The positronium in a mean-field approximation of quantum electrodynamics.

Sok Jérémy
Ceremade, UMR 7534, Université Paris-Dauphine,
Place du Maréchal de Lattre de Tassigny,
75775 Paris Cedex 16, France.

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Abstract

The Bogoliubov-Dirac-Fock (BDF) model is a no-photon, mean-field approximation of quantum electrodynamics. It describes relativistic electrons in the Dirac sea. In this model, a state is fully characterized by its one-body density matrix, an infinite rank nonnegative operator. We prove the existence of the positronium, the bound state of an electron and a positron, represented by a critical point of the energy functional in the absence of external field. This state is interpreted as the ortho-positronium, where the two particles have parallel spins.

Contents

1 Introduction and main results

The Dirac operator

In relativistic quantum mechanics, the kinetic energy of an electron is described by the so-called *Dirac operator* D_0. Its expression is [Tha92]:

$$D_0 := m_e c^2 \beta - i\hbar c \sum_{j=1}^{3} \alpha_j \partial_{x_j} \tag{1}$$

where m_e is the (bare) mass of the electron, c the speed of light and $\hbar$ the reduced Planck constant, β and the α_j's are 4×4 matrices defined as follows:

$$\beta := \begin{pmatrix} \mathrm{Id}_{\mathbb{C}^2} & 0 \\ 0 & -\mathrm{Id}_{\mathbb{C}^2} \end{pmatrix},\ \alpha_j \begin{pmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{pmatrix},\ j \in \{1,2,3\}$$

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

The Dirac operator acts on spinors *i.e.* square-integrable $\mathbb{C}^4$-valued functions:

$$\mathfrak{H} := L^2\big(\mathbb{R}^3, \mathbb{C}^4\big). \tag{2}$$

It corresponds to the Hilbert space associated to one electron. The operator D_0 is self-adjoint on $\mathfrak{H}$ with domain $H^1(\mathbb{R}^3, \mathbb{C}^4)$, but contrary to $-\Delta/2$ in quantum mechanics, it is unbounded from below.

Indeed its spectrum is $\sigma(D_0) = (-\infty, m_e c^2] \cup [m_e c^2, +\infty)$. Dirac postulated that all the negative energy states are already occupied by "virtual electrons", with one electron in each state, and that the uniform filling is unobservable to us. Then, by Pauli's principle real electrons can only have a positive energy.

It follows that the relativistic vacuum, composed by those negatively charged virtual electrons, is a polarizable medium that reacts to the presence of an external field. This phenomenon is called the *vacuum polarization*.

If one turns on an external field that gets strong enough, it leads to a transition of an electron of the Dirac sea from a negative energy state to a positive one. The resulting system – an electron with positive energy plus a hole in the Dirac sea – is interpreted as an electron-positron pair. Indeed the absence of an electron in the Dirac sea is equivalent to the addition of a particle with same mass and opposite charge: the positron.

Its existence was predicted by Dirac in 1931. Although firstly observed in 1929 independently by Skobeltsyn and Chung-Yao Chao, it was recognized in an experiment lead by Anderson in 1932.

Charge conjugation

Following Dirac's ideas, the free vacuum is described by the negative part of the spectrum $\sigma(D_0)$:

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

The correspondence between negative energy states and positron states is given by the *charge conjugation* C [Tha92]. This is an antiunitary operator that maps $\mathrm{Ran}\, P_-^0$ onto $\mathrm{Ran}(1 - P_-^0)$. In our convention [Tha92] it is defined by the formula:

$$\forall\, \psi \in L^2(\mathbb{R}^3),\ \mathrm{C}\psi(x) = i\beta\alpha_2 \overline{\psi}(x), \tag{3}$$

where $\overline{\psi}$ denotes the usual complex conjugation. More precisely:

$$\mathrm{C} \cdot \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_2 \\ \psi_4 \end{pmatrix} = \begin{pmatrix} \overline{\psi}_4 \\ -\overline{\psi}_3 \\ -\overline{\psi}_2 \\ \overline{\psi}_1 \end{pmatrix}. \tag{4}$$

In our convention it is also an *involution*: $\mathrm{C}^2 = \mathrm{id}$. An important property is the following:

$$\forall\, \psi \in L^2, \forall\, x \in \mathbb{R}^3,\ |\mathrm{C}\psi(x)|^2 = |\psi(x)|^2. \tag{5}$$

Positronium

The positronium is the bound state of an electron and a positron. This system was independently predicted by Anderson and Mohorovičić in 1932 and 1934 and was experimentally observed for the first time in 1951 by Martin Deutsch.

It is unstable: depending on the relative spin states of the positron and the electron, its average lifetime in vacuum is 125 ps (para-positronium) or 142 ns (ortho-positronium) (see [Kar04]).

In this paper, we are looking for a positronium state within the Bogoliubov-Dirac-Fock (BDF) model: the state we found can be interpreted as the ortho-positronium where the electron and positron have parallel spins. Our main results are Theorem 1 and 3. In our state, the wave function of the real electron and that of the virtual electron defining the positronium are charge conjugate of each other.

BDF model

The BDF model is a no-photon approximation of quantum electrodynamics (QED) which was introduced by Chaix and Iracane in 1989 [CI89], and studied in many papers [BBHS98, HLS05a, HLS05b, HLS07, HLS09, GLS09, Sok12].

It allows to take into account real electrons together with the Dirac vacuum in the presence of an external field.

This is a Hartree-Fock type approximation in which a state of the system "vacuum + real electrons" is given by an infinite Slater determinant $\psi_1 \wedge \psi_2 \wedge \cdots$. Equivalently, such a state is represented by the projector onto the space spanned by the ψ_j's: its so-called one-body density matrix. For instance P_-^0 represents the free Dirac vacuum.

Here we just give main ideas of the derivation of the BDF model from QED, we refer the reader to [CI89, HLS05a, HLS07] for full details.

Remark 1. To simplify the notations, we choose relativistic units in which, the mass of the electron m_e, the speed of light c and $\hbar$ are set to 1.

Let us say that there is an external density ν, *e.g.* that of some nucleus and let us write $\alpha > 0$ the so-called *fine structure constant* (physically $e^2/(4\pi\varepsilon_0\hbar c)$, where e is the elementary charge and ε_0 the permittivity of free space).

The starting point is the (complicated) Hamiltonian of QED $\mathbb{H}_{\mathrm{QED}}$ that acts on the Fock space of the electron $\mathcal{F}_{\mathrm{elec}}$ [Tha92]. The (formal) difference between the infinite energy of a Hartree-Fock state Ω_P and that of $\Omega_{P_-^0}$, state of the free vacuum taken as a reference state, gives a function of the reduced one-body density matrix $Q := P - P_-^0$.

It can be shown that a projector P is the one-body density matrix of a Hartree-Fock state in $\mathcal{F}_{\mathrm{elec}}$ *iff* $P - P_-^0$ is Hilbert-Schmidt, that is compact such that its singular values form a sequence in ℓ^2.

To get a well-defined energy, one has to impose an ultraviolet cut-off $\Lambda > 0$: we replace $\mathfrak{H}$ by its subspace

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

This procedure gives the BDF energy introduced in [CI89] and studied for instance in [HLS05a, HLS05b].

Notation 1. Our convention for the Fourier transform $\mathscr{F}$ is the following

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

Let us notice that $\mathfrak{H}_\Lambda$ is invariant under D_0 and so under P_-^0.

For the sake of clarity, we will emphasize the ultraviolet cut-off and write Π_Λ for the orthogonal projection onto $\mathfrak{H}_\Lambda$: Π_Λ is the following Fourier multiplier

$$\Pi_\Lambda := \mathscr{F}^{-1}\chi_{B(0,\Lambda)}\mathscr{F}. \tag{6}$$

By means of a thermodynamical limit, Hainzl *et al.* showed in [HLS07] that the formal minimizer and hence the reference state should not be given by $\Pi_\Lambda P_-^0$ but by another projector $\mathcal{P}_-^0$ in $\mathfrak{H}_\Lambda$ that satisfies the self-consistent equation *in* $\mathfrak{H}_\Lambda$:

$$\left\{\begin{array}{rcl} \mathcal{P}_-^0 - \frac{1}{2} & = & -\mathrm{sign}\big(\mathcal{D}^0\big), \\ \mathcal{D}^0 & = & D_0 - \dfrac{\alpha}{2}\dfrac{(\mathcal{P}_-^0 - \frac{1}{2})(x-y)}{|x-y|} \end{array}\right. \tag{7}$$

We have $\mathcal{P}_-^0 = \chi_{(-\infty,0)}(\mathcal{D}^0)$.

In $\mathfrak{H}$, the operator $\mathcal{D}^0$ coincides with a bounded, matrix-valued Fourier multiplier whose kernel is $\mathfrak{H}_\Lambda^\perp \subset \mathfrak{H}$.

The resulting BDF energy $\mathcal{E}^\nu_{\mathrm{BDF}}$ is defined on Hartree-Fock states represented by their one-body density matrix P:

$$\mathscr{N} := \big\{P \in \mathcal{B}(\mathfrak{H}_\Lambda),\ P^* = P^2 = P,\ P - \mathcal{P}_-^0 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\big\}.$$

This energy depends on three parameters: the fine structure constant $\alpha > 0$, the cut-off $\Lambda > 0$ and the external density ν. We assume that ν has finite *Coulomb energy*, that is

$$D(\nu,\nu) := 4\pi\int_{\mathbb{R}^3}\frac{|\widehat{\nu}(k)|^2}{|k|^2}dk. \tag{8}$$

Remark 2. The Coulomb energy coincides with $\iint\limits_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\nu(x)^*\nu(y)}{|x-y|}dxdy$ whenever this integral is well-defined.

Remark 3. The operator $\mathcal{D}^0$ was previously introduced by Lieb *et al.* in [LS00] in another context in the case $\alpha\log(\Lambda)$ small.

Notation 2. We recall that $\mathcal{B}(\mathfrak{H}_\Lambda)$ is the set of bounded operators and $\mathfrak{S}_p(\mathfrak{H}_\Lambda)$ the set of compact operators whose singular values form a sequence in ℓ^p [RS75, Appendix IX.4 Vol II], [Sim79] ($p \geq 1$). In particular $\mathfrak{S}_\infty(\mathfrak{H}_\Lambda)$ is the set $\mathrm{Comp}(\mathfrak{H}_\Lambda)$ of compact operators.

Notation 3. Throughout this paper we write

$$m = \inf\sigma\big(|\mathcal{D}^0|\big) \geq 1, \tag{9}$$

and

$$\mathcal{P}_+^0 := \Pi_\Lambda - \mathcal{P}_-^0 = \chi_{(0,+\infty)}(\mathcal{D}^0). \tag{10}$$

The same symmetry holds for $\mathcal{P}_-^0$ and $\mathcal{P}_+^0$: the charge conjugation C maps $\mathrm{Ran}\,\mathcal{P}_-^0$ onto $\mathrm{Ran}\,\mathcal{P}_+^0$.

Minimizers and critical points

The charge of a state $P \in \mathscr{N}$ is given by the so-called $\mathcal{P}_-^0$-trace of $P - \mathcal{P}_-^0$

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

This trace is well defined as we can check from the formula [HLS05a]

$$(P-\mathcal{P}_-^0)^2 = \mathcal{P}_+^0(P-\mathcal{P}_-^0)\mathcal{P}_+^0 - \mathcal{P}_-^0(P-\mathcal{P}_-^0)\mathcal{P}_-^0. \tag{11}$$

Minimizers of the BDF energy with charge constraint $N \in \mathbb{N}$ corresponds to ground states of a system of N electrons in the presence of an external density ν.

The problem of their existence was studied in several papers [HLS09, Sok12, Sok13]. In [HLS09], Hainzl *et al.* proved that it was sufficient to check binding inequalities and showed existence of ground states in the presence of an external density ν, provided that $N-1<\int\nu$, under technical assumptions on α,Λ.

In [Sok12], we proved that, due to the vacuum polarization, there exists a minimizer for $\mathcal{E}^0_{\rm BDF}$ with charge constraint 1: in other words an electron can bind alone in the vacuum without any external charge (still under technical assumptions on α,Λ).

In [Sok13], the effect of charge screening is studied: due to vacuum polarization, the observed charge of a minimizer $P\neq\mathcal{P}^0_-$ is different from its real charge $\mathrm{Tr}_{\mathcal{P}^0_-}(P-\mathcal{P}^0_-)$.

Here we are looking for a positronium state, that is an electron and a positron in the vacuum without any external density. So we have to study $\mathcal{E}^0_{\rm BDF}$ on

$$\mathscr{M}:=\Big\{P\in\mathscr{N},\ \mathrm{Tr}_{\mathcal{P}^0_-}\left(P-\mathcal{P}^0_-\right)=0\Big\}. \tag{12}$$

From a geometrical point of view $\mathscr{M}$ is a Hilbert manifold and $\mathcal{E}^0_{\rm BDF}$ is a differentiable map on $\mathscr{M}$ (Propositions 1 and 2).

We thus seek a critical point on $\mathscr{M}$, that is some $P\in\mathscr{M},\ P\neq\mathcal{P}^0_-$ such that $\nabla\mathcal{E}^0_{\rm BDF}(P)=0$. We also must ensure that this is a positronium state. A good candidate is a projector P that is obtained from $\mathcal{P}^0_-$ by substracting a state $\psi_-\in\mathrm{Ran}\,\mathcal{P}^0_-$ and adding a state $\psi_+\in\mathrm{Ran}\,\mathcal{P}^0_+$, that is

$$P=\mathcal{P}^0_-+|\psi_+\rangle\langle\psi_+|-|\psi_-\rangle\langle\psi_-|. \tag{13}$$

But there is no reason why such a projector would be a critical point. If it were that would mean that there exists a positronium state in which, apart from the excitation of the virtual electron giving the electron-positron pair, the vacuum is not polarized.

Keeping (13) in mind, we identify a subset $\mathscr{M}_{\mathscr{C}}\subset\mathscr{M}$, made of C-symmetric states.

Definition 1. The set $\mathscr{M}_{\mathscr{C}}$ of C-symmetric states is defined as:

$$\mathscr{M}_{\mathscr{C}}=\{P\in\mathscr{M},\ -\mathrm{C}(P-\mathcal{P}^0_-)\mathrm{C}=P-\mathcal{P}^0_-\}. \tag{14}$$

Remark 4. Let $P\in\mathscr{M}_{\mathscr{C}}$. As $-\mathrm{C}(\mathcal{P}^0_--\mathcal{P}^0_+)\mathrm{C}=\mathcal{P}^0_--\mathcal{P}^0_+$, writing

$$P-\mathcal{P}^0_-=\tfrac{1}{2}\big(P-(\Pi_\Lambda-P)-\mathcal{P}^0_-+\mathcal{P}^0_+\big),$$

there holds:

$$P\in\mathscr{M}_{\mathscr{C}}\Rightarrow P+\mathrm{C}P\mathrm{C}=\Pi_\Lambda, \tag{15}$$

that is

$$\forall\,P\in\mathscr{M}_{\mathscr{C}},\ \mathrm{C}:\mathrm{Ran}\,P\to\mathrm{Ran}(\Pi_\Lambda-P)\text{ is an isometry.}$$

The set $\mathscr{M}_{\mathscr{C}}$ has fine properties: this is a submanifold, invariant under the gradient flow of $\mathcal{E}^0_{\rm BDF}$ (Proposition 3). Moreover it has two connected components $\mathscr{E}_1$ and $\mathscr{E}_{-1}$ (Proposition 4). In particular, any extremum of the BDF energy restricted to $\mathscr{M}_{\mathscr{C}}$ is a critical point on $\mathscr{M}$.

So we are lead to seek a minimizer over each of these connected components: the first ($\mathscr{E}_1$) gives $\mathcal{P}^0_-$, which is the global minimizer over $\mathscr{N}$, but the second gives a non-trivial critical point. It corresponds to the positronium and is a perturbation of a state which can be written as in (13).

Our main Theorems are the following:

Theorem 1. *There exist $\alpha_0,\Lambda_0,L_0>0$ such that if $\alpha\leq\alpha_0,\Lambda^{-1}\leq\Lambda_0^{-1}$, and $\alpha\log(\Lambda)\leq L_0$, then there exists a minimizer of $\mathcal{E}^0_{\rm BDF}$ over $\mathscr{E}_{-1}$. Moreover we have*

$$E_{1,1}:=\inf\{\mathcal{E}^0_{\rm BDF}(P),\ P\in\mathscr{E}_{-1}\}\leq 2m+\frac{\alpha^2 m}{g_1'(0)^2}E_{\rm CP}+\mathcal{O}(\alpha^3),$$

where $E_{\mathrm{CP}} < 0$ is the Choquard-Pekar energy defined as follows [Lie77]:

$$E_{\mathrm{CP}} = \inf\Big\{ \|\nabla\phi\|_{L^2}^2 - D\big(|\phi|^2, |\phi|^2\big),\ \phi \in L^2(\mathbb{R}^3),\ \|\phi\|_{L^2} = 1 \Big\}. \tag{16}$$

Theorem 2. *Under the same assumptions as in Theorem 1, let $\overline{P}$ be a minimizer for $E_{1,1}$. Then there exists an anti-unitary map $A \in \mathbf{A}(\mathfrak{H}_\Lambda)$, and $P^0_{1,1}$ of form (13) such that*

$$\left|\begin{array}{l} \overline{P} = e^A P^0_{1,1} e^A, \\ e^A \psi_\varepsilon = \psi_\varepsilon,\ \varepsilon \in \{+,-\} \text{ and } \psi_- = \mathrm{C}\psi_+, \\ A = \big[\big[A, \mathcal{P}^0_-\big], \mathcal{P}^0_-\big] \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ \|A\|_{\mathfrak{S}_2} \lesssim \alpha, \\ \text{and } \mathrm{C}A\mathrm{C} = A. \end{array}\right. \tag{17}$$

Moreover, the following holds:

$$E_{1,1} = 2m + \frac{\alpha^2 m}{g_1'(0)^2} E_{\mathrm{CP}} + \mathcal{O}(\alpha^3). \tag{18}$$

We emphasize that ψ_+ *does not* represent the electron state.

Theorem 3. *Under the same assumptions as in Theorem 1, let $\overline{P}$ be a minimizer for $E_{1,1}$ and $Q_0 = \overline{P} - \mathcal{P}^0_-$. Let $\overline{\boldsymbol{\pi}}$ be*

$$\overline{\boldsymbol{\pi}} := \chi_{(-\infty,0)}\big(\Pi_\Lambda D_{Q_0} \Pi_\Lambda\big). \tag{19}$$

Then there holds $\mathrm{Ran}\,(\Pi_\Lambda - \overline{\boldsymbol{\pi}}) \cap \mathrm{Ran}\,\overline{P} = \mathbb{C}\psi_e$. The unitary wave function ψ_e satisfies the equation

$$D_{Q_0}\psi_e = \mu_e \psi_e, \tag{20}$$

where μ_e is some constant

$$K_0\alpha^2 \le m - \mu_e \le K_1\alpha^2,\ K_0, K_1 > 0.$$

By C-symmetry $\psi_v := \mathrm{C}\psi_e$ satisfies $D_{Q_0}\psi_v = -\mu_e\psi_v$, and we have

$$\overline{P} = \overline{\boldsymbol{\pi}} + |\psi_e\rangle\langle\psi_e| - |\psi_v\rangle\langle\psi_v|. \tag{21}$$

Moreover the following holds. We split ψ_e into upper spinor $\varphi_e \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ and lower spinor $\chi_e \in L^2(\mathbb{R}^3, \mathbb{C}^2)$ and scale φ_e by $\lambda := \frac{g_1'(0)^2}{\alpha m}$:

$$\widetilde{\varphi}_e(x) := \lambda^{3/2}\varphi_e\big(\lambda x\big).$$

Then in the non-relativistic limit $\alpha \to 0$ (with $\alpha\log(\Lambda)$ kept small), the lower spinor χ_e tends to 0 and, up to translation, $\widetilde{\varphi}_e$ tends to a Pekar minimizer.

Remark 5. As ψ_e and $\psi_v = \mathrm{C}\psi_e$ have antiparallel spins, the state $\overline{P}$ represents one electron in state ψ_e and the absence of one electron in state ψ_v in the Dirac sea, that is an electron and a positron with *parallel spins*.

Remark 6. To prove that $\widetilde{\varphi}_e$ tends to a Pekar minimizer up to translation, it suffices to prove that its Pekar energy tends to E_{CP} [Lie77].

Notation 4. Throughout this paper we write K to mean a constant independent of α, Λ. Its value may differ from one line to the other. We also use the symbol $\lesssim$: $0 \le a \lesssim b$ means there exists $K > 0$ such that $a \le Kb$.

Remarks and notations about $\mathcal{D}^0$

$\mathcal{D}^0$ has the following form [HLS07]:

$$\mathcal{D}^0 = g_0(-i\nabla)\beta - i\boldsymbol{\alpha}\cdot\frac{\nabla}{|\nabla|}g_1(-i\nabla) \tag{22}$$

where g_0 and g_1 are smooth radial functions on $B(0,\Lambda)$ and $\boldsymbol{\alpha} = (\alpha_j)_{j=1}^3$. Moreover we have:

$$\forall\, p \in B(0,\Lambda),\ 1 \le g_0(p),\ \text{and } |p| \le g_1(p) \le |p| g_0(p). \tag{23}$$

Notation 5. For $\alpha\log(\Lambda)$ sufficiently small, we have $m = g_0(0)$ [LL97, Sok12].

Remark 7. In general the smallness of α is needed to ensure technical estimates hold. The smallness of $\alpha\log(\Lambda)$ is needed to get estimates of $\mathcal{D}^0$: in this case $\mathcal{D}^0$ can be obtained by a fixed point scheme [HLS07, LL97], and we have [Sok12, Appendix A]:

$$\begin{gathered} g_0'(0) = 0, \text{ and } \|g_0'\|_{L^\infty}, \|g_0''\|_{L^\infty} \leq K\alpha \\ \|g_1' - 1\|_{L^\infty} \leq K\alpha\log(\Lambda) \leq \tfrac{1}{2} \text{ and } \|g_1''\|_{L^\infty} \lesssim 1. \end{gathered} \tag{24}$$

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2 Description of the model

2.1 The BDF energy

Definition 2. Let $\alpha > 0, \Lambda > 0$ and $\nu \in \mathcal{S}'(\mathbb{R}^3)$ a generalized function with $D(\nu,\nu) < +\infty$. The BDF energy $\mathcal{E}^0_{\rm BDF}$ is defined on $\mathscr{N}$ as follows: for $P \in \mathscr{N}$ we write $Q := P - \mathcal{P}^0_-$ and

$$\begin{cases} \mathcal{E}^0_{\rm BDF}(Q) = \mathrm{Tr}_{\mathcal{P}^0_-}\left(\mathcal{D}^0 Q\right) - \alpha D(\rho_Q,\nu) + \dfrac{\alpha}{2}\Big(D(\rho_Q,\rho_Q) - \|Q\|^2_{\rm Ex}\Big), \\ \forall\, x,y \in \mathbb{R}^3,\ \rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big),\ \|Q\|^2_{\rm Ex} := \displaystyle\iint \frac{|Q(x,y)|^2}{|x-y|}dxdy, \end{cases} \tag{25}$$

where $Q(x,y)$ is the integral kernel of Q.

Remark 8. The term $\mathrm{Tr}_{\mathcal{P}^0_-}\left(\mathcal{D}^0 Q\right)$ is the kinetic energy, $-\alpha D(\rho_Q,\nu)$ is the interaction energy with ν. The term $\dfrac{\alpha}{2}D(\rho_Q,\rho_Q)$ is the so-called *diract term* and $-\dfrac{\alpha}{2}\|Q\|^2_{\rm Ex}$ is the *exchange term*.

1. Let us see that this function is well-defined and more generally that formula (25) is well-defined whenever Q is $\mathcal{P}^0_-$-trace-class [HLS05a, HLS09].

– We start by defining this notion. For any $\varepsilon,\varepsilon' \in \{+,-\}$ and $A \in \mathcal{B}(\mathfrak{H}_\Lambda)$, we write

$$A^{\varepsilon,\varepsilon'} := \mathcal{P}^0_\varepsilon A \mathcal{P}^0_{\varepsilon'}.$$

The set $\mathfrak{S}_1^{\mathcal{P}^0_-}$ of $\mathcal{P}^0_-$-trace class operator is the following Banach space:

$$\mathfrak{S}_1^{\mathcal{P}^0_-} = \left\{Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ Q^{++}, Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda)\right\}, \tag{26}$$

with the norm

$$\|Q\|_{\mathfrak{S}_1^{\mathcal{P}^0_-}} := \|Q^{+-}\|_{\mathfrak{S}_2} + \|Q^{-+}\|_{\mathfrak{S}_2} + \|Q^{++}\|_{\mathfrak{S}_1} + \|Q^{--}\|_{\mathfrak{S}_1}. \tag{27}$$

We have $\mathscr{N} \subset \mathcal{P}^0_- + \mathfrak{S}_1^{\mathcal{P}^0_-}$ thanks to Eq. (11). The closed convex hull of $\mathscr{N} - \mathcal{P}^0_-$ in the $\mathfrak{S}_1^{\mathcal{P}^0_-}$-topology gives

$$\mathcal{K} := \left\{Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ Q^* = Q,\ -\mathcal{P}^0_- \leq Q \leq \mathcal{P}^0_+\right\}$$

and we have [HLS05a, HLS05b]: $\forall\, Q \in \mathcal{K},\ Q^2 \leq Q^{++} - Q^{--}$.

– For Q in $\mathfrak{S}_1^{\mathcal{P}^0_-}$, we show $\mathcal{E}^\nu_{\rm BDF}(Q)$ is well defined. We have

$$\mathcal{P}^0_-(\mathcal{D}^0 Q)\mathcal{P}^0_- = -|\mathcal{D}^0|Q^{--} \in \mathfrak{S}_1(\mathfrak{H}_\Lambda), \text{ because } |\mathcal{D}^0| \in \mathcal{B}(\mathfrak{H}_\Lambda),$$

this proves that the kinetic energy is defined.

– Thanks to the Kato-Seiler-Simon inequality [Sim79, Chapter 4], the operator Q is locally trace-class:

$$\forall\, \phi \in \mathbf{C}_0^\infty(\mathbb{R}^3),\ \phi\Pi_\Lambda \in \mathfrak{S}_2 \text{ so } \phi Q\phi = \phi\Pi_\Lambda Q\phi \in \mathfrak{S}_1(L^2(\mathbb{R}^3)).$$

We recall this inequality states that for all $2 \leq p \leq \infty$ and $d \in \mathbb{N}$, we have

$$\forall\, f, g \in L^p(\mathbb{R}^d),\ f(x)g(-i\nabla) \in \mathfrak{S}_p(\mathfrak{H}_\Lambda) \text{ and } \|f(x)g(-i\nabla)\|_{\mathfrak{S}_p} \leq (2\pi)^{-d/p}\|f\|_{L^p}\|g\|_{L^p}. \tag{28}$$

In particular the *density* ρ_Q of Q, given by the formula

$$\forall\, x \in \mathbb{R}^3,\ \rho_Q(x) := \mathrm{Tr}_{\mathbb{C}^4}\big(Q(x,x)\big)$$

is well defined. In [HLS05a] Hainzl *et al.* prove that its Coulomb energy is finite $D(\rho_Q, \rho_Q) < +\infty$. By Cauchy-Schwartz inequality, $D(\nu, \rho_Q)$ is defined.
– By Kato's inequality

$$\frac{1}{|\cdot|} \leq \frac{\pi}{2}|\nabla|, \tag{29}$$

the exchange term is well-defined: this implies that $\|Q\|_{\mathrm{Ex}}^2 \leq \frac{\pi}{2}\mathrm{Tr}\big(|\nabla|Q^*Q\big)$.
– Furthermore the following holds: if $\alpha < \frac{4}{\pi}$, then the BDF energy is bounded from below on $\mathcal{K}$ [BBHS98, HLS05b, HLS09]. Here we assume it is the case.

2. For $Q \in \mathcal{K}$, its charge is its $\mathcal{P}_-^0$-trace: $q = \mathrm{Tr}_{\mathcal{P}_-^0}(Q)$. So we define charge sectors sets:

$$\forall\, q \in \mathbb{R}^3,\ \mathcal{K}^q := \big\{Q \in \mathcal{K},\ \mathrm{Tr}(Q) = q\big\}.$$

A minimizer of $\mathcal{E}_{\mathrm{BDF}}^\nu$ over $\mathcal{K}$ is interpreted as the polarized vacuum in the presence of ν while minimizer over charge sector $N \in \mathbb{N}$ is interpretreted as the ground state of N electrons in the presence of ν. We define the energy functional E_{BDF}^ν:

$$\forall\, q \in \mathbb{R}^3,\ E_{\mathrm{BDF}}^\nu(q) := \inf\big\{\mathcal{E}_{\mathrm{BDF}}^\nu(Q),\ Q \in \mathcal{K}^q\big\}. \tag{30}$$

We also write:

$$\mathcal{K}_{\mathscr{C}}^0 := \{Q \in \mathcal{K},\ \mathrm{Tr}_{\mathcal{P}_-^0}(Q) = 0,\ -\mathrm{C}Q\mathrm{C} = Q\}. \tag{31}$$

Lemma 1 states that this set is sequentially weakly-$*$ closed in $\mathfrak{S}_1^{\mathcal{P}^0}(\mathfrak{H}_\Lambda)$.
Notation 6. For an operator $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, we write R_Q the operator given by the integral kernel:

$$R_Q(x,y) := \frac{Q(x,y)}{|x-y|}.$$

2.2 Structure of manifold

We define

$$\mathscr{V} = \big\{P - \mathcal{P}_-^0,\ P^* = P^2 = P \in \mathcal{B}(\mathfrak{H}_\Lambda),\ \mathrm{Tr}_{\mathcal{P}_-^0}\big(P - \mathcal{P}_-^0\big) = 0\big\} \subset \mathfrak{S}_2(\mathfrak{H}_\Lambda).$$

Up to adding $\mathcal{P}_-^0$, we deal with

$$\mathscr{M} := \mathcal{P}_-^0 + \mathscr{V} = \big\{P,\ P^* = P^2 = P,\ \mathrm{Tr}_{\mathcal{P}_-^0}\big(P - \mathcal{P}_-^0\big) = 0\big\}.$$

From a geometrical point of view, we recall that these sets are Hilbert manifolds: $\mathscr{V}$ lives in the Hilbert space $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ and $\mathscr{M}$ lives in the affine space $\mathcal{P}_-^0 + \mathfrak{S}_2(\mathfrak{H}_\Lambda)$.

Proposition 1. *The set $\mathscr{M}$ is a Hilbert manifold and for all $P \in \mathscr{M}$,*

$$\mathrm{T}_P\mathscr{M} = \{[A,P],\ A \in \mathcal{B}(\mathfrak{H}_\Lambda),\ A^* = -A \text{ and } PA(1-P) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}. \tag{32}$$

Writing

$$\mathfrak{m}_P := \{A \in \mathcal{B}(\mathfrak{H}_\Lambda),\ A^* = -A,\ PAP = (1-P)A(1-P) = 0 \text{ and } PA(1-P) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)\}, \tag{33}$$

any $P_1 \in \mathscr{M}$ can be written as $P_1 = e^A P e^{-A}$ where $A \in \mathfrak{m}_P$.

The BDF energy $\mathcal{E}^{\nu}_{\mathrm{BDF}}$ is a differentiable function in $\mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$ with:

$$\begin{cases} \forall\, Q, \delta Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ \mathrm{d}\mathcal{E}^{\nu}_{\mathrm{BDF}}(Q)\cdot\delta Q = \mathrm{Tr}_{\mathcal{P}^0_-}\big(D_{Q,\nu}\delta Q\big). \\ D_{Q,\nu} := \mathcal{D}^0 + \alpha\big((\rho_Q-\nu)*\frac{1}{|\cdot|} - R_Q\big). \end{cases} \tag{34}$$

We may rewrite (34) as follows:

$$\forall\, Q, \delta Q \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda),\ \mathrm{d}\mathcal{E}^{\nu}_{\mathrm{BDF}}(Q)\cdot\delta Q = \mathrm{Tr}_{\mathcal{P}^0_-}\big(\Pi_\Lambda D_{Q,\nu}\Pi_\Lambda \delta Q\big) \tag{35}$$

Notation 7. In the case $\nu = 0$ we write $D_Q := D_{Q,0}$.

Proposition 2. *Let (P, v) be in the tangent bundle $\mathrm{T}\mathscr{M}$ and $Q = P - \mathcal{P}^0_-$. Then $[[\Pi_\Lambda D_Q \Pi_\Lambda, P], P]$ is a Hilbert-Schmidt operator in $\mathrm{T}_P\mathscr{M}$ and:*

$$\mathrm{d}\mathcal{E}^0_{BDF}(P)\cdot v = \mathrm{Tr}\Big(\big[\big[\Pi_\Lambda D_Q\Pi_\Lambda, P\big], P\big]v\Big). \tag{36}$$

Remark 9. The operator $[[\Pi_\Lambda D_Q\Pi_\Lambda, P], P]$ is the "projection" of $\Pi_\Lambda D_Q\Pi_\Lambda$ onto $\mathrm{T}_P\mathscr{M}$. It properly defines a vector in the tangent plane which is exactly the *gradient* of $\mathcal{E}^0_{\mathrm{BDF}}$ at the point P.

$$\forall\, P \in \mathscr{M},\ \nabla\mathcal{E}^0_{\mathrm{BDF}}(P) = \big[\big[\Pi_\Lambda D_Q\Pi_\Lambda, P\big], P\big]. \tag{37}$$

We recall $\mathscr{M}_{\mathscr{C}}$ is the set of C-symmetric states (14).

Proposition 3. *The set $\mathscr{M}_{\mathscr{C}}$ is a* submanifold *of $\mathscr{M}$, which is* invariant *under the flow of $\mathcal{E}^0_{BDF}$. For any $P \in \mathscr{M}_{\mathscr{C}}$, writing*

$$\mathfrak{m}_P^{\mathscr{C}} = \{a \in \mathfrak{m}_P,\ \mathrm{C}a\mathrm{C} = a\}, \tag{38}$$

we have

$$\mathrm{T}_P\mathscr{M}_{\mathscr{C}} = \{[a, P],\ a \in \mathfrak{m}_P^{\mathscr{C}}\} = \{v \in \mathrm{T}_P\mathscr{M},\ -\mathrm{C}v\mathrm{C} = v\}. \tag{39}$$

Furthermore, for any $P \in \mathscr{M}_{\mathscr{C}}$ we have

$$\rho_{P-\mathcal{P}^0_-} = 0. \tag{40}$$

Proposition 4. *The set $\mathscr{M}_{\mathscr{C}}$ has two connected components $\mathscr{E}_1$ and $\mathscr{E}_{-1}$:*

$$\forall\, P \in \mathscr{M}_{\mathscr{C}},\ P \in \mathscr{E}_1 \iff \mathrm{Dim}\,\mathrm{Ran}\,P \cap \mathrm{Ran}\,\mathcal{P}^0_+ \equiv 0[2]. \tag{41}$$

In particular, $\mathscr{E}_1$ contains $\mathcal{P}^0_-$ and $\mathscr{E}_{-1}$ contains any $\mathcal{P}^0_- + |\psi\rangle\langle\psi| - |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|$ where $\psi \in \mathrm{Ran}\,\mathcal{P}^0_+$.

We end this section by stating technical results needed to prove Propositions 1,3 and 4.

2.3 Form of trial states

Theorem 4 (Form of trial states)**.** *Let P_1, P_0 be in $\mathscr{N}$ and $Q = P_1 - P_0$. Then there exist $M_+, M_- \in \mathbb{Z}_+$ such that there exist two orthonormal families*

$$\begin{aligned} &(a_1, \dots, a_{M_+}) \cup (e_i)_{i\in\mathbb{N}} && \text{in } \mathrm{Ran}\,\mathcal{P}^0_+, \\ &(a_{-1}, \dots, a_{-M_+}) \cup (e_{-i})_{i\in\mathbb{N}} && \text{in } \mathrm{Ran}\,\mathcal{P}^0_-, \end{aligned}$$

and a nonincreasing sequence $(\lambda_i)_{i\in\mathbb{N}} \in \ell^2$ satisfying the following properties.

1. *The a_i's are eigenvectors for Q with eigenvalue 1 (resp. -1) if $i > 0$ (resp. $i < 0$).*
2. *For each $i \in \mathbb{N}$ the plane $\Pi_i := Span(e_i, e_{-i})$ is spanned by two eigenvectors f_i and f_{-i} for Q with eigenvalues λ_i and $-\lambda_i$.*

3. *The plane* Π_i *is also spanned by two orthogonal vectors* v_i *in* $Ran(1-P)$ *and* v_{-i} *in* $Ran(P)$*. Moreover* $\lambda_i = \sin(\theta_i)$ *where* $\theta_i \in (0, \frac{\pi}{2})$ *is the angle between the two lines* $\mathbb{C}v_i$ *and* $\mathbb{C}e_i$*.*

4. *There holds:*

$$Q = \sum_{i=1}^{M_+} |a_i\rangle\langle a_i| - \sum_{i=1}^{M_-} |a_{-i}\rangle\langle a_{-i}| + \sum_{j\in\mathbb{N}} \lambda_j (|f_j\rangle\langle f_j| - |f_{-j}\rangle\langle f_{-j}|).$$

Remark 10. We have

$$\begin{aligned} Q^{++} &= \sum_{i=1}^{M_+} |a_i\rangle\langle a_i| + \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 |e_j\rangle\langle e_j|, \\ Q^{--} &= -\sum_{i=1}^{M_-} |a_{-i}\rangle\langle a_{-i}| - \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 |e_{-j}\rangle\langle e_{-j}|. \end{aligned} \tag{42}$$

Thanks to Theorem 4, it is possible to characterize C-symmetric states.

Proposition 5. *Let* $\gamma = P - \mathcal{P}^0_-$ *be in* $\mathscr{M}_{\mathscr{C}}$*. For* $-1 \le \mu \le 1$ *and* $A =\in \{\gamma, \gamma^2\}$*, we write*

$$E^A_\mu = Ker(A - \mu).$$

Then for any $\mu \in \sigma(\gamma)$*, we have* $\mathrm{C}E^\gamma_\mu = E^\gamma_{-\mu}$*. Moreover for* $|\mu| < 1$*: if we decompose* $E^\gamma_\mu \oplus E^\gamma_{-\mu}$ *into a sum of planes* Π *as in Theorem 4, then each* Π *is* not C*-invariant and* $\dim E^\gamma_\mu$ *is even. Equivalently* $\dim E^{\gamma^2}_{\mu^2}$ *is divisible by* 4*.*

Moreover there exists a decomposition

$$E^{\gamma^2}_{\mu^2} = \overset{\perp}{\bigoplus_{1\le j\le \frac{N}{2}}} V_{\mu,j} \text{ and } V_{\mu,j} = \Pi^a_{\mu,j} \overset{\perp}{\oplus} \mathrm{C}\Pi^a_{\mu,j}$$

where the $\Pi^a_{\mu,j}$*'s and* $\mathrm{C}\Pi^a_{\mu,j}$*'s are spectral planes described in Theorem 4.*

3 Proof of Theorem 1

3.1 Strategy and tools of the proof

Topologies

The upper bound in (18) comes from minimization over C-symmetric state of form (13).

We prove the existence of the minimizer over $\mathscr{E}_{-1}$ by using a lemma of Borwein and Preiss [BP87, HLS09], a smooth generalization of Ekeland's Lemma [Eke74]: we study the behaviour of a specific minimizing sequence $(P_n)_n$ or equivalently $(P_n - \mathcal{P}^0_- =: Q_n)_n$.

Each element of the sequence satisfies an equation close to the one satisfied by a real minimizer and we show this equation remains in some weak limit.

Remark 11. We recall different topologies over bounded operators, besides the norm topology $\|\cdot\|_{\mathcal{B}}$ [RS75].

1. The so-called *strong topology*, the weakest topology $\mathcal{T}_s$ such that for any $f \in \mathfrak{H}_\Lambda$, the map

$$\begin{aligned} \mathcal{B}(\mathfrak{H}_\Lambda) &\longrightarrow \mathfrak{H}_\Lambda \\ A &\mapsto Af \end{aligned}$$

is continuous.

2. The so-called *weak operator topology*, the weakest topology $\mathcal{T}_{w.o.}$ such that for any $f, g \in \mathfrak{H}_\Lambda$, the map

$$\begin{array}{rcl} \mathcal{B}(\mathfrak{H}_\Lambda) & \longrightarrow & \mathbb{C} \\ A & \mapsto & \langle Af\,,\, g\rangle \end{array}$$

is continuous.

We can also endow $\mathfrak{S}_1^{\mathcal{P}_-^0}$ with its weak-$*$ topology, the weakest topology such that the following maps are continuous:

$$\left|\begin{array}{rcl} \mathfrak{S}_1^{\mathcal{P}_-^0} & \longrightarrow & \mathbb{C} \\ Q & \mapsto & \mathrm{Tr}\big(A_0(Q^{++}+Q^{--})+A_2(Q^{+-}+Q^{-+})\big) \\ \forall\,(A_0,A_2) \in \mathrm{Comp}(\mathfrak{H}_\Lambda)\times\mathfrak{S}_2(\mathfrak{H}_\Lambda). & & \end{array}\right.$$

We emphasize that the weak-$*$ topology is different from the weak topology (where $\mathrm{Comp}(\mathfrak{H}_\Lambda)$ must be replaced by $\mathcal{B}(\mathfrak{H}_\Lambda)$).

The following Lemma is important in our proof.

Lemma 1. *The set $\mathcal{K}^0_{\mathscr{C}}$ (defined in (31)) is weakly-$*$ sequentially closed in $\mathfrak{S}_1^{\mathcal{P}_-^0}(\mathfrak{H}_\Lambda)$.*

We prove this Lemma at the end of this Subsection.

Borwein and Preiss Lemma

We recall this Theorem as stated in [HLS09]:

Theorem 5. *Let $\mathcal{M}$ be a closed subset of a Hilbert space $\mathcal{H}$, and $F : \mathcal{M} \to (-\infty, +\infty]$ be a lower semi-continuous function that is bounded from below and not identical to $+\infty$. For all $\varepsilon > 0$ and all $u \in \mathcal{M}$ such that $F(u) < \inf_{\mathcal{M}} + \varepsilon^2$, there exist $v \in \mathcal{M}$ and $w \in \overline{\mathrm{Conv}(\mathcal{M})}$ such that*

1. *$F(v) < \inf_{\mathcal{M}} + \varepsilon^2$,*
2. *$||u - v||_{\mathcal{H}} < \sqrt{\varepsilon}$ and $||v - w||_{\mathcal{H}} < \sqrt{\varepsilon}$,*
3. *$F(v) + \varepsilon||v - w||^2_{\mathcal{H}} = \min\big\{F(z) + \varepsilon||z - w||^2_{\mathcal{H}},\ z \in \mathcal{M}\big\}$.*

Here we apply this Theorem with $\mathcal{H} = \mathfrak{S}_2(\mathfrak{H}_\Lambda)$, $\mathcal{M} = \mathscr{E}_{-1} - \mathcal{P}^0_-$ and $F = \mathcal{E}^0_{\mathrm{BDF}}$.

The BDF energy is continuous in the $\mathfrak{S}_1^{\mathcal{P}_-^0}$-norm topology, thus its restriction over $\mathscr{V}$ is continuous in the $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$-norm topology.

This subspace $\mathcal{H}$ is closed in the Hilbert-Schmidt norm topology because $\mathscr{V} = \mathscr{M}_{\mathscr{C}}$ is closed in $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$ and $\mathscr{E}_{-1} - \mathcal{P}^0_-$ is closed in $\mathscr{V}$.

Moreover, we have

$$\overline{\mathrm{Conv}(\mathscr{E}_{-1} - \mathcal{P}^0_-)}^{\mathfrak{S}_2} \subset \mathcal{K}^0_{\mathscr{C}}.$$

For every $\eta > 0$, we get a projector $P_\eta \in \mathscr{E}_{-1}$ and $A_\eta \in \mathcal{K}^0_{\mathscr{C}}$ such that P_η that minimizes the functional

$$F_\eta : P \in \mathscr{E}_{-1} \mapsto \mathcal{E}^0_{\mathrm{BDF}}(P - \mathcal{P}^0_-) + \varepsilon\|P - \mathcal{P}^0_- - A_\eta\|^2_{\mathfrak{S}_2}.$$

We write

$$Q_\eta := P_\eta - \mathcal{P}^0_-,\ \Gamma_\eta := Q_\eta - A_\eta,\ \widetilde{D}_{Q_\eta} := \Pi_\Lambda\big(\mathcal{D}^0 - \alpha R_{Q_\eta} + 2\eta\Gamma_\eta\big)\Pi_\Lambda. \tag{43}$$

Studying its differential on $\mathrm{T}_{P_\eta}\mathscr{M}_{\mathscr{C}}$, we get that

$$\big[\widetilde{D}_{Q_\eta}, P_\eta\big] = 0. \tag{44}$$

In particular, by functional calculus, we get that

$$\big[\boldsymbol{\pi}^\eta_-, P_\eta\big] = 0,\ \boldsymbol{\pi}^-_\eta := \chi_{(-\infty,0)}(\widetilde{D}_{Q_\eta}). \tag{45}$$

We also write

$$\boldsymbol{\pi}_\eta^+ := \chi_{(0,+\infty)}(\widetilde{D}_{Q_\eta}) = \Pi_\Lambda - \boldsymbol{\pi}_\eta^-. \tag{46}$$

We can decompose $\mathfrak{H}_\Lambda$ as follows (here R means Ran):

$$\mathfrak{H}_\Lambda = \mathrm{R}(P_\eta)\cap\mathrm{R}(\boldsymbol{\pi}_\eta^-)\overset{\perp}{\oplus}\mathrm{R}(P_\eta)\cap\mathrm{R}(\boldsymbol{\pi}_\eta^+)\overset{\perp}{\oplus}\mathrm{R}(\Pi_\Lambda-P_\eta)\cap\mathrm{R}(\boldsymbol{\pi}_\eta^-)\overset{\perp}{\oplus}\mathrm{R}(\Pi_\Lambda-P_\eta)\cap\mathrm{R}(\boldsymbol{\pi}_\eta^+). \tag{47}$$

We will prove

1. $\operatorname{Ran} P \cap \operatorname{Ran} \boldsymbol{\pi}_\eta^+$ has dimension 1, spanned by a unitary $\psi_\eta \in \mathfrak{H}_\Lambda$.
2. As η tends to 0, up to translation and a subsequence, $\psi_\eta \rightharpoonup \psi_e \neq 0$, $Q_\eta \rightharpoonup \overline{Q}$. There holds $\overline{Q} + \mathcal{P}_-^0 \in \mathscr{E}_{-1}$, ψ_e is a unitary eigenvector of $\Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda$ and

$$\overline{Q} + \mathcal{P}_-^0 = \chi_{(-\infty,0)}\big(\Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda\big) + |\psi_e\rangle\langle\psi_e| - |\mathrm{C}\psi_e\rangle\langle\mathrm{C}\psi_e|.$$

In the following part we write the spectral decomposition of trial states and prove Lemma 1.

Spectral decomposition

Let $(Q_n)_n$ be any minimizing sequence for $E_{1,1}$. We consider the spectral decomposition of the trial states Q_n: thanks to the upper bound, $\operatorname{Dim}\operatorname{Ker}(Q_n - 1) = 1$, as shown in Subsection 3.2.

There exist a *non-increasing* sequence $(\lambda_{j;n})_{j\in\mathbb{N}} \in \ell^2$ of eigenvalues and an orthonormal basis $\mathbf{B}_n$ of $\operatorname{Ran} Q_n$:

$$\mathbf{B}_n := (\psi_n, \mathrm{C}\psi_n) \cup (e^a_{j;n}, e^b_{j;n}, \mathrm{C}e^a_{j;n}, \mathrm{C}e^b_{j;n}),\ \mathcal{P}_-^0\psi_n = \mathcal{P}_-^0 e^\star_{j;n} = 0,\ \star \in \{a,b\}, \tag{48}$$

such that the following holds. We omit the index n:

$$\forall\, j \in \mathbb{N},\quad e^a_{-j} := -\mathrm{C}e^b_j,\ e^b_{-j} := \mathrm{C}e^a_j, \tag{49a}$$

$$\begin{aligned} f^\star_j &:= \sqrt{\tfrac{1-\lambda_j}{2}}e^\star_{-j} + \sqrt{\tfrac{1+\lambda_j}{2}}e^\star_j, \\ f^\star_{-j} &:= -\sqrt{\tfrac{1+\lambda_j}{2}}e^\star_{-j} + \sqrt{\tfrac{1+\lambda_j}{2}}e^\star_j. \end{aligned} \tag{49b}$$

$$\begin{cases} Q_n &= |\psi_n\rangle\langle\psi_n| - |\mathrm{C}\psi_n\rangle\langle\mathrm{C}\psi_n| + \displaystyle\sum_{j\geq 1}\lambda_j q_{j;n} \\ q_{j;n} &= |f^a_j\rangle\langle f^a_j| - |f^a_{-j}\rangle\langle f^a_{-j}| + |f^b_j\rangle\langle f^b_j| - |f^b_{-j}\rangle\langle f^b_{-j}|. \end{cases} \tag{49c}$$

Remark 12. Thanks to the cut-off, the sequences $(\psi_n)_n$ and $(e_{j;n})_n$ are H^1-bounded.

Up to translation and extraction ($(n_k)_k \in \mathbb{N}^{\mathbb{N}}$ and $(x_{n_k})_k \in (\mathbb{R}^3)^{\mathbb{N}}$), we assume that the weak limit of $(\psi_n)_n$ is non-zero (if it were then there would hold $E_{1,1} = 2m$).

We consider the weak limit of each (e_n): by means of a diagonal extraction, we assume that all the $(e_{j,n_k}(\cdot - x_{n_k}))_k$ and $(\psi_{j,n_k}(\cdot - x_{n_k}))_k$, converge along the same subsequence $(n_k)_k$. We also assume that

$$\forall\, j \in \mathbb{N},\ \lambda_{j,n_k} \to \mu_j,\ (\mu_j)_j \in \ell^2,\ (\mu_j)_j \text{ non-increasing}, \tag{50}$$

and that the above convergences also hold in L^2_{loc} and almost everywhere.

Proof of Lemma 1

Let $(Q_n)_n$ be a sequence in $\mathcal{K}^0_{\mathscr{C}}$ that converges to $Q \in \mathcal{K}$ in the weak-$*$ topology of ${\mathfrak{S}_1}^{\mathcal{P}^0_-}$, that is:

$$\forall (G_0, G_2) \in \operatorname{Comp}(\mathfrak{H}_\Lambda) \times \mathfrak{S}_2(\mathfrak{H}_\Lambda) :$$

$$\begin{cases} \operatorname{Tr}(Q_n^{+-}G_2) \underset{n\to+\infty}{\to} \operatorname{Tr}(Q^{+-}G_2) \quad \text{and} \quad \operatorname{Tr}(Q_n^{-+}G_2) \underset{n\to+\infty}{\to} \operatorname{Tr}(Q^{-+}G_2), \\ \operatorname{Tr}(Q_n^{++}G_0) \underset{n\to+\infty}{\to} \operatorname{Tr}(Q^{++}G_0) \quad \text{and} \quad \operatorname{Tr}(Q_n^{--}G_0) \underset{n\to+\infty}{\to} \operatorname{Tr}(Q^{--}G_0). \end{cases}$$

In particular we have $S := \sup_n \|Q_n\|_{\mathfrak{S}_2} < +\infty$ by the uniform boundedness principle. The C-symmetry is a weak-$*$ condition: for all $\phi_1, \phi_2 \in \mathfrak{H}_\Lambda$:

$$\mathrm{Tr}\big(-\mathrm{C}Q_n\mathrm{C}|\phi_1\rangle\langle\phi_2|\big) = -\langle Q_n\mathrm{C}\phi_1\,,\,\mathrm{C}\phi_2\rangle$$

thus $-\mathrm{C}Q\mathrm{C} = Q$. There remains to prove that $\mathrm{Tr}_{\mathcal{P}^0_-}(Q) = 0$.

We consider the spectral decomposition of $P_n := \mathcal{P}^0_- + Q_n$. We know that this is compact perturbation of $\mathcal{P}^0_-$, thus its essential spectrum is $\{0,1\}$ and there exist an ONB of $\mathfrak{H}_\Lambda$:

$$(e_{k;n})_{k=1}^{K_1} \cup (f_{j;n})_{j\in\mathbb{N}} \cup (g_{j;n})_{j\in\mathbb{N}},\ K_1 \in \mathbb{Z}_+$$

and two sequences $(r_{j;n})_j, (s_{j;n})_j$ in $[0, \frac{1}{2})$ that tend to 0, such that

$$P_n = \frac{1}{2}\sum_{k=1}^{K_1} |e_{k;n}\rangle\langle e_{k;n}| + \sum_{j\in\mathbb{N}} \Big\{ r_{j;n}|f_{j;n}\rangle\langle f_{j;n}| + (1-s_{j;n})|g_{j;n}\rangle\langle g_{j;n}|\Big\}.$$

Our aim is to prove we can rewrite P_n as follows:

$$\left|\begin{array}{l} P_n = \overline{P}_n + \overline{\gamma}_n, \\ \overline{\gamma}_n = \displaystyle\sum_j t_{j;n}\big(|\phi_{j;n}\rangle\langle\phi_{j;n}| - |\mathrm{C}\phi_{j;n}\rangle\langle\mathrm{C}\phi_{j;n}|\big), \\ \overline{P}_n \in \mathscr{M}_{\mathscr{C}},\ 2\sum_j t_{j;n} \le \mathrm{Tr}\big(Q_n^{++} - Q_n^{--}\big), \\ (\phi_{j;n})_j \cup (\mathrm{C}\phi_{j;n})_j \text{ orthonormal family.} \end{array}\right. \tag{52}$$

Let us assume this point for the moment. Up to extraction, it is clear that the weak limit $\overline{\gamma}_\infty$ of $(\overline{\gamma}_n)$ has trace 0: the eventual loss of mass of $(\phi_{j;n})_n$ is compensated by that of $(\mathrm{C}\phi_{j;n})_n$: $|\phi_{j;n}(x)|^2 = |\mathrm{C}\phi_{j;n}(x)|^2$ for all $x \in \mathbb{R}^3$. So the weak limit of

$$t_{j;n}\big(|\phi_{j;n}\rangle\langle\phi_{j;n}| - |\mathrm{C}\phi_{j;n}\rangle\langle\mathrm{C}\phi_{j;n}|\big)$$

has trace 0.

The same goes for $\overline{Q}_n := \overline{P}_n - \mathcal{P}^0_-$. We write $S := \limsup_n \mathrm{Tr}_{\mathcal{P}^0_-}(\overline{Q}_n) < +\infty$. We decompose each $\overline{Q}_n$ as in (49) and take the same notations. We may have $D_n := \mathrm{Dim}(\overline{Q}_n^2 - 1) > 2$ but the sequence $(D_n)_n$ is bounded by S. There is at most $\frac{S}{2}$ different $\psi_{j;n}$ in the spectral decomposition of $\overline{Q}_n$ $(j = 1, \dots, \lfloor\frac{S}{2}\rfloor)$.

We study the weak-limit of the $\psi_{j;n}$'s and the $e^\star_{j;n}$'s: there may be a loss of mass. However from (42), we see that the loss of mass in $\psi_{j;n}$ is compensated by that of $\mathrm{C}\psi_{j;n}$, and that of $e^\star_{j;n}$ is compensated by that of $\mathrm{C}e^\star_{j;n}$.

The subscript ∞ means we take the weak limit. If the sequences of eigenvalues $(\lambda_j)_j \in \ell^2$ weakly converges to $(\mu_j)_j \in \ell^2$, then we get that

$$\left\{\begin{array}{l} Q^{++} = \displaystyle\sum_{1\le j\le\lfloor S/2\rfloor} |\psi_{j;\infty}\rangle\langle\psi_{j;\infty}| + \sum_{j\in\mathbb{N}} \mu_j^2\Big\{|e^a_{j,\infty}\rangle\langle e^a_{j,\infty}| + |e^b_{j,\infty}\rangle\langle e^b_{j,\infty}|\Big\} \\ Q^{--} = -\displaystyle\sum_{1\le j\le\lfloor S/2\rfloor} |\psi_{-j;\infty}\rangle\langle\psi_{-j;\infty}| - \sum_{j\in\mathbb{N}} \mu_j^2\Big\{|e^a_{-j,\infty}\rangle\langle e^a_{-j,\infty}| + |e^b_{-j,\infty}\rangle\langle e^b_{-j,\infty}|\Big\} \end{array}\right.$$

where $|\psi_{j,\infty}|^2 = |\psi_{-j,\infty}|^2$ resp. $|e^\star_{j,\infty}|^2 = |e^\star_{-j,\infty}|^2$. Thus

$$\mathrm{Tr}\big(Q^{++} + Q^{--}\big) = 0.$$

Proof of (52) The condition $-\mathrm{C}Q_n\mathrm{C} = Q_n$ is equivalent to $\mathrm{C}P_n\mathrm{C} = \Pi_\Lambda - P_n$, so for any $\mu \in \mathbb{R}$ we have

$$\mathrm{CKer}\,\big(P_n - \mu\big) = \mathrm{Ker}\,\big(P_n - (1-\mu)\big).$$

Up to reindexing the sequences, we can assume that $r_{j;n} = s_{j;n}$ and up to changing the ONB, we can assume that $g_{j;n} = \mathrm{C}f_{j;n}$. Let us remark that

$$\mathrm{C}B_n\mathrm{C} = B_n \text{ where } B_n := \frac{1}{2}\sum_{k=1}^{K_0} |e_{k;n}\rangle\langle e_{k;n}|.$$

As shown in [HLS09, Lemma 15, Appendix B], the condition $Q_n \in \mathfrak{S}_1^{\mathcal{P}_-^0}$ gives

$$\begin{aligned}\mathrm{Tr}\big(Q_n^{++} - Q_n^{--}\big) &= \frac{K_1}{2} + \sum_{j\geq 1}\Big\{r_{j;n}\|\mathcal{P}_+^0 f_{j;n}\|_{L^2}^2 + (1-r_{j;n})\|\mathcal{P}_-^0 f_{j;n}\|_{L^2}^2\Big\} \\ &\quad + \sum_{j\geq 1}\Big\{(1-s_{j;n})\|\mathcal{P}_+^0 g_{j;n}\|_{L^2}^2 + s_{j;n}\|\mathcal{P}_-^0 g_{j;n}\|_{L^2}^2\Big\},\end{aligned}$$

which implies

$$\boxed{\frac{K_1}{2} + \sum_{j\geq 1}(r_{j;n} + s_{j;n}) \leq \mathrm{Tr}_{\mathcal{P}_-^0}(Q_n).}$$

In particular we can write

$$\boxed{\begin{aligned}&P_n = \overline{P}_n + \gamma_n + B_n, \\ &\gamma_n = \sum_{j\geq 1} r_{j:n}\big(|f_{j;n}\rangle\langle f_{j;n}| - |\mathrm{C}f_{j;n}\rangle\langle \mathrm{C}f_{j;n}|\big), \\ &P_n' = \sum_{j\geq 1}|\mathrm{C}f_{j;n}\rangle\langle \mathrm{C}f_{j;n}|.\end{aligned}}$$

Both γ_n and B_n are trace-class, thus $P_n' - \mathcal{P}_-^0 \in \mathfrak{S}_1^{\mathcal{P}_-^0}$. We know that $\mathrm{Tr}_{\mathcal{P}_-^0}(P_n' - \mathcal{P}_-^0)$ is an integer [HLS05a], this gives

$$\frac{K_1}{2} = K_0 \in \mathbb{N}.$$

Let us prove that we can decompose $\mathrm{Ran}\, B_n$ as follows:

$$\mathrm{Ran}\, B_n = F_n \overset{\perp}{\oplus} \mathrm{C}F_n,\ \mathrm{Dim}\, F_n = K_0. \tag{53}$$

This ends the proof: we have

$$B_n = \mathrm{Proj}(\mathrm{C}F_n) + \frac{1}{2}\big(\mathrm{Proj}(F_n) - \mathrm{Proj}(\mathrm{C}F_n)\big)$$

where $\mathrm{Proj}(E)$ is the orthogonal projection onto E. We choose then

$$\boxed{\begin{aligned}&\overline{P}_n := P_n' + \mathrm{Proj}(\mathrm{C}F_n), \\ &\overline{\gamma}_n := \gamma_n + \tfrac{1}{2}\big(\mathrm{Proj}(F_n) - \mathrm{Proj}(\mathrm{C}F_n)\big).\end{aligned}}$$

Let $\phi \in \mathrm{Ran}\, B_n$ with $\mathrm{C}\phi \notin \mathbb{C}\phi$. Else, we take $\phi \perp \phi'$ with

$$\mathrm{C}\phi = e^{i\theta}\phi,\ \mathrm{C}\phi' = e^{i\theta'}\phi',\ \theta, \theta' \in \mathbb{R}.$$

Up to considering $e^{i\theta/2}\phi$ and $e^{i\theta'/2}\phi'$ we may assume that $\mathrm{C}\phi = \phi$, $\mathrm{C}\phi' = \phi'$. Then writing

$$\phi_\pm := \frac{1}{\sqrt{2}}\big(\phi \pm i\phi'\big)$$

we have $\langle \mathrm{C}\phi_+\,,\, \phi_+\rangle = 0$, which is absurd.

Let us consider $\mathrm{Span}(\phi, \mathrm{C}\phi)$ and assume $\|\phi\|_{L^2} = 1$. Thus $z = \langle \mathrm{C}\phi\,,\, \phi\rangle = -re^{i\theta}$ with $0 \leq r \leq 1$. There exist $a, b \in \mathbb{C}$ such that

$$\langle \mathrm{C}(a\phi + b\mathrm{C}\phi)\,,\, a\phi + b\mathrm{C}\phi\rangle = 0.$$

If $r = 0$ we take $a = 1$ and $b = 0$, else it suffices to take $a = r_0 e^{-i\theta/2}$ and $b = r_1 e^{i\theta/2}$ where $r_0, r_1 > 0$ are any number that satisfies

$$\frac{r_0}{r_1} + \frac{r_1}{r_0} = \frac{2}{r}.$$

This is possible because as $0 < r \leq 1$ we have $\frac{2}{r} \geq 2$. By an easy induction, we can write $\mathrm{Ran}\, B_n$ as in (53).

□

3.2 Upper and lower bounds of $E_{1,1}$

Upper bound

We consider trial states of the following form:

$$Q = |\psi\rangle\langle\psi| - |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|,\ \|\psi\|_{L^2} = 1 \text{ and } \mathcal{P}_-^0\psi = 0.$$

The set of these states is written $\mathscr{E}_{-1}^0$. We will prove that the energy of a particular Q gives the upper bound. For such a Q, the BDF energy is simply:

$$2\langle|\mathcal{D}^0|\psi\,,\,\psi\rangle - \frac{\alpha}{2}\iint\frac{|\psi\wedge\mathrm{C}\psi(x,y)|^2}{|x-y|}dxdy. \tag{54}$$

Following [Sok12], we take $\phi_{\mathrm{CP}} \in L^2(\mathbb{R}^3,\mathbb{C})$ the unique positive radial minimizer of the Choquard-Pekar energy. *We know that this minimizer is in the Schwartz class* (here we just need it to be in H^2). We form the spinor:

$$\phi := (\,\phi_{\mathrm{CP}}\ \ 0\ \ 0\ \ 0\,)^{\mathrm{T}},$$

and scale ϕ by a constant $\lambda^{-1} \sim \alpha$ to be chosen later:

$$\phi_\lambda(x) := \lambda^{-3/2}\phi(x/\lambda).$$

We define $\psi_\lambda := \Pi_\Lambda\phi_\lambda$ and write:

$$\psi_+ := \frac{\mathcal{P}_+^0\psi_\lambda}{\|\mathcal{P}_+^0\psi_\lambda\|_{L^2}} \text{ and } \psi_- := \frac{\mathcal{P}_-^0\mathrm{C}\psi_\lambda}{\|\mathcal{P}_-^0\mathrm{C}\psi_\lambda\|_{L^2}} = \mathrm{C}\psi_+. \tag{55}$$

Let us compute the energy of

$$Q_0 := |\psi_+\rangle\langle\psi_+| - |\psi_-\rangle\langle\psi_-|. \tag{56}$$

We have:

$$\begin{aligned}
\|\mathcal{P}_+^0\psi_\lambda\|_{L^2}^2 &= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2\frac{g_0(p)}{2}\big(1+\tfrac{1}{\widetilde{E}(p)}\big)dp,\\
&= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2 g_0(p)\big(1-\tfrac{g_1(p)^2}{4g_0(p)^2}\big)dp + \mathcal{O}(\lambda^{-4}),\\
&= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2\big(m-\tfrac{g_1'(0)^2}{4m}\big)dp + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}),\\
&= 1 - \frac{g_1'(0)^2}{4\lambda^2 m}\|\phi_{\mathrm{CP}}\|_{L^2}^2 + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}).
\end{aligned}$$

Similarly the following holds:

$$\begin{aligned}
\langle|\mathcal{D}^0|\mathcal{P}_+^0\psi_\lambda\,,\,\psi_\lambda\rangle &= \int\limits_{B(0,\Lambda)} \widetilde{E}\,(p)\,\langle\widehat{\mathcal{P}_+^0}(p)\widehat{\psi}_\lambda(p)\,,\,\widehat{\psi}_\lambda(p)\rangle_{\mathbb{R}^3}dp\\
&= \int\limits_{B(0,\Lambda)} |\widehat{\psi_\lambda}(p)|^2\frac{1}{2}\big(g_0(p)+\widetilde{E}\,(p)\,\big)dp\\
&= m + \frac{g_1'(0)^2}{4\lambda^2 m}\|\phi_{\mathrm{CP}}\|_{L^2}^2 + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}).
\end{aligned}$$

Then we estimate:

$$\begin{aligned}
\iint\frac{|\psi_+\wedge\psi_-(x,y)|^2}{|x-y|}dxdy &= 2\Big\{D\big(|\psi_+|^2,|\psi_-|^2\big) - D\big(\psi_+^*\psi_-,\psi_+^*\psi_-\big)\Big\}\\
&= 2\Big\{\tfrac{1}{\lambda}D\big(|\phi_{\mathrm{CP}}|^2,|\phi_{\mathrm{CP}}|^2\big) + \mathcal{O}(\lambda^{-2}) - D\big(\psi_+^*\psi_-,\psi_+^*\psi_-\big)\Big\}\\
&= 2\Big\{\tfrac{1}{\lambda}D\big(|\phi_{\mathrm{CP}}|^2,|\phi_{\mathrm{CP}}|^2\big) + \mathcal{O}(\lambda^{-2})\Big\}.
\end{aligned}$$

Indeed we have:

$$\begin{array}{rcl} \|\psi_+^*\psi_-\|_{L^1} & \lesssim & \|\nabla\psi_\lambda\|_{L^2}\|\psi_\lambda\|_{L^2} = \mathcal{O}(\lambda^{-1}). \\ |\psi_+^*\psi_-| * \frac{1}{|\cdot|} & \leq & |\psi_+|^2 * \frac{1}{|\cdot|} \leq \frac{\pi}{2}\langle|\nabla|\psi_+\,,\,\psi_+\rangle \\ & = & \mathcal{O}(\lambda^{-1}). \end{array}$$

Thus we get that:

$$\mathcal{E}^0_{\rm BDF}(Q_0) = 2m + \frac{g_1'(0)^2}{\lambda^2 m}\|\nabla\phi_{\rm CP}\|_{L^2}^2 - \frac{\alpha}{\lambda}D\big(|\phi_{\rm CP}|^2, |\phi_{\rm CP}|^2\big) + \mathcal{O}((\alpha+\lambda^{-2})\lambda^{-2}). \quad (57)$$

If we *choose*

$$\frac{1}{\lambda} := \frac{\alpha m}{g_1'(0)^2} \quad (58)$$

we get the following upper bound:

$$E_{1,1} \leq \mathcal{E}^0_{\rm BDF}(Q_0) = 2m + \alpha^2\frac{m}{g_1'(0)^2}E_{\rm CP} + \mathcal{O}(\alpha^3). \quad (59)$$

A priori lower bound

Let $Q \in \mathscr{M} - \mathcal{P}^0_-$ be an approximate minimizer such that

$$\mathcal{E}^0_{\rm BDF}(Q) < E_{1,1} + \alpha^2\frac{m}{2g_1'(0)^2}|E_{\rm CP}| < 2m.$$

Our aim is to prove the following

$$\left\{\begin{array}{rcl} E_{1,1} - 2m & \geq & -K\alpha^2, \\ {\rm Tr}\big(|\nabla|Q^2\big) & \leq & K\alpha. \end{array}\right. \quad (60)$$

We have

$$\Big(1 - \alpha\frac{\pi}{4}\Big){\rm Tr}(|\mathcal{D}^0|Q^2) \leq \mathcal{E}^0_{\rm BDF} < 2m \text{ so } \|Q\|^2_{\mathfrak{S}_2} < \frac{2m}{1-\alpha\frac{\pi}{4}} < 3.$$

However $\|Q\|^2_{\mathfrak{S}_2} \geq {\rm Dim\,Ker}(Q^2-1) = 2{\rm Dim\,Ker}(Q-1)$, thus Q has the form written in (49); in particular we have:

$$Q = |\psi\rangle\langle\psi| - |{\rm C}\psi\rangle\langle{\rm C}\psi| + \gamma,\ \psi \in {\rm Ran}(\mathcal{P}^0_+),\ \psi_+ := \psi, \psi_- := {\rm C}\psi \in {\rm Ker}\,\gamma.$$

Let us remark that $\gamma + \mathcal{P}^0_- \in \mathscr{M}$. The energy of Q is:

$$\mathcal{E}^0_{\rm BDF}(Q) = \mathcal{E}^0_{\rm BDF}(\gamma) + 2\langle|\mathcal{D}^0|\psi\,,\,\psi\rangle - \frac{\alpha}{2}\iint\frac{|\psi\wedge{\rm C}\psi(x,y)|^2}{|x-y|}dxdy - \alpha\sum_{\varepsilon\in\{+,-\}}\big(\langle\psi_\varepsilon R_\gamma\,,\,\psi_\varepsilon\rangle\big). \quad (61)$$

We substract $2m$: as $g_0'(0) = 0$ and $\|g_0''\|_{L^\infty} \leq K\alpha$ [Sok12, Appendix A], we have

$$|g_0(p) - m| \leq p^2\int_0^1 |g_0''(tp)|(1-t)dt \leq K\alpha p^2,$$

thus:

$$\begin{aligned} \widetilde{E}\,(p) - m &= \frac{g_1(p)^2 + (g_0(p)-m)(g_0(p)+m)}{\widetilde{E}\,(p)+m} \\ &\leq \frac{g_1(p)^2(1-K\alpha)}{2\widetilde{E}\,(p)}. \end{aligned}$$

Going back to the energy, we have by Cauchy-Schwartz inequality:

$$|\langle\psi_\varepsilon\,,\,R_\gamma\psi_\varepsilon\rangle| \leq \|N[\psi_\varepsilon]\|_{\rm Ex}\|\gamma\|_{\rm Ex},\ N[\psi_\varepsilon] := |\psi_\varepsilon\rangle\langle\psi_\varepsilon|.$$

The quantity $\|N[\psi_\varepsilon]\|^2_{\mathrm{Ex}}$ is simply $D\big(|\psi_\varepsilon|^2,|\psi_\varepsilon|^2\big)$ and we get:

$$(1-K\alpha)\langle \tfrac{g_1^2(-i\nabla)}{|\mathcal{D}^0|}\psi\,,\,\psi\rangle + \mathrm{Tr}(|\mathcal{D}^0|\gamma^2) \leq K_1\alpha^2 + 2\alpha D\big(|\psi|^2,|\psi|^2\big) + \tfrac{3\alpha}{2}\|\gamma\|^2_{\mathrm{Ex}},$$
$$(1-K\alpha)\langle \tfrac{g_1^2(-i\nabla)}{|\mathcal{D}^0|}\psi\,,\,\psi\rangle + \big(1-\tfrac{3\alpha\pi}{4}\big)\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) \leq K_1\alpha^2 + \alpha\pi\langle\,|\nabla|\psi\,,\,\psi\rangle.$$

Now we have:

$$(1-K\alpha)\frac{p^2}{\widetilde{E}\,(p)} \geq 2\alpha|p| \iff p^2 \geq 4\alpha^2(1-K\alpha)\widetilde{E}\,(p)^2\,. \tag{62}$$

We can take $K = \|g_0\|_{L^\infty}$: this inequality holds for

$$|p| \geq r_0 := \frac{2\alpha\|g_0\|_{L^\infty}\sqrt{1-\alpha\|g_0\|_{L^\infty}}}{\sqrt{1-4\alpha^2\|g_1'\|^2_{L^\infty}(1-\alpha\|g_0\|_{L^\infty})}}. \tag{63}$$

If we split $\langle|\nabla\psi|\,,\,\psi\rangle$ at level $|p|=r_0$, we have:

$$\frac{1-\|g_0\|_{L^\infty}\alpha}{2}\langle \tfrac{g_1^2(-i\nabla)}{|\mathcal{D}^0|}\psi\,,\,\psi\rangle + \big(1-\frac{3\alpha\pi}{4}\big)\mathrm{Tr}(|\mathcal{D}^0|\gamma^2) \leq K_1\alpha^2 + \alpha r_0 \lesssim \alpha^2. \tag{64}$$

and

$$\langle|\nabla|\psi\,,\,\psi\rangle \lesssim \alpha. \tag{65}$$

Substituting these estimates in (61), we get:

$$E_{1,1} - 2m \geq \mathcal{E}^0_{\mathrm{BDF}}(Q) - 2m + \alpha^2\frac{m}{2g_1'(0)^2}E_{\mathrm{CP}} \geq -K\alpha^2. \tag{66}$$

Form of a minimizer for $E_{1,1}$

If a minimizer $\overline{P}\in\mathscr{E}_{-1}$ exists, then it satisfies the following:

$$\left|\begin{array}{l}\overline{P} = \mathcal{P}^0_- + \overline{Q} = \mathcal{P}^0_- + |\psi_+\rangle\langle\psi_+| - |\mathrm{C}\psi_+\rangle\langle\mathrm{C}\psi_+| + \gamma\\ \psi_+, \mathrm{C}\psi_+ \in \mathrm{Ker}\,\gamma,\ \mathcal{P}^0_-\psi_+ = 0.\end{array}\right.$$

Moreover the proof of the lower bound ensures that $\|\gamma\|_{\mathfrak{S}_2}\lesssim\alpha$. So let $\mathrm{P}^0_{1,1}$ be:

$$\mathrm{P}^0_{1,1} := \mathcal{P}^0_- + |\psi_+\rangle\langle\psi_+| - |\mathrm{C}\psi_+\rangle\langle\mathrm{C}\psi_+|.$$

Then we have $\|\mathrm{P}^0_{1,1} - \overline{P}\|_{\mathfrak{S}_2} = \|\gamma\|_{\mathfrak{S}_2}\lesssim\alpha$. Using Propositions 1 and 3, we write

$$\overline{P} = e^A\mathrm{P}^0_{1,1}e^{-A},\ A\in\mathfrak{m}^{\mathscr{C}}_{\mathrm{P}^0_{1,1}}$$

where there exist $(\theta_j)_j\in\ell^2$ decreasing and $K_0>0$ such that

$$\|\gamma\|_{\mathfrak{S}_2} = 4\sum_{j=1}^{+\infty}\sin(\theta_j)^2 \leq K_0\alpha^2,\ \text{thus}$$
$$\|A\|^2_{\mathfrak{S}_2} = 4\sum_{j=1}^{\infty}\theta_j^2 \leq \frac{\pi^2}{4}K_0\alpha^2.$$

Assuming Theorem 1, this proves the description of Theorem 2.

3.3 Existence of a minimizer for $E_{1,1}$

We consider a family of almost minimizers $(P_{\eta_n})_n$ of type (43) where $(\eta_n)_n$ is any decreasing sequence. We assume that $\Lambda^2\alpha^{-2}\eta_n$ is small. We also consider the spectral decomposition (49) of any $Q_n := P_{\eta_n} - \mathcal{P}^0_-$.

For short we write $P_n := P_{\eta_n}$ and in general replace the subscript η_n by n.

– We study weak limits of $(Q_n)_n$. We recall that $\mathbb{C}\psi_n = \mathrm{Ker}(Q_n - 1)$, and

$$Q_n = |\psi_n\rangle\langle\psi_n| - |\mathrm{C}\psi_n\rangle\langle\mathrm{C}\psi_n| + \gamma_n,\ \psi_n, \mathrm{C}\psi_n \in \mathrm{Ker}\,\gamma_n. \tag{67}$$

– We first prove that there is no vanishing:

$$\exists A > 0,\ \limsup_n \sup_{z\in\mathbb{R}^3} \int\limits_{B(z,A)} |\psi_n(x)|^2 dx > 0.$$

Indeed, let us assume this is false. Then for any $A > 0$ the following holds:

$$D\big(|\psi_n|^2, |\psi_n|^2\big) \leq \frac{1}{A} + 2\Lambda\Big\{ \sup_{z\in\mathbb{R}^3} \int\limits_{B(z,A)} |\psi_n(x)|^2 dx\Big\}^{1/2},$$

where we have used Cauchy-Schwarz inequality and Hardy inequality. In the limit $n \to +\infty$ and then $A \to +\infty$, we have: $\limsup_n D\big(|\psi_n|^2, |\psi_n|^2\big) = 0$.

There holds *a priori* estimates (60): using Kato's inequality we would get

$$\liminf_n \mathcal{E}^0_{\mathrm{BDF}}(Q_n) \geq 2\liminf_n \langle|\mathcal{D}^0|\psi_n\,,\,\psi_n\rangle + \liminf_n \mathcal{E}^0_{\mathrm{BDF}}(\gamma_n) \geq 2m.$$

Thus, up to translation, we assume that $Q_n \rightharpoonup Q_\infty \neq 0$.

– As the BDF energy is sequential weakly lower continuous [HLS05b], we have

$$E_{1,1} \geq \mathcal{E}^0_{\mathrm{BDF}}(Q_\infty).$$

Our aim is to prove that $Q_\infty + \mathcal{P}^0_- \in \mathscr{M}_{\mathscr{C}}$: in other words that Q_∞ is a minimizer for $E_{1,1}$.

– The spectral decomposition (67) is not the relevant one: let us prove we can describe P_n in function of the spectral spaces of the "mean-field operator" $\widetilde{D}_{Q_n}$: the first step is to prove (69) below.

We recall that Q_n satisfies Eq. (44), that we have the decomposition (47).

The following holds:

$$\begin{aligned}\langle\widetilde{D}_{Q_n}\psi_n\,,\,\psi_n\rangle &= \langle|\mathcal{D}^0|\psi_n\,,\,\psi_n\rangle + \mathcal{O}\big(\alpha\||\nabla|^{1/2}\psi_n\|_{L^2}\||\nabla|^{1/2}Q\|_{\mathfrak{S}_2} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big)\\ &= \langle|\mathcal{D}^0|\psi_n\,,\,\psi_n\rangle + \mathcal{O}(\alpha^2) \geq m - K\alpha^2.\end{aligned}$$

Thus $\mathrm{Ran}\,P_n \cap \mathrm{Ran}\,\boldsymbol{\pi}^n_+ \neq \{0\}$. Let us prove this subspace has dimension 1: we use the minimizing property of Q_n. The condition on the first derivative gives (44), what is the condition on the second derivative ? For any $A \in \mathfrak{m}^{\mathscr{C}}_{P_n}$, expanding $e^A P_n e^{-A} - P_n$ in power of A, we get that the Hessian $\mathrm{Hess}_{P_n}(F_n)$ of $F_n := F_{\eta_n}$ at point P_n is

$$\begin{aligned}&\forall\, V \in \mathrm{T}_{P_n}\mathscr{M}_{\mathscr{C}},\ A = \big[V, P_n\big],\\ &\quad \mathrm{Hess}_{F_n}(P_n; V, V) = \mathrm{Tr}\big(\widetilde{D}_{Q_n}(A^2P_n - AP_nA)\big) + \eta_n\|V\|^2_{\mathfrak{S}_2} - \frac{\alpha}{2}\|V\|^2_{\mathrm{Ex}}.\end{aligned}$$

This Hessian is non-negative. For any unitary $f \perp g$ in $\mathrm{Ran}(\Pi_\Lambda - P_n)$ we choose

$$A := |f\rangle\langle -\mathrm{C}g| - |-\mathrm{C}g\rangle\langle f| + |g\rangle\langle\mathrm{C}f| - |\mathrm{C}f\rangle\langle g| \in \mathfrak{m}^{\mathscr{C}}_{P_n}.$$

As $-\mathrm{C}\widetilde{D}_{Q_n}\mathrm{C} = \widetilde{D}_{Q_n}$, the condition on the Hessian gives

$$2\big(\langle\widetilde{D}_{Q_n}f\,,\,f\rangle + \langle\widetilde{D}_{Q_n}g\,,\,g\rangle\big) + 4\eta_n \geq \frac{\alpha}{2}\big|\big|\,\big[A, P_n\big]\,\big|\big|^2_{\mathrm{Ex}} \geq 0. \tag{68}$$

We have $\mathrm{C}\psi_n \in \mathrm{Ran}(\Pi_\Lambda - P_n)$ and

$$\langle \widetilde{D}_{Q_n} \mathrm{C}\psi_n \, , \, \mathrm{C}\psi_n \rangle = -\langle \widetilde{D}_{Q_n} \psi_n \, , \, \psi_n \rangle \leq -m + K\alpha^2,$$

thus necessarily for n large, there is no plane in $\mathrm{Ran}(\Pi_\Lambda - P_n) \cap \mathrm{Ran}(\boldsymbol{\pi}^n_-)$, equivalently there is no plane in $\mathrm{Ran}\, P_n \cap \mathrm{Ran}\, \boldsymbol{\pi}^n_+$.

There exists a unitary $\psi_{e;n} \in \mathfrak{H}_\Lambda$ that spans $\mathrm{Ran}\, P_n \cap \mathrm{Ran}\, \boldsymbol{\pi}^n_+$. Equivalently $\psi_{v;n} := \mathrm{C}\psi_{e;n}$ spans the other one.

Thus:

$$P_n = |\psi_{e;n}\rangle\langle\psi_{e;n}| + \boldsymbol{\pi}^n_-. \tag{69}$$

- We thus write

$$Q_n = |\psi_{e;n}\rangle\langle\psi_{e;n}| - |\psi_{v;n}\rangle\langle\psi_{v;n}| + \overline{\gamma}_n = \overline{N}_n + \overline{\gamma}_n. \tag{70}$$

As $\mathrm{Ran}\, P_n$ is $\widetilde{D}_{Q_n}$-invariant and that $\widetilde{D}_{Q_n}$ is bounded (with a bound that depends on Λ), necessarily

$$\widetilde{D}_{Q_n} \psi_{e;n} = \mu_n \psi_{e;n}, \ \mu_n \in \mathbb{R}_+.$$

The condition on the Hessian enables us to say that

$$m - \mu_n + 2\eta_n \geq 0.$$

– As for ψ_n, there is no vanishing for $(\psi_{e,n})_n$ for α sufficiently small: decomposing $\psi_+ \in \mathrm{Ran}\, P_n$:

$$\psi_+ = a\psi_{e;n} + \phi, \ \phi \in \mathrm{Ran}\, P_n \cap \mathrm{Ran}\, \boldsymbol{\pi}^n_-,$$

we have

$$|a|^2 \geq \frac{1}{\mu}\big(m + \langle |\widetilde{D}_{Q_n}|\phi \, , \, \phi\rangle - K(\alpha^2 + \eta_n \|\Gamma_n\|_{\mathfrak{S}_2})\big).$$

Provided that μ_n is close to 1, the absence of vanishing for ψ_n implies that of $\psi_{e;n}$.

By Kato's inequality (29):

$$\begin{aligned}\widetilde{D}^2_{Q_n} &\geq |\mathcal{D}^0|\big(1 - 2\alpha \|R_{Q_n}|\mathcal{D}^0|^{-1}\|_{\mathcal{B}} - 4\eta_n \|\Gamma_n\|_{\mathcal{B}}\big)|\mathcal{D}^0| \\ &\geq |\mathcal{D}^0|^2\big(1 - \alpha\|Q_n\|_{\mathrm{Ex}} - 4\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big)\end{aligned}$$

Thus

$$\big|\widetilde{D}_{Q_n}\big| \geq |\mathcal{D}^0|\big(1 - \alpha\|Q_n\|_{\mathrm{Ex}} - 2\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\big) \text{ and } \mu_n \geq 1 - K(\alpha^2 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2}).$$

In the same way we can prove that

$$|\mu_n - m| \lesssim \alpha^2 + \eta_n \|\Gamma_n\|_{\mathfrak{S}_2}$$

So

$$\psi_{e,n} \rightharpoonup \psi_e \neq 0.$$

– We decompose $\overline{\gamma_n} = \boldsymbol{\pi}^n_- - \mathcal{P}^0_- \in \mathscr{E}_1 - \mathcal{P}^0_-$ as in (49): using Cauchy's expansion [HLS05a], we have

$$\boldsymbol{\pi}^n_- - \mathcal{P}^0_- = \frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\omega}{\mathcal{D}^0 + i\omega}\big(2\eta_n\Gamma_n - \alpha\Pi_\Lambda R_{Q_n}\Pi_\Lambda + 2\eta_n\Gamma_n\big)\frac{1}{\widetilde{D}_{Q_n} + i\omega}\Pi_\Lambda. \tag{71}$$

To justify this equality, we remark that $|\widetilde{D}_{Q_n}|$ is uniformly bounded from below: the r.h.s. of (71) is well-defined. Integrating the norm of bounded operator in (71), we get that

$$\|\boldsymbol{\pi}^n_- - \mathcal{P}^0_-\|_{\mathcal{B}} \lesssim \alpha\|Q_n\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2} < 1.$$

In fact, we can also expand in power of $Y_n := -\alpha\Pi_\Lambda R_{Q_n}\Pi_\Lambda + 2\eta_n\Gamma_n$:

$$\left\{\begin{array}{rcl} \boldsymbol{\pi}^n_- - \mathcal{P}^0_- & = & \displaystyle\sum_{j\geq 1} \alpha^j M_j[B_n], \\ M_j[Y_n] & = & \displaystyle -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{d\omega}{\mathcal{D}^0 + i\omega}\Big(Y_n \frac{1}{\mathcal{D}^0 + i\omega}\Big)^j. \end{array}\right. \tag{72}$$

We take the Hilbert-Schmidt norm [HLS05a, Sok12]: as $\|R_{Q_n}\frac{1}{|\nabla|^{1/2}}\|_{\mathfrak{S}_2} \lesssim \|Q\|_{\mathrm{Ex}}$, we have

$$\|\overline{\gamma}_n\|_{\mathfrak{S}_2} \lesssim \alpha\|Q_n\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2} \lesssim \alpha^2. \tag{73}$$

We thus write

$$\overline{\gamma}_n \quad = \quad \sum_{j\geq 1}\lambda_{j;n}q_{j;n},$$

where $q_{j;n}$ has the same form as the one in (49).
– Up to a subsequence, we assume all weak convergences as in Remark (12): the sequence of eigenvalues $(\lambda_{j;n})_n$ tends to $(\mu_j)_j \in \ell^2$ and each $(e^\star_{j;n})_n$ (with $\star \in \{a,b\}$) tends to $e^\star_{j;\infty}$, $(\psi_{e;n})_n$ tends to ψ_e. We also assume that the sequence $(\mu_n)_n$ tends to μ with $0 \leq \mu \leq m$. For shot we write $\psi_v := \mathrm{C}\psi_e$.

– We write $\overline{P} := Q_\infty + \mathcal{P}^0_-$ and $\overline{\boldsymbol{\pi}} := \chi_{(-\infty,0)}(D_{Q_\infty})$. We will prove that

1. $\big[D^{(\Lambda)}_{Q_\infty}, \overline{P}\big] = 0$,
2. $D_{Q_\infty}\psi_e = \mu\psi_e$ and so $\overline{\boldsymbol{\pi}}\psi_e = 0$.
   Moreover $D_{Q_\infty}\mathrm{C}\psi_e = -\mu\mathrm{C}\psi_e$ and $\langle \mathrm{C}\psi_e\,,\,\psi_e\rangle = 0$.
3. $\overline{\boldsymbol{\pi}} = \overline{P} - |\psi_e\rangle\langle\psi_e| + |\mathrm{C}\psi_e\rangle\langle\mathrm{C}\psi_e|$.

Notation 8. We write $D^{(\Lambda)}_{Q_\infty} := \Pi_\Lambda D_{Q_\infty}\Pi_\Lambda$ for short.

This all comes from the fact that

$$\mathrm{s}-\lim_n R_{Q_n} = R_{Q_\infty}. \tag{74}$$

This fact enables us to show

$$\left|\begin{array}{l} R_{Q_n}\psi_{e;n} \rightharpoonup_n R_{Q_\infty}\psi_e \text{ in } L^2, \\ \mathrm{s.op.}-\lim_n \big(\boldsymbol{\pi}^n_- - \mathcal{P}^0_-\big) = \overline{\boldsymbol{\pi}} - \mathcal{P}^0_- \text{ in } \mathcal{B}(\mathfrak{H}_\Lambda), \\ \mathrm{w.op.}-\lim_n P_n = \overline{\boldsymbol{\pi}} - \mathcal{P}^0_- + |\psi_e\rangle\langle\psi_e| - |\psi_v\rangle\langle\psi_v| \text{ in } \mathcal{B}(\mathfrak{H}_\Lambda). \end{array}\right. \tag{75}$$

Indeed for any $f \in \mathfrak{H}_\Lambda$ we have

$$\begin{aligned}\|R_{Q_n}f - R_{Q_\infty}f\|^2_{L^2} &= \int\Big|\int\frac{(Q_n-Q_\infty)(x,y)}{|x-y|}f(y)dy\Big|^2dx \\ &\leq \|f\|^2_{L^2}\Big(\frac{1}{A^2}\|Q_n-Q_\infty\|^2_{\mathfrak{S}_2} + 4\Lambda^2\iint\limits_{B(0,2A)^2}|(Q_n-Q_\infty)(x,y)|^2dxdy\Big) \\ &\quad + 4\Lambda^2\|Q_n-Q_\infty\|^2_{\mathfrak{S}_2}\int\limits_{B(0,A)^c}|f(y)|^2dy.\end{aligned}$$

We have just split as follows: for $x \in \mathbb{R}^3$ we consider

$$\mathbb{R}^3 = B(x,A)^c \sqcup B(x,A)\cap B(0,A) \sqcup B(x,A)\cap B(0,A)^c.$$

Taking the limsup $n \to +\infty$ we get that

$$\forall\, A>0,\ \limsup_n\|R_{Q_n}f - R_{Q_\infty f}\|^2_{L^2} \leq 4\limsup_n\|Q_n\|^2_{\mathfrak{S}_2}\Big(\frac{\|f\|^2_{L^2}}{A^2} + 4\Lambda^2\int\limits_{B(0,A)^c}|f(y)|^2dy\Big),$$

taking the limit $A \to +\infty$ we get that

$$\limsup_n\|R_{Q_n}f - R_{Q_\infty f}\|^2_{L^2} = 0.$$

In particular for any $f \in \mathfrak{H}_\Lambda$

$$\langle R_{Q_n}\psi_{e;n}\,,\,f\rangle = \langle\psi_{e;n}\,,\,R_{Q_n}f\rangle \underset{n\to+\infty}{\longrightarrow} \langle\psi_e\,,\,R_{Q_\infty}f\rangle = \langle R_{Q_\infty}\psi_e\,,\,f\rangle.$$

Thus $\widetilde{D}_{Q_n}\psi_{e;n} \underset{n\to+\infty}{\rightharpoonup} D_{Q_\infty}\psi_e$, and $D_{Q_\infty}\psi_e = \mu\psi_e$.
– Let us prove that

$$\text{s. op.} - \lim_n \boldsymbol{\pi}_-^n = \overline{\boldsymbol{\pi}}. \tag{76}$$

We have

$$R_{Q_n}\frac{1}{\mathcal{D}^0+i\omega}f = R[Q_n - Q_\infty]\frac{1}{\mathcal{D}^0+i\omega}f + R_{Q_\infty}\frac{1}{\mathcal{D}^0+i\omega}f$$

and at fixed ω and f

$$R[Q_n - Q_\infty]\frac{1}{\mathcal{D}^0+i\omega}f \underset{n\to+\infty}{\longrightarrow} 0 \text{ in } L^2.$$

Generally for $J \geq 1$, we expand $\left(R_{Q_n}\frac{1}{\mathcal{D}^0+i\omega}\right)^J$ in power of $R[Q_n - Q_\infty]$ and Q_∞. We get:

$$\forall\, \omega, f,\ \left(R_{Q_n}\frac{1}{\mathcal{D}^0+i\omega}\right)^J \underset{n\to+\infty}{\longrightarrow} 0 \text{ in } L^2.$$

Moreover

$$\begin{aligned}\left|\left|\left(R_{Q_n}\frac{1}{\mathcal{D}^0+i\omega}\right)^J\right|\right|_{L^2} &\leq \widetilde{E}\,(\omega)^{-J/2}\,\|Q_n\tfrac{1}{|\mathcal{D}^0|^{1/2}}\|_{\mathcal{B}}^J\|f\|_{L^2},\\ &\leq \left(\limsup_n \|Q_n\|_{\mathrm{Ex}}\widetilde{E}\,(\omega)^{-1/2}\right)^J\|f\|_{L^2}.\end{aligned}$$

By dominated convergence as

$$u_j\|f\|_{L^2} := \int \frac{d\omega}{\widetilde{E}\,(\omega)^{1+J/2}}\left(\alpha\|Q_n\|_{\mathrm{Ex}} + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\right)^J\|f\|_{L^2} < +\infty, \tag{77}$$

we get

$$M_j[Y_n]f \underset{n\to+\infty}{\longrightarrow} M_j[\alpha R_{Q_\infty}]f \text{ in } L^2.$$

To end this argument we remark that the series $\sum_{j\geq 1} u_j$ is convergent for α and η_n sufficiently small: thus we have

$$\sum_{j\geq 1} M_j[Y_n]f \underset{n\to+\infty}{\longrightarrow} \sum_{j\geq 1} M_j[\alpha R_{Q_\infty}]f \text{ in } L^2,$$

that is (76) holds.
– Thanks to (76), there holds (in the weak operator topology for instance)

$$Q_\infty = \lim_n Q_n = |\psi_e\rangle\langle\psi_e| - |\psi_v\rangle\langle\psi_v| + \overline{\boldsymbol{\pi}} - \mathcal{P}_-^0,$$

that is

$$\overline{P} = |\psi_e\rangle\langle\psi_e| - |\psi_v\rangle\langle\psi_v| + \overline{\boldsymbol{\pi}}. \tag{78}$$

In the weak operator topology we also have

$$\text{w. op.} - \lim_n \left[\widetilde{D}_{Q_n}, Q_n + \mathcal{P}_-^0\right] = \left[D_{Q_\infty}^{(\Lambda)}, Q_\infty + \mathcal{P}_-^0\right],$$

by strong convergence of R_{Q_n} to R_{Q_∞} and norm convergence of $\eta_n\Gamma_n$ to 0.
– There remains to prove that $\|\psi_e\|_{L^2} = 1$. We assume for the moment that we can uniformly separate the μ_n's from the remainder of the positive spectrum $\sigma\left(|\widetilde{D}_{Q_n}|\right)\backslash\{\mu_n\}$. Let us write a_n the bottom of this last set: there exists $\varepsilon > 0$ (of order α^2 in fact) such that for n_0 sufficiently large:

$$\forall n \geq n_0,\ a_n - \mu_n \geq 5\varepsilon. \tag{79}$$

In particular, we can draw a small circle in $\mathbb{C}$ that intersects $\mathbb{R}$ only at points $\mu \pm 2\varepsilon$. We write $\mathcal{C}_\varepsilon$ this circle: it has been chosen such that if $|\mu_n - \mu| \leq \varepsilon$ (true for $n \geq n_1$ where $n_1 \geq n_0$ is sufficiently large),

$$\forall n \geq n_0,\ \mathrm{dist}\big(\mu_n; \mathcal{C}_\varepsilon\big) \geq \varepsilon.$$

By functional calculus we have

$$|\psi_{e;n}\rangle\langle\psi_{e;n}| = \frac{1}{2i\pi}\int_{\mathcal{C}_\varepsilon} \frac{dz}{z - \widetilde{D}_{Q_n}}.$$

We want to substract $\chi_{(\mu-2\varepsilon,\mu+2\varepsilon)}\big(D^{(\Lambda)}_{Q_\infty}\big)$. If (79) is true, then the same holds for the limit $D^{(\Lambda)}_{Q_\infty}$ by strong convergence. Indeed, for any $f \in \mathrm{Ran}\big(\overline{\boldsymbol{\pi}}_+\big)$ (where $\overline{\boldsymbol{\pi}}_+ := \Pi_\Lambda - \overline{\boldsymbol{\pi}}$) we have

$$\|\boldsymbol{\pi}^n_+ f - f\|_{L^2} \to 0.$$

For $f_1 \perp f_2$ in $\mathrm{Ran}\big(\overline{\boldsymbol{\pi}}_+\big)$, there holds

$$\min_j \big(\frac{1}{\|\overline{\boldsymbol{\pi}}^n_+ f_j\|^2_{L^2}}\big)\langle \widetilde{D}_{Q_n}\overline{\boldsymbol{\pi}}^n_+ f_1\ ,\ f_1\rangle + \langle \widetilde{D}_{Q_n}\overline{\boldsymbol{\pi}}^n_+ f_2\ ,\ f_2\rangle \geq a_n + \mu_n$$

– We prove the gap (79) for $D^{(\Lambda)}_{Q_\infty}$ by taking the liminf. Thus, we can isolate the bottom of $\sigma\big(|A|\big)$ for $A = \widetilde{D}_{Q_n}$ or $A = D^{(\Lambda)}_{Q_\infty}$ by the same circle and get

$$|\psi_{e;n}\rangle\langle\psi_{e;n}| - \frac{1}{\|\psi_e\|^2_{L^2}}|\psi_e\rangle\langle\psi_e| = \frac{1}{2i\pi}\int_{\mathcal{C}_\varepsilon} \frac{dz}{z - \widetilde{D}_{Q_n}}\big(\alpha R[Q_\infty - Q_n] + 2\eta_n\Gamma_n\big)\frac{1}{z - D^{(\Lambda)}_{Q_\infty}}.$$

By dominated convergence, this operator strongly converges to 0: this proves

$$\|\psi_e\|_{L^2} = 1.$$

Proof of (79) **and estimate on** $E_{1,1}$ This proof is based on the method of [Sok12]: we know that

$$|m - \mu_n| \leq K\alpha^2$$

and that

$$\widetilde{D}_{Q_n}\psi_{e;n} = \mu_n\psi_{e;n}. \tag{80}$$

In the following, we will get estimates on the Sobolev norms of $\psi_{e;n}$, this will enable us to estimate $\langle \widetilde{D}_{Q_n}\psi_{e;n}\ ,\ \psi_{e;n}\rangle$. We will use estimates on g_0, g_1 written in (24).

Estimate on $\nabla\psi_{e;n}$ From (80) we have

$$\begin{aligned}\|\mathcal{D}^0\psi_{e;n}\|^2_{L^2} - m^2 \leq K\alpha^2 &+ 4\alpha\|Q_n\|_{\mathfrak{S}_2}\|\nabla\psi_{e;n}\|_{L^2} + 4\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}\\ &+2\|\nabla\psi_{e;n}\|^2_{L^2}\big(\alpha\|Q_n\|^2_{\mathfrak{S}_2} + 4\eta^2_n\|\Gamma_n\|^2_{\mathfrak{S}_2}\big)\end{aligned}$$

and $\|\nabla\psi_{e;n}\|^2_{L^2} \lesssim \alpha^2$. In the same way, for n sufficiently large, we can prove that

$$\langle\, |\nabla|^3\psi_{e;n}\ ,\ \psi_{e;n}\rangle \lesssim \alpha^3.$$

We multiply (80) by $|\nabla|^{1/2}$ and take the L^2-norm. We can drop all terms with $2\eta_n\Gamma_n$ because all the operators that we consider are bounded in $\mathfrak{H}_\Lambda$ and $\eta_n\|\Gamma_n\|_{\mathfrak{S}_2}$ tends to 0 as n tends to $+\infty$. We just have to deal with $|\nabla|^{1/2}R_{Q_n}\psi_{e;n}$. We recall that in Fourier space, the following holds [HLS05a]

$$\forall\, Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda), p, q \in \mathbb{R}^3,\ \mathscr{F}\big(R_Q; p, q\big) = \frac{1}{2\pi}\int_{\mathbb{R}^3}\frac{d\ell}{|\ell|^2}\widehat{Q}(p - \ell, q - \ell).$$

So, writing $\mathfrak{A}_n$ the operator whose Fourier transform is given by the integral kernel

$$\mathscr{F}\big(\mathfrak{A}_n; p, q\big) := |p - q|^{1/2}|\widehat{Q}(p, q)|,$$

we have

$$\Big|\mathscr{F}\big([|\nabla|^{1/2}, R_{Q_n}]\big)\Big| \leq \mathscr{F}\big(R_{\mathfrak{A}_n}; p, q\big).$$

By Hardy's inequality, we have

$$\big|\big|[|\nabla|^{1/2}, R_{Q_n}]\psi_{e;n}\big|\big|_{L^2} \leq 4\| \, |\nabla|^{1/2} Q_n\|_{\mathfrak{S}_2} \|\nabla\psi_{e;n}\|_{L^2} \lesssim \alpha^{3/2}.$$

As

$$\|R_{Q_n}|\nabla|^{1/2}\psi_{e;n}\|_{L^2} \leq \frac{\pi}{2}\| \, |\nabla|^{1/2} Q_n\|_{\mathfrak{S}_2} \|\nabla\psi_{e;n}\|_{L^2} \lesssim \alpha^{3/2},$$

we have $\| \, |\nabla|^{1/2} R_{Q_n}\psi_{e;n}\|_{L^2} \lesssim \alpha^{3/2}$ and

$$\langle \, |\nabla||\mathcal{D}^0|^2\psi_{e;n} \, , \, \psi_{e;n}\rangle - m^{\langle}|\nabla|\psi_{e;n} \, , \, \psi_{e;n}\rangle \lesssim \alpha^3. \tag{81}$$

Estimates on $\chi_{e;n}$ We scale (80) by α^{-1}, that is we consider

$$\underline{\psi_{e;n}}(x) := \alpha^{-3/2}\psi_{e;n}(\tfrac{x}{\alpha}), \ x \in \mathbb{R}^3.$$

This enables us to get an estimate of the lower spinor of $\psi_{e;n}$. We write

$$\psi_{e;n} =: \begin{pmatrix} \varphi_{e;n} \\ \chi_{e;n} \end{pmatrix} \in L^2(\mathbb{R}^3, \mathbb{C}^2)^2$$

For short we also write

$$\mathbf{g}_1(p) := g_1(p)\tfrac{p}{|p|}, \ p \in \mathbb{R}^3.$$

We write

$$\underline{Q_n}(x,y) := \alpha^{-3}\underline{Q_n}\big(\frac{x}{\alpha}, \frac{y}{\alpha}\big) \text{ and } \underline{\Gamma_n}(x,y) := \alpha^{-3}\underline{\Gamma_n}\big(\frac{x}{\alpha}, \frac{y}{\alpha}$$

The upper and lower spinors $\underline{\varphi_{e;n}}$ and $\underline{\chi_{e;n}}$ of $\underline{\psi_{e;n}}$ satisifies

$$\underline{\chi_{e;n}} = \frac{\mathbf{g}_1\big(\frac{-i\nabla}{\alpha}\big)\cdot\boldsymbol{\sigma}}{\alpha^2(\mu_n + g_0\big(\frac{i\nabla}{\alpha}\big))}\underline{\varphi_{e;n}} + \big(-\alpha^2 R_{\underline{Q_n}}\underline{\psi_{e;n}} + 2\alpha\eta_n\underline{\Gamma_n}\underline{\psi_{e;n}}\big)_{\downarrow}. \tag{82}$$

By Hardy's inequality, we get that

$$\|\chi_{e;n}\|_{L^2} = \|\underline{\chi_{e;n}}\|_{L^2} \lesssim \alpha.$$

As there holds:

$$\langle -\Delta\chi_{e;n} \, , \, \chi_{e;n}\rangle \leq \| \, |\nabla|^{3/2}\chi_{e;n}\|_{L^2}\sqrt{\|\chi_{e;n}\|_{L^2}\|\nabla\chi_{e;n}\|_{L^2}}$$

we also get the following (rough) estimate

$$\|\chi_{e;n}\|_{L^2} \lesssim \alpha^{4/3}.$$

Estimate on $E_{1,1}$ Using (24), we have (here $g_\star$ means $g_\star(-i\nabla)$)

$$\begin{aligned}
\langle \mathcal{D}^0\psi_{e;n} \, , \, \psi_{e;n}\rangle &= \langle g_0\psi_{e;n} \, , \, \psi_{e;n}\rangle + 2\mu_n\langle \tfrac{g_1^2}{(g_0+\mu_n)^2}\phi_{e;n} \, , \, \phi_{e;n}\rangle + \mathcal{O}\big(\alpha(\alpha^2 + \eta_n\|\Gamma_n\|_{\mathfrak{S}_2})\big) \\
&= \langle g_0\psi_{e;n} \, , \, \psi_{e;n}\rangle + 2m\langle \tfrac{g_1^2}{(g_0+m)^2}\phi_{e;n} \, , \, \phi_{e;n}\rangle + \mathcal{O}\big(\alpha^3\big), \\
&= m + \frac{g_1'(0)^2}{2m}\|\nabla\phi_{e;n}\|_{L^2}^2 + \mathcal{O}\big(\alpha^3\big).
\end{aligned}$$

As $\psi_{v;n} = \mathrm{C}\psi_{e;n}$, we have

$$\frac{1}{2}\iint \frac{|\psi_{e;n}\wedge\psi_{v;n}(x,y)|^2}{|x-y|}dxdy = D\big(|\varphi_{e;n}|^2, |\varphi_{e;n}|^2\big) + \mathcal{O}(\alpha^3).$$

Using (73), we finally get for n sufficiently large

$$\langle \widetilde{D}_{Q_n}\psi_{e;n} \, , \, \psi_{e;n}\rangle = m + \frac{g_1'(0)^2}{2m}\|\nabla\phi_{e;p}\|_{L^2}^2 - \alpha D\big(|\varphi_{e;n}|^2, |\varphi_{e;n}|^2\big) + \mathcal{O}(\alpha^3). \tag{83}$$

As $\|\varphi_{e;n}\|_{L^2}^2 = 1 - K\alpha^2$, we get

$$E_{1,1} \geq \mathcal{E}^0_{\mathrm{BDF}}(Q_\infty) = 2m + \frac{\alpha^2 m}{g_1'(0)^2}\mathcal{E}_{\mathrm{CP}}\big(\widetilde{\varphi_{e;n}}\big) + \mathcal{O}(\alpha^3),$$

where $\mathcal{E}_{\mathrm{CP}}$ denotes the Pekar energy [LL97] and $\widetilde{\varphi_{e;n}}$ is the scaling of $\varphi_{e;n}$ by $\frac{g_1'(0)^2}{\alpha m}$.

We already have an upper bound of $E_{1,1}$: it has the same expansion with $\mathcal{E}_{\mathrm{CP}}\big(\varphi_{e;n}\big)$ replaced by the smallest possible value E_{CP}. As there holds

$$\mathcal{E}_{\mathrm{CP}}\big(\underline{\varphi_{e;n}}\big) \geq (1 - \|\chi_{e;n}\|_{L^2}^2)^3 E_{\mathrm{CP}}$$

we thus have

$$\mathcal{E}_{\mathrm{CP}}\big(\underline{\varphi_{e;n}}\big) = E_{\mathrm{CP}} + \mathcal{O}(\alpha), \tag{84}$$

and

$$\mu_n = m + 2m\frac{\alpha^2}{g_1'(0)^2}E_{\mathrm{CP}} + \mathcal{O}(\alpha^3). \tag{85}$$

Thus $\mu_n < m$ for α sufficiently small. Are there other eigenvalues in $(0, m)$? As the Hessians are non-negative (see (68)), we have

$$\sigma\,|\widetilde{D}_{Q_n}| \subset [\mu_n - 2\eta_n, +\infty)$$

Let $\xi_n \perp \psi_n$ in $\mathrm{Ran} \in (\boldsymbol{\pi}_+^n)$ and $s_n \in (\mu_n - 2\eta_n, m)$ such that

$$\widetilde{D}_{Q_n}\xi_n = s_n\xi_n.$$

By the same method as before used for $\psi_{e;n}$, we can prove the following:

$$\begin{array}{l|l} \|\nabla\xi_n\|_{L^2} \lesssim \alpha, & \|\,|\nabla|^{3/2}\xi_n\|_{L^2} \lesssim \alpha^{3/2}, \\ \|(\xi_n)_\downarrow\|_{L^2} \lesssim \alpha, & \|\nabla(\xi_n)_\downarrow\|_{L^2} \lesssim \alpha^{4/3}. \end{array}$$

The arrow $\downarrow$ means we take the lower spinor (which is in $L^2(\mathbb{R}^3, \mathbb{C}^2)$). In particular we have

$$s_n = \langle \widetilde{D}_{Q_n}\xi_n\,,\,\xi_n\rangle = m + \frac{g_1'(0)^2}{2m}\|\nabla\xi_n\|_{L^2}^2 - \alpha D(\xi_n^*\psi_{e;n}; \xi_n^*\psi_{e;n}) + \mathcal{O}(\alpha^{8/3}).$$

Remark 13. We have lost $\alpha^{1/3}$ due to the rough estimate $\|\nabla(\xi_n)_\downarrow\|_{L^2} \lesssim \alpha^{4/3}$. We can prove that this quantity is of order α^2, but the proof is technical.

Estimate on $\underline{\psi_{e;n}}$ We know that $\underline{\psi_{e;n}}$ is close to a Pekar minimizer: its Pekar energy is

$$E_{CP} + \mathcal{O}(\alpha^{2/3}).$$

For α sufficiently small, we know that this gives information about the distance between $\underline{\psi_{e;n}}$ and the manifold $\mathscr{P}$ of Pekar minimizer [Len09]:

$$\mathrm{dist}_{H^1}(\underline{\psi_{e;n}}, \mathscr{P})^2 \leq K\mathcal{E}_{\mathrm{CP}}(\underline{\psi_{e;n}}) - E_{\mathrm{CP}}.$$

The notation dist_{H^1} means the distance in the H^1-norm.

This result is stated in $L^2(\mathbb{R}^3, \mathbb{C})$, but it is not hard to prove it is also true in $L^2(\mathbb{R}^3, \mathbb{C}^4)$: in this case $\mathscr{P}$ is isomorphic to $\mathbb{R}^3 \times \mathbb{S}^3$ (and not simply to $\mathbb{R}^3 \times \mathbb{S}^1$).

If $\underline{\xi_n}$ denotes the scaling of ξ_n by $\frac{g_1'(0)^2}{2\alpha m}$, there holds

$$\frac{g_1'(0)^2}{2\alpha^2 m}(s_n - m) = \|\nabla\underline{\xi_n}\|_{L^2}^2 - D\big(\underline{\xi_n}^*\underline{\psi_{e;n}}, \underline{\xi_n}^*\underline{\psi_{e;n}}\big) + \mathcal{O}(\alpha^{2/3}). \tag{86}$$

Eventually by replacing $\underline{\psi_{e;n}}$ by its projection ϕ^n_{CP} onto $\mathscr{P}$, we also have

$$\frac{g_1'(0)^2}{2\alpha^2 m}(s_n - m) = \|\nabla\underline{\xi_n}\|_{L^2}^2 - D\big(\underline{\xi_n}^*\phi^n_{\mathrm{CP}}, \underline{\xi_n}^*\phi^n_{\mathrm{CP}}\big) + \mathcal{O}(\alpha^{1/3}). \tag{87}$$

Proof of (79) We just have to study the spectrum of $\sigma(-\Delta - R(|\phi^n_{\rm CP}\rangle\langle\phi^n_{\rm CP}|))$, and precisely its negative eigenvalues. Its smallest eigenvalue is $E_{\rm CP}$ with eigenvector $\phi^n_{\rm CP}$. Now we seek the second smallest eigenvalue, that is

$$F_{\rm CP} := \inf\Big\{\langle\big(-\Delta - R(|\phi^n_{\rm CP}\rangle\langle\phi^n_{\rm CP}|)\big)f\,,\,f\rangle,\ f\perp\phi^n_{\rm CP}\in H^1,\ \|f\|_{L^2}=1\Big\}. \quad (88)$$

By studying a minimizing sequence, we get

$$F_{\rm CP} > E_{\rm CP}. \quad (89)$$

By continuity the same holds for the spectrum of $-\Delta - R(|\underline{\psi_{e;n}}\rangle\langle\underline{\psi_{e;n}}|)$: for α sufficiently small (and n sufficiently big) its smallest eigenvalue t_n has multiplicity one and its second smallest eigenvalue $\widetilde{t_n}$ is away from t_n, uniformly in α (and n):

$$\widetilde{t}_n - t_n > \frac{F_{\rm CP}-E_{\rm CP}}{2} > 0.$$

As a consequence, we get from (86) the following:

$$s_n - \mu_n \geq \frac{\alpha^2 m}{g_1'(0)^2}\big(F_{\rm CP}-E_{\rm CP}\big) + \mathcal{O}(\alpha^{7/3}), \quad (90)$$

and (79) holds.

3.4 Proof of Theorems 2 and 3

In fact, it suffices to follow the proof of Theorem 1: instead of having an almost minimizer, we deal with a real minimizer $\overline{P} = \overline{Q} + \mathcal{P}^0_-$. Technically speaking, we just have to drop the term $\eta_n\Gamma_n$ in the equations and by the same method we prove the following.

1. There exist $0<\mu<m$ and a wave function $\psi_e\in\mathfrak{H}_\Lambda$ such that

$$\begin{cases} \overline{P} = |\psi_e\rangle\langle\psi_e| - |{\rm C}\psi_e\rangle\langle{\rm C}\psi_e| + \chi_{(-\infty,0)}\big(\Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda\big), \\ \Pi_\Lambda D_{\overline{Q}}\Pi_\Lambda\psi_e = \mu\psi_e. \end{cases} \quad (91)$$

2. We have $\|\,|\nabla|^3\psi_e\|_{L^2}\lesssim\alpha^{3/2}$. Splitting ψ_e into upper and lower spinors φ_e and χ_e, we have $\|\chi_e\|_{L^2}\lesssim\alpha$. We write $\widetilde{\varphi_e}(x) := \lambda^{3/2}\varphi_e(\lambda x)$ with $\lambda = \frac{g_1'(0)^2}{\alpha m}$. The following holds:

$$\begin{cases} E_{1,1} &= 2m + \frac{\alpha^2 m}{g_1'(0)^2}\mathcal{E}_{\rm CP}\big(\widetilde{\varphi_e}\big) + \mathcal{O}(\alpha^3) \\ &= 2m + \frac{\alpha^2 m}{g_1'(0)^2}{\rm E}_{\rm CP} + \mathcal{O}(\alpha^3), \\ \mu &= m + 2m\frac{\alpha^2}{g_1'(0)^2}E_{\rm CP} + \mathcal{O}(\alpha^3). \end{cases} \quad (92)$$

3. In the limit $\alpha\to 0$ we have

$$\lim_{\alpha\to0}\|\chi_e\|_{L^2} = 0 \text{ and } \lim_{\alpha\to0}\mathcal{E}_{\rm CP}\big(\widetilde{\varphi_e}\big) = {\rm E}_{\rm CP}.$$

The *geometrical* description of a minimizer of Theorem 2 has already been proved at the end of Subsection 3.2 under the assumption of existence.

4 Proofs on results on the variational set

4.1 On the manifold $\mathscr{M}$: Theorem 4, Propositions 1, 2

Proof of Theorem 4

– As Q is a compact self-adjoint operator, we apply the spectral theorem and write

$$Q = \sum_{i\in\mathbb{Z}^*} \mu_i |b_i\rangle\langle b_i|,$$

where $(\mu_i)_{i\in\mathbb{N}}$ (resp. $(\mu_i)_{i\in\mathbb{Z}^*_-}$) is the non-increasing sequence of positive eigenvalues of Q (resp. increasing sequence of negative eigenvalues).

It is clear that $-1 \leq Q \leq 1$. If $Q\psi = \psi$, then necessarily $P_1\psi = \psi$ and $P_0\psi = 0$, analogously if $Q\psi = -\psi$, then $P_1\psi = 0$ and $P_0\psi = \psi$.

Up to index translation we have:

$$A := Q - \Big\{ \sum_{i=1}^{M_+} |a_i\rangle\langle a_i| - \sum_{i=1}^{M_-} |a_{-i}\rangle\langle a_{-i}| \Big\} = \sum_{i\in\mathbb{Z}^*} \mu_i |b_i\rangle\langle b_i| = A_p - A_n, \tag{93}$$

where A_p is the sum over positive i and $-A_n$ over negative i.

Notation 9. For short, for any $\mu \in \mathbb{R}$ and any self-adjoint operator S, we write $E^S_\mu = \mathrm{Ker}(S-\mu)$ the spectral subspace of S.

Furthermore, for an operator B we write

$$B^{\varepsilon_1\ \varepsilon_2} = P_0(\varepsilon_1) B P_0(\varepsilon_2),\ \varepsilon_i = \pm,\ P_0(-) = P_0,\ P_0(+) = 1 - P_0.$$

– We know that

$$Q^{++} - Q^{--} = Q^2 = \sum_{i=1}^{M_+} |a_i\rangle\langle a_i| + \sum_{i=1}^{M_-} |a_{-i}\rangle\langle a_{-i}| + \sum_{i\in\mathbb{Z}^*} \mu_i^2 |b_i\rangle\langle b_i|.$$

In particular $[Q^2, P_0] = 0$ and all the spectral subspaces of Q^2 are P_0-invariant. For any $\mu > 0$,

$$E^{Q^2}_{\mu^2} = E^Q_\mu \overset{\perp}{\oplus} E^Q_{-\mu} = E^{Q^{++}}_{\mu^2} \overset{\perp}{\oplus} E^{Q^{--}}_{-\mu^2}.$$

For $i \in \mathbb{N}$, let c_i be a unitary eigenvector for Q^{++} with eigenvalue $0 < \mu_i^2 < 1$. We write

$$c_i = c_p + c_n,\ c_p \in \mathrm{Ran}(A_p),\ c_n \in \mathrm{Ran}(A_n).$$

We have $A_p c_p = \mu_i c_p$ and $A_n c_n = -\mu_i c_n$. Moreover $c_n \neq 0$, otherwise $(1-P_0)c_p = c_p$ and

$$A c_p = \mu_i c_p = ((1-P_0) - (1-P_1))c_p \ i.e.\ (1-P_1)c_p = (1-\mu_i)c_p.$$

This would give $\mu_i = 1$ or $\mu_i = 0$. By the same argument $c_p \neq 0$. We have $P_0 c_p = -P_0 c_n$ and this vector is non-zero, otherwise $(1-P_0)c_p = c_p$. Thus the two-dimensional plane $\Pi = \mathrm{Span}(c_p, c_n)$ is in $E^{Q^2}_{\mu_i^2}$ and there exists an orthonormal basis $(e_+ = c_i, e_-)$ of Π such that $P_0 e_- = e_-$ (and $(1-P_0)c_i = c_i$).

We write $c_p = ||c_p|| d_p$ and $c_n = ||c_n|| d_n$ and up to a phase, we have:

$$c_i = \cos(\phi) d_p + \sin(\phi) d_n.$$

There holds:

$$Q^2 c_i = \mu_i^2 c_i = A_p c_i = \mu_i (1-P_0)(\cos(\phi) d_p + \sin(\phi) d_n) = \mu_i(\cos(\phi)^2 - \sin(\phi)^2) c_i,$$

and $\mu_i = \cos(2\phi)$. We have

$$E^{Q^2}_{\mu_i^2} = \Pi \overset{\perp}{\oplus} R.$$

– By induction over the dimension of the remainder $\mathrm{Dim}(R \cap E^{Q^{++}}_{\mu_i^2})$, we can decompose $E^{Q^2}_{\mu_i^2}$ as a sum of orthogonal planes: by symmetry there holds $\mathrm{Dim}\, E^{Q^{++}}_{\mu_i^2} = \mathrm{Dim}\, E^{Q^{--}}_{\mu_i^2}$. Each plane Π is invariant under the action of Q and $\mathcal{P}^0_-$ and so also

under that $P = Q + \mathcal{P}^0_-$. Therefore, there also exists an orthonormal basis (v_+, v_-) of Π such that $P_1 v_- = v_-$ and $(1 - P_1)v_+ = v_+$. Up to a phase we suppose that

$$v_- = \cos(\theta)e_- + \sin(\theta)e_+ \text{ and } v_+ = -\sin(\theta)e_- + \cos(\theta)e_+,\ \theta \in (0, \tfrac{\pi}{2}). \tag{94}$$

In the plane Π we thus have:

$$Q|_\Pi = |v_-\rangle\langle v_-| - |e_-\rangle\langle e_-|.$$

Such an operator has eigenvalues $\pm\sin(\theta)$ with eigenvectors

$$\begin{cases} f_+ = \sqrt{\frac{1-\sin(\theta)}{2}}e_- + \sqrt{\frac{1+\sin(\theta)}{2}}e_+ & \text{associated to } \sin(\theta), \\ f_- = -\sqrt{\frac{1+\sin(\theta)}{2}}e_- + \sqrt{\frac{1-\sin(\theta)}{2}}e_+ & \text{associated to } -\sin(\theta) \end{cases} \tag{95}$$

□

Proof of Proposition 1 In general, let P_1 and P_2 be two orthogonal projectors in $\mathfrak{H}_\Lambda$. If $P_2 = UP_1U^{-1}$ where U is a unitary operator, we have:

$$P_2 - P_1 \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \iff [U, P_1]U^{-1} \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \textit{ i.e. } [U, P_1] \in \mathfrak{S}_2(\mathfrak{H}_\Lambda). \tag{96}$$

– For any $P_1 \in \mathscr{M}$ and any $P_2 \in \mathscr{M}$ with $\|P_1 - P_2\|_{\mathcal{B}} < 1$, we can decompose $P_2 - P_1$ as in Theorem 4 but with P_1 as new reference (the decomposition is the same but with $e_j \in \mathrm{Ran}\,(1 - P_1)$ and $e_{-j} \in \mathrm{Ran}\,P_1$):

$$\begin{cases} P_2 - P_1 = \sum_{j\in\mathbb{N}} (|v_{-j}\rangle\langle v_{-j}| - |e_{-j}\rangle\langle e_{-j}|),\ v_{-j} = \cos(\theta_j)e_{-j} + \sin(\theta_j)e_j \\ P_2 v_{-j} = v_{-j},\ P_1 e_{-j} = e_{-j}, P_1 e_j = 0 \text{ and } \sum_{j\in\mathbb{N}} \sin(\theta_j)^2 < +\infty. \end{cases}$$

Above we have $\theta_j \in (0, \frac{\pi}{2})$ for all $j \in \mathbb{N}$. Let A be defined as follows:

$$A = \sum_{j\in\mathbb{N}} \theta_j (|e_j\rangle\langle e_{-j}| - |e_{-j}\rangle\langle e_j|),\ \theta_j \in (0, \tfrac{\pi}{2}),$$

then we have $P_2 = e^A P_1 e^{-A}$, $A^* = -A$ and

$$[A, P_1] = \sum_{j\in\mathbb{N}} \theta_j (|e_j\rangle\langle e_{-j}| + |e_{-j}\rangle\langle e_j|) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda). \tag{97}$$

Furthermore $[\exp(A), P_1] \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$: for all $k \in \mathbb{N}$, there holds:

$$[A^k, P_1] = \sum_{j=0}^{k-1} A^j [A, P_1] A^{k-1-j},$$

and

$$\|[\exp(A), P_1]\|_{\mathfrak{S}_2} \leq \sum_{k=1}^{+\infty} \frac{1}{k!} \big\{ k \|[A, P_1]\|_{\mathfrak{S}_2} \|A\|_{\mathcal{B}}^{k-1} \big\} = \|[A, P_1]\|_{\mathfrak{S}_2} \exp \|A\|_{\mathcal{B}}. \tag{98}$$

Let us call this A the *canonical* antiunitary operator $L_{P_1}(P_2)$ associated to P_2: we will see it does not depend on the choice of eigenvectors e_j.

Remark 14. In the case $\|P_2 - P_1\|_{\mathcal{B}} = 1$, we have $1, -1 \in \sigma(P_2 - P_1)$: indeed $P_2 - P_1$ may be decomposed as in (93) with $M_+ = M_-$ because $\mathrm{Tr}(P_2 - P_1) = 0$.

We still have $P_2 = e^A P_1 e^{-A}$ with

$$A = \sum_{i=1}^{M_+} \frac{\pi}{2} \Big(|a_i\rangle\langle a_{-i}| - |a_{-i}\rangle\langle a_i| \Big) + \sum_{j\geq 1} \theta_j \Big(|e_j\rangle\langle e_{-j}| - |e_{-j}\rangle\langle e_j| \Big), \tag{99}$$

where $a_i, e_j \in \mathrm{Ran}(1 - P_1)$ and $a_{-i}, e_{-j} \in \mathrm{Ran}\,P_1$ form an orthonormal family as in the decomposition of Theorem 4 (in particular the non-zero eigenvalues in $(-1, 1)$ are the $\pm\sin(\theta_i)$).

– Let $(\mathfrak{m}_{P_1}, \|\cdot\|_{\mathfrak{S}_2})$ be the set of compact operators:

$$\mathfrak{m}_{P_1} := \{a \in \mathcal{B}(\mathfrak{H}_\Lambda),\ ((1-P_1)aP_1)^* = -P_1a(1-P_1) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ (1-P_1)a(1-P_1) = P_1P_1 = 0\}.$$

Remark 15. As we consider operators in $\mathcal{B}(\mathfrak{H}_\Lambda)$ we can replace 1 by Π_Λ in the definition.

The map Φ_{P_1}

$$\Phi_{P_1} : \begin{array}{ccc} (\mathfrak{m}_{P_1}, 0) & \longrightarrow & (\mathscr{M}, P_1) \\ a & \mapsto & e^a P_1 e^{-a} \end{array} \tag{100}$$

is differentiable and we have:

$$\forall A \in \mathfrak{m}_{P_1},\ \mathrm{d}\Phi_{P_1}(P_1) \cdot A = [A, P_1].$$

This map

$$\mathrm{d}\Phi_{P_1} : \mathfrak{m}_{P_1} \to \{[A, P_1],\ A \in \mathfrak{m}_{P_1}\} =: \mathrm{Ran}(\mathrm{d}\Phi_{P_1})$$

is invertible with inverse

$$\mathrm{d}\Phi_{P_1}^{-1} : v \in \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \mapsto [v, P_1] \in \mathfrak{m}_{P_1}.$$

This proves that in a neighbourhood of P_1, the corresponding part of $\mathscr{M}$ is the graph of some function $\mathcal{F}_{P_1}$.

Indeed, if we see the set

$$\mathcal{P}_-^0 + \mathfrak{S}_2(\mathfrak{H}_\Lambda) = P_1 + \mathfrak{S}_2(\mathfrak{H}_\Lambda)$$

as an affine space with associated vector space $\mathfrak{S}_2(\mathfrak{H}_\Lambda)$, then we have

$$\mathfrak{S}_2(\mathfrak{H}_\Lambda) = \mathfrak{m}_{P_1} \overset{\perp}{\oplus} \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \overset{\perp}{\oplus} \{u \in \mathfrak{S}_2(\mathfrak{H}_\Lambda),\ P_1u(1-P_1) = (1-P_1)uP_1 = 0\}.$$

We decompose any $Q \in \mathfrak{S}_2(\mathfrak{H}_\Lambda)$ with respect to $\mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \oplus (\mathrm{Ran}(\mathrm{d}\Phi_{P_1}))^\perp$:

$$Q = v[P_1; Q] + w[P_1; Q] \in \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \oplus (\mathrm{Ran}(\mathrm{d}\Phi_{P_1}))^\perp.$$

In a neighbourhood $\mathcal{V}_{P_1}$ of P_1, the set $\mathcal{V}_{P_1} \cap \mathscr{M}$ is a portion of the graph of

$$\mathcal{F}_{P_1} : v \in \mathrm{Ran}(\mathrm{d}\Phi_{P_1}) \mapsto P_1 + w\big[P_1; e^{[v,P_1]}P_1e^{-[v,P_1]} - P_1\big] \in P_1 + (\mathrm{Ran}\,\mathrm{d}\Phi_{P_1})^\perp.$$

– Thus for any $P_1 \in \mathscr{M}$, there exists a neighbourhood $\mathcal{V}_{P_1} \ni P_1$ such that $\mathscr{M} \cap \mathcal{V}_{P_1}$ is a manifold with $\mathrm{T}_{P_1}\mathscr{M} = \mathrm{Ran}(\mathrm{d}\Phi_{P_1})$. To conclude $\mathscr{M}$ is a proper manifold, it suffices to compare the neighbourhood of $\mathscr{M}$ (or prove that $\mathscr{M}$ is connected): for $P_1, P_3 \in \mathscr{M}$, we use Remark 14 and write $P_3 = e^A P_1 e^{-A}$ with $A \in \mathfrak{m}_{P_1}$. Then it is clear that the map

$$\mathfrak{T}(P_1, P_3) : \begin{array}{ccc} (\mathscr{M}, P_1) & \longrightarrow & (\mathscr{M}, P_3) \\ P & \mapsto & e^A P e^{-A} \end{array}$$

is an isometry and that its differential $\mathfrak{t}(P_1, P_3)$ is an isometry that maps $\mathrm{T}_{P_1}\mathscr{M}$ onto $\mathrm{T}_{P_3}\mathscr{M}$. The map $t \in [0,1] \mapsto e^{tA}P_1e^{-tA} \in \mathscr{M}$ links P_1 and P_3.

Moreover the map

$$L_{P_1} : \begin{array}{ccc} \{P \in \mathscr{M},\ \|P - P_1\|_{\mathcal{B}} < 1\} & \longrightarrow & \mathfrak{m}_{P_1} \\ P & \mapsto & A \end{array}$$

is locally invertible around P_1 with (local) inverse Φ_{P_1}.

More generally, we can prove that the restriction of Φ_{P_1} to the $a \in \mathfrak{m}_{P_1}$ with $\|a\|_{\mathcal{B}} < \frac{\pi}{2}$ is one-to-one: it suffices to consider the spectral decomposition of a and link spectral subspaces with rotations.

□

Proof of proposition 2

Remark 16. 1. We recall that if P_1 and P_2 are two projectors such that $P_1 - P_2$ is Hilbert-Schmidt, then

$$A \in \mathfrak{S}_1^{P_1} \iff A \in \mathfrak{S}_1^{P_2} \text{ and } \mathrm{Tr}_{P_1}(A) = \mathrm{Tr}_{P_2}(A). \tag{101}$$

2. For any $A \in \mathcal{B}$ and any projector P we have:

$$[[A, P], P] = (1 - P)AP + PA(1 - P). \tag{102}$$

If we restrict $\mathcal{E}_{\mathrm{BDF}}$ to $\mathscr{M}$, using (101) and (102) we get that for $(P, v) \in \mathrm{T}\mathscr{M}$:

$$\mathrm{d}\mathcal{E}^0_{\mathrm{BDF}}(P) \cdot v = \mathrm{Tr}_P(\Pi_\Lambda D_{P-\mathcal{P}^0_-}\Pi_\Lambda v) = \mathrm{Tr}_P\big([[\Pi_\Lambda D_{P-\mathcal{P}^0_-}\Pi_\Lambda, P], P]v\big). \tag{103}$$

We write $Q = P - \mathcal{P}^0_-$, $\boldsymbol{\pi} = \chi_{(-\infty,0)}(\Pi_\Lambda D_Q \Pi_\Lambda)$ and $\Gamma = P - \boldsymbol{\pi}$. We have:

$$\begin{aligned} P\Pi_\Lambda D_Q\Pi_\Lambda(1 - P) &= (\boldsymbol{\pi} + \Gamma)\Pi_\Lambda D_Q\Pi_\Lambda(1 - \boldsymbol{\pi} - \Gamma), \\ &= \boldsymbol{\pi} - \Pi_\Lambda D_Q\Pi_\Lambda\Gamma + \Gamma\Pi_\Lambda D_Q\Pi_\Lambda(1 - \boldsymbol{\pi}) - \Gamma\Pi_\Lambda D_Q\Pi_\Lambda\Gamma. \end{aligned}$$

Thus

$$[[\Pi_\Lambda D_Q\Pi_\Lambda, P], P] = |\Pi_\Lambda D_Q\Pi_\Lambda|\Gamma + \Gamma|\Pi_\Lambda D_Q\Pi_\Lambda| - 2\Gamma\Pi_\Lambda D_Q\Pi_\Lambda\Gamma. \tag{104}$$

We have:

$$\begin{aligned} |\Pi_\Lambda D_Q\Pi_\Lambda|^2 &= \Pi_\Lambda(\mathcal{D}^0)^2 + \alpha\big(\Pi_\Lambda B_Q\Pi_\Lambda\mathcal{D}^0 + \mathcal{D}^0\Pi_\Lambda B_Q\Pi_\Lambda\big) + \alpha^2(\Pi_\Lambda B_Q\Pi_\Lambda)^2 \\ &\leq \Pi_\Lambda(\mathcal{D}^0)^2\Big(1 + \alpha\|\Pi_\Lambda B_Q\Pi_\Lambda \mathrm{inv}(\mathcal{D}^0)\|_{\mathcal{B}}\Big)^2, \\ &\leq \Pi_\Lambda(\mathcal{D}^0)^2\Big(1 + \alpha K\|V_Q\tfrac{\Pi_\Lambda}{\sqrt{1-\Delta}}\|_{\mathcal{B}} + \|R_Q\tfrac{\Pi_\Lambda}{\sqrt{1-\Delta}}\|_{\mathcal{B}}\Big)^2. \end{aligned}$$

We have $\Gamma = (P - \mathcal{P}^0_-) + (\mathcal{P}^0_- - \boldsymbol{\pi}) \in \mathfrak{S}_1^{\mathcal{P}^0_-}(\mathfrak{H}_\Lambda)$. So the following holds:

$$\big|\big|\,|\Pi_\Lambda D_Q\Pi_\Lambda|\Gamma\big|\big|_{\mathfrak{S}_2} \lesssim E(\Lambda)^{1/2}\|\,|\mathcal{D}^0|^{1/2}\Gamma\|_{\mathfrak{S}_2}(1 + \alpha(\sqrt{D(\rho_Q, \rho_Q)} + \||\mathcal{D}^0|^{1/2}Q\|_{\mathfrak{S}_2}))^2,$$

and

$$\|\Gamma\Pi_\Lambda D_Q\Pi_\Lambda\Gamma\|_{\mathfrak{S}_2} \leq 2\big|\big|\,|\Pi_\Lambda D_Q\Pi_\Lambda|^{1/2}\Gamma\big|\big|^2_{\mathfrak{S}_2} < +\infty.$$

□

4.2 On the manifold $\mathscr{M}_{\mathscr{C}}$: Propositions 3, 4 and 5

Proof of Proposition 3
Let $P_1, P_2 \in \mathscr{M}_{\mathscr{C}}$ such that $\|P_2 - P_1\|_{\mathcal{B}} < 1$. Thanks to Theorem 4, we know that P_2 can be written as $P_2 = e^A P_1 e^{-A}$ where $A \in \mathcal{B}(\mathfrak{H}_\Lambda)$ is antiunitary and

$$P_1AP_1 = (1 - P_1)A(1 - P_1).$$

– Taking into account the C-symmetry we can say more: thanks to (15) we can follow the proof of Proposition 5 with $\mathcal{P}^0_-$ replaced by P_1. This gives

$$\mathrm{C}A\mathrm{C} = A. \tag{105}$$

Indeed there exist $\mathcal{J} \subset \mathbb{Z}^*$ with $-\mathcal{J} = \mathcal{J}$ and $(e_j)_{j\in J}$ in $\mathfrak{H}_\Lambda^{\mathcal{J}}$ such that

1. $(e_j)_j \cup (Ce_j)_j$ is an orthonormal basis for $\mathrm{Ran}(P_2 - P_1)$,
2. for all $j \in \mathcal{J}$, $j > 0$: $P_1e_j = 0$ and $P_1e_{-j} = e_{-j}$,
3. each 4-dimensional space $\mathrm{Span}(e_j, e_{-j}, \mathrm{C}e_j, \mathrm{C}e_{-j})$ is spanned by four eigenvectors $f_j \perp \mathrm{C}f_{-j}$ with eigenvalue $\sin(\theta_i) > 0$ and $f_{-j} \perp \mathrm{C}f_j$ with eigenvalue $-\sin(\theta_i)$.

Then A is defined as follows:

$$A = \sum_{j\in\mathcal{J}} \theta_j \Big(|e_j\rangle\langle e_{-j}| - |e_{-j}\rangle\langle e_j| - |\mathrm{C}e_{-j}\rangle\langle \mathrm{C}e_j| + |\mathrm{C}e_j\rangle\langle \mathrm{C}e_{-j}| \Big)$$

It is easy to check (105) from this formula. Reciprocally, let $A \in \mathfrak{m}_P$ be an antiunitary map satisfying (105). Then we know that $e^A P e^{-A} \in \mathscr{M}$. Moreover we have $-\mathrm{C}e^A\mathrm{C} = -e^A$. It follows that

$$\begin{aligned} -\mathrm{C}(e^A P e^{-A} - P)\mathrm{C} &= \mathrm{C}e^A\mathrm{C}(-\mathrm{C}P\mathrm{C})\mathrm{C}e^{-A}\mathrm{C} + \mathrm{C}P\mathrm{C}, \\ &= e^A(-(\Pi_\Lambda - P))e^{-A} + (\Pi_\Lambda - P), \\ &= -\Pi_\Lambda + e^A P e^{-A} + \Pi_\Lambda - P = e^A P e^{-A} - P. \end{aligned}$$

In other words $e^A P e^{-A} \in \mathscr{M}_{\mathscr{C}}$. Thus Φ_{P_1} (*cf* (100)) is a local isomorphism from $(\mathfrak{m}_{P_1}, 0)$ to $(\mathscr{M}, P_1)$, and its restriction

$$\Phi^{\mathscr{C}}_{P_1} : \begin{array}{ccc} \mathfrak{m}^{\mathscr{C}}_{P_1} & \longrightarrow & \mathscr{M}_{\mathscr{C}} \\ a & \mapsto & e^a P_1 e^{-a} \end{array}$$

is well-defined and is a local isomorphism from $(\mathfrak{m}^{\mathscr{C}}_{P_1}, 0)$ to $(\mathscr{M}_{\mathscr{C}}, P)$. There remains to prove that for any $P_1, P_2 \in \mathscr{M}_{\mathscr{C}}$, there exists an isometry of $\mathfrak{S}_2$, that maps $\mathfrak{m}^{\mathscr{C}}_{P_1}$ onto $\mathfrak{m}^{\mathscr{C}}_{P_2}$. If $\|P_1 - P_2\|_{\mathcal{B}} < 1$, this isometry is given by

$$\phi^0_{\mathscr{C}}(P_1, P_2) : X \in \mathfrak{S}_2(\mathfrak{H}_\Lambda) \mapsto \exp(L_{P_1}(P_2))\, X \exp(-L_{P_1}(P_2)) \in \mathfrak{S}_2(\mathfrak{H}_\Lambda).$$

The restriction is:

$$\phi_{\mathscr{C}}(P_1, P_2) : X \in \mathfrak{m}^{\mathscr{C}}_{P_1} \mapsto \exp(L_{P_1}(P_2))\, a \exp(-L_{P_1}(P_2)),$$

indeed, as $\mathrm{C}L_{P_1}(P_2)\mathrm{C} = L_{P_1}(P_2)$ we have $\mathrm{C}\phi_{\mathscr{C}}(P_1, P_2; a)\mathrm{C} = \phi_{\mathscr{C}}(P_1, P_2; a)$. If $\|P_1 - P_2\|_{\mathcal{B}} = 1$ then we can write

$$P_2 - P_1 = \sum_{k=1}^{K} \big(|a_k\rangle\langle a_k| - |\mathrm{C}a_k\rangle\langle \mathrm{C}a_k| \big) + \gamma(P_1, P_2),$$

where $(a_k)_k \cup (\mathrm{C}a_k)_k$ is an orthonormal family which is orthogonal to $\operatorname{Ran}\gamma(P_1, P_2)$ and $\|\gamma(P_1, P_2)\|_{\mathcal{B}} < 1$. We also have $P_1 \mathrm{C}a_k = \mathrm{C}a_k$ and $P_1 a_k = 0$. We define

$$\begin{cases} P_{12} & := \quad P_1 + \displaystyle\sum_{k=1}^{K} \big(|a_k\rangle\langle a_k| - |\mathrm{C}a_k\rangle\langle \mathrm{C}a_k| \big) \in \mathscr{M}_{\mathscr{C}}, \\ U_{12} & := \quad \displaystyle\sum_{k=1}^{K} \big(|\mathrm{C}a_k\rangle|a_k\rangle - |a_k\rangle\langle \mathrm{C}a_k| \big) \in \mathbf{U}(\mathfrak{H}_\Lambda). \end{cases}$$

Then $\|P_2 - P_{12}\|_{\mathcal{B}} < 1$ and $U_{12} P_1 U_{12}^* = -U_{12} P_1 U_{12} = P_{12}$. Moreover

$$\phi_{\mathscr{C}, P_1, P_{12}} : \begin{array}{ccc} \mathfrak{m}^{\mathscr{C}}_{P_1} & \longrightarrow & \mathfrak{m}^{\mathscr{C}}_{P_{12}} \\ a & \mapsto & U_{12} a U_{12}^{-1} \end{array}$$

is well-defined and is an isometry. Indeed, as $\mathrm{C}U_{12}\mathrm{C} = -U_{12}$, we get that

$$\mathrm{C}U_{12} a U_{12}^{-1}\mathrm{C} = U_{12} a U_{12}^{-1}.$$

This proves the isometric isomorphisms

$$\left| \begin{array}{ccccc} \mathfrak{S}_2(\mathfrak{H}_\Lambda) & \xrightarrow[\phi^0_{\mathscr{C}}(P_1, P_{12})]{\simeq} & \mathfrak{S}_2(\mathfrak{H}_\Lambda) & \xrightarrow[\phi^0_{\mathscr{C}}(P_{12}, P_2)]{\simeq} & \mathfrak{S}_2(\mathfrak{H}_\Lambda), \\ \mathfrak{m}^{\mathscr{C}}_{P_1} & \xrightarrow[\phi_{\mathscr{C}}(P_1, P_{12})]{\simeq} & \mathfrak{m}^{\mathscr{C}}_{P_{12}} & \xrightarrow[\phi_{\mathscr{C}}(P_{12}, P_2)]{\simeq} & \mathfrak{m}^{\mathscr{C}}_{P_2}. \end{array} \right.$$

So $\mathscr{M}_{\mathscr{C}}$ is a submanifold and the characterization of the tangent planes (39) follows from that of $\mathscr{M}$.
– Let us show that $\mathscr{M}_{\mathscr{C}}$ is invariant under the flow of $\mathcal{E}^0_{\rm BDF}$: it suffices to show that for any $P \in \mathscr{M}_{\mathscr{C}}$, the gradient $\nabla\mathcal{E}^0_{\rm BDF}(P)$ (*cf* (37)) is in $\mathrm{T}_P\mathscr{M}_{\mathscr{C}}$. For a C-symmetric state P, we write $Q := P - \mathcal{P}^0_-$.

That the density ρ_Q vanishes is clear from (107) and the fact that for any $\psi \in \mathfrak{H}_\Lambda$ and $x \in \mathbb{R}^3$ we have $|\mathrm{C}\psi(x)|^2 = |\psi(x)|^2$. From (4), we get that for $-\mathrm{C}Q\mathrm{C} = Q$ there holds:

$$-\mathrm{C}Q\mathrm{C}(x,y) = Q(x,y) \text{ so } -\mathrm{C}R_Q\mathrm{C}(x,y) = R_Q(x,y) = \frac{Q(x,y)}{|x-y|}.$$

As $-\mathrm{C}\mathcal{D}^0\mathrm{C} = \mathcal{D}^0$, it follows that:

$$-\mathrm{C}\big(\mathcal{D}^0 + \alpha(\rho_Q * \tfrac{1}{|\cdot|} - R_Q)\big)\mathrm{C} = -\mathrm{C}(\mathcal{D}^0 - \alpha R_Q)\mathrm{C} = \mathcal{D}^0 - \alpha R_Q. \tag{106}$$

We remark that $[\Pi_\Lambda, \mathrm{C}] = 0$, and $\mathrm{C}P\mathrm{C} = 1 - P$ and $\mathrm{C}(1-P)\mathrm{C} = P$. Thus

$$\begin{aligned}
-\mathrm{C}\big[\big[\Pi_\Lambda D_Q \Pi_\Lambda; P\big]; P\big]\mathrm{C} &= -\mathrm{C}\big(P\Pi_\Lambda D_Q\Pi_\Lambda(1-P) + (1-P)\Pi_\Lambda D_Q\Pi_\Lambda P\big)\mathrm{C} \\
&= (1-P)\big(-\Pi_\Lambda \mathrm{C} D_Q \mathrm{C}\Pi_\Lambda\big)P + P\big(-\Pi_\Lambda \mathrm{C} D_Q \mathrm{C}\Pi_\Lambda\big)(1-P) \\
&= (1-P)\Pi_\Lambda D_Q\Pi_\Lambda P + P\Pi_\Lambda D_Q\Pi_\Lambda(1-P) \\
&= \big[\big[\Pi_\Lambda D_Q\Pi_\Lambda; P\big]; P\big].
\end{aligned}$$

Proof of Proposition 4 Let $c : t \in [0,1] \mapsto c(t) \in \mathscr{M}_{\mathscr{C}}$ be a continuous map such that $c(0) = 0$ and $\|c(1)\|_{\mathcal{B}} = 1$. By Theorem 4 and Proposition 5, any $c(t)$ has the following form:

$$\begin{aligned}
c(t) = &\sum_{j\in\mathbb{N}} \lambda_j\big(|f_j(t)\rangle\langle f_j(t)| - |f_{-j}(t)\rangle\langle f_{-j}(t)| + |\mathrm{C}f_{-j}(t)\rangle\langle \mathrm{C}f_{-j}(t)| - |\mathrm{C}f_j(t)\rangle\langle f_j(t)|\big) \\
&+ \sum_{j=1}^{N(t)} \big(|a_j(t)\rangle\langle a_j(t)| - |\mathrm{C}a_j(t)\rangle\langle \mathrm{C}a_j(t)|\big),
\end{aligned}$$

where $(a_j)_j \cup (\mathrm{C}a_j)_j \cup (f_j)_j \cup (\mathrm{C}f_j)$ is an orthonormal family and $(\lambda_j)_j$ is the sequence of positive eigenvalues lesser than 1. Each plane $\mathrm{Span}(f_j, f_{-j})$ (resp. $\mathrm{Span}(\mathrm{C}f_j, \mathrm{C}f_{-j})$) is spanned by $e_j \in \mathrm{Ran}(\mathcal{P}^0_+)$ and $e_{-j} \in \mathrm{Ran}(\mathcal{P}^0_-)$ (resp. $\mathrm{C}e_{-j} \in \mathrm{Ran}(\mathcal{P}^0_+)$ and $\mathrm{C}e_j \in \mathrm{Ran}(\mathcal{P}^0_-)$).

Let t_0 be $\inf\{t \in [0,1],\ \|c(t)\|_{\mathcal{B}} = 1\}$. For any $t \in [0,1]$ and any $\mu \in \sigma(c(t))\backslash\{1,0\}$, $4 \,|\, \mathrm{Dim}\, E^{c(t)^2}_{\mu^2}$. In particular, for $t < t_0$ the number

$$J(c(t)) = \mathrm{Dim} \bigoplus_{\frac{1}{2}<\mu\leq 1} E^{c(t)^2}_{\mu^2} \text{ is divisible by 4.}$$

By continuity, $J(c(t))$ is divisible by 4 for any t : the variations of J follow the variations of the λ_i's (λ_i equals $\sin(\widehat{\mathbb{C}v_j, \mathbb{C}e_j})$ in the notations of Theorem 4). Such an eigenvalue is associated to 4-dimensional spaces of type $\mathrm{Span}(f_j, f_{-j}, \mathrm{C}f_j, \mathrm{C}f_{-j})$ and each of them has a basis made of four eigenvectors in $E^{c(t)^2}_{\lambda_i^2}$.

Thus $4 \,|\, J(c(1))$ and for any unitary $\psi \in \mathrm{Ran}\,\mathcal{P}^0_+$, there is no continuous path in $\mathscr{M}_{\mathscr{C}}$ that links 0 and $Q_\psi = |\psi\rangle\langle\psi| - |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|$. It is then straightforward to prove that for any $\gamma \in \mathscr{M}_{\mathscr{C}}$, if $4 \,|\, J(\gamma)$ then there exists a path that links 0 and γ else there exists a path that links Q_ψ and γ. □

Proof of Proposition 5

A direct computation shows that for any $\psi \in L^2$:

$$\mathrm{C}|\psi\rangle\langle\psi|\mathrm{C} = |\mathrm{C}\psi\rangle\langle\mathrm{C}\psi|. \tag{107}$$

By Theorem 4, for $\mu \in \sigma(\gamma) \cap (0,1)$, there exist $N \in \mathbb{N}$ and N orthogonal planes $\Pi_\mu^1, \dots \Pi_\mu^N$ such that

$$E_{\mu^2}^{\gamma^2} = E_\mu^\gamma \overset{\perp}{\oplus} E_{-\mu}^\gamma = \bigoplus_{1 \le j \le N} \Pi_\mu^j,$$

where each plane is γ-invariant with $\gamma|_{\Pi_\mu} = |v_-\rangle\langle v_-| - |e_-\rangle\langle e_-|$ with $Pv_= v_-$ and $\mathcal{P}_-^0 e_- = e_-$. The expression of its eigenvectors f_+ and f_- are written in (95), where $e_+ \in \operatorname{Ran} \mathcal{P}_+^0$ is chosen such that $v_- = \cos(\theta)e_- + \sin(\theta)e_+$.

As C is *isometric*, then necessarily $E_{\mu^2}^{\gamma^2}$ is C-invariant, and $\mathrm{C}\Pi_\mu^j$ is some plane $\widetilde{\Pi}_\mu^j$ in $E_{\mu^2}^{\gamma^2}$, γ-*invariant* (there holds $\mu = \sin(\widehat{\mathbb{C}v_-, \mathbb{C}e_-})$). Let us show that $\Pi_\mu^j \neq \widetilde{\Pi}_\mu^j$. Indeed, using (95) this would imply that $\mathrm{C}e_- = e^{i\phi_1}e_+$ and $\mathrm{C}e_+ = e^{i\phi_2}e_-$ for some $\phi_1, \phi_2 \in \mathbb{R}$ and

$$-(|\mathrm{C}e_-\rangle\langle \mathrm{C}e_+| + |\mathrm{C}e_+\rangle\langle \mathrm{C}e_-|) = |e_-\rangle\langle e_+| + |e_+\rangle\langle e_-|.$$

In particular there would hold $-e^{i(\phi_1-\phi_2)} = 1$ that is $\phi_1 - \phi_2 \equiv \pi[2\pi]$. However C is an involution so $\mathrm{C}^2 e_+ = e_+$ and $e^{i(\phi_1-\phi_2)}e_+ = e_+$: this gives $\phi_1 - \phi_2 \equiv 0[2\pi]$ and contradicts the previous result.

Thus the two planes are different and the 4-dimensional space V_μ they span is C and γ-invariant: $E_{\mu^2}^{\gamma^2} = V_\mu \overset{\perp}{\oplus} W_\mu$. By induction over $\operatorname{Dim} W_\mu$, we get that $2N$ is divisible by 4, that is N is even. We obtain $\frac{N}{2}$ such V_μ, written V_μ^j.

In each V_μ^j, let $u_j^a \perp u_j^b$ be two unitary eigenvectors associated to μ. Thus $\mathrm{C}u_j^a \perp \mathrm{C}u_j^b$ are two eigenvectors associated to $-\mu$. We use Theorem 4 to decompose $V_\mu^j = \Pi^a \overset{\perp}{\oplus} \Pi^b$ with

$$\left| \begin{array}{l} \forall \star \in \{a,b\},\ \Pi_\star = \mathrm{Span}(u_j^\star, u_{-j}^\star) = \mathrm{Span}(e_j^\star, e_{-j}^\star) \\ \gamma u_{\pm j}^\star = \pm\mu u_\pm^\star,\ \mathcal{P}_\mp^0 e_{\pm j}^\star = 0. \end{array} \right.$$

We may assume (95) holds for both planes. Our aim is to prove that up to a phase, $\mathrm{C}u_{\pm j}^a = u_\mp^b$. *A priori* there exist $\phi_0, \phi_1, \phi_2, \theta \in [-\pi, \pi)$ such that

$$\left| \begin{array}{l} \mathrm{C}u_j^a = e^{i\phi_1}\cos(\theta)u_{-j}^a + e^{i\phi_2}\sin(\theta)u_{-j}^b, \\ \mathrm{C}u_j^b = -e^{i(\phi_1+\phi_0)}\sin(\theta)u_{-j}^a + e^{i(\phi_2+\phi_0)}\cos(\theta)u_{-j}^b. \end{array} \right.$$

We may assume $\cos(\theta), \sin(\theta) > 0$. Using (95), and writing $\overline{\phi}_k = \phi_k + \phi_0$, $k \in \{1,2\}$, we get

$$\begin{array}{r|l} \mathrm{C}e_j^a = -e^{i\phi_1}\cos(\theta)e_{-j}^a - e^{i\phi_2}\sin(\theta)e_{-j}^b, & \mathrm{C}e_j^b = e^{i\overline{\phi}_1}\sin(\theta)e_{-j}^a - e^{i\overline{\phi}_2}\cos(\theta)e_{-j}^b, \\ \mathrm{C}e_{-j}^a = e^{i\phi_1}\cos(\theta)e_j^a + e^{i\phi_2}\sin(\theta)e_j^b, & \mathrm{C}e_{-j}^b = -e^{i\overline{\phi}_1}\sin(\theta)e_j^a + e^{i\overline{\phi}_2}\cos(\theta)e_j^b. \end{array}$$

Applying C to $\mathrm{C}e_j^a$ we get

$$e_j^a = e^{i(\overline{\phi}_1-\phi_2)}\big(\sin(\theta)^2 - e^{i(\phi_2-\overline{\phi}_1)}\cos(\theta)^2\big)e_j^a - e^{i\phi_0}\frac{\sin(2\theta)}{2}\big(e^{i(\phi_2-\overline{\phi}_1)}+1\big)e_j^b.$$

Thus $\sin(\theta) = 1$ and $\overline{\phi}_1 - \phi_2 \equiv 0[2\pi]$. This gives:

$$E_{\mu^2}^{\gamma^2} = \overset{\perp}{\underset{1 \le j \le \frac{N}{2}}{\oplus}} V_\mu^j \text{ and } V_\mu^j = \Pi_{\mu,j}^a \overset{\perp}{\oplus} \mathrm{C}\Pi_{\mu,j}^a, \tag{108}$$

where each $\Pi_{\mu,j}^a$ and $\mathrm{C}\Pi_{\mu,j}^a$ is a spectral plane described in Theorem 4. □

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