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# NON ANALYTICITY OF THE GROUND STATE ENERGY OF THE HAMILTONIAN FOR HYDROGEN ATOM IN NONRELATIVISTIC QED

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ABSTRACT. We derive the ground state energy up to the fourth order in the fine structure constant  $\alpha$  for the translation invariant Pauli-Fierz Hamiltonian for a spinless electron coupled to the quantized radiation field. As a consequence, we obtain the non-analyticity of the ground state energy of the Pauli-Fierz operator for a single particle in the Coulomb field of a nucleus.

#### 1. Introduction

We study the translation invariant Pauli-Fierz Hamiltonian describing a spinless electron interacting with the quantized electromagnetic radiation field.

In the last fifteen years, a large number of rigorous results were obtained concerning the spectral properties of Pauli-Fierz operators, starting with the pioneering works of Bach, Fröhlich and Sigal [5, 3, 4]. In particular, the ground state energy were intensively studied ([15], [19], [17], [12], [9], [8], [16], [14]).

One of the problems recently discussed is the existence of an expansion in powers of the fine structure constant  $\alpha$  for the ground state energy of Pauli-Fierz operators. The very first results in this direction are due to Pizzo [20] and later on Bach, Fröhlich and Pizzo [2], where the operator for the Hydrogen atom is considered. In [2], a sophisticated rigorous renormalization group analysis is developed in order to determine the ground state energy, up to any arbitrary precision in powers of  $\alpha$ , with an expansion of the form

$$\varepsilon_0 + \sum_{k=1}^{2N} \varepsilon(k) \alpha^{k/2} + o(\alpha^N),$$

for any given N, where the coefficients  $\varepsilon_k(\alpha)$  may diverge as  $\alpha \to 0$ , but are smaller in magnitude than any power of  $\alpha^{-1}$ . The recursive algorithms developed in [2] are highly complex, and explicitly computing the ground state energy to any subleading order of  $\alpha$  is an extensive task. In the physical model where the photon form factor in the quantized electromagnetic vector potential contains the critical frequency space singularity responsible for the infamous infrared problem, it is expected that the rate of divergence of some of these coefficient functions  $\varepsilon_k(\alpha)$  is proportional to  $\log \alpha^{-1}$ . However, this is not explicitly exhibited in the current literature; for instance, it can a priori not be ruled out that terms involving logarithmic corrections cancel mutually. Moreover, for some models with a mild infrared behavior [14], the ground state energy is proven to be analytic in  $\alpha$  (see also [18]).

In a recent paper [7] Chen, Vougalter and the present authors study the binding energy for Hydrogen atom, which is the difference between the infimum  $\Sigma_0$  of the spectrum of the translationally invariant operator and the infimum  $\Sigma$  of the

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spectrum of the operator with Coulomb potential. It is shown in [7] that the binding energy as the form

(1) 
$$\Sigma_0 - \Sigma = \frac{\alpha^2}{4} + e^{(1)}\alpha^3 + e^{(2)}\alpha^4 + e^{(3)}\alpha^5 \log \alpha^{-1} + o(\alpha^5 \log \alpha^{-1}),$$

where the coefficients  $e^{(1)}$ ,  $e^{(2)}$  and  $e^{(3)}$  are independent of  $\alpha$  and explicitly computed. A natural question thus arose in the community, to know wether the logarithmic divergent term in (1) stemmed from  $\Sigma$ ,  $\Sigma_0$  or both. This question can not be answered on the basis of the computations done in [7], because we did not compute separately the value of  $\Sigma$  and  $\Sigma_0$ , but their difference.

Although the value of  $\Sigma_0$  was known up to the order  $\alpha^3$  from earlier work [6], this did not allow us to answer the above question.

In the work at hand, we compute the infimum  $\Sigma_0$  of the spectrum of the translationally invariant operator, up to the order  $\alpha^4$  with error  $\mathcal{O}(\alpha^5)$ , derive  $\Sigma$  up to the order  $\alpha^4$ , and show that the logarithmic term in (1) is related to  $\Sigma$  and not to  $\Sigma_0$ .

#### 2. The model

We study a non-relativistic free spinless electron interacting with the quantized electromagnetic field in Coulomb gauge. The Hilbert space accounting for the pure states of the electron is given by  $L^2(\mathbb{R}^3)$ , where we neglect its spin. The Fock space of the transverse photons is

$$\mathfrak{F} = \bigoplus_{n \in \mathbb{N}} \mathfrak{F}_n,$$

where the *n*-photon space  $\mathfrak{F}_n = \bigotimes_s^n \left(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2\right)$  is the symmetric tensor product of *n* copies of one-photon Hilbert spaces  $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$ . The factor  $\mathbb{C}^2$  accounts for the two independent transversal polarizations of the photon. On  $\mathfrak{F}$ , we introduce creation and annihilation operators  $a_{\lambda}^*(k)$ ,  $a_{\lambda}(k)$  satisfying the distributional commutation relations

$$[a_{\lambda}(k), a_{\lambda'}^*(k')] = \delta_{\lambda,\lambda'} \delta(k-k'), [a_{\lambda}^{\sharp}(k), a_{\lambda'}^{\sharp}(k')] = 0,$$

where  $a_{\lambda}^{\sharp}$  denotes either  $a_{\lambda}$  or  $a_{\lambda}^{*}$ . There exists a unique unit ray  $\Omega_{f} \in \mathfrak{F}$ , the Fock vacuum, which satisfies  $a_{\lambda}(k) \Omega_{f} = 0$  for all  $k \in \mathbb{R}^{3}$  and  $\lambda \in \{1, 2\}$ .

The Hilbert space of states of the system consisting of both the electron and the radiation field is given by

$$\mathfrak{H}:=L^2(\mathbb{R}^3)\otimes \mathfrak{F}$$
.

We shall use units such that  $\hbar = c = 1$ , and where the mass of the electron equals m = 1/2. The electron charge is then given by  $e = \sqrt{\alpha}$ .

The Hamiltonian of the system is given by

$$T = I_{el} \otimes H_f + : (i\nabla_x \otimes I_f - \sqrt{\alpha}A(x))^2 :,$$

where :  $(\cdots)$  : denotes normal ordering. The free photon field energy operator  $H_f$  is given by

$$H_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| a_{\lambda}^*(k) a_{\lambda}(k) dk.$$

The magnetic vector potential is

$$A(x) = A^{-}(x) + A^{+}(x),$$

where

(2) 
$$A^{-}(x) = \sum_{\lambda=1} \int_{\mathbb{R}^{3}} \frac{\kappa(|k|)}{2\pi |k|^{1/2}} \varepsilon_{\lambda}(k) e^{ikx} \otimes a_{\lambda}(k) dk$$

is the part of A(x) containing the annihilation operators, and  $A^+(x) = (A^-(x))^*$ . The vectors  $\varepsilon_{\lambda}(k) \in \mathbb{R}^3$  are the two orthonormal polarization vectors perpendicular to k,

$$\varepsilon_1(k) = \frac{(k_2, -k_1, 0)}{\sqrt{k_1^2 + k_2^2}}$$
 and  $\varepsilon_2(k) = \frac{k}{|k|} \wedge \varepsilon_1(k)$ .

In (2), the function  $\kappa$  implements an ultraviolet cutoff on the momentum k. We assume  $\kappa$  to be of class  $C^1$ , with compact support in  $\{|k| \leq \Lambda\}$ ,  $0 \leq \kappa \leq 1$  and  $\kappa = 1$  for  $|k| < \Lambda - 1$ .

The ground state energy of T is denoted by

$$\Sigma_0 := \inf \operatorname{spec}(T)$$
.

We note that this system is translationally invariant; that is, T commutes with the operator of total momentum

$$P_{tot} = p_{el} \otimes I_f + I_{el} \otimes P_f,$$

where  $p_{el}$  and  $P_f$  denote respectively the electron and the photon momentum operators

Therefore, for fixed value  $p \in \mathbb{R}^3$  of the total momentum, the restriction of T to the fibre space  $\mathbb{C} \otimes \mathfrak{F}$  is given by (see e.g. [10])

(3) 
$$T(p) = : (p - P_f - \sqrt{\alpha}A(0))^2 : +H_f,$$

where by abuse of notation, we dropped all tensor products involving the identity operators  $I_f$  and  $I_{el}$ . Henceforth, we will write

$$A^{\pm} := A^{\pm}(0)$$
.

It is proven in [1, 10] that

$$\Sigma_0 = \inf \operatorname{spec}(T(0))$$
 is an eigenvalue of the operator  $T(0)$ .

We are now in position to state our first main result.

On  $\mathfrak F$  we define respectively the positive bilinear form and its associated seminorm

(4) 
$$\langle v, w \rangle_* := \langle v, (H_f + P_f^2) w \rangle, \quad ||v||_* := \langle v, v \rangle_*^{\frac{1}{2}}.$$

**Theorem 2.1** (Ground state energy of T and T(0)). We have

(5) 
$$\Sigma_0 = d^{(0)}\alpha^2 + d^{(1)}\alpha^3 + d^{(2)}\alpha^4 + \mathcal{O}(\alpha^5) ,$$

with

$$d^{(0)} := -\|\Phi_2\|_*^2$$

$$d^{(1)} := 2\|A^{-}\Phi_{2}\|^{2} - 4\|\Phi_{3}\|_{*}^{2} - 4\|\Phi_{1}\|_{*}^{2}$$

$$d^{(2)} := -\left(\frac{2\|A^-\Phi_2\|^2 - 4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2}{\|\Phi_2\|_*}\right)^2$$

$$+8 \operatorname{Re} \langle \Phi_1, A^- \cdot A^- \Phi_3 \rangle + 8 \|A^- \Phi_1\|^2 + 8 \|A^- \Phi_3\|^2 - 16 \|\tilde{\Phi}_2\|_*^2 - 16 \|\Phi_4\|_*^2 + \|\Phi_2\|^2 \|\Phi_2\|_*^2$$

and

$$\Phi_{2} := -(H_{f} + P_{f}^{2})^{-1}A^{+} \cdot A^{+}\Omega_{f}, 
\Phi_{3} := -(H_{f} + P_{f}^{2})^{-1}P_{f} \cdot A^{+}\Phi_{2}, 
\Phi_{1} := -(H_{f} + P_{f}^{2})^{-1}P_{f} \cdot A^{-}\Phi_{2}, 
(6)$$

$$\tilde{\Phi}_{2} := -P_{\Phi_{2}}^{\perp}(H_{f} + P_{f}^{2})^{-1}\left(P_{f} \cdot A^{+}\Phi_{1} + P_{f} \cdot A^{-}\Phi_{3} + \frac{1}{2}A^{+} \cdot A^{-}\Phi_{2}\right) 
\Phi_{4} := -(H_{f} + P_{f}^{2})^{-1}\left(P_{f} \cdot A^{+}\Phi_{3} + \frac{1}{4}A^{+} \cdot A^{+}\Phi_{2}\right),$$

where  $P_{\Phi_2}^{\perp}$  is the orthogonal projection onto  $\{\varphi \in \mathfrak{F} \mid \langle \varphi, \Phi_2 \rangle_* = 0\}.$ 

The proof of Theorem 2.1 is postponed to Section 4. The proof of the upper bound is derived in subsection 4.1 using a bona fide trial function, whereas the most difficult part, namely the proof of the lower bound, is given in subsection 4.2.

Corollary 2.1 (non analyticity of inf spec(H)). The Pauli-Fierz Hamiltonian for an electron interacting with a Coulomb electrostatic field and coupled to the quantized radiation field is

$$H:=T-\frac{\alpha}{|x|}.$$

Its ground state energy  $\Sigma := \inf \operatorname{spec}(H)$  fulfills

$$\Sigma = \tilde{d}^{(0)}\alpha^2 + \tilde{d}^{(1)}\alpha^3 + \tilde{d}^{(2)}\alpha^4 + \tilde{d}^{(3)}\alpha^5 \log \alpha^{-1} + o(\alpha^5 \log \alpha^{-1}),$$

where

$$\tilde{d}^{(0)} = d^{(0)} - \frac{1}{4}, \quad \tilde{d}^{(1)} = d^{(1)} - e^{(1)}, \quad \tilde{d}^{(2)} = d^{(2)} - e^{(2)}, \quad \tilde{d}^{(3)} = -e^{(3)},$$

with

$$e^{(1)} = \frac{2}{\pi} \int_0^\infty \frac{\kappa^2(t)}{1+t} dt,$$

$$\begin{split} e^{(2)} &= \frac{2}{3} \operatorname{Re} \sum_{i=1}^{3} \langle (A^{-})^{i} (H_{f} + P_{f}^{2})^{-1} A^{+} . A^{+} \Omega_{f}, (H_{f} + P_{f}^{2})^{-1} (A^{+})^{i} \Omega_{f} \rangle \\ &+ \frac{1}{3} \sum_{i=1}^{3} \| (H_{f} + P_{f}^{2})^{-\frac{1}{2}} \Big( 2A^{+} . P_{f} (H_{f} + P_{f}^{2})^{-1} (A^{+})^{i} - P_{f}^{i} (H_{f} + P_{f}^{2})^{-1} A^{+} . A^{+} \Big) \Omega_{f} \|^{2} \\ &- \frac{2}{3} \sum_{i=1}^{3} \| A^{-} (H_{f} + P_{f}^{2})^{-1} (A^{+})^{i} \Omega_{f} \|^{2} + 4a_{0}^{2} \| Q_{1}^{\perp} (-\Delta - \frac{1}{|x|} + \frac{1}{4})^{-\frac{1}{2}} \Delta u_{1} \|^{2}, \\ &a_{0} = \int \frac{k_{1}^{2} + k_{2}^{2}}{4\pi^{2} |k|^{3}} \frac{2}{|k|^{2} + |k|} \kappa(|k|) \, \mathrm{d}k_{1} \mathrm{d}k_{2} \mathrm{d}k_{3}, \\ &e^{(3)} = -\frac{1}{3\pi} \| (-\Delta - \frac{1}{|x|} + \frac{1}{4})^{\frac{1}{2}} \nabla u_{1} \|^{2}, \end{split}$$

and  $Q_1^{\perp}$  is the projection onto the orthogonal complement to the ground state  $u_1$  of the Schrödinger operator  $-\Delta - \frac{1}{|x|}$ .

*Proof.* This is a direct consequence of the above Theorem 2.1 and [7, Theorem 2.1].

The next main result gives an approximate ground state of T(0). Let  $\Psi$  be the ground state of T(0), normalized by the condition

(7) 
$$\langle \Psi, \Omega_f \rangle = 1$$
.

The existence of  $\Psi$  was proved in [1, 10]. We decompose the state  $\Psi$  according to its  $\langle \cdot, \cdot \rangle_*$ -projections in the direction of  $\Phi_1$ ,  $\Phi_2$ ,  $\tilde{\Phi}_2$ ,  $\Phi_3$  and  $\Phi_4$  and its orthogonal part R. This gives

(8) 
$$\Psi = \Omega_f + 2\eta_1 \alpha^{\frac{3}{2}} \Phi_1 + \eta_2 \alpha \Phi_2 + \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2 + 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3 + \eta_4 \alpha^2 \Phi_4 + R ,$$

where the coefficients  $\eta_i$  (i = 1, 2, 3, 4) and  $\tilde{\eta}_2$ , and the vector R are uniquely determined by the conditions

(9) 
$$\langle \Phi_i, \Phi_j \rangle_* = \|\Phi_j\|_*^2 \delta_{ij}, \quad \langle \Phi_i, \tilde{\Phi}_2 \rangle_* = 0, \langle \Phi_j, R \rangle_* = 0, \quad \langle \tilde{\Phi}_2, R \rangle_* = 0, \quad \langle \Omega_f, R \rangle = \langle \Omega_f, \Phi_j \rangle = 0,$$

for i, j = 1, 2, 3, 4.

**Theorem 2.2** (Ground state of T(0)). Let  $\Psi$  be the ground state of T(0), normalized by the condition  $\langle \Psi, \Omega_f \rangle = 1$ . Then

$$\Psi = \Omega_f + 2\alpha^{\frac{3}{2}}\Phi_1 + \alpha(1 - \beta\alpha)\Phi_2 + 4\alpha^2\tilde{\Phi}_2 + 2\alpha^{\frac{3}{2}}\Phi_3 + 4\alpha^2\Phi_4 + \tilde{R} ,$$

$$with \ \beta := \frac{2\|A^-\Phi_2\|^2 - 4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2}{\|\Phi_2\|_*^2} ,$$

$$\tilde{R} := R + 2(\eta_1 - 1)\alpha^{\frac{3}{2}}\Phi_1 + (\eta_2 - (1 - \beta\alpha))\alpha\Phi_2 + 2(\eta_3 - 1)\alpha^{\frac{3}{2}}\Phi_3 + (\tilde{\eta}_2 - 4)\alpha^2\tilde{\Phi}_2 + (\eta_4 - 4)\alpha^2\Phi_4 ,$$

where the coefficients  $\eta_j$  (j=1,2,3,4) and  $\tilde{\eta}_2$  satisfy that there exists a finite constant c such that for all  $\alpha$ ,  $|\eta_{1,3}-1|^2 \leq c\alpha$ ,  $|\eta_2-1|^2 \leq c\alpha^2$ ,  $|\tilde{\eta}_2-4|^2 \leq c\alpha$ , and  $|\eta_4-4|^2 \leq c\alpha$ , and with

$$\|\tilde{R}\|, \|R\| = \mathcal{O}(\alpha), \quad and \quad \|\tilde{R}\|_*, \|R\|_* = \mathcal{O}(\alpha^2).$$

The proof of this theorem is given in subsection 4.3.

#### 3. Photon number and field energy bounds

In order to derive the ground state energy for T(0), we need to derive some a priori expected photon number bound and expected field energy bound for the ground state.

As a consequence of Theorem 3.2 in [6], we have the following bound for the \*-norm of the remainder R of the ground state  $\Psi$ , as defined by (8).

**Proposition 3.1.** There exists  $c < \infty$  such that

(11) 
$$\langle (H_f + P_f^2)R, R \rangle \le c(1 + |\tilde{\eta}_2|^2 + |\eta_4|^2)\alpha^4.$$

*Proof.* In [6, Theorem 3.2] it is shown that for  $\eta_1$ ,  $\eta_2$  and  $\eta_3$  given by (8) and (9), and for  $r := \Psi - \Omega_f - 2\eta_1\alpha^{\frac{3}{2}}\Phi_1 - \eta_2\alpha\Phi_2 - 2\eta_3\alpha^{\frac{3}{2}}\Phi_3$ , we have  $||r||_* = \mathcal{O}(\alpha^2)$ . Therefore, using the decomposition (8) concludes the proof.

#### Proposition 3.2. Let

(12) 
$$\Theta := \Psi - \alpha \eta_2 \Phi_2 - 2\alpha^{\frac{3}{2}} \eta_1 \Phi_1 - 2\alpha^{\frac{3}{2}} \eta_3 \Phi_3 - \Omega_f,$$

where the vectors  $\Phi_i$  (i = 1, 2, 3) are defined in (6) in Theorem 2.1 and the coefficients  $\eta_i$  (i = 1, 2, 3) are given by the decomposition of  $\Psi$  according to (8) and the conditions (9).

Then

(13) 
$$\langle \Theta, N_f \Theta \rangle = \mathcal{O}(\alpha^3).$$

*Proof.* According to [6, Theorem 3.2], we have

Now we write

$$\langle \Theta, N_f \Theta \rangle = \int_{|k| < \alpha} \|a_{\lambda}(k)\Theta\|^2 dk + \int_{|k| > \alpha} \|a_{\lambda}(k)\Theta\|^2 dk .$$

The second term in the right hand side of (15) is bounded as follows

$$(16) \quad \int_{|k| > \alpha} \|a_{\lambda}(k)\Theta\|^{2} dk = \int_{|k| > \alpha} \frac{1}{|k|} |k| \|a_{\lambda}(k)\Theta\|^{2} dk \le \alpha^{-1} \|H_{f}^{\frac{1}{2}}\Theta\|^{2} = \mathcal{O}(\alpha^{3}) ,$$

where we used (14). For the first term in the right hand side of (15), we write (17)

$$\begin{split} & \int_{|k| < \alpha} \|a_{\lambda}(k)\Theta\|^{2} \mathrm{d}k = \int_{|k| < \alpha} \|a_{\lambda}(k) \left(\Psi - \alpha \eta_{2} \Phi_{2} - 2\alpha^{\frac{3}{2}} \eta_{1} \Phi_{1} - 2\alpha^{\frac{3}{2}} \eta_{3} \Phi_{3}\right) \|^{2} \mathrm{d}k \\ & \leq 4 \left( \int_{|k| < \alpha} \|a_{\lambda}(k)\Psi\|^{2} \mathrm{d}k + \alpha^{2} |\eta_{2}|^{2} \int_{|k| < \alpha} \|a_{\lambda}(k)\Phi_{2}\|^{2} \mathrm{d}k \right. \\ & \quad + \alpha^{3} |\eta_{1}|^{2} \int_{|k| < \alpha} \|a_{\lambda}(k)\Phi_{1}\|^{2} \mathrm{d}k + \alpha^{3} |\eta_{3}|^{2} \int_{|k| < \alpha} \|a_{\lambda}(k)\Phi_{3}\|^{2} \mathrm{d}k \right) \,. \end{split}$$

Straightforward computations shows that the last three terms in the right hand side of (17) are  $\mathcal{O}(\alpha^3)$ . To estimate the first integral in the right hand side of (17) we follow the strategy used in the proof of [6, Proposition 3.1] as explained below.

For  $\sigma > 0$ , let  $T_{\sigma}(p)$  denote the fiber Hamiltonian regularized by an infrared cutoff implemented by replacing the ultraviolet cutoff function  $\kappa$  of (2) by a  $C^1$  function  $\kappa_{\sigma}$  with  $\kappa_{\sigma} = \kappa$  on  $[\sigma, \infty)$ ,  $\kappa_{\sigma}(0) = 0$ , and  $\kappa_{\sigma}$  monotonically increasing on  $[0, \sigma]$ . Then,  $E_{\sigma}(p) := \inf \operatorname{spec}(T_{\sigma}(p))$  is a simple eigenvalue with eigenvector  $\Psi_{\sigma}(p) \in \mathfrak{F}$  [1, 10]. If p = 0, one has  $\nabla_p E_{\sigma}(p = 0) = 0$  (see [1, 10]). In Formula (6.11) of [11], it is shown that

(18) 
$$a_{\lambda}(k)\Psi_{\sigma}(0) = (A) + (B),$$

where from (6.12) of [11], it follows that

(19) 
$$\| (A) \| \le C(k) |\nabla_p E_{\sigma}(0)| = 0,$$

and that

$$(20) \quad (B) = -\sqrt{\alpha} \frac{\kappa_{\sigma}(|k|)}{|k|^{\frac{1}{2}}} \frac{1}{T_{\sigma}(k) - E_{\sigma}(0) + |k|} (T_{\sigma}(0) - E_{\sigma}(0)) \epsilon_{\lambda}(k) \cdot \nabla_{p} \Psi_{\sigma}(0),$$

if the electron spin is zero. Thus it follows immediately from (6.19) in [11] that

$$||a_{\lambda}(k)\Psi_{\sigma}(0)|| \leq c\sqrt{\alpha} \frac{\kappa_{\sigma}(|k|)}{|k|} \left| \frac{1}{m_{ren,\sigma}} - 1 \right| ||\Psi_{\sigma}(0)|| \leq c\alpha \frac{\kappa_{\sigma}(|k|)}{|k|} ||\Psi_{\sigma}(0)||,$$

for spin zero, where  $m_{ren,\sigma}$  is the renormalized electron mass for p = 0 (see [1, 10]), defined by

(21) 
$$\frac{1}{m_{ren,\sigma}} = 1 - 2 \frac{\nabla_p \Psi_{\sigma}(0), (T_{\sigma}(0) - E_{\sigma}(0)) \nabla_p \Psi_{\sigma}(0) \rangle}{\|\Psi_{\sigma}(0)\|^2} .$$

As proved in [1, 10],  $1 < m_{ren,\sigma} < 1 + c\alpha$  uniformly in  $\sigma \ge 0$ . Therefore, one can write

(22) 
$$\int_{|k| < \alpha} \|a_{\lambda}(k)\Psi\|^{2} dk = \lim_{\sigma \to 0} \int_{|k| < \alpha} \|a_{\lambda}(k)\Psi_{\sigma}\|^{2} dk$$
$$\leq \lim_{\sigma \to 0} \int_{|k| < \alpha} c \alpha \frac{\kappa_{\sigma}(|k|)}{|k|} \|\Psi_{\sigma}(0)\|^{2} dk = \mathcal{O}(\alpha^{3}) ,$$

where  $\Psi = s - \lim_{\sigma \searrow 0} \Psi_{\sigma}(0)$  (see [1]). The inequalities (16) and (22) conclude the proof.

A straightforward consequence of this result is

Corollary 3.1. For  $\Theta$  defined as in (12) by  $\Theta = \Psi - \alpha \eta_2 \Phi_2 - 2\alpha^{\frac{3}{2}} \eta_1 \Phi_1 - 2\alpha^{\frac{3}{2}} \eta_3 \Phi_3 - \Omega_f$ , we have

#### 4. Proof of Theorem 2.1

We introduce the following notations:

$$\tilde{\Phi}_{2} = \tilde{\Phi}_{2}^{(1)} + \tilde{\Phi}_{2}^{(2)} + \tilde{\Phi}_{2}^{(3)} 
:= \left(P_{\Phi_{2}}^{\perp} (H_{f} + P_{f}^{2})^{-1} P_{f} \cdot A^{+} \Phi_{1}\right) + \left(P_{\Phi_{2}}^{\perp} (H_{f} + P_{f}^{2})^{-1} P_{f} \cdot A^{-} \Phi_{3}\right) 
+ \left(P_{\Phi_{2}}^{\perp} (H_{f} + P_{f}^{2})^{-1} \frac{1}{2} A^{+} \cdot A^{-} \Phi_{2}\right),$$

(25) 
$$\Phi_4 = \Phi_4^{(1)} + \Phi_4^{(2)} := \left( (H_f + P_f^2)^{-1} P_f \cdot A^+ \Phi_3 \right) + \left( \frac{1}{4} (H_f + P_f^2)^{-1} A^+ \cdot A^+ \Phi_2 \right).$$

For  $n \in \mathbb{N}$  we also define  $\Gamma^{(n)}$  as the orthogonal projection onto the *n*-photon space  $\mathfrak{F}_n$  of the Fock space  $\mathfrak{F}$ , whereas  $\Gamma^{(\geq n)}$  shall denote the orthogonal projection onto  $\bigoplus_{k>n} \mathfrak{F}_k$ .

Finally, we set

(26) 
$$R_i := \Gamma^{(i)} R$$
, for  $i = 1, 2, 3, 4$ , and  $R_{>k} := \Gamma^{(\geq k)} R$ .

4.1. **Proof of the upper bound.** The proof of the upper bound in Theorem 2.1 is easily obtained by picking the trial function

(27) 
$$\Psi^{\text{trial}} := \Omega_f + 2\alpha^{\frac{3}{2}} \Phi_1 + \alpha \left( 1 - \alpha \frac{2\|A^- \Phi_2\|^2 - 4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2}{\|\Phi_2\|_*^2} \right) \Phi_2 + \alpha^2 \tilde{\Phi}_2 + 2\alpha^{\frac{3}{2}} \Phi_3 + \alpha^2 \Phi_4.$$

We then compute  $\langle \Psi^{\rm trial}, T(0)\Psi^{\rm trial}\rangle/\|\Psi^{\rm trial}\|^2$ . A straightforward computation yields

$$\begin{split} &\langle \Psi^{\rm trial},\, T(0)\Psi^{\rm trial}\rangle \\ &= -\alpha^2 \|\Phi_2\|_*^2 \, + \, \alpha^3 \Big( 2\|A^-\Phi_2\|^2 - 4\|\Phi_3\|_*^2 - 4\|\Phi_1\|_*^2 \Big) \\ &+ \, \alpha^4 \Big( 8{\rm Re}\, \langle \Phi_1,\, A^-\cdot A^-\Phi_3\rangle + 8\|A^-\Phi_1\|^2 + 8\|A^-\Phi_3\|^2 - 16\|\tilde{\Phi}_2\|_*^2 - 16\|\Phi_4\|_*^2 \Big) \\ &- \alpha^4 \left( \frac{-4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2 + 2\|A^-\Phi_2\|^2}{\|\Phi_2\|_*} \right)^2 + \mathcal{O}(\alpha^5) \,. \end{split}$$

Since  $\|\Psi^{\text{trial}}\|^2 = 1 + \alpha^2 \|\Phi_2\|^2 + \mathcal{O}(\alpha^3)$ , we thus obtain

$$\inf \operatorname{spec}(T(0)) \leq \frac{\langle \Psi^{\operatorname{trial}}, T(0)\Psi^{\operatorname{trial}} \rangle}{\|\Psi^{\operatorname{trial}}\|^{2}}$$

$$= -\alpha^{2} \|\Phi_{2}\|_{*}^{2} + \alpha^{3} \left(2\|A^{-}\Phi_{2}\|^{2} - 4\|\Phi_{3}\|_{*}^{2} - 4\|\Phi_{1}\|_{*}^{2}\right) + \alpha^{4} \left(8\operatorname{Re}\langle\Phi_{1}, A^{-} \cdot A^{-}\Phi_{3}\rangle\right)$$

$$+ 8\|A^{-}\Phi_{1}\|^{2} + 8\|A^{-}\Phi_{3}\|^{2} - 16\|\tilde{\Phi}_{2}\|_{*}^{2} - 16\|\Phi_{4}\|_{*}^{2} + \|\Phi_{2}\|^{2}\|\Phi_{2}\|_{*}^{2}\right)$$

$$- \alpha^{4} \left(\frac{-4\|\Phi_{1}\|_{*}^{2} - 4\|\Phi_{3}\|_{*}^{2} + 2\|A^{-}\Phi_{2}\|^{2}}{\|\Phi_{2}\|_{*}}\right)^{2} + \mathcal{O}(\alpha^{5}),$$

which concludes the proof of the upper bound.

#### 4.2. Proof of the lower bound. Since

$$T(0) = H_f + : (-P_f - \alpha^{\frac{1}{2}}A(0))^2 :$$

$$= (H_f + P_f^2) + \alpha^{\frac{1}{2}}(P_f \cdot A^+ + A^+ \cdot P_f) + \alpha^{\frac{1}{2}}(P_f \cdot A^- + A^- \cdot P_f) + \alpha(A^+)^2 + \alpha(A^-)^2 + 2\alpha A^+ \cdot A^-$$
we obtain

(28) 
$$\langle \Psi, T(0)\Psi \rangle = \operatorname{Re} \langle \Psi, \alpha^{\frac{1}{2}} P_f \cdot A^- \Psi \rangle + \operatorname{Re} \langle \Psi, 2\alpha A^- \cdot A^- \Psi \rangle + \langle \Psi, 2\alpha A^+ \cdot A^- \Psi \rangle + \langle \Psi, (H_f + P_f^2) \Psi \rangle$$

As in (8)-(9), we decompose the ground state  $\Psi$  of T(0) as follows

$$\Psi = \Omega_f + 2\eta_1 \alpha^{\frac{3}{2}} \Phi_1 + \eta_2 \alpha \Phi_2 + \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2 + 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3 + \eta_4 \alpha^2 \Phi_4 + R .$$

Each term in the right hand side of (28) are estimated respectively in Lemmata A.2-A.5.

We thus collect all terms that occur in Lemmata A.2-A.5, regroup them according to the following rearrangement, and estimate them separately

(29) 
$$\langle \Psi, T(0)\Psi \rangle = (I) + (II) + (III) + (IV) + (V) + \text{ positive terms}$$

where the positive terms are a part of  $\langle \Psi, (H_f + P_f^2)\Psi \rangle$  and

- (I) = Terms with a pre-factor  $\alpha^2$  involving a remainder term  $R_i$ ,
- (II) = Terms with a pre-factor  $\alpha^2$  not involving remainder terms R,
- (III) = Terms with a pre-factor  $\alpha^3$ ,
- (IV) = Terms with a prefactor  $\alpha^4$ ,
- (V) = Terms with a pre-factor  $\alpha^5$  and the terms  $\mathcal{O}(\alpha^5)$ .

• Terms with a pre-factor  $\alpha^2$  involving a remainder term  $R_i$ .

$$(I) := -8\alpha^{2} \operatorname{Re} \eta_{1} \langle \tilde{\Phi}_{2}^{(1)}, R_{2} \rangle_{*} - 8\alpha^{2} \operatorname{Re} \eta_{3} \langle \tilde{\Phi}_{2}^{(2)}, R_{2} \rangle_{*} - 8\alpha^{2} \operatorname{Re} \eta_{2} \langle \tilde{\Phi}_{2}^{(3)}, R_{2} \rangle_{*} - 8\alpha^{2} \operatorname{Re} \eta_{2} \langle \Phi_{4}^{(2)}, R_{4} \rangle_{*} - 8\alpha^{2} \operatorname{Re} \eta_{3} \langle \Phi_{4}^{(1)}, R_{4} \rangle_{*}$$

• Terms with a pre-factor  $\alpha^2$  not involving remainder terms R:

(30) 
$$(II) := -\alpha^{2} 2\operatorname{Re} \bar{\eta}_{2} \|\Phi_{2}\|_{*}^{2} + \alpha^{2} |\eta_{2}|^{2} \|\Phi_{2}\|_{*}^{2}$$
$$= -\alpha^{2} \|\Phi_{2}\|_{*}^{2} + \alpha^{2} \left( (\operatorname{Re} \eta_{2}) - 1)^{2} + (\operatorname{Im} \eta_{2})^{2} \right)$$
$$\geq -\alpha^{2} \|\Phi_{2}\|_{*}^{2} + \alpha^{2} \left( (\operatorname{Re} \eta_{2}) - 1)^{2} \right).$$

• Terms with a pre-factor  $\alpha^3$ .

$$(III) := \alpha^{3} \left( -8\operatorname{Re} \eta_{1} \bar{\eta}_{2} \|\Phi_{1}\|_{*}^{2} + 4|\eta_{1}|^{2} \|\Phi_{1}\|_{*}^{2} \right.$$

$$\left. - 8\operatorname{Re} \eta_{3} \bar{\eta}_{2} \|\Phi_{3}\|_{*}^{2} + 4|\eta_{3}|^{2} \|\Phi_{3}\|_{*}^{2} + 2|\eta_{2}| \|A^{-}\Phi_{2}\|^{2} \right)$$

$$= 4\alpha^{3} \|\Phi_{1}\|_{*}^{2} \left( |\eta_{1} - \eta_{2}|^{2} - |\eta_{2}|^{2} \right)$$

$$+ 4\alpha^{3} \|\Phi_{3}\|_{*}^{2} \left( |\eta_{3} - \eta_{2}|^{2} - |\eta_{2}|^{2} \right) + 2\alpha^{3} \|A^{-}\Phi_{2}\|^{2} + \mathcal{O}(\alpha^{5}).$$

Since from Lemma A.1 we have  $\eta_2 = 1 + \mathcal{O}(\alpha)$ , we get  $(\operatorname{Im} \eta_2)^2 = \mathcal{O}(\alpha^2)$  and  $(\operatorname{Re} \eta_2)^2 - 1 = 2(\operatorname{Re} \eta_2 - 1) + \mathcal{O}(\alpha^2)$ , and thus  $|\eta_2|^2 = 1 + 2(\operatorname{Re} \eta_2 - 1) + \mathcal{O}(\alpha^2)$ . Together with (31), this yields

(32) 
$$(III) = \alpha^{3} (-4\|\Phi_{1}\|_{*}^{2} - 4\|\Phi_{3}\|_{*}^{2} + 2\|A^{-}\Phi_{2}\|^{2})$$

$$+ 2\alpha^{3} (\operatorname{Re} \eta_{2} - 1)(-4\|\Phi_{1}\|_{*}^{2} - 4\|\Phi_{3}\|_{*}^{2} + 2\|A^{-}\Phi_{2}\|^{2})$$

$$+ 4\alpha^{3} \|\Phi_{1}\|_{*}^{2} |\eta_{1} - \eta_{2}|^{2} + 4\alpha^{3} \|\Phi_{3}\|_{*}^{2} |\eta_{3} - \eta_{2}|^{2} + \mathcal{O}(\alpha^{5}).$$

The first term in the right hand side of (32) is the  $\alpha^3$  term in the equality (5), thus we leave it as it is. The last line in (32), which is positive, shall be used later to estimate the terms (I) and (IV).

The second term in the right hand side of (32) is estimated together with the term  $\alpha^2 \|\Phi_1\|_*^2 (\operatorname{Re} \eta_2 - 1)^2$  obtained in the lower bound (30) for (II). We obtain

$$2\alpha^{3}(\operatorname{Re}\eta_{2}-1)(2\|A^{-}\Phi_{2}\|^{2}-4\|\Phi_{1}\|_{*}^{2}-4\|\Phi_{3}\|_{*}^{2})+\alpha^{2}\|\Phi_{2}\|_{*}^{2}(\operatorname{Re}\eta_{2}-1)^{2}$$

$$=\alpha^{2}\left(\alpha\frac{2\|A^{-}\Phi_{2}\|^{2}-4\|\Phi_{1}\|_{*}^{2}-4\|\Phi_{3}\|_{*}^{2}}{\|\Phi_{2}\|_{*}}+(\operatorname{Re}\eta_{2}-1)\|\Phi_{2}\|_{*}\right)^{2}$$

$$-\alpha^{4}\left(\frac{2\|A^{-}\Phi_{2}\|^{2}-4\|\Phi_{1}\|_{*}^{2}-4\|\Phi_{3}\|_{*}^{2}}{\|\Phi_{2}\|_{*}}\right)^{2}$$

$$\geq-\alpha^{4}\left(\frac{2\|A^{-}\Phi_{2}\|^{2}-4\|\Phi_{1}\|_{*}^{2}-4\|\Phi_{3}\|_{*}^{2}}{\|\Phi_{2}\|_{*}}\right)^{2}.$$

• Collecting estimates (30), (32) and (33) yields

$$(II) + (III) \ge -\alpha^2 \|\Phi_2\|_*^2 + \alpha^3 \left(2\|A^-\Phi_2\|^2 - 4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2\right)$$

$$-\alpha^4 \left(\frac{2\|A^-\Phi_2\|^2 - 4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2}{\|\Phi_2\|_*}\right)^2$$

$$+ 4\alpha^3 \|\Phi_1\|_*^2 |\eta_1 - \eta_2|^2 + 4\alpha^3 \|\Phi_3\|_*^2 |\eta_3 - \eta_2|^2 + \mathcal{O}(\alpha^5).$$

• Terms with a pre-factor  $\alpha^4$ .

$$\begin{split} &(35)\\ &(IV) := \\ &-8\alpha^4 \Big( \mathrm{Re}\, \eta_1 \bar{\eta_2} \langle \tilde{\Phi}_2^{(1)}, \tilde{\Phi}_2 \rangle_* + \mathrm{Re}\, \eta_3 \bar{\eta_2} \langle \tilde{\Phi}_2^{(2)}, \tilde{\Phi}_2 \rangle_* + \mathrm{Re}\, \eta_2 \bar{\eta_2} \langle \tilde{\Phi}_2^{(3)}, \tilde{\Phi}_2 \rangle_* \Big) + |\tilde{\eta}_2|^2 \alpha^4 \|\tilde{\Phi}_2\|_*^2 \\ &-8\alpha^4 \Big( \mathrm{Re}\, \eta_2 \bar{\eta}_4 \langle \Phi_4^{(2)}, \Phi_4 \rangle_* + \mathrm{Re}\, \eta_3 \bar{\eta}_4 \langle \Phi_4^{(1)}, \Phi_4 \rangle_* \Big) + |\eta_4|^2 \alpha^4 \|\Phi_4\|_*^2 \\ &+8\alpha^4 \mathrm{Re}\, \eta_1 \bar{\eta}_3 \langle \Phi_1, A^- \cdot A^- \Phi_3 \rangle + 8|\eta_1|^2 \alpha^4 \|A^- \Phi_1\|^2 + 8|\eta_3|^2 \alpha^4 \|A^- \Phi_3\|^2 \;. \end{split}$$

Let us first remark that in this expression, we have terms with pre-factor  $\tilde{\eta}_2$  and positive terms with pre-factor  $|\tilde{\eta}_2|^2$ , therefore, this implies that  $\tilde{\eta}_2$  is uniformly bounded in  $\alpha$  for a minimizer. The same remarks hold for  $\eta_4$ . Thus, there exists  $c < \infty$  independent on  $\alpha$  such that

$$|\tilde{\eta}_2| \le c, \quad |\eta_4| \le c.$$

Now, we add to the term (IV) half of the positive term  $4\alpha^3 \|\Phi_1\|_*^2 |\eta_1 - \eta_2|^2 + 4\alpha^3 \|\Phi_3\|_*^2 |\eta_3 - \eta_2|^2$  obtained in the lower bound (34) for (II) + (III), and we split the resulting expression in three parts as follows

(37) 
$$(IV) + 2\alpha^{3} \|\Phi_{1}\|_{*}^{2} |\eta_{1} - \eta_{2}|^{2} + 2\alpha^{3} \|\Phi_{3}\|_{*}^{2} |\eta_{3} - \eta_{2}|^{2}$$

$$=: (IV)^{(1)} + (IV)^{(2)} + (IV)^{(3)} + (IV)^{(4)} ,$$

where

(38)

$$(IV)^{(1)} := -8\alpha^{4} \left( \operatorname{Re} \eta_{1} \bar{\eta}_{2} \langle \tilde{\Phi}_{2}^{(1)}, \tilde{\Phi}_{2} \rangle_{*} + \operatorname{Re} \eta_{3} \bar{\eta}_{2} \langle \tilde{\Phi}_{2}^{(2)}, \tilde{\Phi}_{2} \rangle_{*} + \operatorname{Re} \eta_{2} \bar{\eta}_{2} \langle \tilde{\Phi}_{2}^{(3)}, \tilde{\Phi}_{2} \rangle_{*} \right)$$
$$+ |\tilde{\eta}_{2}|^{2} \alpha^{4} ||\tilde{\Phi}_{2}||_{*}^{2} + 2\alpha^{3} ||\Phi_{1}||_{*}^{2} |\eta_{1} - \eta_{2}|^{2} + \alpha^{3} ||\Phi_{3}||_{*}^{2} |\eta_{3} - \eta_{2}|^{2},$$

(39) 
$$(IV)^{(2)} := -8\alpha^4 \left( \operatorname{Re} \eta_2 \bar{\eta}_4 \langle \Phi_4^{(2)}, \Phi_4 \rangle_* + \operatorname{Re} \eta_3 \bar{\eta}_4 \langle \Phi_4^{(1)}, \Phi_4 \rangle_* \right) + |\eta_4|^2 \alpha^4 ||\Phi_4||_*^2 + \alpha^3 ||\Phi_3||_*^2 |\eta_3 - \eta_2|^2,$$

and

$$(40) \quad (IV)^{(3)} := 8\alpha^4 \operatorname{Re} \eta_1 \bar{\eta}_3 \langle \Phi_1, A^- \cdot A^- \Phi_3 \rangle + 8|\eta_1|^2 \alpha^4 ||A^- \Phi_1||^2 + 8|\eta_3|^2 \alpha^4 ||A^- \Phi_3||^2 + \alpha^3 ||\Phi_1||_*^2 |\eta_1 - \eta_2|^2 + \alpha^3 ||\Phi_3||_*^2 |\eta_3 - \eta_2|^2$$

Using from Lemma A.1 that  $\eta_2 = 1 + \mathcal{O}(\alpha)$  and the fact that  $\eta_4$  is bounded uniformly in  $\alpha$  (see (36)) yields

$$(41) (IV)^{(2)} = -8\alpha^4 \left( \operatorname{Re} \eta_2 \bar{\eta}_4 \langle \Phi_4^{(2)}, \Phi_4 \rangle_* + \operatorname{Re} \eta_2 \bar{\eta}_4 \langle \Phi_4^{(1)}, \Phi_4 \rangle_* \right)$$

$$-8\alpha^4 \operatorname{Re} (\eta_3 - \eta_2) \bar{\eta}_4 \langle \Phi_4^{(1)}, \Phi_4 \rangle_* + \alpha^3 \|\Phi_3\|_*^2 |\eta_3 - \eta_2|^2 + |\eta_4|^2 \alpha^4 \|\Phi_4\|_*^2$$

$$= -8\alpha^4 \left( \operatorname{Re} \eta_2 \bar{\eta}_4 \langle \Phi_4^{(2)}, \Phi_4 \rangle_* + \operatorname{Re} \eta_2 \bar{\eta}_4 \langle \Phi_4^{(1)}, \Phi_4 \rangle_* \right) - c\alpha^5 |\eta_4|^2 + |\eta_4|^2 \alpha^4 \|\Phi_4\|_*^2$$

$$\geq -16\alpha^4 \|\Phi_4\|_*^2 - c\alpha^5.$$

The term  $(IV)^{(1)}$  is treated as follows

(42)

$$(IV)^{(1)} = -8\alpha^{4} \operatorname{Re} (\eta_{1} - \eta_{2}) \bar{\eta}_{2}^{2} \langle \tilde{\Phi}_{2}^{(1)}, \tilde{\Phi}_{2} \rangle_{*} + 2\alpha^{3} \|\Phi_{1}\|_{*}^{2} |\eta_{1} - \eta_{2}|^{2}$$

$$-8\alpha^{4} \operatorname{Re} (\eta_{3} - \eta_{2}) \bar{\eta}_{2}^{2} \langle \tilde{\Phi}_{2}^{(2)}, \tilde{\Phi}_{2} \rangle_{*} + \alpha^{3} \|\Phi_{3}\|_{*}^{2} |\eta_{3} - \eta_{2}|^{2}$$

$$-8\alpha^{4} \operatorname{Re} \eta_{2} \bar{\eta}_{2}^{2} \langle \tilde{\Phi}_{2}^{(1)}, \tilde{\Phi}_{2} \rangle_{*} - 8\alpha^{4} \operatorname{Re} \eta_{2} \bar{\eta}_{2}^{2} \langle \tilde{\Phi}_{2}^{(2)}, \tilde{\Phi}_{2} \rangle_{*} - 8\alpha^{4} \operatorname{Re} \eta_{2} \bar{\eta}_{2}^{2} \langle \tilde{\Phi}_{2}^{(3)}, \tilde{\Phi}_{2} \rangle_{*}$$

$$+ |\tilde{\eta}_{2}|^{2} \alpha^{4} \|\tilde{\Phi}_{2}\|_{*}^{2}.$$

Since  $\tilde{\eta}_2$  is bounded (see (36)), the first line and the second line in the right hand side are of the order  $\alpha^5$ . In addition, replacing  $\eta_2$  by  $1 + \mathcal{O}(\alpha)$  (see Lemma A.1) in the third line of (42) yields

$$(43) (IV)^{(1)} = \\ -8\alpha^{4} \operatorname{Re} \left( \bar{\eta_{2}} \langle \tilde{\Phi}_{2}^{(1)}, \tilde{\Phi}_{2} \rangle_{*} + \bar{\eta_{2}} \langle \tilde{\Phi}_{2}^{(2)}, \tilde{\Phi}_{2} \rangle_{*} + \bar{\eta_{2}} \langle \tilde{\Phi}_{2}^{(3)}, \tilde{\Phi}_{2} \rangle_{*} \right) + |\tilde{\eta}_{2}|^{2} \alpha^{4} ||\tilde{\Phi}_{2}||_{*}^{2} + \mathcal{O}(\alpha^{5}) \\ = -8\alpha^{4} \operatorname{Re} \tilde{\eta_{2}} ||\tilde{\Phi}_{2}||_{*}^{2} + |\tilde{\eta}_{2}|^{2} \alpha^{4} ||\tilde{\Phi}_{2}||_{*}^{2} + \mathcal{O}(\alpha^{5}) \\ \geq -16\alpha^{4} ||\tilde{\Phi}_{2}||_{*}^{2} + \mathcal{O}(\alpha^{5}).$$

Eventually, we estimate the term  $(IV)^{(3)}$ . We have

(44)

$$(IV)^{(3)} = 8\alpha^4 \operatorname{Re} \eta_1 \bar{\eta}_3 \langle \Phi_1, A^- \cdot A^- \Phi_3 \rangle + \frac{1}{2}\alpha^3 \|\Phi_1\|_*^2 |\eta_1 - \eta_2|^2 + \frac{1}{2}\alpha^3 \|\Phi_3\|_*^2 |\eta_3 - \eta_2|^2$$

$$+ 8|\eta_1|^2 \alpha^4 \|A^- \Phi_1\|^2 + \frac{1}{2}\alpha^3 \|\Phi_1\|_*^2 |\eta_1 - \eta_2|^2$$

$$+ 8|\eta_3|^2 \alpha^4 \|A^- \Phi_3\|^2 + \frac{1}{2}\alpha^3 \|\Phi_3\|_*^2 |\eta_3 - \eta_2|^2$$

The first line in (44) is estimated as

$$8\alpha^{4}\operatorname{Re}\eta_{1}\bar{\eta}_{3}\langle\Phi_{1}, A^{-}\cdot A^{-}\Phi_{3}\rangle + \frac{1}{2}\alpha^{3}\|\Phi_{1}\|_{*}^{2}|\eta_{1} - \eta_{2}|^{2} + \frac{1}{2}\alpha^{3}\|\Phi_{3}\|_{*}^{2}|\eta_{3} - \eta_{2}|^{2}$$

$$= 8\alpha^{4}\operatorname{Re}(\eta_{1} - \eta_{2})\bar{\eta}_{3}\langle\Phi_{1}, A^{-}\cdot A^{-}\Phi_{3}\rangle + \frac{1}{2}\alpha^{3}\|\Phi_{1}\|_{*}^{2}|\eta_{1} - \eta_{2}|^{2}$$

$$+ 8\alpha^{4}\operatorname{Re}\eta_{2}(\bar{\eta}_{3} - \bar{\eta}_{2})\langle\Phi_{1}, A^{-}\cdot A^{-}\Phi_{3}\rangle + \frac{1}{2}\alpha^{3}\|\Phi_{3}\|_{*}^{2}|\eta_{3} - \eta_{2}|^{2}$$

$$+ 8\alpha^{4}\operatorname{Re}|\eta_{2}|^{2}\langle\Phi_{1}, A^{-}\cdot A^{-}\Phi_{3}\rangle$$

$$\geq -c\alpha^{5} + 8\alpha^{4}\operatorname{Re}\langle\Phi_{1}, A^{-}\cdot A^{-}\Phi_{3}\rangle$$

where we used again  $|\eta_2|^2 = 1 + \mathcal{O}(\alpha)$  and  $|\eta_3| = \mathcal{O}(1)$ . The second line in (44) is estimated as

$$8|\eta_1|^2\alpha^4||A^-\Phi_1||^2 + \frac{1}{2}\alpha^3||\Phi_1||_*^2|\eta_1 - \eta_2|^2$$

$$(46) = 8|\eta_{2}|^{2}\alpha^{4}||A^{-}\Phi_{1}||^{2} + 8(|\eta_{1}|^{2} - |\eta_{2}|^{2})\alpha^{4}||A^{-}\Phi_{1}||^{2} + \frac{1}{2}\alpha^{3}||\Phi_{1}||_{*}^{2}|\eta_{1} - \eta_{2}|^{2}$$

$$\geq 8\alpha^{4}||A^{-}\Phi_{1}||^{2} + \mathcal{O}(\alpha^{5}) - 96|\eta_{1} - \eta_{2}|\alpha^{4}||A^{-}\Phi_{1}||^{2} + \frac{1}{2}\alpha^{3}||\Phi_{1}||_{*}^{2}|\eta_{1} - \eta_{2}|^{2}$$

$$\geq 8\alpha^{4}||A^{-}\Phi_{1}||^{2} + \mathcal{O}(\alpha^{5}).$$

Similarly, the third line in (44) is estimated by

$$(47) 8|\eta_3|^2\alpha^4||A^-\Phi_3||^2 + \frac{1}{2}\alpha^3||\Phi_3||_*^2|\eta_3 - \eta_2|^2 \ge 8\alpha^4||A^-\Phi_3||^2 + \mathcal{O}(\alpha^5).$$

Collecting (45), (46) and (47) yields

$$(48) (IV)^{(3)} \ge 8\alpha^4 \operatorname{Re} \langle \Phi_1, A^- \cdot A^- \Phi_3 \rangle + 8\alpha^4 \|A^- \Phi_1\|^2 + 8\alpha^4 \|A^- \Phi_3\|^2 + \mathcal{O}(\alpha^5).$$

This inequality, together with (37), (41) and (43) gives

$$(49)$$

$$(IV) + 2\alpha^{3} \|\Phi_{1}\|_{*}^{2} |\eta_{1} - \eta_{2}|^{2} + 2\alpha^{3} \|\Phi_{3}\|_{*}^{2} |\eta_{3} - \eta_{2}|^{2}$$

$$\geq \alpha^{4} \left( 8 \operatorname{Re} \langle \Phi_{1}, A^{-} \cdot A^{-} \Phi_{3} \rangle + 8 \|A^{-} \Phi_{1}\|^{2} + 8 \|A^{-} \Phi_{3}\|^{2} - 16 \|\Phi_{2}\|_{*}^{2} - 16 \|\Phi_{4}\|_{*}^{2} \right)$$

$$+ \mathcal{O}(\alpha^{5}).$$

• Next, we can treat the term (I). For that sake, we add the remaining other half of the positive term  $4\alpha^3\|\Phi_1\|_*^2|\eta_1-\eta_2|^2+4\alpha^3\|\Phi_3\|_*^2|\eta_3-\eta_2|^2$  obtained in the lower bound (34) for (II)+(III). Writing  $\eta_1=(\eta_1-\eta_2)+\eta_2,\,\eta_3=(\eta_3-\eta_2)+\eta_2,\,\eta_2=1+\mathcal{O}(\alpha)$  and using the fact that  $\langle \tilde{\Phi}_2^{(1)},R_2\rangle_*+\langle \tilde{\Phi}_2^{(2)},R_2\rangle_*+\langle \tilde{\Phi}_2^{(3)},R_2\rangle_*=\langle \tilde{\Phi}_2,R_2\rangle_*=0$ , we get, following the same arguments as for the estimate of (IV)

(50) 
$$(I) + 2\alpha^3 \|\Phi_1\|_{\star}^2 |\eta_1 - \eta_2|^2 + 2\alpha^3 \|\Phi_3\|_{\star}^2 |\eta_3 - \eta_2|^2 = \mathcal{O}(\alpha^5).$$

• Terms with a pre-factor  $\alpha^5$  and the terms  $\mathcal{O}(\alpha^5)$ . Collecting these terms yields the following result

(51) 
$$(V) := -c\alpha^5(|\eta_1|^2 + |\eta_2|^2 + |\eta_3|^2 + |\eta_4|^2 + |\tilde{\eta}_2|^2) + \mathcal{O}(\alpha^5) = \mathcal{O}(\alpha^5).$$

The last equality holds since  $\eta_1$ ,  $\eta_2$ , and  $\eta_3$  are bounded (Lemma A.1) and since we proved in (36) that  $\tilde{\eta}_2$  and  $\eta_4$  are also bounded.

• Collecting (34), (49) (50) and (51) thus gives

$$\begin{split} &\langle \Psi, T(0)\Psi \rangle = (I) + (II) + (III) + (IV) + (V) \\ &\geq -\alpha^2 \|\Phi_2\|_*^2 + \alpha^3 \Big( 2\|A^-\Phi_2\|^2 - 4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2 \Big) \\ &- \alpha^4 \left( \frac{-4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2 + 2\|A^-\Phi_2\|^2}{\|\Phi_2\|_*} \right)^2 \\ &+ \alpha^4 \Big( 8\text{Re} \, \langle \Phi_1, A^- \cdot A^-\Phi_3 \rangle + 8\|A^-\Phi_1\|^2 + 8\|A^-\Phi_3\|^2 - 16\|\Phi_2\|_*^2 - 16\|\Phi_4\|_*^2 \Big) + \mathcal{O}(\alpha^5) \,. \end{split}$$

We conclude the proof of the lower bound for  $\inf \operatorname{spec}(T(0))$  by computing

(53) 
$$\|\Psi\|^{2} = 1 + \|2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1} + R_{1}\|^{2} + \|\eta_{2}\alpha\Phi_{2} + \tilde{\eta}_{2}\alpha^{2}\tilde{\Phi}_{2} + R_{2}\|^{2} + \|2\eta_{3}\alpha^{\frac{3}{2}}\Phi_{3} + R_{3}\|^{2} + \|\alpha^{2}\eta_{4}\Phi_{4} + R_{4}\|^{2} = 1 + \alpha^{2}\|\Phi_{2}\|^{2} + \mathcal{O}(\alpha^{3}) ,$$

where we used that  $\eta_1$ ,  $\eta_3$ ,  $\tilde{\eta_2}$ , and  $\eta_4$  are bounded (Lemma A.1 and (36)), that  $\eta_2 = 1 + \mathcal{O}(\alpha)$  (Lemma A.1), and as a consequence of Corollary 3.1 that the following holds:  $||R_1||$ ,  $||R_2||$ ,  $||R_3||$ ,  $||R_{>4}|| = \mathcal{O}(\alpha^{\frac{3}{2}})$ .

4.3. **Proof of Theorem 2.2.** The proof of (10) is a consequence of the fact that inf spec $(T(0)) = \langle \Psi, T(0)\Psi \rangle / \|\Psi\|^2$  and the value of  $\langle \Psi^{\text{trial}}, T(0)\Psi^{\text{trial}} \rangle / \|\Psi^{\text{trial}}\|^2$  coincide up to  $\mathcal{O}(\alpha^5)$  for  $\Psi^{\text{trial}} := \Omega_f + 2\alpha^{\frac{3}{2}}\Phi_1 + \alpha\left(1 - \alpha\frac{2\|A^-\Phi_2\|^2 - 4\|\Phi_1\|_*^2 - 4\|\Phi_3\|_*^2}{\|\Phi_2\|_*^2}\right)\Phi_2 + \alpha^2\tilde{\Phi}_2 + 2\alpha^{\frac{3}{2}}\Phi_3 + \alpha^2\Phi_4.$ 

The properties for  $\eta_1$ , 3 and  $\eta_2$  were already established in [6] as reminded in Lemma A.1. The properties for  $\tilde{\eta}_2$  and  $\eta_4$  come from the fact that  $\tilde{\eta}_2$  and  $\eta_4$  minimize (52) up to  $\mathcal{O}(\alpha^5)$ .

The equality  $||R||_* = \mathcal{O}(\alpha^2)$  is given by Proposition 3.1. The equality  $||\tilde{R}||_* = \mathcal{O}(\alpha^2)$  is a consequence of  $||R||_* = \mathcal{O}(\alpha^2)$ , the definition (10) for  $\tilde{R}$ , and the \*-orthogonalities in (9).

Finally, Corollary 3.1 proves  $||R|| = \mathcal{O}(\alpha)$ , which in turn implies  $||\tilde{R}|| = \mathcal{O}(\alpha)$ . Acknowledgments

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#### Appendix

A.1. Estimates on  $\eta_1$ ,  $\eta_2$  and  $\eta_3$ . In the following lemma, we give an estimate of the coefficients  $\eta_1$ ,  $\eta_2$  and  $\eta_3$  that occur in the decomposition (8) of  $\Psi$ .

Lemma A.1. We have

(54) 
$$\eta_1 = 1 + \mathcal{O}(\alpha^{\frac{1}{2}}), \quad \eta_3 = 1 + \mathcal{O}(\alpha^{\frac{1}{2}}), \quad and \quad \eta_2 = 1 + \mathcal{O}(\alpha)$$

*Proof.* This is a direct consequence on the estimates of  $\eta_1$ ,  $\eta_2$  and  $\eta_3$  for the approximate ground state up to the order  $\alpha^3$  derived in [6], since, due to the conditions (9), the coefficients  $\eta_1$ ,  $\eta_2$  and  $\eta_3$  in the decomposition (8) of  $\Psi$  are the same as the coefficients  $\eta_1$ ,  $\eta_2$  and  $\eta_3$  in the decomposition [6, (10)]. Note that there was a misprint in the estimates provided in [6] for  $|\eta_1 - 1|$ ,  $|\eta_2 - 1|$  and  $|\eta_3 - 1|$ , since a square was missing. One should read in [6, Theorem 3.2],  $|\eta_{1,3} - 1|^2 \le c\alpha$  and  $|\eta_2 - 1|^2 \le c\alpha^2$ .

A.2. Estimate of the term Re  $\langle \Psi, 4\alpha^{\frac{1}{2}}P_f \cdot A^-\Psi \rangle$ . Throughout this appendix, we shall always use the decomposition of  $\Psi$  given by (8)-(9) and (24)-(25).

Lemma A.2. We have

$$\operatorname{Re} \langle \Psi, 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \Psi \rangle + \frac{1}{8} \langle (H_{f} + P_{f}^{2}) R, R \rangle$$

$$\geq -8\alpha^{3} \operatorname{Re} \eta_{1} \bar{\eta}_{2} \|\Phi_{1}\|_{*}^{2} - 8\alpha^{3} \operatorname{Re} \eta_{2} \bar{\eta}_{3} \|\Phi_{3}\|_{*}^{2}$$

$$(55) \quad -8\alpha^{4} \operatorname{Re} \tilde{\eta}_{2} \bar{\eta}_{1} \langle \tilde{\Phi}_{2}, \tilde{\Phi}_{2}^{(1)} \rangle_{*} - 8\alpha^{4} \operatorname{Re} \tilde{\eta}_{2} \bar{\eta}_{3} \langle \tilde{\Phi}_{2}, \tilde{\Phi}_{2}^{(2)} \rangle_{*} - 8\alpha^{4} \operatorname{Re} \eta_{3} \bar{\eta}_{4} \langle \Phi_{4}^{(1)}, \Phi_{4} \rangle_{*}$$

$$-8\alpha^{2} \operatorname{Re} \eta_{1} \langle \tilde{\Phi}_{2}^{(1)}, R_{2} \rangle_{*} - 8\alpha^{2} \operatorname{Re} \eta_{3} \langle \tilde{\Phi}_{2}^{(2)}, R_{2} \rangle_{*} - 8\operatorname{Re} \eta_{3} \alpha^{2} \langle \Phi_{4}^{(1)}, R_{4} \rangle_{*}$$

$$-c(1 + |\eta_{2}|^{2} + |\tilde{\eta}_{2}|^{2} + |\eta_{4}|^{2})\alpha^{5}.$$

*Proof.* Using the decomposition (8)-(9) of the ground state  $\Psi$ , we obtain

$$\begin{split} & \operatorname{Re} \langle \Psi, \, 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \Psi \rangle = \\ & \operatorname{Re} \langle R_{1}, \, (4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \eta_{2} \alpha \Phi_{2} + 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \tilde{\eta}_{2} \alpha^{2} \tilde{\Phi}_{2} + 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} R_{2}) \rangle \\ & + \operatorname{Re} \langle 2\eta_{1} \alpha^{\frac{3}{2}} \Phi_{1}, \, (4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \eta_{2} \alpha \Phi_{2} + 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \tilde{\eta}_{2} \alpha^{2} \tilde{\Phi}_{2} + 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} R_{2}) \rangle \\ & + \operatorname{Re} \langle \eta_{2} \alpha^{2} \Phi_{2}, \, (4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} 2\eta_{3} \alpha^{\frac{3}{2}} \Phi_{3} + 4P_{f} \cdot A^{-} R_{3}) \rangle \\ & + \operatorname{Re} \langle \tilde{\eta}_{2} \alpha^{2} \tilde{\Phi}_{2}, \, (4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} 2\eta_{3} \alpha^{\frac{3}{2}} \Phi_{3} + 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} R_{3}) \rangle \\ & + \operatorname{Re} \langle R_{2}, \, (4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} 2\eta_{3} \alpha^{\frac{3}{2}} \Phi_{3} + 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} R_{3}) \rangle \\ & + \operatorname{Re} \langle 2\eta_{3} \alpha^{\frac{3}{2}} \Phi_{3}, \, (4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \eta_{4} \alpha^{2} \Phi_{4} + 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} R_{4}) \rangle \\ & + \operatorname{Re} \langle R_{3}, \, (4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \eta_{4} \alpha^{2} \Phi_{4} + 4\operatorname{Re} \alpha^{\frac{1}{2}} P_{f} \cdot A^{-} R_{4}) \rangle + \operatorname{Re} \langle \Gamma^{(\geq 4)} \Psi, \, 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \Gamma^{(\geq 5)} \Psi \rangle \; . \end{split}$$

For each value of n, we collect separately the terms in the right hand side of this equality that stem from Re  $\langle \Gamma^{(n)}\Psi, 4\alpha^{\frac{1}{2}}P_f \cdot A^-\Gamma^{(n+1)}\Psi \rangle$ . For estimating some of these terms, like in (57) or (58), we shall add a term like  $\epsilon \langle H_f R, R \rangle$  or  $\epsilon \langle P_f^2 R, R \rangle$  borrowed from the left hand side of (55).

- For n=0 there is no contribution.
- For n = 1, we obtain the terms

(56) 
$$\operatorname{Re} \langle R_1, 4\alpha^{\frac{1}{2}} P_f \cdot A^- \eta_2 \alpha \Phi_2 \rangle = -4\alpha^{\frac{3}{2}} \operatorname{Re} \bar{\eta}_2 \langle R_1, \Phi_1 \rangle_* = 0 ,$$

where we used the  $\langle \cdot, \cdot \rangle_*$ -orthogonality of  $R_1$  and  $\Phi_1$  given by (9),

(57) 
$$\operatorname{Re} \langle R_{1}, 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} \tilde{\eta}_{2} \alpha^{2} \tilde{\Phi}_{2} \rangle + \frac{1}{16} \langle P_{f}^{2} R_{1}, R_{1} \rangle$$

$$\geq -4 \| P_{f} R_{1} \| \| A^{-} \tilde{\Phi}_{2} \| \alpha^{\frac{5}{2}} |\tilde{\eta}_{2}| + \frac{1}{16} \| P_{f} R_{1} \|^{2}$$

$$= (\frac{1}{4} \| P_{f} R_{1} \| - 8\alpha^{\frac{5}{2}} |\tilde{\eta}_{2}| \| A^{-} \tilde{\Phi}_{2} \|)^{2} - 64 \| A^{-} \tilde{\Phi}_{2} \|^{2} |\tilde{\eta}_{2}|^{2} \alpha^{5}$$

$$\geq -c |\tilde{\eta}_{2}|^{2} \alpha^{5}.$$

Note that we shall use the above argument several times in this proof, as well as in the proof of the other lemmata of this Appendix. We shall not give details again in these other cases.

We also have the following terms

(58) 
$$\operatorname{Re} \langle R_{1}, 4\alpha^{\frac{1}{2}} P_{f} \cdot A^{-} R_{2} \rangle + \frac{1}{16} \langle P_{f}^{2} R_{1}, R_{1} \rangle + \frac{1}{16} \langle H_{f} R_{2}, R_{2} \rangle \\ \geq -c\alpha^{\frac{1}{2}} \|P_{f} R_{1}\|^{2} - c\alpha^{\frac{1}{2}} \|A^{-} R_{2}\|^{2} + \frac{1}{16} \langle P_{f}^{2} R_{1}, R_{1} \rangle + \frac{1}{16} \langle H_{f} R_{2}, R_{2} \rangle \geq 0 ,$$

where we used from [15, Lemma A4] the inequality  $||A^-R_2|| \le c||H_f^{\frac{1}{2}}R_2||$ ,

(59) 
$$\operatorname{Re} \langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 4\alpha^{\frac{1}{2}}P_{f} \cdot A^{-}\eta_{2}\alpha\Phi_{2} \rangle = 8\alpha^{3}\operatorname{Re}\eta_{1}\bar{\eta}_{2}\langle\Phi_{1}, P_{f} \cdot A^{-}\Phi_{2}\rangle$$
$$= -8\alpha^{3}\operatorname{Re}\eta_{1}\bar{\eta}_{2}\|\Phi_{1}\|_{*}^{2},$$

(60) 
$$\operatorname{Re} \langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 4\alpha^{\frac{1}{2}}P_{f}\cdot A^{-}\tilde{\eta}_{2}\alpha^{2}\tilde{\Phi}_{2}\rangle = 8\alpha^{4}\operatorname{Re}\eta_{1}\bar{\tilde{\eta}_{2}}\langle\Phi_{1}, P_{f}\cdot A^{-}\tilde{\Phi}_{2}\rangle$$
$$= -8\alpha^{4}\operatorname{Re}\eta_{1}\bar{\tilde{\eta}_{2}}\langle\tilde{\Phi}_{2}^{(1)}, \tilde{\Phi}_{2}\rangle_{*},$$

and

(61) 
$$\operatorname{Re} \langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 4\alpha^{\frac{1}{2}}P_{f} \cdot A^{-}R_{2} \rangle = 8\alpha^{2}\operatorname{Re} \eta_{1}\langle (H_{f} + P_{f}^{2})P_{f} \cdot A^{+}\Phi_{1}, P_{\Phi_{2}}^{\perp}R_{2} \rangle_{*} \\
= -8\alpha^{2}\operatorname{Re} \eta_{1}\langle \tilde{\Phi}_{2}^{(1)}, R_{2} \rangle_{*}.$$

- For n=2, we obtain the terms

(62) 
$$\operatorname{Re} \langle \eta_2 \alpha \Phi_2, 4\alpha^{\frac{1}{2}} P_f \cdot A^{-2} \eta_3 \alpha^{\frac{3}{2}} \Phi_3 \rangle = -8\alpha^3 \operatorname{Re} \eta_2 \bar{\eta}_3 \|\Phi_3\|_{*}^2,$$

(63) 
$$\operatorname{Re} \langle \eta_2 \alpha^2 \Phi_2, 4P_f \cdot A^- R_3 \rangle = -4\alpha^{\frac{3}{2}} \operatorname{Re} \eta_2 \langle \Phi_3, R_3 \rangle_* = 0,$$

(64) 
$$\operatorname{Re}\langle \tilde{\eta}_{2}\alpha^{2}\tilde{\Phi}_{2}, 4\alpha^{\frac{1}{2}}P_{f}\cdot A^{-}2\eta_{3}\alpha^{\frac{3}{2}}\Phi_{3}\rangle = -8\alpha^{4}\operatorname{Re}\tilde{\eta}_{2}\bar{\eta}_{3}\langle \tilde{\Phi}_{2}, \tilde{\Phi}_{2}^{(2)}\rangle_{*},$$

(65) 
$$\operatorname{Re} \langle \eta_2 \alpha^2 \tilde{\Phi}_2, 4\alpha^{\frac{1}{2}} P_f \cdot A^- R_3 \rangle + \frac{1}{32} \langle P_f^2 R_3, R_3 \rangle \ge -c |\eta_2|^2 \alpha^5,$$

where we used from [15, Lemma A4] that  $||A^-R_3|| \le c||H_f^{\frac{1}{2}}R_3||$ ,

(66) 
$$\operatorname{Re} \langle R_2, 4\alpha^{\frac{1}{2}} P_f \cdot A^{-2} \eta_3 \alpha^{\frac{3}{2}} \Phi_3 \rangle = -8\alpha^2 \operatorname{Re} \bar{\eta}_3 \langle R_2, \tilde{\Phi}_2^{(2)} \rangle_*,$$

and

(67) 
$$\operatorname{Re} \langle R_2, 4\alpha^{\frac{1}{2}} P_f \cdot A^- R_3 \rangle + \frac{1}{16} \langle P_f^2 R_2, R_2 \rangle + \frac{1}{32} \langle H_f R_3, R_3 \rangle \ge 0$$

with similar argument as for (58) for the last inequality.

- For n=3, we obtain the terms

(68) 
$$\operatorname{Re} \langle 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3, 4\alpha^{\frac{1}{2}} P_f \cdot A^- \eta_4 \alpha^2 \Phi_4 \rangle = -8\alpha^4 \operatorname{Re} \eta_3 \bar{\eta}_4 \langle \Phi_4^{(1)}, \Phi_4 \rangle_*,$$

(69) 
$$\operatorname{Re} \langle 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3, 4\alpha^{\frac{1}{2}} P_f \cdot A^- R_4 \rangle = -8 \operatorname{Re} \eta_3 \alpha^2 \langle \Phi_4^{(1)}, R_4 \rangle_*,$$

(70) 
$$\operatorname{Re} \langle R_3, 4\alpha^{\frac{1}{2}} P_f \cdot A^- \eta_4 \alpha^2 \Phi_4 \rangle + \frac{1}{32} \langle P_f^2 R_3, R_3 \rangle \ge -c |\eta_4|^2 \alpha^5,$$

and

(71) 
$$\operatorname{Re} \langle R_3, 4\operatorname{Re} \alpha^{\frac{1}{2}} P_f \cdot A^- R_4 \rangle + \frac{1}{32} \langle P_f^2 R_3, R_3 \rangle + \frac{1}{32} \langle H_f R_4, R_4 \rangle \ge 0.$$

- All contributions to the terms with  $n \ge 4$ , give

(72) 
$$\operatorname{Re} \langle \Gamma^{(\geq 4)} \Psi, 4\alpha^{\frac{1}{2}} P_f \cdot A^{-} \Gamma^{(\geq 5)} \Psi \rangle + \frac{1}{16} \langle H_f \Gamma^{(\geq 5)} \Psi, \Gamma^{(\geq 5)} \Psi \rangle \\ \geq -c\alpha \|P_f \Gamma^{(\geq 4)} \Psi\|^2 = -c\alpha^5 (1 + |\tilde{\eta}_2|^2 + |\eta_4|^2),$$

where we used (11) of Proposition 3.1.

Collecting the inequalities (56)-(72) conclude the proof of the Lemma.

# A.3. Estimate of the term $\operatorname{Re} \langle \Psi, 2\alpha A^- \cdot A^- \Psi \rangle$ .

Lemma A.3. We have

(73) 
$$\operatorname{Re} \langle \Psi, 2\alpha A^{-} \cdot A^{-}\Psi \rangle + \frac{1}{8} \langle (H_{f} + P_{f}^{2})R, R \rangle$$

$$\geq -2 \alpha^{2} \operatorname{Re} \bar{\eta}_{2} \|\Phi_{2}\|_{*}^{2} - 8 \alpha^{2} \operatorname{Re} \eta_{2} \langle \Phi_{4}^{(2)}, R_{4} \rangle_{*}$$

$$+ 8 \alpha^{4} \operatorname{Re} \eta_{1} \bar{\eta}_{3} \langle \Phi_{1}, A^{-} \cdot A^{-}\Phi_{3} \rangle - 8 \alpha^{4} \operatorname{Re} \eta_{2} \bar{\eta}_{4} \langle \Phi_{4}^{(2)}, \Phi_{4} \rangle_{*}$$

$$- c(1 + |\eta_{1}|^{2} + |\eta_{3}|^{2} + |\tilde{\eta}_{2}|^{2} + |\eta_{4}|^{2}) \alpha^{5}$$

*Proof.* Using the decomposition (8)-(9) of the ground state  $\Psi$  yields

$$\operatorname{Re} \langle \Psi, 2\alpha A^- \cdot A^- \Psi \rangle$$

= Re 
$$\langle \Omega_f, (2\alpha A^- \cdot A^- \eta_2 \alpha \Phi_2 + 2\alpha A^- \cdot A^- \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2 + 2\alpha A^- \cdot A^- R_2) \rangle$$

+ Re 
$$\langle 2\eta_1 \alpha^{\frac{3}{2}} \Phi_1, (2\alpha A^- \cdot A^- 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3 + 2\alpha A^- \cdot A^- R_3) \rangle$$

+ Re 
$$\langle R_1, (2\alpha A^- \cdot A^- 2n_3\alpha^{\frac{3}{2}}\Phi_3 + 2\alpha A^- \cdot A^- R_3) \rangle$$

+ Re 
$$\langle \eta_2 \alpha \Phi_2, (2\alpha A^- \cdot A^- \eta_4 \alpha^2 \Phi_4 + 2\alpha A^- \cdot A^- R_4) \rangle$$

+ Re 
$$\langle \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2, (2\alpha A^- \cdot A^- \eta_4 \alpha^2 \Phi_4 + 2 \operatorname{Re} \alpha A^- \cdot A^- R_4) \rangle$$

+ Re 
$$\langle R_2, (2\alpha A^- \cdot A^- \eta_4 \alpha^2 \Phi_4 + 2\alpha A^- \cdot A^- R_4) \rangle$$
 + Re  $\langle 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3, 2\alpha A^- \cdot A^- R_5 \rangle$ 

$$+\operatorname{Re}\langle R_3, 2\alpha A^-\cdot A^-R_5\rangle\rangle + \operatorname{Re}\langle \Gamma^{n\geq 4}\Psi, 2\alpha A^-\cdot A^-R_{\geq 6}\rangle$$
.

We collect in this expression the different contributions in Re  $\langle \Gamma^{(n)}\Psi, 2\alpha A^- \cdot A^-\Gamma^{(n+2)}\Psi \rangle$  for each value of n. We shall use throughout this proof very similar arguments to those used in the proof of Lemma A.2.

- For n = 0, we have the terms

(74) 
$$\operatorname{Re} \langle \Omega_f, 2\alpha A^- \cdot A^- \eta_2 \alpha \Phi_2 \rangle = -2 \alpha^2 \operatorname{Re} \eta_2 \|\Phi_2\|_{*}^2,$$

(75) 
$$\operatorname{Re} \langle \Omega_f, 2\alpha A^- \cdot A^- \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2 \rangle = -2\alpha^3 \operatorname{Re} \bar{\tilde{\eta}_2} \langle \Phi_2, \tilde{\Phi}_2 \rangle_* = 0,$$

and

(76) 
$$\operatorname{Re} \langle \Omega_f, 2\alpha A^- \cdot A^- R_2 \rangle = -2\alpha \operatorname{Re} \langle \Phi_2, R_2 \rangle_* = 0,$$

- For n = 1, we have the terms

(77) 
$$\operatorname{Re} \langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 2\alpha A^{-} \cdot A^{-}2\eta_{3}\alpha^{\frac{3}{2}}\Phi_{3} \rangle = 8 \alpha^{4} \operatorname{Re} \eta_{1}\bar{\eta}_{3} \langle \Phi_{1}, A^{-} \cdot A^{-}\Phi_{3} \rangle,$$

(78) 
$$\operatorname{Re} \langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 2\alpha A^{-}\cdot A^{-}R_{3}\rangle + \frac{1}{32}\langle H_{f}R_{3}, R_{3}\rangle \geq -c|\eta_{1}|^{2}\alpha^{5},$$

(79) 
$$\operatorname{Re} \langle R_{1}, 2\alpha A^{-} \cdot A^{-} 2\eta_{3}\alpha^{\frac{3}{2}}\Phi_{3} \rangle + \frac{1}{32} \langle H_{f}R_{1}, R_{1} \rangle \\ = \operatorname{Re} \langle H_{f}^{\frac{1}{2}}R_{1}, H_{f}^{-\frac{1}{2}} 2\alpha A^{-} \cdot A^{-} 2\eta_{3}\alpha^{\frac{3}{2}}\Phi_{3} \rangle + \frac{1}{32} \langle H_{f}R_{1}, R_{1} \rangle \geq -c|\eta_{3}|^{2}\alpha^{5},$$

and, using (13) of Proposition 3.2 and [15, Lemma A4]

(80)

$$\operatorname{Re} \langle R_{1}, 2\alpha A^{-} \cdot A^{-} R_{3} \rangle + \frac{1}{32} \langle H_{f} R_{3}, R_{3} \rangle^{5} \geq -c\alpha \|A^{+} R_{1}\| \|H_{f}^{\frac{1}{2}} R_{3}\| + \frac{1}{32} \|H_{f}^{\frac{1}{2}} R_{3}\|^{2}$$

$$\geq (-c\alpha^{2} \|A^{+} R_{1}\|^{2} - \frac{1}{32} \|H_{f}^{\frac{1}{2}} R_{3}\|^{2}) + \frac{1}{32} \|H_{f}^{\frac{1}{2}} R_{3}\|^{2}$$

$$\geq -c\alpha^{2} (\|R_{1}\|^{2} + \|H_{f}^{\frac{1}{2}} R_{1}\|^{2}) \geq -c\alpha^{5} (1 + |\tilde{\eta}_{2}|^{2} + |\eta_{4}|^{2})$$

- For n=2, we have the terms

(81) 
$$\operatorname{Re} \langle \eta_2 \alpha \Phi_2, 2\alpha A^- \cdot A^- \eta_4 \alpha^2 \Phi_4 \rangle = -8\alpha^4 \operatorname{Re} \eta_2 \bar{\eta}_4 \langle \Phi_4^{(2)}, \Phi_4 \rangle_*,$$

(82) 
$$\operatorname{Re} \langle \eta_2 \alpha \Phi_2, 2\alpha A^- \cdot A^- R_4 \rangle = -8\alpha^2 \operatorname{Re} \eta_2 \langle \Phi_4^{(2)}, R_4 \rangle_*,$$

(83) 
$$\operatorname{Re} \langle \tilde{\eta}_{2} \alpha^{2} \tilde{\Phi}_{2}, 2\alpha A^{-} \cdot A^{-} \eta_{4} \alpha^{2} \Phi_{4} \rangle \geq -c \, \alpha^{5} (|\tilde{\eta}_{2}|^{2} + |\eta_{4}|^{2})$$

(84) 
$$\operatorname{Re} \langle \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2, 2\operatorname{Re} \alpha A^- \cdot A^- R_4 \rangle \ge -c \alpha^5 (1 + |\tilde{\eta}_2|^2 + |\eta_4|^2),$$

using  $||A^-R_4|| \le c ||H_f^{\frac{1}{2}}R_4|| \le c\alpha^5(1+|\tilde{\eta_2}|^2+|\eta_4|^2)$  (respectively [15, Lemma A4] and Proposition 3.1). We also have the terms

(85) 
$$\operatorname{Re} \langle R_{2}, 2\alpha A^{-} \cdot A^{-} \eta_{4} \alpha^{2} \Phi_{4} \rangle + \frac{1}{32} \langle H_{f} R_{2}, R_{2} \rangle \\ = \operatorname{Re} \langle H_{f}^{\frac{1}{2}} R_{2}, 2\alpha H_{f}^{-\frac{1}{2}} A^{-} \cdot A^{-} \eta_{4} \alpha^{2} \Phi_{4} \rangle + \frac{1}{32} \langle H_{f} R_{2}, R_{2} \rangle \geq -c |\eta_{4}|^{2} \alpha^{6}$$

and

(86)

$$\operatorname{Re} \langle R_2, 2\alpha A^- \cdot A^- R_4 \rangle + \frac{1}{32} \langle H_f R_4, R_4 \rangle \ge -c\alpha^2 \|A^+ R_2\|^2$$

$$\ge -c\alpha^2 (\|H_f R_2\|^2 + \|R_2\|^2) \ge -c\alpha^2 (\|R_2\|_*^2 + \|\Theta\|^2 + |\tilde{\eta}_2|^2 \|\alpha^2 \tilde{\Phi}_2\|^2 + |\eta_4|^2 \|\alpha^2 \Phi_4\|^2)$$

$$\ge -c\alpha^5 (1 + |\tilde{\eta}_2|^2 + |\eta_4|^2),$$

for  $\Theta$  defined by (12) and using from (23) of Corollary 3.1 that  $\|\Theta\|^2 = \mathcal{O}(\alpha^3)$  and from (11) of Proposition 3.1 that  $\|R_2\|_*^2 \leq c\alpha^4(1+|\tilde{\eta_2}|^2+|\eta_4|^2)$ .

- For  $n \geq 3$  we collect all the terms as follows

(87) 
$$\operatorname{Re} \langle 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3, 2\alpha A^- \cdot A^- R_5 \rangle + \frac{1}{32} \langle H_f R_5, R_5 \rangle \ge -c |\eta_3|^2 \alpha^5,$$

(88) 
$$\operatorname{Re}\langle R_3, 2\alpha A^- \cdot A^- R_5 \rangle + \frac{1}{32}\langle H_f R_5, R_5 \rangle \ge -c\alpha^5,$$

using (23) of Corollary 3.1 in the last inequality. Finally, we get

(89) Re 
$$\langle \Gamma^{n\geq 4}\Psi, 2\alpha A^- \cdot A^- R_{\geq 6} \rangle + \frac{1}{32} \langle H_f R_{\geq 6}, R_{\geq 6} \rangle \geq -c\alpha^5 (1 + |\tilde{\eta_2}|^2 + |\eta_4|^2),$$

Collecting (74)-(89) yields the result.

# A.4. Estimate of the term $\langle \Psi, 2\alpha A^+ \cdot A^- \Psi \rangle$ .

Lemma A.4. We have

(90)

$$\langle \Psi, 2\alpha A^{+} \cdot A^{-} \Psi \rangle + \frac{1}{8} \langle (H_{f} + P_{f}^{2})R, R \rangle \geq -8\alpha^{2} \operatorname{Re} \bar{\eta}_{2} \langle R_{2}, \tilde{\Phi}_{2}^{(3)} \rangle_{*} + 2|\eta_{2}|^{2} \alpha^{3} ||A^{-} \Phi_{2}||^{2} + 8\alpha^{4} |\eta_{1}|^{2} ||A^{-} \Phi_{1}||^{2} + 8\alpha^{4} |\eta_{3}|^{2} ||A^{-} \Phi_{3}||^{2} - 8\alpha^{4} \operatorname{Re} \tilde{\eta}_{2} \eta_{2} \langle \tilde{\Phi}_{2}, \tilde{\Phi}_{2}^{(3)} \rangle_{*} - c\alpha^{5} (1 + |\eta_{1}|^{2} + |\eta_{3}|^{2} + |\tilde{\eta}_{2}|^{2}).$$

*Proof.* With the decomposition (8)-(9) of  $\Psi$  we get

$$\langle \Psi, 2\alpha A^{+} \cdot A^{+} \Psi \rangle = \langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 2\alpha A^{+} \cdot A^{-}2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1} \rangle + 2\operatorname{Re}\langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 2\alpha A^{+} \cdot A^{-}R_{1}\rangle + \langle \eta_{2}\alpha\Phi_{2}, 2\alpha A^{+} \cdot A^{-}\eta_{2}\alpha\Phi_{2} \rangle + 2\operatorname{Re}\langle \eta_{2}\alpha\Phi_{2}, 2\alpha A^{+} \cdot A^{-}\tilde{\eta}_{2}\alpha^{2}\tilde{\Phi}_{2}\rangle$$

$$+ \langle \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2, 2\alpha A^+ \cdot A^- \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2 \rangle + \langle R_2, 2\alpha A^+ \cdot A^- R_2 \rangle + 2 \operatorname{Re} \langle R_2, 2\alpha A^+ \cdot A^- \eta_2 \Phi_2 \rangle$$

$$+2\operatorname{Re}\langle R_2, 2\alpha A^+ \cdot A^- \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2^{(2)} \rangle + \langle 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3, 2\alpha A^+ \cdot A^- 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3 \rangle$$

$$+2\operatorname{Re}\left\langle 2\eta_{3}\alpha^{\frac{3}{2}}\Phi_{3},2\alpha A^{+}\cdot A^{-}R_{3}\right\rangle +\left\langle R_{3},2\alpha A^{+}\cdot A^{-}R_{3}\right\rangle +\left\langle \Gamma^{(\geq4)}\Psi,2\alpha A^{+}\cdot A^{-}\Gamma^{(\geq4)}\Psi\right\rangle .$$

For each value of n, we next collect in the above equality the different contributions of  $\langle \Gamma^{(n)}\Psi, 2\alpha A^+ \cdot A^-\Gamma^{(n)}\Psi \rangle$ .

- For n = 0, there is no term.
- For n = 1, we have

(91) 
$$\langle 2\eta_1 \alpha^{\frac{3}{2}} \Phi_1, 2\alpha A^+ \cdot A^- 2\eta_1 \alpha^{\frac{3}{2}} \Phi_1 \rangle = 8|\eta_1|^2 \alpha^4 ||A^- \Phi_1||^2,$$

and

(92) 
$$2\operatorname{Re}\langle 2\eta_{1}\alpha^{\frac{3}{2}}\Phi_{1}, 2\alpha A^{+}\cdot A^{-}R_{1}\rangle + \frac{1}{32}\langle H_{f}R_{1}, R_{1}\rangle \geq -c|\eta_{1}|^{2}\alpha^{5}.$$

- For n=2, we obtain

(93) 
$$\langle \eta_2 \alpha \Phi_2, 2\alpha A^+ \cdot A^- \eta_2 \alpha \Phi_2 \rangle = 2|\eta_2|^2 \alpha^3 ||A^- \Phi_2||^2,$$

(94) 
$$2\operatorname{Re}\langle \eta_2 \alpha \Phi_2, 2\alpha A^+ \cdot A^- \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2 \rangle = -8\operatorname{Re} \eta_2 \tilde{\eta}_2 \alpha^4 \langle \tilde{\Phi}_2^{(3)}, \tilde{\Phi}_2 \rangle_*,$$

(95) 
$$\langle \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2, 2\alpha A^+ \cdot A^- \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2 \rangle = 4\alpha^5 |\tilde{\eta}_2|^2 ||A^- \tilde{\Phi}_2||^2,$$

$$\langle R_2, 2\alpha A^+ \cdot A^- R_2 \rangle \ge 0,$$

(97) 
$$2\operatorname{Re}\langle R_2, 2\alpha A^+ \cdot A^- \eta_2 \Phi_2 \rangle = -8\alpha^2 \operatorname{Re} \bar{\eta}_2 \langle R_2, \tilde{\Phi}_2^{(3)} \rangle_*,$$

and

(98) 
$$2\operatorname{Re}\langle R_2, 2\alpha A^+ \cdot A^- \tilde{\eta}_2 \alpha^2 \tilde{\Phi}_2^{(2)} \rangle + \frac{1}{32} \langle H_f R_2, R_2 \rangle \ge -c |\tilde{\eta}_2|^2 \alpha^5.$$

- For n=3, we have

(99) 
$$\langle 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3, 2\alpha A^+ \cdot A^- 2\eta_3 \alpha^{\frac{3}{2}} \Phi_3 \rangle = 8\alpha^4 |\eta_3|^2 ||A^- \Phi_3||^2,$$

(100) 
$$2\operatorname{Re}\langle 2\eta_3\alpha^{\frac{3}{2}}\Phi_3, 2\alpha A^+ \cdot A^-R_3\rangle + \frac{1}{32}\langle H_fR_3, R_3\rangle \ge -|\eta_3|^2\alpha^5,$$

and

$$\langle R_3, 2\alpha A^+ \cdot A^- R_3 \rangle \ge 0,$$

- For n > 4, we obtain

(102) 
$$\langle \Gamma^{(\geq 4)} \Psi, 2\alpha A^+ \cdot A^- \Gamma^{(\geq 4)} \Psi \rangle \geq 0.$$

Collecting (91)-(102) concludes the proof of the lemma.

## A.5. Computation of the term $\langle \Psi, H_f + P_f^2 \Psi \rangle$ .

Lemma A.5. We have

(103) 
$$\langle (H_f + P_f^2)\Psi, \Psi \rangle = |\eta_2|^2 \alpha^2 ||\Phi_2||_*^2 + 4|\eta_1|^2 \alpha^3 ||\Phi_1||_*^2 + 4|\eta_3|^2 \alpha^3 ||\Phi_3||_*^2 + |\tilde{\eta}_2|^2 \alpha^4 ||\tilde{\Phi}_2||_*^2 + |\eta_4|^2 \alpha^4 ||\Phi_4||_*^2 + ||R||_*^2 .$$

*Proof.* Using the decomposition (8) of  $\Psi$  and using the whole set of orthogonalities with respect to  $\langle \cdot, \cdot \rangle_*$  given in (9), we obtain that all crossed terms are zero. The proof is thus straightforward.

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