^{++}Q^{+-}\zeta^{-+}V^{++}$ These operators are difficult to handle. We use Lemma 10 (Appendix A). First:

$$\zeta^{+-}Q^{-+}\zeta^{++}V^{++} = \big(\zeta^{+-}\frac{1}{|D_0|^{\frac{\varepsilon_\Lambda}{4}}}\big)\big(|D_0|^{\frac{\varepsilon_\Lambda}{4}}Q^{-+}\zeta^{++}|D_0|^{\frac{1}{2}+\frac{\varepsilon_\Lambda}{4}}\big)\big(\frac{1}{|D_0|^{\frac{1}{2}+\frac{\varepsilon_\Lambda}{4}}}V^{++}\big) \in \mathfrak{S}_1,$$

with norm $\mathcal{O}((\log(\Lambda))^{3/2}\|\nabla\zeta\|_{L^3}\|V\|_{L^6}\||D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2})$. We used the KSS inequality and Hölder-type inequality for $\mathfrak{S}_p$. Similarly we can show that $\zeta^{++}Q^{+-}\zeta^{-+}V^{++} \in \mathfrak{S}_1$.

Then by density of $\mathfrak{S}_1$ in $\mathfrak{S}_2$, we approximate $\big(|D_0|^{\frac{\varepsilon_\Lambda}{4}}Q^{-+}\zeta^{++}|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}\big)$ by trace-class operators enabling us to say that:

$$\mathrm{Tr}(\zeta^{+-}Q^{-+}\zeta^{++}V^{++}) = \mathrm{Tr}\Big(\big(|D_0|^{\frac{\varepsilon_\Lambda}{4}}Q^{-+}\zeta^{++}|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}\big)\big(\frac{1}{|D_0|^{\frac12+\frac{\varepsilon_\Lambda}{4}}}V^{++}\big)\big(\zeta^{+-}\frac{1}{|D_0|^{\frac{\varepsilon_\Lambda}{4}}}\big)\Big).$$

Let us show that $Q^{-+}\zeta^{++}V^{++}\zeta^{+-} \in \mathfrak{S}_1$. It suffices to show $\frac{1}{|D_0|^{a[\Lambda]}}V^{++}\eta^{+-} \in \mathfrak{S}_2$. We go in Fourier space and used formula (113) to show $[V, P_+^0 e^{-sE|D_0|}] \in \mathfrak{S}_2$.

$$\mathscr{F}([V, P_+^0 e^{-sE|D_0|}]; p, q) = \frac{1}{(2\pi)^{3/2}}\widehat{V}(p-q)\big(P_+^0(q)e^{-sE(q)} - P_-^0(p)e^{-sE(p)}\big);$$

then (*cf* Appendix A)

$$\begin{aligned}
P_+^0(q)e^{-sE(q)} - P_-^0(p)e^{-sE(p)} &= (P_+^0(q) - P_+^0(p))e^{-sE(q)} + P_+^0(p)(e^{-sE(q)} - e^{-sE(p)}) \\
\big|P_+^0(q) - P_+^0(p)\big| &\lesssim \frac{|p-q|}{\max(E(p), E(q))} \\
\big|e^{-sE(q)} - e^{-sE(p)}\big| &= s|E(p) - E(q)|\frac{|e^{-sE(q)} - e^{-sE(p)}|}{s|E(p) - E(q)|} \\
&\le s|p-q|\min(e^{-sE(p)}, e^{-sE(q)}) \\
&\le s|p-q|(e^{-sE(p)} + e^{-sE(q)}).
\end{aligned}$$

By easy computation: $\|[V, P_+^0 e^{-sE|D_0|}]\|_{\mathfrak{S}_2} \lesssim s^{-1/2}e^{-s/\sqrt{2}}\|\nabla V\|_{L^2}$:

$$\int_{s=0}^{+\infty}\|[V, P_+^0 e^{-s|D_0|}]\boldsymbol{\alpha}\cdot\nabla\zeta e^{-s|D_0|}\|_{\mathfrak{S}_2}ds \lesssim \|\nabla\zeta\|_{L^\infty}\|\nabla V\|_{L^2}\int_0^{+\infty}\frac{e^{-s}ds}{s^{1/2}}.$$

At last there remains to show:

$$\mathcal{A}[V,\zeta] = \int_0^{+\infty}\frac{e^{-s|D_0|}}{|D_0|^{a[\Lambda]}}P_+^0\big(V\boldsymbol{\alpha}\cdot\nabla\zeta\big)P_-^0 e^{-s|D_0|}ds \in \mathfrak{S}_2,$$

as in Appendix A it suffices to go in Fourier space and remark $\|V\partial_j\zeta\|_{L^2} \le \|V\|_{L^6}\|\partial_j\zeta\|_{L^3}$:

$$\|\mathcal{A}[V,\zeta]\|_{\mathfrak{S}_2} \lesssim \sqrt{\log(\Lambda)}\|V\nabla\zeta\|_{L^2} \lesssim \sqrt{\log(\Lambda)}\|V\|_{L^6}\|\partial_j\zeta\|_{L^3}.$$

The case of $\zeta^{++}Q^{+-}\zeta^{-+}V^{++}$ is similar: first we prove by density that

$$\mathrm{Tr}(\zeta^{++}Q^{+-}\zeta^{-+}V^{++}) = \mathrm{Tr}(\zeta^{-+}V^{++}\zeta^{++}Q^{+-}),$$

and we get *in fine*

$$\begin{aligned}
&\|\rho[\zeta^{++}Q^{+-}\zeta^{-+}V^{++}]\|_{\mathcal{C}} + \|\rho[\zeta^{-+}Q^{+-}\zeta^{-+}V^{++}]\|_{\mathcal{C}} \\
&\qquad\lesssim (\sqrt{\log(\Lambda)}\|\nabla\zeta\|_{L^3} + \|\nabla\zeta\|_{L^\infty})(\|\zeta P_+^0|D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2} + \|\nabla\zeta\|_{L^\infty}\|Q\|_{\mathfrak{S}_2}).
\end{aligned} \tag{114}$$

□

D.2 Estimates on the localised operator γ

Here γ is the vacuum part of a (hypothetical) minimizer of $E^0_{\mathrm{BDF}}(2)$ or a minimizer of $E^0_{\mathrm{BDF}}(1)$. Our aim is to prove:

Proposition 8. *Let ζ be a smooth function with:*

$$\begin{cases} \|\nabla\zeta\|_{L^\infty}, \|\partial_j\partial_k\zeta\|_{L^\infty} < +\infty,\ j,k \in \{1,2,3\} \\ \|\zeta v'\|_{L^6}, \|\zeta\nabla v'\|_{L^2}, \|\zeta\gamma\|_{Ex}, \|\zeta R_N\|_{\mathfrak{S}_2} < +\infty. \end{cases}$$

Then there holds:

$$\begin{aligned}
\|\zeta|\mathbf{D}|^{1/2}\gamma\|_{\mathfrak{S}_2} &\lesssim c^{-1/2}\|\zeta\nabla v'\|_{L^2} + \alpha(\|\zeta\gamma\|_{Ex} + \|\zeta R_N\|_{\mathfrak{S}_2}) \\
&\quad + \alpha^2(\|\zeta\nabla v'\|_{L^2} + \|\zeta v'\|_{L^6} + \|\zeta\gamma\|_{Ex} + \|\zeta R_N\|_{\mathfrak{S}_2})^2 \\
&\quad + \big\{\|\nabla\zeta\|_{L^\infty} + \textstyle\sum_{1\le j,k\le 3}\|\partial_j\partial_k\zeta\|_{L^\infty}\big\}\big\{\alpha(\|\rho'_\gamma\|_{\mathcal{C}} + \||\nabla|^{1/2}\gamma'\|_{\mathfrak{S}_2})\big\}.
\end{aligned} \tag{115}$$

The same holds for $\||D_0|^{\widetilde{a}}\gamma\|_{\mathfrak{S}_2}$ with $\widetilde{a} \in \{\frac12, a[\Lambda]\}$.
We can replace $\|\zeta\gamma\|_{Ex} + \|\zeta R_N\|_{\mathfrak{S}_2}$ by $\|\gamma'\|_{Ex}$ and put $P^0_\pm\gamma$ instead of γ.

D.2.1 Idea of the proof

We will focus on the Cauchy expansion of γ: $\gamma = \sum_{j=1}^{+\infty} \alpha^j Q_j(\gamma', \rho'_\gamma)$.

As shown in [6, 20, 22], we substitute $P^0_\pm(\rho'_\gamma * \frac{1}{|\cdot|})P^0_\mp$ by its expression (94) whenever it is necessary (in $Q_{0,1}, Q_{0,3}, Q_{0,5}$)

We multiply γ by $|D_0|^{\tilde{\alpha}}$ (or $|\mathbf{D}|^{1/2}$) and then by ζ. We consider $\frac{|D_0|^{\tilde{\alpha}}}{\mathbf{D}+i\eta}$ (or $\frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}$) as a whole operator and we then commute ζ with this operator and maybe some P^0_ε and $\frac{1}{D_0+i\omega}$ (if it was necessary to use (94)) in order to stick ζ with a $v\rho'_\gamma * \frac{1}{|\cdot|}$, a R'_γ or a $\partial_j\rho'_\gamma * \frac{1}{|\cdot|}$ (if (94) was used). For instance in the case of $Q_{0,1}$:

$$\begin{aligned} Q^{+-}_{0,1} &= \int_{-\infty}^{+\infty} \frac{|\mathbf{D}|^{1/2}P^0_+}{\mathbf{D}+i\eta} v' \frac{P^0_-}{\mathbf{D}+i\eta} \\ &= \frac{i}{2\pi} \iint\limits_{\mathbb{R}\times\mathbb{R}} \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \frac{1}{D_0+i\omega} \boldsymbol{\alpha}\cdot\nabla v' \frac{P^0_-}{D_0+i\omega} \frac{d\eta d\omega}{\mathbf{D}+i\eta}. \end{aligned} \tag{116}$$

We multiply by ζ and under the integral sign:

$$\begin{aligned} \zeta \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \frac{1}{D_0+i\omega} \boldsymbol{\alpha}\cdot\nabla v' &= \Big[\zeta, \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}\Big] \frac{1}{D_0+i\omega} \boldsymbol{\alpha}\cdot\nabla v' + \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \Big[\zeta, \frac{1}{D_0+i\omega}\Big] \boldsymbol{\alpha}\cdot\nabla v' \\ &\quad + \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta} \frac{1}{D_0+i\omega} \zeta\boldsymbol{\alpha}\cdot\nabla v'. \end{aligned} \tag{117}$$

We treat the first two terms in Section D.2.2. For the latter we go in Fourier space and up to a constant the kernel of its Fourier transform is:

$$\frac{\overline{E}_p^{1/2}}{\overline{E}_p + \overline{E}_q} \frac{P^0_+(p)}{E(p)+E(q)} \big(\mathscr{F}(\zeta\boldsymbol{\alpha}\cdot\nabla v'; p-q)\big) P^0_-(q).$$

In particular its Hilbert-Schmidt norm is $\mathcal{O}(\sqrt{\log(\Lambda)}\|\zeta\nabla v'_{\rho_\gamma}\|_{L^2})$.

Doing the same for the other $Q_{k,\ell}$, we get terms with commutators treated in D.2.2 and other terms with $\zeta v'_{\rho_\gamma}$, $\zeta\boldsymbol{\alpha}\cdot\nabla v'$ and $\zeta R_{\gamma'} = R_{\zeta\gamma'}$. In particular taking the $\|\cdot\|_{\mathfrak{S}_2}$ under the integral sign, we get the following estimates on those terms.

$$\mathcal{O}\Big(c^{-1/2}\|\zeta\nabla v'\|_{L^2} + \alpha\|\zeta\gamma'\|_{\mathrm{Ex}} + \alpha^2(\|\zeta\nabla v'\|_{L^2} + \|\zeta v'\|_{L^6} + \|\zeta\gamma'\|_{\mathrm{Ex}})^2\Big). \tag{118}$$

Remark 20. The term $\|\zeta\gamma'\|_{\mathrm{Ex}}$ is due to Ineq. (51) (l.h.s). Moreover we can deal with γ and N in γ' differently. Indeed as $R_N \in \mathfrak{S}_2$, $\|\zeta\gamma'\|_{\mathrm{Ex}}$ can be replaced by $K(\|\zeta\gamma\|_{\mathrm{Ex}} + \|\zeta R_N\|_{\mathfrak{S}_2})$.

Remark 21. The term $\mathcal{T}[\zeta, v'] := \zeta\boldsymbol{\alpha}\cdot\nabla v'$ appears in $P^0_{-\varepsilon}v'P^0_\varepsilon$, that equals up to a multiplicative constant to

$$\int_{\omega=-\infty}^{+\infty} \frac{d\omega}{D_0+i\omega} \mathcal{T}[\zeta, v'] \frac{P^0_\varepsilon}{D_0+i\omega}.$$

Up to a constant its Fourier transform is

$$\frac{P^0_{-\varepsilon}(p)\widehat{\mathcal{T}}(p-q)P^0_\varepsilon(q)}{E(p)+E(q)},$$

and we deal with this term as $\widehat{P^0_{-\varepsilon}}(p)\widehat{v'}(p-q)\widehat{P^0_\varepsilon}(q)$ in [7, 20, 22].

D.2.2 Commutating ζ

We recall here that $[\zeta, P_\varepsilon^0]$ is treated in (94), Appendix A.

In the same spirit of Lemma 10, we have the following Lemma.

Lemma 11. *Let $\eta \in \mathbb{R}$ and ζ smooth with*

$$\|\nabla\zeta\|_{L^\infty}, \|\partial_j\partial_k\zeta\|_{L^\infty} < +\infty, k, j \in \{1,2,3\}.$$

Then there holds:

$$\Big|\Big|\Big[\zeta, \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}\Big]|\mathbf{D}+i\eta|^{7/12}\Big|\Big|_{\mathcal{B}} \lesssim \|\nabla\zeta\|_{L^\infty} + \sum_{1\leq j,k\leq 3}\|\partial_j\partial_k\zeta\|_{L^\infty}.$$

Remark 22. We can do the same with $|D_0|^{a[\Lambda]}$ or $|D_0|^{1/2}$ instead of $|\mathbf{D}|^{1/2}$ by using the following formula [17, p. 87]:

$$|D_0|^a = \frac{\sin(a\pi)}{\pi}\int_{s=0}^{+\infty}\frac{ds}{s^{1-a}}\frac{|D_0|}{|D_0|+s},\ a = a[\Lambda], 1/2.$$

Here we show the proof for $|\mathbf{D}|^{1/2}$ because it enables us to localise the kinetic energy. But we can replace every $|D_0|^{a[\Lambda]}$ by $|\mathbf{D}|^{1/2}$ and vice-versa.

There is also:

Lemma 12. *There exists $K > 0$ such that for any $\eta \in \mathbb{R}$ and any smooth function ζ with $\|\nabla\zeta\|_{L^\infty} < +\infty$:*

$$\Big|\Big[\zeta, \frac{1}{D_0+i\omega}\Big](x-y)\Big| \leq K\|\nabla\zeta\|_{L^\infty}\frac{e^{-E(\eta)/2(x-y)}}{|x-y|}. \tag{119}$$

Remark 23. We recall that up to some constant $\frac{1}{a^2-\Delta}(x-y) = \sqrt{\frac{\pi}{2}}\frac{e^{-a|x-y|}}{|x-y|}$ [16].
– The interesting fact here is that by taking the commutator of ζ and some function of $-i\nabla$ we gain some exponent for η or ω. Thus by using KSS inequalities under the integral sign we get the following estimates for the term with commutators:

$$\mathcal{O}\Big(\big(\|\nabla\zeta\|_{L^\infty} + \sum_{1\leq j,k\leq 3}\|\partial_j\partial_k\zeta\|_{L^\infty}\big)\big(\alpha(\|\rho'_\gamma\|_{\mathfrak{C}} + \||\nabla|^{1/2}\gamma\|_{\mathfrak{S}_2} + \|\nabla N\|_{\mathfrak{S}_2})\big)\Big) \tag{120}$$

Proof of Lemma 11: We decompose $\zeta = \zeta^{++} + \zeta^{+-} + \zeta^{-+} + \zeta^{--}$. We write for each term $\zeta^{\varepsilon\varepsilon'}$, $\varepsilon, \varepsilon' \in \{+,-\}$:

$$\Big[\zeta^{\varepsilon\varepsilon'}, \frac{|\mathbf{D}|^{1/2}}{\mathbf{D}+i\eta}\Big] = [\zeta^{\varepsilon\varepsilon'}, |\mathbf{D}|^{1/2}]\frac{1}{\mathbf{D}+i\eta} + |\mathbf{D}|^{1/2}\Big[\zeta^{\varepsilon\varepsilon'}, \frac{1}{\mathbf{D}+i\eta}\Big].$$

It follows that:

$$|\mathbf{D}|^{1/2}\Big[\zeta^{\varepsilon\varepsilon'}, \frac{1}{\mathbf{D}+i\eta}\Big] = \frac{|\mathbf{D}|^{1/2}P_\varepsilon^0}{\mathbf{D}+i\eta}[\mathbf{D},\zeta]\frac{P_{\varepsilon'}^0}{\mathbf{D}+i\eta}. \tag{121}$$

The term $|\mathbf{D}|^{1/2}\Big[\zeta^{\varepsilon\varepsilon'}, \frac{1}{\mathbf{D}+i\eta}\Big]$ By simple computation we have:

$$\begin{aligned}[\mathbf{D},\zeta] &= \Big(1-\frac{\Delta}{\Lambda^2}\Big)(-i\boldsymbol{\alpha}\cdot\nabla\zeta) + \frac{(-\Delta\zeta)}{\Lambda^2}D_0 + 2\nabla\zeta\cdot\frac{\nabla D_0}{\Lambda^2}\\ &= (-i\boldsymbol{\alpha}\cdot\nabla\zeta) - \sum_{j=1}^3\Big(\frac{\partial_j}{\Lambda^2}(-i\boldsymbol{\alpha}\cdot\nabla\partial_j\zeta) - 2(\partial_j^2\zeta)\frac{D_0}{\Lambda^2}\Big)\\ &+(-\Delta\zeta)\frac{D_0}{\Lambda^2} - \sum_{j=1}^3\frac{\partial_j}{\Lambda}\Big((-i\boldsymbol{\alpha}\cdot\nabla\zeta)\frac{\partial_j}{\Lambda} - (\partial_j\zeta)\frac{D_0}{\Lambda}\Big).\end{aligned} \tag{122}$$

Then there holds:

$$\|\frac{|D_0|}{\Lambda|\mathbf{D}|^{1/3}}\|_{\mathcal{B}} \lesssim 1. \tag{123}$$

Thus substituting in (121), on the right of derivatives of ζ, there is still an operator $\frac{1}{|\mathbf{D}+i\eta|^{2/3}}$ available for some KSS inequality. The $\|\cdot\|_{\mathcal{B}}-$norm of the operator on their left is $\mathcal{O}(\overline{E}_\eta^{-1/6})$. The $\|\cdot\|_{\mathcal{B}}-$norm of derivatives of ζ are $\mathcal{O}(\|\nabla\zeta\|_{L^\infty}+\|\Delta\zeta\|_{L^\infty})$.

The term $[\zeta^{\varepsilon\varepsilon'},|\mathbf{D}|^{1/2}]\frac{1}{\mathbf{D}+i\eta}$ By symmetry it suffices to study ζ^{++} and ζ^{+-}. First:

$$[\zeta^{++},|\mathbf{D}|^{1/2}]\tfrac{1}{\mathbf{D}+i\eta} \quad = \tfrac{1}{\pi}\int_0^{+\infty}\sqrt{s}ds\frac{P_+^0}{\mathbf{D}+s}[\mathbf{D},\zeta]\frac{P_+^0}{\mathbf{D}+s}\frac{1}{\mathbf{D}+i\eta}.$$

Once again, if we replace $[\mathbf{D},\zeta]$ by its expression in (122), we see that taking $|\mathbf{D}+i\eta|^{-1/4}$ from $\frac{1}{\mathbf{D}+i\eta}$, there remains $\frac{|\mathbf{D}+i\eta|^{1/4}}{\mathbf{D}+i\eta}$ for some KSS inequality.

This enables us to get a finite integral over the s variable:

$$\int_0^{+\infty}\frac{\sqrt{s}ds}{(1+s)^{2/3}}\frac{1}{(1+s)^{11/12}}<+\infty.$$

At last:

$$\begin{aligned}[\zeta^{+-},|\mathbf{D}|^{1/2}]\frac{1}{\mathbf{D}+i\eta} &= -\frac{1}{\pi}\int_0^{+\infty}\sqrt{s}ds\frac{P_+^0}{|\mathbf{D}|+s}(\zeta\mathbf{D}+\mathbf{D}\zeta)\frac{P_-^0}{|\mathbf{D}|+s}\frac{1}{\mathbf{D}+i\eta}\\ &= -\frac{1}{\pi}\int_0^{+\infty}\sqrt{s}ds\frac{P_+^0}{|\mathbf{D}|+s}(2\zeta\mathbf{D}+[\mathbf{D},\zeta])\frac{P_-^0}{|\mathbf{D}|+s}\frac{1}{\mathbf{D}+i\eta}.\end{aligned}$$

The term with $[\mathbf{D},\zeta]$ is dealt with as before. There remains:

$$\int_0^{+\infty}\frac{\sqrt{s}ds}{|\mathbf{D}|+s}\zeta^{+-}\frac{\mathbf{D}}{|\mathbf{D}|+s}\frac{1}{\mathbf{D}+i\eta}. \tag{124}$$

We write (*cf* (94)):

$$\zeta^{+-}=P_+^0[\zeta,P_-^0]=\frac{P_+^0}{2\pi}\int_{-\infty}^{+\infty}\frac{d\omega}{\mathbf{D}+i\omega}[\mathbf{D},\zeta]\frac{1}{\mathbf{D}+i\omega}, \tag{125}$$

and substitute ζ^{+-} by this expression in (124). We must compensate $\frac{|D_0|}{\Lambda}$ on the left side of ζ and $\frac{|D_0|\mathbf{D}}{\Lambda}$ on its right side: we use $\frac{1}{|\mathbf{D}+i\omega|^{1/3}}$ on the left side and $\{|\mathbf{D}+i\omega|^{1/2}|\mathbf{D}+i\eta|^{5/12}(|\mathbf{D}|+s)^{5/12}\}^{-1}$ on the right side: there remains $\frac{1}{|\mathbf{D}+i\eta|^{7/12}}$ for some KSS inequality and:

$$\int_{s=0}^{+\infty}\int_{\omega=-\infty}^{+\infty}\frac{\sqrt{s}dsd\omega}{(1+s)^{19/12}E(\omega)^{7/6}}<+\infty.$$

Proof of lemma 12: This is straightforward because everything is computable:

$$\frac{1}{D_0+i\eta}=\frac{D_0-i\eta}{E(\eta)^2-\Delta}.$$

However $\frac{1}{E(\eta)^2-\Delta}(x-y)=\frac{e^{-E(\eta)|x-y|}}{4\pi|x-y|}$ so it is clear that:

$$\Big|\frac{1}{D_0+i\eta}(x-y)\Big|\lesssim\frac{e^{-E(\eta)|x-y|/2}}{|x-y|^2}.$$

In Direct space we use $|\zeta(x)-\zeta(y)|\leq\|\nabla\zeta\|_{L^\infty}|x-y|$ and

$$\Big|\Big[\zeta,\frac{1}{D_0+i\omega}\Big](x-y)\Big|\lesssim\|\nabla\zeta\|_{L^\infty}\frac{e^{-E(\eta)/2(x-y)}}{|x-y|}$$

D.2.3 Localisation of $\nabla v_{\rho'_\gamma}$ and R_N

We recall that $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$ is the following function:

$$\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}(x) := \left\{1 - \xi_{c\lambda\mathrm{R}_g}^2(x - cz_1) - \xi_{c\lambda\mathrm{R}_g}^2(x - cz_2)\right\}^{-1/2},\ \lambda_0 < \lambda < 2^{-1}.$$

We will take $\lambda_0 \leq \lambda \leq 3^{-1}$ ($\lambda_0(L, \mathrm{R}_g)$ is defined in (82)). More generally except for $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\partial v\|_{L^2}, \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)} v\|_{L^6}$, the estimates are true with ζ instead of $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}$ in the case where ζ is $\zeta(x) = \zeta_0(x/A)$ with $0 \leq \zeta_0 \leq 1$ fixed . This part gives estimates with respect to ζ_0 and A.

Notation 12. We write $\theta_1^1(x) := \sqrt{1 - \xi_1^2(x)}$, it is clear that

$$\|\nabla \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\|_{L^\infty} \leq \frac{\|\nabla\theta_1^1\|_{L^\infty}}{c\lambda\mathrm{R}_g} \text{ and so on.}$$

Proposition 9. *Let $\gamma + N$ be a minimizer for $E^0(2)$ (or $E^0(1)$), $\rho \in L^1 \cap L^2$ (*e.g. *$\rho = \rho_\gamma, \rho_N$) and $\lambda_0 \leq \lambda < 2^{-1}$. With the previous notations, there holds:*

$$\left\{\begin{array}{rl}
\|\boldsymbol{\eta}_{cR_g}^{(\lambda)} R[N_j]\|_{\mathfrak{S}_2}^2 & \lesssim \|\nabla\psi_j\|_{L^2}^2 \displaystyle\int_x (\boldsymbol{\eta}_{cR_g}^{(\lambda)})^2(x)|\psi_j(x)|^2 dx \lesssim \left\{(\lambda R_g)^2 c^2\right\}^{-1}, \\
\|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\gamma\|_{Ex} & \lesssim \|\nabla\theta_1^1\|_{L^\infty}(c\lambda R_g)^{-1}\||D_0|^{1/2}\gamma\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}, \\
\|\boldsymbol{\eta}_{cR_g}^{(\lambda)} v_\rho\|_{L^6} & \lesssim \|(\nabla\boldsymbol{\eta}_{cR_g}^{(\lambda)})v_\rho\|_{L^2} + \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\nabla v_\rho\|_{L^2}, \\
\|(\nabla\boldsymbol{\eta}_{cR_g}^{(\lambda)})v_\rho\|_{L^2} & \lesssim \|\rho\|_{L^1}\|\nabla|\nabla|\boldsymbol{\theta}_1^1\|_{L^2}(c\lambda R_g)^{-1/2}, \\
\|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\partial_j v_\rho\|_{L^2} & \lesssim \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\rho\,\boldsymbol{\eta}_{cR_g}^{(\lambda/2)}\|_{\mathcal{C}} + \|\rho\|_{L^1}\Big(\frac{\|\nabla\theta_1^1\|_{L^\infty}^{1/4}}{(c\lambda R_g)^{1/2}} + \frac{\|\nabla\theta_1^1\|_{L^\infty}}{(c\lambda R_g)^{3/4}}\Big) \\
& \quad + \|\rho\|_{L^2}^{1/6}\|\rho\|_{L^1}^{5/6}\frac{\|\nabla\theta_1^1\|_{L^\infty}^{3/4}}{(c\lambda R_g)^{1/2}} + \|\rho\|_{L^1}\Big(\frac{1 + \|\nabla\theta_1^1\|_{L^\infty}}{(c\lambda R_g)^{1/2}}\Big).
\end{array}\right. \tag{126}$$

Moreover if we write $\gamma = \alpha Q_{0,1} + \alpha Q_{1,0} + \alpha^2\widetilde{Q}_2$, $\rho_N = n$ we also have:

$$\left\{\begin{array}{rl}
\|\boldsymbol{\eta}_{cR_g}^{(\lambda)}\rho_\gamma\|_{\mathcal{C}} & \lesssim \frac{\alpha}{c\lambda R_g}\|\nabla\theta_1^1\|_{L^\infty}(\|n\|_{\mathcal{C}} + \|\alpha\rho_{1,0} + \alpha^2\widetilde{\rho}_2\|_{L^{6/5}}) \\
& \quad + L\|\boldsymbol{\eta}_{cR_g}^{(\lambda)} n\|_{\mathcal{C}} + \|\boldsymbol{\eta}_{cR_g}^{(\lambda)}(\alpha\rho_{1,0} + \alpha^2\widetilde{\rho}_2)\|_{\mathcal{C}}.
\end{array}\right. \tag{127}$$

We recall that $\|\rho\|_{L^{6/5}} \lesssim \|\rho\|_{L^2}^{1/3}\|\rho\|_{L^1}^{2/3}$.

Proof: We will write $v_\rho = v$ for convenience.

The term $\|\boldsymbol{\eta}_{c\mathbf{R}_g}^{(\lambda)} R_N\|_{\mathfrak{S}_2}$

$$\begin{aligned}
\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)} N_j\|_{\mathfrak{S}_2}^2 &= \iint \frac{(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2(x)|\psi_j(x)|^2|\psi_j(y)|^2}{|x-y|^2}dxdy \\
&= \int_x dx(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2(x)|\psi_j(x)|^2\int_y \frac{|\psi_j(y)|^2}{|x-y|^2}dy \\
&\leq 4\|\nabla\psi_j\|_{L^2}^2\int_x(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2(x)|\psi_j(x)|^2dx \lesssim \frac{1}{(\lambda\mathrm{R}_g)^2}\frac{1}{c^2}
\end{aligned}$$

where we have used Lemma 7.

The term $\|\boldsymbol{\eta}_{c\mathbf{R}_g}^{(\lambda)}\gamma\|_{\mathbf{Ex}}$

$$\begin{aligned}
\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\|_{\mathrm{Ex}} &\leq \sqrt{\tfrac{\pi}{2}}\||D_0|^{1/2}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\gamma\|_{\mathfrak{S}_2} \\
&\leq \sqrt{\tfrac{\pi}{2}}\big(\|[|D_0|^{1/2}, \boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}]\gamma\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}\big) \\
&\lesssim \|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}\|_{L^\infty}\||D_0|^{1/2}\gamma\|_{\mathfrak{S}_2} + \|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2},
\end{aligned}$$

and we can treat $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{1/2}\gamma\|_{\mathfrak{S}_2}$ as $\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)}|D_0|^{a[\Lambda]}\gamma\|_{\mathfrak{S}_2}$.

The term $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathbf{R}_g} v\|_{L^6}$ We use the Sobolev inequality:

$$\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} v\|_{L^6} \quad \lesssim \|(\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}) v\|_{L^2} + \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \nabla v\|_{L^2}.$$

We get a term $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \nabla v\|_{L^2}$ we will treat later.

– For the term $\|(\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}) v\|_{L^2}$, we use the fact that $\rho * \frac{1}{|\cdot|}$ is L^3_w with weak norm of order $\|\rho\|_{L^1}$ [23] and we use rearrangement inequalities [16]: $\int |fg| \leq \int |f|_* |g|_*$ and $\|\nabla |f|_*\|_{L^2} \leq \|\nabla |f|\|_{L^2}$.

$$\begin{aligned}
\|(\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}) v\|^2_{L^2} &= \int |\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2 |v|^2 \leq \int (|\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2)_* (|v|^2)_* \\
&\lesssim \int (|\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2)_*(x) \frac{\|\rho\|^2_{L^1}}{|x|^2} dx \\
&\lesssim \|\rho\|^2_{L^1} \|\nabla \sqrt{(|\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2)_*}\|^2_{L^2} = \|\rho\|^2_{L^1} \|\nabla (\sqrt{|\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|^2})_*\|^2_{L^2} \\
&\lesssim \|\rho\|^2_{L^1} \|\nabla |\nabla \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}|\|^2_{L^2} \lesssim \|\rho\|^2_{L^1} \frac{\|\nabla |\nabla|\theta^1_1\|^2_{L^2}}{c\lambda \mathrm{R}_g}.
\end{aligned}$$

– For the term $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \partial_j v\|_{L^2}$, we write:

$$\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \partial_j v(x) = \int \frac{(y_j - x_j)}{|x-y|^3} (\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(x) - \boldsymbol{\eta}^{(y)}_{c\mathrm{R}_g}) \rho(y) dy + (\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \rho) * \Big(\partial_j \frac{1}{|\,\cdot\,|}\Big). \tag{128}$$

The last term will give $\|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \rho\|_{\mathcal{C}}$. From this point, due to the particular form of $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}$ there holds:

$$\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} = \boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g} \text{ so } \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \rho\|_{\mathcal{C}} = \|\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g} \rho\, \boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g}\|_{\mathcal{C}}. \tag{129}$$

Let us treat the first term of (128). More generally we take $\zeta(x) = \zeta_0(x/A)$ and we use the properties of $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}$ at the very end.

Taking the squared norm we have:

$$\iint \rho(x)\rho(x) dx dy \int \frac{(\zeta(t) - \zeta(x))(\zeta(t) - \zeta(y))(t_j - x_j)(t_j - y_j)}{|t-x|^3 |t-y|^3} dt.$$

We split at level $|x-y| = \sqrt{A}$: first if $|x-y| \geq \sqrt{A}$, then

$$\begin{aligned}
&\iint\limits_{|x-y| \geq \sqrt{A}} \frac{|\rho(x)||\rho(y)|}{|x-y|^{1/2}} \int \frac{\|\nabla \zeta\|^{1/2}_{L^\infty} dt}{|t|^{7/4} |t - \mathbf{e}|^{7/4}} \\
&\qquad \leq \frac{\|\nabla \zeta\|^{1/2}_{L^\infty}}{\sqrt{A}} \|\rho\|^2_{L^1} \lesssim \frac{L^2 \|\nabla \zeta_0\|^{1/2}_{L^\infty}}{A}.
\end{aligned}$$

If $|x-y| \leq \sqrt{A}$ then there holds $|x-y| \|\nabla \zeta\|_{L^\infty} \leq \|\nabla \zeta_0\|_{L^\infty} \frac{1}{\sqrt{A}}$, thus $\zeta(x) = \zeta(y) + \zeta(x) - \zeta(y)$ and we substitute in the integral over t. We split $\mathbb{R}^3$ in three: $|t-x| < |x-y|/2$, $|t-y| < |x-y|/2$ and the remainder domain.

a. For the first ball $B(x, |x-y|/2) = B_x$:

$$\int_{B_x} \frac{|\zeta(x) - \zeta(t)||\zeta(y) - \zeta(t)|}{|t-x|^2 |t-y|^2} dt \leq \frac{\|\nabla \zeta_0\|^2_{L^\infty}}{A^{3/2}} \int_{B_x} \frac{dt}{|t-x|^2 |t-y|} \quad \lesssim \frac{\|\nabla \zeta_0\|^2_{L^\infty}}{A^{3/2}}.$$

b. The same holds for the ball B_y. c. For the remainder domain C_{xy}:

c.1. we first deal with the term $(\zeta(y) - \zeta(x)(\zeta(t) - \zeta(y))$:

$$\begin{aligned}
\int\limits_{t \in C_{xy}} dt \frac{|(\zeta(x) - \zeta(y))(\zeta(t) - \zeta(y))|}{|x-t|^2 |y-t|^2} \quad &\leq \frac{(\|\nabla \zeta_0\|_{L^\infty})^{3/2}}{A} \int \frac{dt}{|x-t|^2 |y-t|^{3/2}} \\
&\lesssim \frac{(\|\nabla \zeta_0\|_{L^\infty})^{3/2}}{A} \frac{1}{|x-y|^{1/2}}
\end{aligned}$$

$$\text{and:} \iint \frac{|\rho(x)||\rho(y)|}{|x-y|^{1/2}}dxdy \lesssim \|\rho\|_{L^2}^{1/3}\|\rho\|_{L^1}^{5/3} \lesssim L^2 c^{-1/2}.$$

We used above the Hardy-Littlewood-Sobolev inequality [16, Theorem 4.3].
c.2. At last we must handle the term $(\zeta(t)-\zeta(x))^2$:

$$\iint\limits_{|x-y|\leq\sqrt{A}} \rho(x)\rho(y)dxdy \int\limits_{t\in C_{xy}} \frac{(\zeta(t)-\zeta(y))^2(t_j-y_j)(t_j-x_j)}{|x-t|^3|y-t|^3}dt.$$

As $t\in C_{xy}$ we can replace $|x-t|^{-2}$ by $K|y-t|^{-2}$.

$$\int\limits_{t\in C_{xy}} \frac{(\zeta(t)-\zeta(y))^2}{|t-y|^4}dt \quad \leq \int_t \frac{(\zeta(t)-\zeta(y))^2}{|t-y|^4}dt.$$

We use now the properties of the function $\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}$. It is easy to see that no matter where $y\in\mathbb{R}^3$ is, this last integral is $\mathcal{O}((c\lambda\mathrm{R}_g)^{-1}K(\theta_1^1))$. Indeed let Ext be the domain defined by $\mathrm{Ext}=\{y\in\mathbb{R}^3 : f(y):=\mathrm{dist}(y,\{\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\neq 1\})>2c\lambda\mathrm{R}_g\}$.
c.2.1. If $y\in\mathrm{Ext}$, then it is clear that the previous integral is an

$$\mathcal{O}\Big(\frac{(c\lambda\mathrm{R}_g)^3}{f(y)^4}\Big)=\mathcal{O}\big(\frac{1}{c\lambda\mathrm{R}_g}\big).$$

c.2.2. Else we split $\mathbb{R}^3$ at level $|t-y|=2c\lambda\mathrm{R}_g$:

$$\int\limits_{|t-y|\leq 2c\lambda\mathrm{R}_g} dt\frac{(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(t)-\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(y))^2}{|t-y|^4} \lesssim \frac{\|\nabla\theta_1^1\|_{L^\infty}^2}{(c\lambda\mathrm{R}_g)^2}(c\lambda\mathrm{R}_g)=\mathcal{O}\big(\frac{\|\nabla\theta_1^1\|_{L^\infty}^2}{c\lambda\mathrm{R}_g}\big).$$

$$\int\limits_{|t-y|>2c\lambda\mathrm{R}_g} dt\frac{(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(t)-\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(y))^2}{|t-y|^4} \leq \int\limits_{|t-y|>2c\lambda\mathrm{R}_g} \frac{dt}{|t-y|^4}=\mathcal{O}\Big(\frac{1}{c\lambda\mathrm{R}_g}\Big).$$

Proof of (127) To begin with we remark that by the Hardy-Littlewood-Sobolev inequality [16]: $\|\rho\|_{\mathcal{C}}\lesssim\|\rho\|_{L^{6/5}}$. Then we use formula (56) of ρ_γ. We write

$$\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(x)\check{F}_\Lambda*\rho(x)=\int_y(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(x)-\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}(y))\check{F}_\Lambda(x-y)\rho(y)dy+\check{F}_\Lambda*(\boldsymbol{\eta}^{(\lambda)}_{c\mathrm{R}_g}\rho)(x).$$

So it suffices to show $\||\cdot|\check{F}_\Lambda\|_{L^1}\lesssim\alpha$ to end the proof: this is precisely (54)-(55), applied with $\ell=1$ to $\check{F}_\Lambda$ (true if α is less than some $K(\ell=1)$). □

D.2.4 Proof of Lemma 9

We write ξ instead of $\xi_j^{(\frac{1}{3})}$ and Q instead of γ' for convenience.

First remark: for any $\varepsilon,\varepsilon'\in\{+,-\}$:

$$P^0_\varepsilon\xi P^0_\varepsilon Q P^0_{\varepsilon'}\xi P^0_{\varepsilon'}=[P^0_\varepsilon,\xi]Q^{\varepsilon\,\varepsilon'}[\xi,P^0_{\varepsilon'}]+[P^0_\varepsilon,\xi]Q^{\varepsilon\,\varepsilon'}\xi+\xi Q^{\varepsilon\,\varepsilon'}[\xi,P^0_{\varepsilon'}]+\xi Q^{\varepsilon\,\varepsilon'}\xi. \quad (130)$$

This gives the error term between $\xi Q\xi$ and $\xi[Q]$. We estimate their density as in Section D.1, that is by duality.

Second remark: $\partial_j\xi^{(\lambda)}=(\partial_j\xi)\boldsymbol{\eta}^{(\lambda/2)}_{c\mathrm{R}_g}$.

As in this section, by using (94), it is clear that

$$\|[P^0_\varepsilon,\xi]Q^{\varepsilon\,\varepsilon'}[\xi,P^0_{\varepsilon'}]\|_{\mathcal{C}}\lesssim\||D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2}\|\xi\|_{L^6}^2\lesssim\frac{\||D_0|^{a[\Lambda]}Q\|_{\mathfrak{S}_2}}{(c\mathrm{R}_g)^2}.$$

We can drop terms involving the density of these operators.

We write:

$$\xi^{+-}=\frac{i}{2\pi}\int_{-\infty}^{+\infty}\frac{1}{D_0+i\omega}(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)})^2(\boldsymbol{\alpha}\cdot\nabla\xi)\frac{d\omega}{D_0+i\omega}.$$

We commute $\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}$ with $(D_0+i\omega)^{-1}$ on the right and on the left. As shown before there holds:

$$\Big|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}(x)-\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}(y))\frac{1}{D_0+i\omega}(x-y)\Big|\lesssim\frac{e^{-E(\omega)|x-y|/2}}{|x-y|}\|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{L^\infty}.$$

So taking KSS inequalities under the integral sign we obtain for instance:

$$\begin{aligned}&\mathrm{Tr}\big(P_-^0\xi Q\xi^{+-}VP_-^0\big)=\mathrm{Tr}\Big(P_-^0\xi Q\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\xi^{+-}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}VP_-^0\Big)\\&+\mathcal{O}\Big(\|V\|_{L^6}\|Q|D_0|^{1/2}\|_{\mathfrak{S}_2}\|\nabla\xi\|_{L^3}\|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{L^\infty}\int_{\mathbb{R}}\frac{d\omega}{E(\omega/2)^{5/4}}\Big)\\&+\mathcal{O}\Big(\|\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{L^\infty}^2\|V\|_{L^6}\|\nabla\xi\|_{L^3}\|Q\|_{\mathfrak{S}_2}\int_{\mathbb{R}}\frac{d\omega}{E(\omega/2)^2}\Big).\end{aligned}$$

There remains the first trace. First of all, for any V Schwartz, we can show as in Section D.1 that the operator is trace-class with norm controlled by

$$\sqrt{\log(\Lambda)}\|\nabla(\xi\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}V)\|_{L^2}\||D_0|^{1/2}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}Q^{+-}\|_{\mathfrak{S}_2}+\|\nabla\xi\|_{L^\infty}\|\nabla(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}V)\|_{L^2}\|QP_+^0\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\|_{\mathfrak{S}_2}.$$

We have *a priori* $\|\nabla(\xi\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}V)\|_{L^2}\lesssim\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\nabla V\|_{L^2}+\|\nabla(\xi\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)})\|_{L^3}\|V\|_{L^6}$.
In particular:

$$\|[P_\varepsilon^0,\xi]Q^{\varepsilon\,\varepsilon'}\xi\|_{\mathcal{C}}\lesssim\sqrt{\log(\Lambda)}\||D_0|^{1/2}\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}Q^{\varepsilon'\,\varepsilon}\|_{\mathfrak{S}_2}\lesssim\frac{L}{\sqrt{c\lambda\mathrm{R}_g}}.$$

We use now the fact that we want the trace *for a particular* V, namely $\rho[\xi Q\xi]*\frac{1}{|\cdot|}$. So as in Proposition 9, the function $(\xi^2\rho_\gamma')*\frac{1}{|\cdot|}$ is in L^3_w and

$$\|(\nabla\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)})\big[(\xi^2\rho_\gamma')*\tfrac{1}{|\cdot|}\big]\|_{L^2}\lesssim\frac{\sqrt{2}}{\sqrt{\lambda c\mathrm{R}_g}}\|\rho_\gamma'\|_{L^1}\lesssim\frac{\sqrt{2}}{\sqrt{\lambda c\mathrm{R}_g}}.$$

Then we write $(\xi^2\rho_\gamma')*\frac{1}{|\cdot|}=\rho_\gamma'*\frac{1}{|\cdot|}-((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2\rho_\gamma')*\frac{1}{|\cdot|}$ and

$$\begin{aligned}\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\nabla\big[(\xi^2\rho_\gamma')*\tfrac{1}{|\cdot|}\big]\|_{L^2}&\lesssim\|\nabla((\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2\rho_\gamma')*\tfrac{1}{|\cdot|}\|_{L^2}+\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\nabla(\rho_\gamma')*\tfrac{1}{|\cdot|}\|_{L^2}\\&\lesssim\|(\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda)})^2\rho_\gamma'\|_{\mathcal{C}}+\sum_{j=1}^3\|\boldsymbol{\eta}_{c\mathrm{R}_g}^{(\lambda/2)}\partial_j v_{\rho_\gamma}'\|_{L^2},\end{aligned}$$

and those terms are dealt with Propositions 9 and 8.

Putting everything together, we get an error term of order:

$$\sqrt{\log(\Lambda)}\times\frac{1}{c\sqrt{\mathrm{R}_g}}\times\frac{1}{\sqrt{c\mathrm{R}_g}}=\mathcal{O}\Big(\frac{L}{c\mathrm{R}_g}\Big).$$

References

[1] V. Bach, J.-M. Barbaroux, B. Helffer, and H. Siedentop. On the stability of the relativistic electron-positron field. *Comm. Math. Phys*, 201:445–460, 1998.

[2] É. Cancès, A. Deleurence, and M. Lewin. A new approach to the modelling of local defects in crystals: the reduced Hartree-Fock case. *Commun. Math. Phys.*, 281:129–177, 2008.

[3] P. Chaix and D. Iracane. From quantum electrodynamics to mean-field theory: I. the Bogoliubov-Dirac-Fock formalism. *J. Phys. B: At. Mol. Opt. Phys.*, 22:3791–3814, 1989.

[4] M. Esteban and É. Séré. Nonrelativistic limit of the Dirac-Fock equations. *Ann. Henri Poincaré*, pages 941–961, 2001.

[5] R. L. Frank, E. H. Lieb, R. Seiringer, and L. Thomas. Stability and absence of binding for multi-polaron systems. *Publ. Math. IHES*, 113(1):39–67, 2011.

[6] Ph. Gravejat, M. Lewin, and É. Séré. Ground state and charge renormalization in a nonlinear model of relativistic atoms. *Comm. Math. Phys*, 286, 2009.

[7] C. Hainzl, M. Lewin, and É. Séré. Existence of a stable polarized vacuum in the Bogoliubov-Dirac-Fock approximation. *Comm. Math. Phys*, 257, 2005.

[8] C. Hainzl, M. Lewin, and É. Séré. Self-consistent solution for the polarized vacuum in a no-photon QED model. *J. Phys. A: Math and Gen.*, 38(20):4483–4499, 2005.

[9] C. Hainzl, M. Lewin, and É. Séré. Existence of atoms and molecules in the mean-field approximation of no-photon quantum electrodynamics. *Arch. Rational Mech. Anal*, 192(3):453–499, 2009.

[10] C. Hainzl and H. Siedentop. Non-perturbative mass and charge renormalization in relativistic no-photon quantum electrodynamics. *Comm. Math. Phys.*, 243(2):241–260, 2003.

[11] E. Lenzmann. Uniqueness of ground states for pseudo-relativistic Hartree equations. *Analysis and PDE*, 1(3):1–27, 2009.

[12] M. Lewin. Geometric methods for nonlinear many-body quantum systems. *J. Funct. Anal.*, 260:3535–3595, 2011.

[13] M. Lewin and N. Rougerie. Derivation of Pekar's polarons from a microscopic of quantum crystals. *SIAM J. Math. Anal.*, 2011.

[14] M. Lewin and N. Rougerie. On the binding of polarons in a mean-field quantum crystal. *ESAIM Control Optim. Calc. Var.*, 2012.

[15] E. H. Lieb. Existence and uniqueness of the minimizing solution of Choquard's nonlinear equation. *Studies in Applied Mathematics*, 57:93–105, October 1977.

[16] E. H. Lieb and M. Loss. *Analysis*. AMS, 1997.

[17] E. H. Lieb and R. Seiringer. *The stability of matter in quantum mechanics*. Cambridge University Press, Cambridge, 2010.

[18] M. Reed and B. Simon. *Methods of Modern Mathematical Physics*, volume I-II. Academic Press Inc., 1975.

[19] B. Simon. *Trace Ideals and their Applications*, volume 35 of *London Mathematical Society Lecture Notes Series*. Cambridge University Press, 1079.

[20] J. Sok. Charge renormalisation in a mean-field approximation of QED, 2013. preprint, http://arxiv.org/abs/1311.6575.

[21] J. Sok. Existence of ground state of an electron in the BDF approximation. *Rev. Math. Phys.*, 26(5), 2014.

[22] J. Sok. *Modèle de champ moyen en électrodynamique quantique*. PhD thesis, Université Paris-Dauphine, 2014.

[23] E. Stein. *Singular Integrals and Differentiability of Functions*. Princeton University Press, 1970.

[24] B. Thaller. *The Dirac Equation*. Springer Verlag, 1992.

[25] G. N. Watson. *A treatise on the theory of Bessel functions*. Cambridge University Press, 1922.