QUANTITATIVE ESTIMATES ON THE HYDROGEN GROUND STATE ENERGY IN NON-RELATIVISTIC QED

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Abstract. In this paper, we determine the exact expression for the hydrogen ground state energy in the Pauli-Fierz model up to the order $O(\alpha^5 \log \alpha^{-1})$, where α denotes the finestructure constant, and prove rigorous bounds on the remainder term of the order $o(\alpha^5 \log \alpha^{-1})$. As a consequence, we prove that the ground state energy is not a real analytic function of α, and verify the existence of logarithmic corrections to the expansion of the ground state energy in powers of α, as conjectured in the recent literature.

1. Introduction

For a hydrogen-like atom consisting of an electron interacting with a static nucleus of charge eZ, described by the Schrödinger Hamiltonian $-\Delta - \frac{\alpha Z}{|x|}$,

$$\inf \sigma(-\Delta) - \inf \sigma(-\Delta - \frac{\alpha Z}{|x|}) \;=\; \frac{(Z\alpha)^2}{4} \;.$$

corresponds to the binding energy necessary to remove the electron to spatial infinity.

The interaction of the electron with the quantized electromagnetic field is accounted for by adding to $-\Delta - \frac{\alpha Z}{|x|}$ the photon field energy operator H_f, and an operator $I(\alpha)$ which describes the coupling of the electron to the quantized electromagnetic field; the small parameter α is the fine structure constant. Thereby, one obtains the Pauli-Fierz Hamiltonian described in detail in Section 2. In this case, determining the binding energy

$$\inf \sigma\big(\, -\Delta + H_f + I(\alpha)\,\big) - \inf \sigma\big(\, -\Delta - \frac{\alpha Z}{|x|} + H_f + I(\alpha)\,\big) \qquad (1)$$

is a very hard problem. A main obstacle emerges from the fact that the ground state energy is not an isolated eigenvalue of the Hamiltonian, and can not be determined with ordinary perturbation theory. Furthermore, the photon form factor in the quantized electromagnetic vector potential occurring in the interaction term $I(\alpha)$ contains a critical frequency space singularity that is responsible for the infamous infrared problem in quantum electrodynamics. As a consequence, quantities such as the ground state energy do not exist as a convergent power series in the fine structure constant α with coefficients independent of α.

In recent years, several rigorous results addressing the computation of the binding energy have been obtained, [14, 13, 8]. In particular, the coupling to the photon field has been shown to increase the binding energy of the electron to the nucleus, and that up to normal ordering, the leading term is $\frac{(\alpha Z)^2}{4}$ [12, 14, 8].

Moreover, for a model with scalar bosons, the binding energy is determined in [13], in the first subleading order in powers of α, up to α^3, with error term

$\alpha^3 \log \alpha^{-1}$. This result has inspired the question of a possible emergence of logarithmic terms in the expansion of the binding energy; however, this question has so far remained open.

In [2], a sophisticated rigorous renormalization group analysis is developed in order to determine the ground state energy (and the renormalized electron mass) up to any arbitrary precision in powers of α, with an expansion of the form

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

(for any given N) where the coefficients $\varepsilon_k(\alpha)$ diverge as $\alpha \to 0$, but are smaller in magnitude than any positive power of α^{-1}. The recursive algorithms developed in [2] are highly complex, and explicitly computing the ground state energy to any subleading order in powers of α is an extensive task. While it is expected that the rate of divergence of these coefficient functions is proportional to a power of $\log \alpha^{-1}$, 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.

The goal of the current paper is to develop an alternative method (as a continuation of [4]) that determines the binding energy up to several subleading orders in powers of α, with rigorous error bounds, and proving the presence of terms logarithmic in α.

The main result established in the present paper (for $Z = 1$) states that the binding energy can be estimated as

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

where $e^{(i)}$ $(i = 1, 2, 3)$ are independent of α, $e^{(1)} > 0$, and $e^{(3)} \neq 0$. Their explicit values are given in Theorem 2.1.

As a consequence, we conclude that the binding energy is *not analytic* in α. In addition, our proof clarifies how the logarithmic factor in $\alpha^5 \log \alpha^{-1}$ is linked to the infrared singularity of the photon form factor in the interaction term $I(\alpha)$. We note that for some models with a mild infrared behavior, [10], the ground state energy is proven to be analytic in α.

Organization of the proof. Our proof of the expression (3) for the hydrogen binding energy involves the following main steps:

Since the binding energy (1) involves the ground state energy of the self-energy operator $T = -\Delta + H_f + I(\alpha)$, it is necessary to determine the value of $\inf \sigma(T)$. This was achieved in [4] (see also Lemma A.7), using in particular the fact that $\inf \sigma(T) = \inf \sigma(T(0))$ [9, 6], where $T(0)$ is the restriction of T to total momentum $P = 0$ (see details in Section 2, (7)).

The derivation of (3) requires both a lower and an upper bound for the binding energy. This is accomplished in three steps.

The first term in the expansion for the binding energy is the Coulomb term $\frac{\alpha^2}{4}$; it can be recovered with an approximate ground state containing no photon, and with an electronic part given by the ground state u_α of the Schrödinger-Coulomb operator $-\Delta - \frac{\alpha}{|x|}$. The first step, described in Section 4, thus consists of estimating the contribution to the binding energy stemming from states orthogonal to u_α with respect to the quadratic form for $-\Delta - \frac{\alpha}{|x|} + H_f + I(\alpha)$.

The next two steps consist of estimating the binding energy up to the order α^3 (Theorem 5.2, Section 5), and subsequently to the order $\alpha^5 \log \alpha^{-1}$ (Theorem 6.1, Section 6).

One of the key ingredient to control some of the error terms occurring in both the upper and lower bounds, is an estimate on the expected photon number for the ground state Ψ of the total hamiltonian $-\Delta - \frac{\alpha Z}{|x|} + H_f + I(\alpha)$. Such a bound is derived in Section 3 and yields $\langle \Psi, N_f \Psi \rangle = \mathcal{O}(\alpha^2 \log \alpha^{-1})$, where N_f is the photon number operator.

In Section 2, we give a detailed introduction of the model and state the main results. In the Appendix, we provide some technical lemmata used in the derivation of the binding energy.

2. The model

We study a scalar electron interacting with the quantized electromagnetic field in the Coulomb gauge, and with the electrostatic potential generated by a fixed nucleus. The Hilbert space accounting for the Schrödinger electron is given by $\mathfrak{H}_{el} = L^2(\mathbb{R}^3)$. The Fock space of photon states is given by

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

where the n-photon space $\mathfrak{F}_n = \bigotimes_s^n \big(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2 \big)$ 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

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

where $a_\lambda^\sharp$ denotes either a_λ or a_λ^*. 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

$$\mathfrak{H} \; := \; \mathfrak{H}_{el} \, \otimes \, \mathfrak{F}.$$

We 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 $e = \sqrt{\alpha}$, where the fine structure constant α will here be considered as a small parameter.

Let $x \in \mathbb{R}^3$ be the position vector of the electron and let $y_i \in \mathbb{R}^3$ be the position vector of the i-th photon.

We consider the normal ordered Pauli-Fierz Hamiltonian on $\mathfrak{H}$ for Hydrogen,

$$:\big(i\nabla_x \otimes I_f - \sqrt{\alpha} A(x) \big)^2 : + V(x) \otimes I_f + I_{el} \otimes H_f . \tag{4}$$

where $: \cdots :$ denotes normal ordering, corresponding to the subtraction of a normal ordering constant $c_{\text{n.o.}} \alpha$, with $c_{\text{n.o.}} I_f := [A^+(x), A^-(x)]$ is independent of x.

The electrostatic potential $V(x)$ is the Coulomb potential for a static point nucleus of charge $e = \sqrt{\alpha}$ (i.e., $Z = 1$)

$$V(x) = -\frac{\alpha}{|x|}.$$

We will describe the quantized electromagnetic field by use of the Coulomb gauge condition.

The operator that couples an electron to the quantized vector potential is given by

$$A(x)=\sum_{\lambda=1,2}\int_{\mathbb{R}^3}\frac{\chi_\Lambda(|k|)}{2\pi|k|^{1/2}}\varepsilon_\lambda(k)\Big[e^{ikx}\otimes a_\lambda(k)+e^{-ikx}\otimes a_\lambda^*(k)\Big]\mathrm{d}k$$

where by the Coulomb gauge condition, $\mathrm{div}A=0$.

The vectors $\varepsilon_\lambda(k)\in\mathbb{R}^3$ are the two orthonormal polarization vectors perpendicular to k,

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

The function χ_Λ implements an *ultraviolet cutoff* on the wavenumbers k. We assume χ_Λ to be of class C^1, with compact support in $\{|k|\le\Lambda\}$, $\chi_\Lambda\le 1$ and $\chi_\Lambda=1$ for $|k|\le\Lambda-1$. For convenience, we shall write

$$A(x)\;=\;A^-(x)\;+\;A^+(x),$$

where

$$A^-(x)\;=\;\sum_{\lambda=1,2}\int_{\mathbb{R}^3}\frac{\chi_\Lambda(|k|)}{2\pi|k|^{1/2}}\,\varepsilon_\lambda(k)\,\mathrm{e}^{ikx}\,\otimes\,a_\lambda(k)\,\mathrm{d}k$$

is the part of $A(x)$ containing the annihilation operators, and $A^+(x)=(A^-(x))^*$.

The photon field energy operator H_f is given by

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

We will, with exception of our discussion in Section 3, study the unitarily equivalent Hamiltonian

$$H=U\Big(:\big(i\nabla_x\otimes I_f-\sqrt{\alpha}A(x)\big)^2:+V(x)\otimes I_f+I_{el}\otimes H_f\Big)U^*\;,\tag{5}$$

where the unitary transform U is defined by

$$U=\mathrm{e}^{iP_f.x},$$

and

$$P_f=\sum_{\lambda=1,2}\int k\,a_\lambda^*(k)a_\lambda(k)\mathrm{d}k$$

is the photon momentum operator. We have

$$Ui\nabla_xU^*=i\nabla_x+P_f\quad\text{and}\quad UA(x)U^*=A(0)\;.$$

In addition, the Coulomb operator V, the photon field energy H_f, and the photon momentum P_f remain unchanged under the action of U. Therefore, in this new system of variables, the Hamiltonian reads as follows

$$H=\;:\big((i\nabla_x\otimes I_f-I_{el}\otimes P_f)-\sqrt{\alpha}A(0)\big)^2:+H_f-\frac{\alpha}{|x|}\;,\tag{6}$$

where : ... : denotes again the normal ordering. Notice that the operator H can be rewritten, taking into account the normal ordering and omitting, by abuse of notations, the operators I_{el} and I_f,

$$\begin{aligned}H=&(-\Delta_x-\frac{\alpha}{|x|})+(H_f+P_f^2)-2\mathrm{Re}\,(i\nabla_x.P_f)\\&-2\sqrt{\alpha}(i\nabla_x-P_f).A(0)+2\alpha A^+(0).A^-(0)+2\alpha\mathrm{Re}\,(A^-(0))^2\;.\end{aligned}$$

For a free spinless electron coupled to the quantized electromagnetic field, the self-energy operator T is given by

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

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.

Let $\mathfrak{H}_P \cong \mathbb{C} \otimes \mathfrak{F}$ denote the fibre Hilbert space corresponding to conserved total momentum P.

For fixed value P of the total momentum, the restriction of T to the fibre space $\mathfrak{H}_P$ is given by (see e.g. [6])

$$T(P) = \ :(P - P_f - \sqrt{\alpha}A(0))^2 : + H_f \tag{7}$$

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

$$A^{\pm} \equiv A^{\pm}(0) \ .$$

Moreover, we denote

$$\Sigma_0 = \inf \sigma(T) \quad \text{and} \quad \Sigma = \inf \sigma(H) = \inf \sigma(T + V).$$

It is proven in [1, 6] that $\Sigma_0 = \inf \sigma(T(0))$ is an eigenvalue of the operator $T(0)$.

Our main result is the following theorem.

Theorem 2.1. *The binding energy fulfills*

$$\Sigma_0 - \Sigma = \frac{1}{4}\alpha^2 + e^{(1)}\alpha^3 + e^{(2)}\alpha^4 + e^{(3)}\alpha^5 \log \alpha^{-1} + o(\alpha^5 \log \alpha^{-1}), \tag{8}$$

where

$$e^{(1)} = \frac{2}{\pi}\int_0^\infty \frac{\chi_\Lambda^2(t)}{1+t}\mathrm{d}t,$$

$$\begin{aligned} e^{(2)} = &\frac{2}{3}\,\mathrm{Re} \sum_{i=1}^{3} \langle (A^-)^i (H_f + P_f^2)^{-1} A^+.A^+\Omega_f , (H_f + P_f^2)^{-1}(A^+)^i \Omega_f \rangle \\ &+ \frac{1}{3}\sum_{i=1}^{3} \|(H_f + P_f^2)^{-\frac{1}{2}} \Big(2A^+.P_f(H_f + P_f^2)^{-1}(A^+)^i - P_f^i(H_f + P_f^2)^{-1}A^+.A^+\Big)\Omega_f\|^2 \\ &- \frac{2}{3}\sum_{i=1}^{3} \|A^-(H_f + P_f^2)^{-1}(A^+)^i\Omega_f\|^2 + 4a_0^2 \|Q_1^\perp(-\Delta - \frac{1}{|x|} + \frac{1}{4})^{-\frac{1}{2}}\Delta u_1\|^2, \end{aligned}$$

$$a_0 = \int \frac{k_1^2 + k_2^2}{4\pi^2|k|^3}\,\frac{2}{|k|^2 + |k|}\chi_\Lambda(|k|)\,\mathrm{d}k_1\mathrm{d}k_2\mathrm{d}k_3,$$

$$e^{(3)} = -\frac{1}{3\pi}\|(-\Delta - \frac{1}{|x|} + \frac{1}{4})^{\frac{1}{2}}\nabla u_1\|^2,$$

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

3. Bounds on the expected photon number

Lemma 3.1. *Let*

$$K \;=\; (i\nabla - \sqrt{\alpha}A(x))^2 \;+\; H_f \;-\; \frac{\alpha}{|x|} \;=\; v^2 + H_f - \frac{\alpha}{|x|}\;,$$

be the Pauli-Fierz operator defined without normal ordering, where $v = i\nabla - \sqrt{\alpha}A(x)$*. Let* $\Psi \in \mathcal{H}$ *denote the ground state of* K*,*

$$K\,\Psi \;=\; E\,\Psi\;,$$

normalized by

$$\|\,\Psi\,\| \;=\; 1\;.$$

Let

$$N_f \;:=\; \sum_{\lambda=1,2}\int a_\lambda^*(k)\,a_\lambda(k)\,\mathrm{d}k$$

denote the photon number operator. Then, there exists a constant c *independent of* α*, such that for any sufficiently small* $\alpha > 0$*, the estimate*

$$\langle \Psi\,,\,N_f\,\Psi\rangle \;\le\; c\,\alpha^2\,\log\alpha^{-1}$$

is satisfied.

Proof. Using

$$[a_\lambda(k), H_f] = |k|, \quad \text{and} \quad [a_\lambda(k), v] = \frac{\epsilon(k)}{2\pi|k|^{\frac12}}\chi_\lambda(k)\mathrm{e}^{ik.x}$$

and the pull-through formula,

$$\begin{aligned} a_\lambda(k)E\Psi \;&=\; a_\lambda(k)K\Psi \\ &=\; \Big[(H_f + |k|)a_\lambda(k) - \frac{1}{|x|}a_\lambda(k) + [v, a_\lambda(k)]v + v[v, a_\lambda(k)]\Big]\Psi\;, \end{aligned}$$

we get

$$a_\lambda(k)\,\Psi \;=\; -\,\frac{\sqrt{\alpha}\chi_\Lambda(|k|)}{2\pi\sqrt{|k|}}\,\frac{2}{K+|k|-E}\,\Big(\Big(i\nabla - \sqrt{\alpha}A(x)\Big)\cdot\epsilon_\lambda(k)\mathrm{e}^{ik.x}\Big)\,\Psi\;. \tag{9}$$

From (9), we obtain

$$\begin{aligned} \Big\|\,a_\lambda(k)\Psi\,\Big\|^2 \;&\le\; \frac{\alpha\,\chi_\Lambda(|k|)}{|k|}\,\Big\|\,\frac{1}{K+|k|-E}\,\Big\|^2\,\Big\|\,\Big(i\nabla - \sqrt{\alpha}A(x)\Big)\Psi\,\Big\|^2 \\ &\le\; \frac{\alpha\,\chi_\Lambda(|k|)}{|k|^3}\,\Big[\big\langle\Psi\,,\,K\,\Psi\big\rangle \;+\; \big\langle\Psi\,,\,\frac{\alpha}{|x|}\,\Psi\big\rangle\Big]\;, \end{aligned}$$

since $K - E \ge 0$, and $\big(i\nabla - \sqrt{\alpha}A(x)\big)^2 \le (K + \frac{\alpha}{|x|})$. We have

$$\big\langle\Psi\,,\,K\,\Psi\big\rangle \le c\,\alpha. \tag{10}$$

Moreover, for the normal ordered hamiltonian defined in (4), we have

$$\begin{aligned} :K: \;&= -\Delta_x - 4\sqrt{\alpha}\mathrm{Re}\,\big(i\nabla_x.A^-(x)\big) + \alpha : A(x)^2 : + H_f - \frac{\alpha}{|x|} \\ &\ge (1 - c\sqrt{\alpha})(-\Delta_x) + \alpha : A(x)^2 : + (1 - c\sqrt{\alpha})H_f - \frac{\alpha}{|x|} \\ &\ge -c\alpha^2 - \frac12\Delta_x - \frac{\alpha}{|x|} \end{aligned} \tag{11}$$

where in the last inequality we used (see e.g. [11])

$$\alpha : A(x) :^2 + (1 - c\sqrt{\alpha}) H_f \geq -c\alpha^2.$$

Inequalities (10), (11) and

$$-\frac{1}{4}\Delta_x - \frac{\alpha}{|x|} \geq -4\alpha^2$$

imply

$$-\frac{1}{4}\langle \Delta_x \Psi, \Psi \rangle \leq c\alpha^2 \|\Psi\|^2.$$

Thus,

$$\Big\langle \Psi \, , \, \frac{\alpha}{|x|}\Psi \Big\rangle \leq \langle -\Delta_x \Psi, \Psi \rangle + \frac{1}{4}\alpha^2 \|\Psi\|^2 \leq (c + \frac{1}{4})\alpha^2 \|\Psi\|^2. \tag{12}$$

Collecting (10), (12) and (9) we find

$$\Big\| a_\lambda(k)\Psi \Big\| \ \leq \ \frac{c\,\alpha\,\chi_\Lambda(|k|)}{|k|^{\frac{3}{2}}} \ . \tag{13}$$

This a priori bound exhibits the L^2-critical singularity in frequency space. It does not take into consideration the exponential localization of the ground state due to the confining Coulomb potential, and appears in a similar form for the free electron.

To account for the latter, we use the following two results from the work of Griesemer, Lieb, and Loss, [11]. Equation (58) in [11] provides the bound

$$\Big\| a_\lambda(k)\Psi \Big\| \ < \ \frac{c\,\sqrt{\alpha}\,\chi_\Lambda(|k|)}{|k|^{\frac{1}{2}}} \Big\| \, |x|\Psi \, \Big\| \ .$$

Moreover, Lemma 6.2 in [11] states that

$$\Big\| \, \exp[\beta|x|]\Psi \, \Big\|^2 \ \leq \ c \, \Big[1 + \frac{1}{\Sigma_0 - E - \beta^2} \Big] \, \| \, \Psi \, \|^2 \ ,$$

for any

$$\beta^2 \ < \ \Sigma_0 - E \ = \ O(\alpha^2) \ .$$

For the 1-electron case, Σ_0 is the electron self-energy, and E is the ground state of $: K :$. Choosing $\beta = O(\alpha)$,

$$\begin{aligned} \| \, |x|\Psi \, \| \quad &\leq \quad \| |x|^4 \Psi \|^{\frac{1}{4}} \, \|\Psi\|^{\frac{3}{4}} \leq \frac{(4!)^{\frac{1}{4}}}{\beta} \, \Big\| \, \exp[\beta|x|]\Psi \, \Big\|^{\frac{1}{4}} \|\Psi\|^{\frac{3}{4}} \\ &\leq \quad \frac{c}{\beta} \Big[1 + \frac{1}{\Sigma_0 - E - \beta^2} \Big]^{\frac{1}{8}} \, \| \, \Psi \, \| \\ &\leq \quad c_1 \alpha^{-\frac{5}{4}} \ . \end{aligned}$$

Notably, this bound only depends on the binding energy of the potential.

Thus,

$$\Big\| a_\lambda(k)\Psi \Big\| < \frac{c\alpha^{-\frac{3}{4}}\chi_\Lambda(|k|)}{|k|^{\frac{1}{2}}} \ . \tag{14}$$

We see that binding to the Coulomb potential weakens the infrared singularity by a factor $|k|$, but at the expense of a large constant factor α^{-2}. For the free electron, this estimate does not exist.

Using (13) and (14), we find

$$\begin{aligned}\langle\, \Psi\,,\, N_f\, \Psi\,\rangle \;&=\; \int \mathrm{d}k \,\Big\|\, a_\lambda(k)\Psi\,\Big\|^2\\ &\le\; \int_{|k|<\delta} \mathrm{d}k\, \frac{c\,\alpha^{-\frac{3}{2}}}{|k|} \;+\; \int_{\delta\le|k|\le\Lambda} \mathrm{d}k\, \frac{c\,\alpha^2}{|k|^3}\\ &\le\; c\,\alpha^{-\frac{3}{2}}\,\delta^2 \;+\; c'\,\alpha^2\,\log\frac{1}{\delta}\\ &\le\; c\,\alpha^{\frac{9}{4}} \;+\; c''\,\alpha^2\,\log\alpha^{-1}\;.\end{aligned}$$

for $\delta = \alpha^{\frac{15}{8}}$. This proves the lemma. □

4. Estimates on the quadratic form for states orthogonal to the ground state of the Schrödinger operator

Throughout this paper, we will denote by Γ^n the projection onto the n-th photon sector (without distinction for the n-photon sector of $\mathfrak{F}$ and the n-photon sector of $\mathfrak{H}$). We also define $\Gamma^{\geq n} = 1 - \sum_{j=0}^{n-1}\Gamma^j$.

Starting with this section, we study the Hamiltonian H defined in (6), written in relative coordinates. In particular, $i\nabla_x$ now stands for the operator unitarily equivalent to the operator of total momentum, which, by abuse of notation, will be denoted by P.

Let

$$u_\alpha(x) = \frac{1}{\sqrt{8\pi}}\alpha^{3/2}\mathrm{e}^{-\alpha|x|/2} \tag{15}$$

be the normalized ground state of the Schrödinger operator

$$h_\alpha := -\Delta_x - \frac{\alpha}{|x|}.$$

We will also denote by $-e_0 = -\frac{\alpha^2}{4}$ and $-e_1 = -\frac{\alpha^2}{16}$ the two lowest eigenvalues of this operator.

Theorem 4.1. *Assume that $\Phi\in\mathfrak{H}$ fulfils $\langle\Gamma^k\Phi, u_\alpha\rangle_{L^2(\mathbb{R}^3,\mathrm{d}x)} = 0$, for all $k\geq 0$. Then there exists $\nu>0$ and $\alpha_0>0$ such that for all $0<\alpha<\alpha_0$*

$$\langle H\Phi,\,\Phi\rangle \geq (\Sigma_0 - e_0)\|\Phi\|^2 + \delta\|\Phi\|^2 + \nu\|H_f^{\frac{1}{2}}\Phi\|^2, \tag{16}$$

where $\delta = (e_0-e_1)/2 = \frac{3}{32}\alpha^2$.

Remark 4.1. *All photons with momenta larger than the ultraviolet cutoff do not contribute to lower the energy. More precisely, due to the cutoff function $\chi_\Lambda(|k|)$ in the definition of $A(x)$, and since we have*

$$H = (i\nabla_x - P_f)^2 - 2\sqrt{\alpha}\mathrm{Re}\,(i\nabla_x - P_f).A(0) + \alpha : A(0)^2 : + H_f - \frac{\alpha}{|x|},$$

it follows that for any given normalized state $\Phi\in\mathfrak{H}$, there exists a normalized state $\Phi_{\leq\Lambda}$ such that $\forall x\in\mathbb{R}^3$, for all $n\in\{1,2,\ldots\}$, for all $((k_1,\lambda_1),\ (k_2,\lambda_2),\ldots,\ (k_n,\lambda_n))\in \big((\mathbb{R}^3\setminus\{k,\ |k|\leq\Lambda+1\})\times\{1,2\}\big)^n$, we have

$$\Gamma^n\Phi_{\leq\Lambda}(x,(k_1,\lambda_1),\ (k_2,\lambda_2),\ldots,\ (k_n,\lambda_n)) = 0 \tag{17}$$

and

$$\langle\Phi_{\leq\Lambda}, H\Phi_{\leq\Lambda}\rangle \leq \langle\Phi, H\Phi\rangle \quad \textit{and} \quad \langle\Phi_{\leq\Lambda}, T\Phi_{\leq\Lambda}\rangle \leq \langle\Phi, T\Phi\rangle.$$

A key consequence of this remark is that throughout the paper, all states will be implicitly assumed to fulfill condition (17)*. This is crucial for the proof of Corollary 4.2.*

To prove Theorem 4.1, we first need the following Lemma.

Lemma 4.1. *There exists $c_0 > 0$ such that for all α small enough we have*

$$H - \frac{1}{2}(P - P_f)^2 - \frac{1}{2}H_f \geq -c_0\alpha^2.$$

A straightforward consequence of this lemma is the following result.

Corollary 4.1. *Let Ψ^{GS} be the normalized ground state of H. Then*

$$\langle H_f \Psi^{GS}, \Psi^{GS}\rangle \leq 2c_0\alpha^2\|\Psi^{GS}\|^2 \tag{18}$$

Proof. This follows from $\langle H\Psi^{\mathrm{GS}}, \Psi^{\mathrm{GS}}\rangle \leq (\Sigma_0 - e_0)\|\Psi^{\mathrm{GS}}\|^2 < 0$. □

Moreover, from Theorem 4.1 and Lemma 4.1, we obtain

Corollary 4.2. *Assume that $\Phi \in \mathfrak{H}$ is such that $\langle \Gamma^n\Phi, u_\alpha\rangle_{L^2(\mathbb{R}^3,\mathrm{d}x)} = 0$ holds for all $n \geq 0$. Then, for ν and δ defined in Theorem 4.1, there exists $\zeta > 0$, and $\alpha_0 > 0$ such that for all $0 < \alpha < \alpha_0$ we have*

$$\langle H\Phi,\, \Phi\rangle \geq (\Sigma_0 - e_0)\|\Phi\|^2 + M[\Phi], \tag{19}$$

where

$$M[\Phi] := \frac{\delta}{2}\|\Phi\|^2 + \frac{\nu}{2}\|H_f^{\frac{1}{2}}\Phi\|^2 + \zeta\|(P - P_f)\Phi\|^2 + \zeta\|\Gamma^{n\leq 4}P\Phi\|^2. \tag{20}$$

Proof. According to Remark 4.1, there exists $\widetilde{c} > 1$ such that the operator inequality $P_f^2\Gamma^{n\leq 4} \leq \widetilde{c}H_f\Gamma^{n\leq 4}$ holds on the set of states for which (17) is satisfied. The value of $\widetilde{c}$ only depends on the ultraviolet cutoff Λ. Thus,

$$\|\Gamma^{n\leq 4}P\Phi\|^2 \leq 2\|(P - P_f)\Phi\|^2 + 2\|\Gamma^{n\leq 4}P_f\Phi\|^2 \leq 2\|(P - P_f)g\|^2 + 2\widetilde{c}\|H_f^{\frac{1}{2}}\Gamma^{n\leq 4}\Phi\|^2,$$

which yields

$$\|(P - P_f)\Phi\|^2 \geq \frac{1}{2}\|\Gamma^{n\leq 4}P\Phi\|^2 - \widetilde{c}\|H_f^{\frac{1}{2}}\Gamma^{n\leq 4}\Phi\|^2\ .$$

Therefore, it suffices to prove Corollary 4.2 with $M[\Phi]$ replaced by

$$\widetilde{M}[\Phi] := \frac{\delta}{2}\|\Phi\|^2 + \frac{3}{4}\nu\|H_f^{\frac{1}{2}}\Phi\|^2 + 2\zeta\|(P - P_f)\Phi\|^2, \tag{21}$$

and ζ small enough so that $\widetilde{c}\zeta < \frac{\nu}{4}$.

Now we consider two cases. Let $c_1 := \max\{8c_0, 8\delta/\alpha^2\}$.

If $\|(P - P_f)\Phi\|^2 \leq c_1\alpha^2\|\Phi\|^2$, Theorem 4.1 and the above remark imply (19).

If $\|(P - P_f)\Phi\|^2 > c_1\alpha^2\|\Phi\|^2$, Lemma 4.1 implies that

$$\begin{aligned}
\langle H\Phi, \Phi\rangle &\geq \frac{1}{2}\langle (P - P_f)^2\Phi, \Phi\rangle + \frac{1}{2}\langle H_f\Phi, \Phi\rangle - c_0\alpha^2\|\Phi\|^2 \\
&\geq \frac{1}{4}\langle (P - P_f)^2\Psi^\perp, \Psi^\perp\rangle + \frac{1}{2}\langle H_f\Phi, \Phi\rangle + \frac{1}{8}\|(P - P_f)\Phi\|^2 \\
&\geq \frac{1}{4}\langle (P - P_f)^2\Phi, \Phi\rangle + \frac{1}{2}\langle H_f\Phi, \Phi\rangle + \frac{c_1\alpha^2}{8}\|\Phi\|^2\ ,
\end{aligned}$$

which concludes the proof since $\Sigma_0 - e_0 < 0$. □

Proof of Lemma 4.1. Recall the notation $A^{\pm} \equiv A^{\pm}(0)$. The following holds.

$$
\begin{aligned}
& H - \frac{1}{2}(P-P_f)^2 - \frac{1}{2}H_f \\
& = \frac{1}{2}(P-P_f)^2 - \frac{\alpha}{|x|} - 2\sqrt{\alpha}\mathrm{Re}\,((P-P_f).A(0)) + 2\alpha \mathrm{Re}\,(A^-)^2 + 2\alpha A^+.A^- + \frac{1}{2}H_f,
\end{aligned}
$$

$$\frac{1}{4}(P-P_f)^2 - \frac{\alpha}{|x|} \geq -4\alpha^2. \tag{22}$$

and

$$2\sqrt{\alpha}|\langle (P-P_f).A(0)\psi,\psi\rangle| \leq 2\sqrt{\alpha}\|(P-P_f)\psi\|^2 + 2\sqrt{\alpha}\|A^-\psi\|^2 \ . \tag{23}$$

By the Schwarz inequality, there exists c_1 independent of α such that

$$\|A^-\psi\|^2 \leq c_1 \|H_f^{\frac{1}{2}}\psi\|^2. \tag{24}$$

Inequalities (23)-(24) imply that for small α,

$$2\sqrt{\alpha}|\langle (P-P_f).A(0)\psi,\psi\rangle| \leq \frac{1}{4}\|(P-P_f)\psi\|^2 + \frac{1}{4}\langle H_f\psi,\psi\rangle. \tag{25}$$

Moreover using (24) and

$$\|A^+\psi\|^2 \leq c_2\|\psi\|^2 + c_3\|H_f^{\frac{1}{2}}\psi\|^2 \,, \tag{26}$$

we arrive at

$$
\begin{aligned}
\alpha\langle (A^-)^2\psi,\psi\rangle &= \alpha\langle A^-\psi, A^+\psi\rangle \leq \epsilon\|A^-\psi\|^2 + \epsilon^{-1}\alpha^2\|A^+\psi\|^2 \\
& \leq \epsilon c_1\|H_f^{\frac{1}{2}}\psi\|^2 + \epsilon^{-1}\alpha^2(c_2\|\psi\|^2 + c_3\|H_f^{\frac{1}{2}}\psi\|^2)\,.
\end{aligned} \tag{27}
$$

Collecting the inequalities (22), (25) and (27) with $\epsilon < 1/(8c_1)$ and α small enough, completes the proof. □

Proof of Theorem 4.1: Let $\Phi := \Phi_1 + \Phi_2 := \chi(|P| < \frac{p_c}{2})\Phi + \chi(|P| \geq \frac{p_c}{2})\Phi$, where $P = i\nabla_x$ is the total momentum operator (due to the transformation (5)) and $p_c = \frac{1}{3}$ is a lower bound on the norm of the total momentum for which [6, Theorem 3.2] holds.

Since P commutes with the translation invariant operator $H + \frac{\alpha}{|x|}$, we have for all $\epsilon \in (0,1)$,

$$
\begin{aligned}
\langle H\Phi,\Phi\rangle &= \langle H\Phi_1,\Phi_1\rangle + \langle H\Phi_2,\Phi_2\rangle - 2\mathrm{Re}\,\langle \frac{\alpha}{|x|}\Phi_1,\Phi_2\rangle \\
&\geq \langle H\Phi_1,\Phi_1\rangle + \langle H\Phi_2,\Phi_2\rangle - \epsilon\langle \frac{\alpha}{|x|}\Phi_1,\Phi_1\rangle - \epsilon^{-1}\langle \frac{\alpha}{|x|}\Phi_2,\Phi_2\rangle.
\end{aligned} \tag{28}
$$

- First, we have the following estimate

$$
\begin{aligned}
& : (P - P_f - \sqrt{\alpha}A(0))^2 : + H_f \\
& = (P-P_f)^2 - 2\mathrm{Re}\,(P-P_f).\sqrt{\alpha}A(0) + \alpha : A(0)^2 : + H_f \\
& \geq (1-\sqrt{\alpha})(P-P_f)^2 + (\alpha - \sqrt{\alpha}) : A(0)^2 : + H_f - c_{\mathrm{n.o.}}\sqrt{\alpha} \\
& \geq (1-\sqrt{\alpha})(P-P_f)^2 + (1-\mathcal{O}(\sqrt{\alpha}))H_f - \mathcal{O}(\sqrt{\alpha})
\end{aligned}
$$

where in the last inequality we used (24) and (26). Therefore

$$\begin{aligned} &\langle (H - \epsilon^{-1}\frac{\alpha}{|x|})\Phi_2, \Phi_2\rangle \geq \langle (\frac{1-\sqrt{\alpha}}{2}(P-P_f)^2 - (1+\epsilon^{-1})\frac{\alpha}{|x|})\Phi_2, \Phi_2\rangle \\ &\quad + \Big\langle \left(\frac{1-\sqrt{\alpha}}{2}(P-P_f)^2 + (1-\mathcal{O}(\sqrt{\alpha}))H_f - \mathcal{O}(\sqrt{\alpha})\right)\Phi_2, \Phi_2 \Big\rangle \end{aligned} \tag{29}$$

The lowest eigenvalue of the Schrödinger operator $-(1-\mathcal{O}(\sqrt{\alpha}))\frac{\Delta}{2} - \frac{(1+\epsilon^{-1})\alpha}{|x|}$ is larger than $-c_\epsilon \alpha^2$. Thus, using (29) and denoting

$$L := \frac{1-\sqrt{\alpha}}{2}(P-P_f)^2 + (1-\mathcal{O}(\sqrt{\alpha}))H_f - \mathcal{O}(\sqrt{\alpha}) - c_\epsilon\alpha^2 \ ,$$

we get

$$\langle H\Phi_2, \Phi_2) - \epsilon^{-1}\langle \frac{\alpha}{|x|}\Phi_2, \Phi_2\rangle \geq (L\Phi_2, \Phi_2\rangle. \tag{30}$$

Now we have the following alternative: Either $|P_f| < \frac{p_c}{3}$, in which case we have $\langle L\Phi_2, \Phi_2\rangle \geq (\frac{p_c^2}{24} - \mathcal{O}(\sqrt{\alpha}))\|\Phi_2\|^2$, or $|P_f| \geq \frac{p_c}{3}$, in which case, using $\Phi_2 = \chi(|P| > \frac{p_c}{2})\Phi_2$ and $H_f \geq |P_f|$, we have $L \geq (\frac{p_c}{6} - \mathcal{O}(\sqrt{\alpha}))\|\Phi_2\|^2$. In both cases, this yields the bound

$$\langle L\Phi_2, \Phi_2\rangle \geq \frac{p_c^2}{48}\|\Phi_2\|^2 \geq (\Sigma_0 - e_0 + \frac{7}{8}(e_0 - e_1))\|\Phi_2\|^2 \tag{31}$$

since, for α small enough, the right hand side tends to zero, whereas p_c is a constant independent of α. Inequalities (30) and (31) yield

$$\langle H\Phi_2, \Phi_2\rangle - \epsilon^{-1}\langle \frac{\alpha}{|x|}\Phi_2, \Phi_2\rangle \geq (\Sigma_0 - e_0 + \frac{7}{8}(e_0 - e_1))\|\Phi_2\|^2. \tag{32}$$

• For $T(P)$ being the self-energy operator with fixed total momentum P defined in (7), we have from [6, Theorem3.2 (B)]

$$\left| \inf \sigma(T(P)) - \frac{P^2}{2} - \inf \sigma(T(0)) \right| \leq \frac{c_0 \alpha P^2}{2}.$$

Therefore

$$\langle T(P)\Phi_1, \Phi_1\rangle \geq (1 - o_\alpha(1))(P^2\Phi_1, \Phi_1\rangle + \Sigma_0\|\Phi_1\|^2. \tag{33}$$

If $\|\Phi_2\|^2 \geq 8\|\Phi_1\|^2$, using (33) yields

$$\begin{aligned} &\langle H\Phi_1, \Phi_1\rangle - \epsilon\langle \frac{\alpha}{|x|}\Phi_1, \Phi_1\rangle \\ &\geq (1 - o_\alpha(1))(P^2\Phi_1, \Phi_1\rangle - \langle (1+\epsilon)\frac{\alpha}{|x|}\Phi_1, \Phi_1\rangle + \Sigma_0\|\Phi_1\|^2 \\ &\geq (\Sigma_0 - (1 + \mathcal{O}(\alpha) + \mathcal{O}(\epsilon))e_0)\,\|\Phi_1\|^2. \end{aligned} \tag{34}$$

Therefore, together with $\|\Phi_2\|^2 \geq 8\|\Phi_1\|^2$ and (32), for α and ϵ small enough this implies

$$\langle H\Phi, \Phi\rangle \geq (\Sigma_0 - e_0)\|\Phi\|^2 + \frac{3}{4}(e_0 - e_1)\|\Phi\|^2. \tag{35}$$

If $\|\Phi_2\|^2 < 8\|\Phi_1\|^2$, we have, from (33)

$$\begin{aligned}&\langle H\Phi_1,\Phi_1\rangle - \epsilon\langle \frac{\alpha}{|x|}\Phi_1,\Phi_1\rangle\\ \geq&(1-o_\alpha(1))(P^2\Phi_1,\Phi_1\rangle - \langle(1+\epsilon)\frac{\alpha}{|x|}\Phi_1,\Phi_1\rangle + \Sigma_0\|\Phi_1\|^2\\ \geq&(1+o_\alpha(1)+\mathcal{O}(\epsilon))\Bigg(-e_0\sum_{k=0}^{\infty}\|\langle\Gamma^k\Phi_1,u_\alpha\rangle_{L^2(\mathbb{R}^3,\mathrm{d}x)}\|^2+e_1(\|\Phi_1\|^2\\ &-\sum_{k=0}^{\infty}\|\langle\Gamma^k\Phi_1,u_\alpha\rangle_{L^2(\mathbb{R}^3,\mathrm{d}x)}\|^2)\Bigg)+\Sigma_0\|\Phi_1\|^2.\end{aligned} \tag{36}$$

Now, by orthogonality of Φ and u_α in the sense that for all k, $\langle\Gamma^k\Phi,u_\alpha\rangle_{L^2(\mathbb{R}^3,\mathrm{d}x)}=0$, we get

$$\begin{aligned}\sum_{k=0}^{\infty}\|\langle u_\alpha,\Gamma^k\Phi_1\rangle\|^2=\sum_{k=0}^{\infty}\|\langle u_\alpha,\Gamma^k\Phi_2\rangle\|^2 &\leq \|\Phi_2\|^2\|u_\alpha\chi(|P|\geq\frac{p_c}{2})\|^2\\ &\leq 8\|\Phi_1\|^2\|u_\alpha\chi(|P|\geq\frac{p_c}{2})\|^2 \to_{\alpha\to0} 0\end{aligned} \tag{37}$$

Thus, for α and ϵ small enough, (36), (37) and (32) imply also (35) in that case.

- Let $\widetilde{c}=\max\{\delta,|c_0|\alpha^2\}$.

If $\langle H_f\Phi,\Phi\rangle < 8\widetilde{c}\|\Phi\|^2$, (16) follows from (35) with $\nu=\delta/(16\widetilde{c})$.

If $\langle H_f\Phi,\Phi\rangle \geq 8\widetilde{c}\|\Phi\|^2$, using Lemma 4.1, we obtain

$$\begin{aligned}\langle H\Phi,\Phi\rangle &\geq \frac12\langle H_f\Phi,\Phi\rangle - c_0\alpha^2\|g\|^2 \geq \frac14\langle H_f\Phi,\Phi\rangle+\widetilde{c}\|\Phi\|^2\\ &\geq \frac14\langle H_f\Phi,\Phi\rangle + \delta\|\Phi\|^2+(\Sigma_0-e_0)\|\Phi\|^2,\end{aligned} \tag{38}$$

since $\Sigma_0-e_0\leq 0$, which yields (16) with $\nu=\frac14$.

This concludes the proof of (16).

5. Estimate of the binding energy up to α^3 term

Definition 5.1. *Let u_α be the normalized ground state of*

$$h_\alpha := -\Delta - \frac{\alpha}{|x|}\ .$$

We define the projection $\Psi^{u_\alpha}\in\mathfrak{F}$ of the normalized ground state Ψ^{GS} of H, onto u_α as follows

$$\Psi^{GS}=u_\alpha\Psi^{u_\alpha}+\Psi^\perp,$$

where for all $k\geq 0$,

$$\langle u_\alpha,\Gamma^k\Psi^\perp\rangle_{L^2(\mathbb{R}^3,\mathrm{d}x)}=0. \tag{39}$$

Definition 5.2. *Let*

$$\begin{aligned}\Phi_*^2 &:= -(H_f+P_f^2)^{-1}A^+\cdot A^+\Omega_f\\ \Phi_*^3 &:= -(H_f+P_f^2)^{-1}P_f\cdot A^+\Phi_*^2\\ \Phi_*^1 &:= -(H_f+P_f^2)^{-1}P_f\cdot A^-\Phi_*^2\end{aligned}$$

where evidently, the state Φ_*^i contains i photons.

Definition 5.3. *On $\mathfrak{F}$, we define the positive bilinear form*

$$\langle v\,,\,w\,\rangle_{*}\;:=\;\langle\,v\,,\,(H_f+P_f^2)\,w\,\rangle, \tag{40}$$

and its associated semi-norm $\|v\|_{*}=\langle v,v\rangle_{*}^{1/2}$.

We will also use the same notation for this bilinear forms on $\mathfrak{F}_n$, $\mathfrak{H}$ and $\mathfrak{H}_n$.

Similarly, we define the bilinear form $\langle\,.\,,\,.\,\rangle_{\sharp}$ on $\mathfrak{H}$ as

$$\langle\,u\,,\,v\,\rangle_{\sharp}:=\langle\,u\,,\,(H_f+P_f^2+h_\alpha+e_0)\,v\,\rangle$$

and its associated semi-norm $\|v\|_{\sharp}=\langle v,v\rangle_{\sharp}^{1/2}$.

Definition 5.4. *Let*

$$\Phi_{*}^{u_\alpha}:=2\alpha^{\frac12}\nabla u_\alpha.(H_f+P_f^2)^{-1}A^{+}\Omega_f\ , \tag{41}$$

and

$$\Phi_{\sharp}^{u_\alpha}:=2\alpha^{\frac12}\nabla u_\alpha.(H_f+P_f^2+h_\alpha+e_0)^{-1}A^{+}\Omega_f\ . \tag{42}$$

Remark 5.1. *The function $\Phi_{*}^{u_\alpha}$ is not a vector in the Fock space $\mathfrak{H}$ because of the infrared singularity of the photon form factor. However, $H_f^{\gamma}\Phi_{*}^{u_\alpha}$ belongs to $\mathfrak{H}$, for any $\gamma>0$.*

Theorem 5.1 (A priori estimate on the binding energy)**.** *We have*

$$\Sigma\le\Sigma_0-e_0-\|\Phi_{\sharp}^{u_\alpha}\|_{\sharp}^2+\mathcal{O}(\alpha^4) \tag{43}$$

Proof. Using the trial function in $\mathfrak{H}$

$$\Phi^{\mathrm{trial}}:=u_\alpha(\Omega_f+2\alpha^{\frac32}\Phi_{*}^1+\alpha\Phi_{*}^2+2\alpha^{\frac32}\Phi_{*}^3)+\Phi_{\sharp}^{u_\alpha}\ ,$$

and from [4, Theorem 3.1],

$$\Sigma_0=-\alpha^2\|\Phi_{*}^2\|_{*}^2+\alpha^3(2\|A^{-}\Phi_{*}^2\|^2-4\|\Phi_{*}^1\|_{*}^2-4\|\Phi_{*}^3\|_{*}^2)+\mathcal{O}(\alpha^4)\ ,$$

the result follows straightforwardly. □

We decompose the function Ψ^{u_α} defined in Definition 5.1 as follows.

Definition 5.5. *Let*

$$\Psi^{u_\alpha}:=\Gamma^0\Psi^{u_\alpha}+2\eta_1\alpha^{\frac32}\Phi_{*}^1+\eta_2\alpha\Phi_{*}^2+2\eta_3\alpha^{\frac32}\Phi_{*}^3+\Delta_{*}^{u_\alpha},$$

where $\Gamma^0\Delta_{*}^{u_\alpha}=0$, $\langle\Phi_{*}^i,\Gamma^i\Delta_{*}^{u_\alpha}\rangle_{*}=0$ (i=1,2,3), and Φ_{*}^1, Φ_{*}^2, Φ_{*}^3 are given in Definition 5.2.

We further decompose $\Psi^{\perp}$ into two parts.

Definition 5.6. *Let*

$$\Psi^{\perp}=:\kappa_1\Phi_{\sharp}^{u_\alpha}+\Delta_{\sharp}^{\perp},$$

with $\langle\Phi_{\sharp}^{u_\alpha},\Gamma^1\Delta_{\sharp}^{\perp}\rangle_{\sharp}=0$.

To establish the estimate of the binding energy up to the α^3 term, we will compute $\langle H\Psi^{\mathrm{GS}},\Psi^{\mathrm{GS}}\rangle$ according to the decomposition of Ψ^{GS} introduced in Definitions 5.1 to 5.6. Using

$$H=(P^2-\frac{\alpha}{|x|})\;+\;T(0)\;-\;2\mathrm{Re}\,P\cdot(P_f+\sqrt{\alpha}A(0)),$$

and due to the orthogonality of u_α and $\Psi^{\perp}$, we obtain

$$\langle H\Psi^{\mathrm{GS}},\Psi^{\mathrm{GS}}\rangle=\langle Hu_\alpha\Psi^{u_\alpha},u_\alpha\Psi^{u_\alpha}\rangle+\langle H\Psi^{\perp},\Psi^{\perp}\rangle-4\mathrm{Re}\,\langle P.(P_f+\sqrt{\alpha}A(0))u_\alpha\Psi^{u_\alpha},\Psi^{\perp}\rangle. \tag{44}$$

We will estimate separately each term in (44).

5.1. Estimate of the term $\langle Hu_\alpha \Psi^{u_\alpha}, u_\alpha \Psi^{u_\alpha}\rangle$.

Lemma 5.1.

$$\begin{aligned}\langle Hu_\alpha \Psi^{u_\alpha}, u_\alpha \Psi^{u_\alpha}\rangle \geq & - e_0 \|\Psi^{u_\alpha}\|^2 - \alpha^2 \|\Phi_*^2\|_*^2 \|\Gamma^0 \Psi^{u_\alpha}\|^2 + \alpha^2 |\eta_2 - \Gamma^0 \Psi^{u_\alpha}|^2 \|\Phi_*^2\|_*^2 \\ & + \alpha^3 |\eta_2|^2 \left(2\|A^- \Phi_*^2\|^2 - 4\|\Phi_*^1\|_*^2 - 4\|\Phi_*^3\|_*^2\right) \\ & + 4\alpha^3 \left(|\eta_1 - \eta_2|^2 \|\Phi_*^1\|_*^2 + |\eta_3 - \eta_2|^2 \|\Phi_*^3\|_*^2\right) \\ & + c\alpha^4 \log \alpha^{-1} \left(|\eta_1|^2 + |\eta_2|^2 + |\eta_3|^2 + \|\Gamma^0 \Psi^{u_\alpha}\|^2\right) + \frac{1}{2}\|\Delta_*^{u_\alpha}\|_*^2.\end{aligned}$$

Proof. The proof is a trivial modification of the one given for the lower bound in [4, Theorem 3.1]. The only modification is that we have a slightly weaker estimate in Lemma 3.1 on the photon number for the ground state. This is accounted for by replacing the term of order α^4 in [4, Theorem 3.1] by a term of order $\alpha^4 \log \alpha^{-1}$. In addition, we need to use the equality $\langle P.(P_f + \sqrt{\alpha} A(0)) u_\alpha \Psi^{u_\alpha}, u_\alpha \Psi^{u_\alpha}\rangle = 0$, due to the symmetry of u_α. □

5.2. Estimates for the cross term $-4\mathrm{Re}\,\langle P.(P_f + \sqrt{\alpha} A(0)) u_\alpha \Psi^{u_\alpha}, \Psi^\perp\rangle$.

Lemma 5.2 ($-4\mathrm{Re}\,\langle P.P_f u_\alpha \Psi^{u_\alpha}, \Psi^\perp\rangle$ term)**.**

$$-4\mathrm{Re}\,\langle P.P_f u_\alpha \Psi^{u_\alpha}, \Psi^\perp\rangle \geq -c\alpha^4 (|\eta_1|^2 + |\eta_2|^2 + |\eta_3|^2) - \epsilon \|H_f^{\frac{1}{2}} \Delta_\sharp^\perp\|^2 - c\alpha \|H_f^{\frac{1}{2}} \Delta_*^{u_\alpha}\|^2.$$

Proof. • For $n = 1$ photon,

$$\langle P.P_f \Gamma^1 u_\alpha \Psi^{u_\alpha}, \Psi^\perp\rangle = \langle P.P_f (\eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \Gamma^1 \Delta_*^{u_\alpha}) u_\alpha, \kappa_1 \Phi_\sharp^{u_\alpha} + \Gamma^1 \Delta_\sharp^\perp\rangle. \tag{45}$$

Obviously

$$|\langle P.P_f (\eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \Gamma^1 \Delta_*^{u_\alpha}) u_\alpha, \Gamma^1 \Delta_\sharp^\perp\rangle| \leq \epsilon \|H_f^{\frac{1}{2}} \Gamma^1 \Delta_\sharp^\perp\|^2 + c\alpha^5 |\eta_1|^2 + c\alpha^2 \|H_f^{\frac{1}{2}} \Gamma^1 \Delta_*^{u_\alpha}\|^2. \tag{46}$$

Due to Lemma A.4 holds $\|H_f^{\frac{1}{2}} (\Phi_\sharp^{u_\alpha} - \Phi_*^{u_\alpha})\|^2 = \mathcal{O}(\alpha^5)$, which implies

$$\begin{aligned}&|\langle P.P_f (\eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \Gamma^1 \Delta_*^{u_\alpha}) u_\alpha, \kappa_1 \Phi_\sharp^{u_\alpha}\rangle| \leq |\kappa_1|^2 c\alpha^5 + c|\eta_1|^2 \alpha^5 + c\alpha^2 \|H_f^{\frac{1}{2}} \Gamma^1 \Delta_*^{u_\alpha}\|^2 \\ &+ |\langle P.P_f (\eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \Gamma^1 \Delta_*^{u_\alpha}) u_\alpha, \kappa_1 \Phi_*^{u_\alpha}\rangle|.\end{aligned} \tag{47}$$

For the last term on the right hand side of (47), due to the orthogonality of $\frac{\partial u_\alpha}{\partial x_i}$ and $\frac{\partial u_\alpha}{\partial x_j}$, $i \neq j$, and the equality $\|\frac{\partial u_\alpha}{\partial x_i}\| = \|\frac{\partial u_\alpha}{\partial x_j}\|$, holds

$$\begin{aligned}&|\langle P.P_f (\eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \Gamma^1 \Delta_*^{u_\alpha}) u_\alpha, \kappa_1 \Phi_*^{u_\alpha}\rangle| = \sum_{i=1}^3 \|\frac{\partial u_\alpha}{\partial x_i}\|^2 |\langle \eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \Gamma^1 \Delta_*^{u_\alpha}, \kappa_1 P_f^i (A^+ \Omega_f)^i\rangle| \\ &= c|\langle \eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \Gamma^1 \Delta_*^{u_\alpha}, \kappa_1 A^+.P_f \Omega_f\rangle| = 0.\end{aligned} \tag{48}$$

• For $n = 2$ photons,

$$\begin{aligned}|\langle P.P_f \Gamma^2 u_\alpha \Psi^{u_\alpha}, \Psi^\perp\rangle| &= |\langle P.P_f (\eta_2 \alpha \Phi_*^2 + \Gamma^2 \Delta_*^{u_\alpha}) u_\alpha, \Gamma^2 \Delta_\sharp^\perp\rangle| \\ &\leq c\alpha^4 |\eta_2|^2 + \epsilon \|H_f^{\frac{1}{2}} \Gamma^2 \Delta_\sharp^\perp\|^2 + \alpha \|H_f^{\frac{1}{2}} \Gamma^2 \Delta_*^{u_\alpha}\|^2.\end{aligned}$$

• For $n = 3$ photons, a similar estimate yields

$$|\langle P.P_f\Gamma^3 u_\alpha \Psi^{u_\alpha}, \Psi^\perp\rangle| = |\langle P.P_f(\eta_3\alpha^{\frac{3}{2}}\Phi_*^3 + \Gamma^3\Delta_*^{u_\alpha})u_\alpha, \Gamma^3\Delta_\sharp^\perp\rangle|$$
$$\leq c\alpha^4|\eta_3|^2 + \epsilon\|H_f^{\frac{1}{2}}\Gamma^3\Delta_\sharp^\perp\|^2 + \alpha\|H_f^{\frac{1}{2}}\Gamma^3\Delta_*^{u_\alpha}\|^2.$$

• For $n \geq 4$ photons,

$$|\langle P.P_f\Gamma^{n\geq 4}u_\alpha\Psi^{u_\alpha}, \Psi^\perp\rangle| \leq \epsilon\|H_f^{\frac{1}{2}}\Gamma^{n\geq 4}\Delta_\sharp^\perp\|^2 + \alpha\|H_f^{\frac{1}{2}}\Gamma^{n\geq 4}\Delta_*^{u_\alpha}\|^2.$$

□

Lemma 5.3 ($-4Re\langle\sqrt{\alpha}P.A(0)u_\alpha\Psi^{u_\alpha}, \Psi^\perp\rangle$ term)**.**

$$-4\mathrm{Re}\,\langle\sqrt{\alpha}P.A(0))u_\alpha\Psi^{u_\alpha}, \Psi^\perp\rangle \geq -2\mathrm{Re}\,\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha}\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 - \epsilon\|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 - \epsilon\alpha^2\|\Delta_\sharp^\perp\|^2$$
$$-c\alpha\|H_f^{\frac{1}{2}}\Delta_*^{u_\alpha}\|^2 - c\alpha^4(|\eta_1|^2 + |\eta_2|^2 + |\eta_3|^2 + |\kappa_1|^2) + \mathcal{O}(\alpha^5\log\alpha^{-1}).$$

Proof. We first estimate the term

$$\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+u_\alpha\Psi^{u_\alpha}, \Psi^\perp\rangle = \alpha\mathrm{Re}\sum_{n=0}^{\infty}\langle P.A^+u_\alpha\Gamma^n\Psi^{u_\alpha}, \Gamma^{n+1}\Psi^\perp\rangle.$$

• For $n = 0$ photon, using the orthogonality $\langle\Phi_\sharp^{u_\alpha}, \Gamma^1\Delta_\sharp^\perp\rangle_\sharp = 0$, yields

(49)

$$-\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+\Gamma^0u_\alpha\Psi^{u_\alpha}, \kappa_1\Phi_\sharp^{u_\alpha} + \Gamma^1\Delta_\sharp^\perp\rangle = -\frac{1}{2}\mathrm{Re}\,\left((\Gamma^0\Psi^{u_\alpha})\langle\Phi_\sharp^{u_\alpha}, \kappa_1\Phi_\sharp^{u_\alpha} + \Gamma^1\Delta_\sharp^\perp\rangle_\sharp\right)$$
$$= -\frac{1}{2}\mathrm{Re}\,\left(\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha}\langle\Phi_\sharp^{u_\alpha}, \Phi_\sharp^{u_\alpha}\rangle_\sharp\right)\ .$$

• For $n \geq 1$ photons,

(50)
$$|\sum_{n\geq 2}\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+\Gamma^n u_\alpha\Delta_*^{u_\alpha}, \Gamma^{n+1}\Delta_\sharp^\perp\rangle| \leq c\alpha^3\|\Delta_*^{u_\alpha}\|^2 + \epsilon\|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2$$
$$\leq \epsilon\|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 + c\alpha^5(|\eta_1|^2 + |\eta_2|^2 + |\eta_3|^2) + \mathcal{O}(\alpha^5\log\alpha^{-1}),$$

where we used from Lemma 3.1 that $\|\Delta_*^{u_\alpha}\|^2 \leq \mathcal{O}(\alpha^2\log\alpha^{-1}) + c\alpha^3(|\eta_1|^2 + |\eta_3|^2) + c\alpha^2|\eta_2|^2$. We also have

(51)
$$|\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P(2\eta_1\alpha^{\frac{3}{2}}\Phi_*^1 + \eta_2\alpha\Phi_*^2 + 2\eta_3\alpha^{\frac{3}{2}}\Phi_*^3)u_\alpha, A^-\Delta_\sharp^\perp\rangle|$$
$$\leq \epsilon\|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 + c(\alpha^6|\eta_1|^2 + \alpha^5|\eta_2|^2 + \alpha^6|\eta_3|^2).$$

We next estimate the term $2\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^-u_\alpha\Psi^{u_\alpha}, \Psi^\perp\rangle$. We first get

(52)
$$|\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P.A^-\Delta_*^{u_\alpha}u_\alpha, \Delta_\sharp^\perp\rangle| \leq \epsilon\alpha^2\|\Delta_\sharp^\perp\|^2 + c\alpha\|H_f^{\frac{1}{2}}\Delta_*^{u_\alpha}\|^2.$$

Then we write

(53)
$$|\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle(2\eta_1\alpha^{\frac{3}{2}}A^-\Phi_*^1 + 2\eta_3\alpha^{\frac{3}{2}}A^-\Phi_*^3)\nabla u_\alpha, \Delta_\sharp^\perp\rangle| \leq \epsilon\alpha^2\|\Delta_\sharp^\perp\|^2 + c\alpha^4(|\eta_1|^2 + |\eta_3|^2).$$

We also have

(54)
$$|\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle\eta_2\alpha A^-\Phi_*^2.\nabla u_\alpha, \kappa_1\Phi_\sharp^{u_\alpha}\rangle|$$
$$= |\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle\eta_2\alpha H_f^{-\frac{1}{2}}A^-\Phi_*^2.\nabla u_\alpha, H_f^{\frac{1}{2}}\kappa_1\Phi_\sharp^{u_\alpha}\rangle| \leq c\alpha^4(|\eta_2|^2 + |\kappa_1|^2),$$

since $H_f^{-\frac{1}{2}}A^-\Phi_*^2 \in L^2(\mathbb{R}^3)$ and $\|H_f^{\frac{1}{2}}\Phi_\sharp^{u_\alpha}\| = \mathcal{O}(\alpha^{\frac{3}{2}})$. Finally we get

$$
\begin{aligned}
&|\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle \eta_2\alpha A^-\Phi_*^2.\nabla u_\alpha, \Gamma^1\Delta_\sharp^\perp\rangle| \\
&= |\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle \eta_2\alpha H_f^{-\frac{1}{2}}A^-\Phi_*^2.\nabla u_\alpha, H_f^{\frac{1}{2}}\Gamma^1\Delta_\sharp^\perp\rangle| \leq \epsilon\|H_f^{\frac{1}{2}}\Gamma^1\Delta_\sharp^\perp\|^2 + c\alpha^5|\eta_2|^2.
\end{aligned}
\tag{55}
$$

Collecting (49) to (55) concludes the proof. □

5.3. **Estimate for the term $\langle H\Psi^\perp, \Psi^\perp\rangle$.**

Lemma 5.4.

$$
\langle H\Psi^\perp, \Psi^\perp\rangle \geq (\Sigma_0 - e_0)\|\Delta_\sharp^\perp\|^2 - c\alpha^4|\kappa_1|^2 + \frac{1}{2}M[\Delta_\sharp^\perp] + |\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2,
\tag{56}
$$

where $M[\ .\ ]$ is defined in Corollary 4.2

Proof. Recall that

$$
\begin{aligned}
H &= (P^2 - \frac{\alpha}{|x|}) + (H_f + P_f^2) - 2\mathrm{Re}\ (P.P_f) \\
&- 2\sqrt{\alpha}(P - P_f).A(0) + 2\alpha A^+.A^- + 2\alpha\mathrm{Re}\,(A^-)^2\ .
\end{aligned}
$$

Due to the orthogonality $\langle \Phi_\sharp^{u_\alpha}, \Delta_\sharp^\perp\rangle_\sharp = 0$ we get

$$
\begin{aligned}
&\langle H\Psi^\perp, \Psi^\perp\rangle \\
&= \langle Hr, r\rangle + |\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 - e_0|\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|^2 - e_0\kappa_1\langle\Delta_\sharp^\perp, \Phi_\sharp^{u_\alpha}\rangle + 2\alpha|\kappa_1|^2\|A^-\Phi_\sharp^{u_\alpha}\|^2 \\
&- 2\mathrm{Re}\,\langle P.P_f\Phi_\sharp^{u_\alpha}, \Phi_\sharp^{u_\alpha}\rangle + 2\alpha\mathrm{Re}\,\langle A^-.A^-\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle - 4\sqrt{\alpha}\mathrm{Re}\,\langle P.A^-\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle \\
&- 4\sqrt{\alpha}\mathrm{Re}\,\langle P.A^+\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle + 4\mathrm{Re}\,\sqrt{\alpha}\langle P_f.A(0)\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle + 4\alpha\mathrm{Re}\,\langle A^+.A^-\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle \\
&- 4\mathrm{Re}\,\langle P.P_f\Phi_\sharp^{u_\alpha}, \Delta_\sharp^\perp\rangle.
\end{aligned}
\tag{57}
$$

For the first term on the right hand side of (57), we have, from Corollary 4.2

$$
\langle H\Delta_\sharp^\perp, \Delta_\sharp^\perp\rangle \geq (\Sigma_0 - e_0)\|\Delta_\sharp^\perp\|^2 + M[\Delta_\sharp^\perp].
\tag{58}
$$

According to Lemma A.3, we obtain

$$
-e_0\kappa_1\langle\Delta_\sharp^\perp, \Phi_\sharp^{u_\alpha}\rangle - e_0|\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|^2 \geq -\epsilon\alpha^2\|\Delta_\sharp^\perp\|^2 - c|\kappa_1|^2\alpha^5\log\alpha^{-1}.
\tag{59}
$$

The next term, namely $2\alpha|\kappa_1|^2\|A^-\Phi_\sharp^{u_\alpha}\|^2$, is positive.

Due to the symmetry in x-variable,

$$
\langle P.P_f\Phi_\sharp^{u_\alpha}, \Phi_\sharp^{u_\alpha}\rangle = 0.
\tag{60}
$$

The term $2\alpha\mathrm{Re}\,\langle A^-.A^-\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle$ is estimated as

$$
2\alpha\mathrm{Re}\,\langle A^-.A^-\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle \geq -c\alpha^2\|\kappa_1\Phi_\sharp^{u_\alpha}\|^2 - \frac{1}{4}\nu\|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 = -\frac{1}{4}\nu\|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 - c|\kappa_1|^2\alpha^5\log\alpha^{-1}.
\tag{61}
$$

Due to Lemma A.3 and [11, Lemma A4],

$$
|\alpha^{\frac{1}{2}}\langle A^-\Delta_\sharp^\perp, P\kappa_1\Phi_\sharp^{u_\alpha}\rangle| \leq \frac{\nu}{8}\|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 + c|\kappa_1|^2\alpha^6\log\alpha^{-1}.
\tag{62}
$$

The next term we have to estimate fulfils

$$
|\alpha^{\frac{1}{2}}\langle P.A^+\Delta_\sharp^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle| \leq \epsilon\|P\Gamma^0\Delta_\sharp^\perp\|^2 + c\alpha|\kappa_1|^2\|A^-\Phi_\sharp^{u_\alpha}\|^2 \leq \epsilon\|(P-P_f)\Delta_\sharp^\perp\|^2 - c|\kappa_1|^2\alpha^4.
\tag{63}
$$

We have

(64)

$$\mathrm{Re}\,\sqrt{\alpha}\langle P_f.A(0)\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle=\mathrm{Re}\,\sqrt{\alpha}\langle P_f.A^-\Gamma^2\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle+\mathrm{Re}\,\sqrt{\alpha}\langle P_f.A^+\Gamma^0\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle$$
$$=\mathrm{Re}\,\sqrt{\alpha}\langle P_f.A^-\Gamma^2\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle+\mathrm{Re}\,\sqrt{\alpha}\langle A^+.P_f\Gamma^0\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle$$

Obviously, $\langle A^+.P_f\Gamma^0\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle=0$, and the first term is bounded by

$$\begin{aligned}|\mathrm{Re}\,\sqrt{\alpha}\langle P_f.A^-\Gamma^2\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle|&\le\epsilon\|H_f^{\frac12}\Gamma^2\Delta_\sharp^\perp\|^2+c\alpha|\kappa_1|^2\|P_f\Phi_\sharp^{u_\alpha}\|^2\\&\le\epsilon\|H_f^{\frac12}\Gamma^2\Delta_\sharp^\perp\|^2+c|\kappa_1|^2\alpha^4.\end{aligned}\tag{65}$$

For the term $\alpha\mathrm{Re}\,\langle A^+.A^-\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle$ we obtain

(66)

$$\alpha\mathrm{Re}\,\langle A^+.A^-\Delta_\sharp^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle\ge-c\alpha^2\|H_f^{\frac12}\kappa_1\Phi_\sharp^{u_\alpha}\|^2|\kappa_1|^2-\epsilon\|H_f^{\frac12}\Delta_\sharp^\perp\|^2=-c\alpha^5|\kappa_1|^2-\epsilon\|H_f^{\frac12}\Delta_\sharp^\perp\|^2.$$

According to (214) of Lemma A.3, the last term we have to estimate fulfils

(67)

$$\mathrm{Re}\,\langle P.P_f\kappa_1\Phi_\sharp^{u_\alpha},\Delta_\sharp^\perp\rangle\le\epsilon\|H_f^{\frac12}\Gamma^1\Delta_\sharp^\perp\|^2+c\|P|P_f|^{\frac12}\kappa_1\Phi_\sharp^{u_\alpha}\|^2\le\epsilon\|H_f^{\frac12}\Gamma^1\Delta_\sharp^\perp\|^2+c\alpha^5|\kappa_1|^2.$$

Collecting the estimates (57) to (67) yields (56). □

5.4. **Upper bound on the binding energy up to the order α^3.**

Theorem 5.2. *1) Let $\Sigma=\inf\sigma(H)$. Then*

$$\Sigma=\Sigma_0-e_0-\|\Phi_*^{u_\alpha}\|_*^2+\mathcal{O}(\alpha^4),\tag{68}$$

$$\Sigma_0=-\alpha^2\|\Phi_*^2\|_*^2+\alpha^3(2\|A^-\Phi_*^2\|^2-4\|\Phi_*^1\|_*^2-4\|\Phi_*^3\|_*^2)+\mathcal{O}(\alpha^4),$$

and $\Phi_*^{u_\alpha}$ defined by (41).

2) For the components $\Delta_\sharp^\perp$, Ψ^{u_α}, $\Delta_*^{u_\alpha}$ of the ground state Ψ^{GS}, and the coefficients η_1, η_2, η_3 and κ_1 defined in Definitions 5.1-5.5, holds

$$\|\Delta_\sharp^\perp\|^2=\mathcal{O}(\alpha^{\frac{33}{16}}),\ \|H_f^{\frac12}\Delta_\sharp^\perp\|^2=\mathcal{O}(\alpha^4),\ \|(P-P_f)\Delta_\sharp^\perp\|^2=\mathcal{O}(\alpha^4),\tag{69}$$

$$\|\Psi^{u_\alpha}\|^2\ge1-c\alpha^2,\ \|\Gamma^0\Psi^{u_\alpha}\|^2\ge1-c\alpha^2,\tag{70}$$

$$\|\Delta_*^{u_\alpha}\|_*^2=\mathcal{O}(\alpha^4),\ \|\Delta_*^{u_\alpha}\|^2=\mathcal{O}(\alpha^{\frac{33}{16}}),\tag{71}$$

$$|\eta_{1,3}-1|^2\le c\alpha,\ |\eta_2-1|^2\le c\alpha^2,\ |\kappa_1-1|^2\le c\alpha\ .\tag{72}$$

Proof. • *Step 1:* We first show that (68) holds with an error estimate of the order $\alpha^4\log\alpha^{-1}$.

Collecting Lemmata 5.1, 5.2, 5.3 and Lemma 5.4 yields

(73)

$$\begin{aligned}&\langle H\Psi^{\mathrm{GS}},\Psi^{\mathrm{GS}}\rangle\\&\ge-e_0\|\Psi^{u_\alpha}\|^2-\alpha^2\|\Phi_*^2\|_*^2|\Gamma^0\Psi^{u_\alpha}|^2+\alpha^3|\eta_2|^2(2\|A^-\Phi_*^2\|^2-4\|\Phi_*^1\|_*^2-4\|\Phi_*^3\|_*^2)\\&+\alpha^2|\eta_2-\Gamma^0\Psi^{u_\alpha}|^2\|\Phi_*^2\|_*^2+4\alpha^3(|\eta_1-\eta_2|^2\|\Phi_*^1\|_*^2+|\eta_3-\eta_2|^2\|\Phi_*^3\|_*^2)\\&-c\alpha^4\log\alpha^{-1}(|\eta_1|^2+|\eta_2|^2+|\eta_3|^2+\|\Gamma^0\Psi^{u_\alpha}\|^2)+\frac14\|\Delta_*^{u_\alpha}\|_*^2\\&+|\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+(\Sigma_0-e_0)\|\Delta_\sharp^\perp\|^2+\frac14M[\Delta_\sharp^\perp]-c\alpha^4|\kappa_1|^2\\&-2\mathrm{Re}\,(\kappa_1\Gamma^0\Psi^{u_\alpha})\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+\mathcal{O}(\alpha^5\log\alpha^{-1}).\end{aligned}$$

We first estimate

$$
\begin{aligned}
&|\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 - 2\mathrm{Re}\,(\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha})\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 - c\alpha^4|\kappa_1|^2 \\
&\geq -\|\Phi_\sharp^{u_\alpha}\|_\sharp^2|\Gamma^0\Psi^{u_\alpha}|^2 + \frac{|\overline{\kappa_1} - \Gamma^0\Psi^{u_\alpha}|^2}{2}\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 + \mathcal{O}(\alpha^4).
\end{aligned}
\tag{74}
$$

Moreover, since $|\Gamma^0\Psi^{u_\alpha}| \leq 1$, we replace in (73) $-\alpha^2\|\Phi_*^2\|_*^2|\Gamma^0\Psi^{u_\alpha}|^2$ by $-\alpha^2\|\Phi_*^2\|_*^2$ and in (74) $-\|\Phi_\sharp^{u_\alpha}\|_\sharp^2|\Gamma^0\Psi^{u_\alpha}|^2$ by $-\|\Phi_\sharp^{u_\alpha}\|_\sharp^2$. In addition, using the inequalities

$$
|\eta_2-\eta_j|^2 \geq \frac{1}{2}|\eta_j-\Gamma^0\Psi^{u_\alpha}|^2 - |\eta_2-\Gamma^0\Psi^{u_\alpha}|^2 \quad \text{and} \quad |\eta_j|^2 \leq 2|\eta_j-\Gamma^0\Psi^{u_\alpha}|^2+2 \tag{75}
$$

for $j = 1, 2, 3$ yields that for some $c > 0$,

$$
\begin{aligned}
&\langle H\Psi^{\mathrm{GS}}, \Psi^{\mathrm{GS}}\rangle \\
&\geq -e_0\|\Psi^{u_\alpha}\|^2 - \alpha^2\|\Phi_*^2\|_*^2 + \alpha^3|\eta_2|^2(2\|A^-\Phi_*^2\|^2 - 4\|\Phi_*^1\|_*^2 - 4\|\Phi_*^3\|_*^2) - \|\Phi_\sharp^{u_\alpha}\|_\sharp^2 \\
&+ c\alpha^2|\eta_2 - \Gamma^0\Psi^{u_\alpha}|^2\|\Phi_*^2\|_*^2 + c\alpha^3(|\eta_1 - \Gamma^0\Psi^{u_\alpha}|^2 + |\eta_3 - \Gamma^0\Psi^{u_\alpha}|^2) + c\alpha^3|\kappa_1 - \Gamma^0\Psi^{u_\alpha}|^2 \\
&+ \frac{1}{4}\|\Delta_*^{u_\alpha}\|_*^2 + (\Sigma_0 - e_0)\|\Delta_\sharp^\perp\|^2 + \frac{1}{4}M[\Delta_\sharp^\perp] + \mathcal{O}(\alpha^4\log\alpha^{-1}).
\end{aligned}
\tag{76}
$$

Comparing this expression with (43) of Theorem 5.1 gives

$$
\Sigma = \Sigma_0 - e_0 - \|\Phi_\sharp^{u_\alpha}\|_\sharp^2 + \mathcal{O}(\alpha^4\log\alpha^{-1}). \tag{77}
$$

Finally, by Lemma A.4, we can replace $\|\Phi_\sharp^{u_\alpha}\|_\sharp$ by $\|\Phi_*^{u_\alpha}\|_*$ in (77).

• *Step 2:* We now show that the error term does not contain any $\log\alpha^{-1}$ term, by deriving improved estimates on the photon number for $\Delta_\sharp^\perp$ and $\Delta_*^{u_\alpha}$.

From (76) we obtain

$$
\|\Delta_*^{u_\alpha}\|_*^2 = \mathcal{O}(\alpha^4\log\alpha^{-1}) \quad \text{and} \quad \|H_f^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 = \mathcal{O}(\alpha^4\log\alpha^{-1}). \tag{78}
$$

This last two relations enable us to improve the estimates on the expected photon number as follows

$$
\|N^{\frac{1}{2}}\Delta_*^{u_\alpha}\|^2 = \mathcal{O}(\alpha^{\frac{33}{16}}) \tag{79}
$$

$$
\|N^{\frac{1}{2}}\Delta_\sharp^\perp\|^2 = \mathcal{O}(\alpha^{\frac{33}{16}}) \tag{80}
$$

To see this, we note that from Definition 5.1, we have

$$
\|a_\lambda(k)\Psi^{u_\alpha}\|^2 \leq \|a_\lambda(k)\Psi^{\mathrm{GS}}\|^2 \leq \frac{c\alpha^{-\frac{3}{2}}\chi_\Lambda(|k|)}{|k|},
$$

where in the last inequality, we used (14). Taking into account that

$$
\Delta_*^{u_\alpha} = \Psi^{u_\alpha} - 2\alpha^{\frac{3}{2}}\Phi_*^1 - \alpha\Phi_*^2 - 2\alpha^{\frac{3}{2}}\Phi_*^3,
$$

where

$$
\|a_\lambda(k)\Phi_*^1\|^2 \leq \frac{c\chi_\Lambda(|k|)}{|k|}\ ,\ \|a_\lambda(k)\Phi_*^2\|^2 \leq \frac{c\chi_\Lambda(|k|)(1 + |\log|k|\,|)}{|k|}
$$

$$
\|a_\lambda(k)\Phi_*^3\|^2 \leq \frac{c\chi_\Lambda(|k|)}{|k|}\,,
$$

we arrive at

$$
\|a_\lambda(k)\Delta_*^{u_\alpha}\|^2 \leq \frac{c\alpha^{-\frac{3}{2}}\chi_\Lambda(|k|)(1 + |\log|k|\,|)}{|k|}.
$$

For the expected photon number of $\Delta_*^{u_\alpha}$ thus holds

$$\begin{aligned}\|N^{\frac{1}{2}}\Delta_*^{u_\alpha}\|^2 &= \sum_\lambda \int \|a_\lambda(k)\Delta_*^{u_\alpha}\|^2 \mathrm{d}k \\ &\leq \sum_\lambda \int_{|k|\leq\alpha^{\frac{15}{8}}} \frac{c\alpha^{-\frac{3}{2}}(1+|\log|k||)}{|k|}\mathrm{d}k + \int_{|k|>\alpha^{\frac{15}{8}}} |k|^{-1}\,|k|\,\|a_\lambda(k)\Delta_*^{u_\alpha}\|^2\mathrm{d}k \\ &\leq c\alpha^{\frac{17}{8}} + c\alpha^{-\frac{15}{8}}\|H_f^{\frac{1}{2}}\Delta_*^{u_\alpha}\|^2 \leq c\alpha^{\frac{33}{16}}.\end{aligned}$$

The relation (80) can be proved similarly using

$$\|a_\lambda(k)\Phi_\sharp^{u_\alpha}\|^2 \leq c\frac{\alpha^{-1}}{|k|}\ .$$

We are now in position to finish the proof of Theorem 5.2. First we see that according to (79) and (80), we have

$$\|N^{\frac{1}{2}}\Psi^{u_\alpha}\|^2 = \mathcal{O}(\alpha^2),$$

which implies that in Lemma 5.1 we can replace the term $c\alpha^4\log\alpha^{-1}(|\eta_1|^2+|\eta_2|^2+|\eta_3|^2+|\Gamma^0\Psi^{u_\alpha}|^2)$ with $c\alpha^4(|\eta_1|^2+|\eta_2|^2+|\eta_3|^2+|\Gamma^0\Psi^{u_\alpha}|^2)$ and consequently in (76) and (77), the term $\mathcal{O}(\alpha^4\log\alpha^{-1})$ can be replaced by $\mathcal{O}(\alpha^4)$. This proves (68). The estimates (69)-(72) follow from (68) and (76) with $\mathcal{O}(\alpha^4\log\alpha^{-1})$ replaced with $\mathcal{O}(\alpha^4)$. □

6. Estimate of the binding energy up to $\alpha^5\log\alpha^{-1}$ term

Theorem 6.1 (Upper bound up to the order $\alpha^5\log\alpha^{-1}$ for the binding energy)**.** *For α small enough, we have*

$$\Sigma_0 - \Sigma \geq \frac{1}{4}\alpha^2 + e^{(1)}\alpha^3 + e^{(2)}\alpha^4 + e^{(3)}\alpha^5\log\alpha^{-1} + o(\alpha^5\log\alpha^{-1}), \tag{81}$$

where $e^{(1)}$, $e^{(2)}$ and $e^{(3)}$ are defined in Theorem 2.1.

Definition 6.1. *1) Pick*

$$\kappa_2 = \begin{cases} \alpha^{-1}\frac{\langle\Psi^\perp,\Phi_*^2\Gamma^0\Psi^\perp\rangle_\sharp}{\langle\Phi_*^2\Gamma^0\Psi^\perp,\Phi_*^2\Gamma^0\Psi^\perp\rangle_\sharp} & \textit{if } \|\Gamma^0\Psi^\perp\| > \alpha^{\frac{3}{2}}, \\ 0 & \textit{if } \|\Gamma^0\Psi^\perp\| \leq \alpha^{\frac{3}{2}}\ . \end{cases}$$

2) We split $\Psi^\perp$ into $\Psi_1^\perp$ and $\Psi_2^\perp$ as follows: $\forall n\geq 0$, $\Gamma^n\Psi^\perp = \Gamma^n\Psi_1^\perp + \Gamma^n\Psi_2^\perp$ and for $n=0$,

$$\Gamma^0\Psi_1^\perp = \Gamma^0\Psi^\perp \quad \textit{and} \quad \Gamma^0\Psi_2^\perp = 0,$$

for $n=1$,

$$\Gamma^1\Psi_1^\perp = \kappa_1\Phi_\sharp^{u_\alpha} \quad \textit{and} \quad \langle\Gamma^1\Psi_2^\perp,\Phi_\sharp^{u_\alpha}\rangle_\sharp = 0,$$

for $n=2$,

$$\begin{aligned}\Gamma^2\Psi_1^\perp &= \alpha\kappa_2\Phi_*^2\Gamma^0\Psi_1^\perp + \sum_{i=1}^3 \alpha\kappa_{2,i}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}, \\ &\quad \textit{with } W_i = P_f^i\Phi_*^2 - 2A^+.P_f(H_f+P_f^2)^{-1}(A^+)^i\Omega_f, \\ \Gamma^2\Psi_2^\perp &= \Gamma^2\Psi^\perp - \Gamma^2\Psi_1^\perp,\ \textit{with } \langle\Gamma^2\Psi_2^\perp,(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\rangle_\sharp = 0\ (i=1,2,3), \\ &\quad \textit{and } \langle\Gamma^2\Psi_2^\perp,\Phi_*^2\Gamma^0\Psi_1^\perp\rangle_\sharp = 0,\end{aligned}$$

for $n=3$,

$$\begin{aligned}
&\Gamma^3\Psi_1^\perp = \alpha\kappa_3(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha},\\
&\Gamma^3\Psi_2^\perp = \Gamma^3\Psi^\perp - \Gamma^3\Psi_1^\perp,\ \langle\Gamma^3\Psi_2^\perp,(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\rangle_\sharp = 0,
\end{aligned}$$

and for $n\geq 4$,

$$\Gamma^n\Psi_1^\perp = 0 \quad \textit{and} \quad \Gamma^n\Psi_2^\perp = \Gamma^n\Psi^\perp.$$

Lemma 6.1. *The following a priori estimates hold*

$$\begin{aligned}
&\kappa_1 = 1+\mathcal{O}(\alpha^{\frac12}),\\
&|\kappa_2|\,\|\Gamma^0\Psi_1^\perp\| = \mathcal{O}(\alpha),\\
&\kappa_{2,i} = \mathcal{O}(1),\ (i=1,2,3),\\
&\|\Gamma^0\Psi_1^\perp\| = \mathcal{O}(\alpha),\\
&\|P\Gamma^0\Psi_1^\perp\| = \mathcal{O}(\alpha^2).
\end{aligned}$$

Proof. To derive these estimates, we use Theorem 5.2.

The first equality is a consequence of (72).

To derive the next two estimates, we first notice that (69) yields

$$\begin{aligned}
\|P\Gamma^2\Delta_\sharp^\perp\|^2 &\leq 2\|(P-P_f)\Delta_\sharp^\perp\|^2 + 2\|P_f\Gamma^2\Delta_\sharp^\perp\|^2\\
&\leq 2\|(P-P_f)\Delta_\sharp^\perp\|^2 + 2c\|H_f^{\frac12}\Gamma^2\Delta_\sharp^\perp\|^2 = \mathcal{O}(\alpha^4),
\end{aligned}$$

therefore, using again (69), we obtain

$$\|(h_\alpha+e_0)^{\frac12}\Gamma^2\Delta_\sharp^\perp\|^2 \leq \|P\Gamma^2\Delta_\sharp^\perp\|^2 + e_0\|\Gamma^2\Delta_\sharp^\perp\|^2 = \mathcal{O}(\alpha^4),$$

and thus, using from (69) that $\|H_f^{\frac12}\Gamma^2\Delta_\sharp^\perp\|^2 = \mathcal{O}(\alpha^4)$, we get

$$\|\Gamma^2\Delta_\sharp^\perp\|_\sharp^2 = \|\Gamma^2\Psi^\perp\|_\sharp^2 = \mathcal{O}(\alpha^4). \tag{82}$$

We then write, using (82) and the $\langle\,\cdot\,,\,\cdot\,\rangle_\sharp$-orthogonality of $\Gamma^2\Psi_1^\perp$ and $\Gamma^2\Psi_2^\perp$,

$$\|\Gamma^2\Psi_1^\perp\|_\sharp^2 \leq \|\Gamma^2\Psi^\perp\|_\sharp^2 = \mathcal{O}(\alpha^4). \tag{83}$$

Since $\|\Gamma^2\Psi_1^\perp\|_\sharp \leq \|\Gamma^2\Psi_1^\perp\|_*$, and using (206) of Lemma A.1, we obtain

$$\begin{aligned}
\mathcal{O}(\alpha^4) &= \|\Gamma^2\Psi_1^\perp\|_*^2 = \|\alpha\kappa_2\Phi_*^2\Gamma^0\Psi_1^\perp\|_*^2 + \|\alpha\sum_i\kappa_{2,i}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\|_*^2\\
&= \alpha^2\|\Phi_*^2\|_*^2|\kappa_2|^2\|\Gamma^0\Psi_1^\perp\|^2 + \frac{\alpha^2}{3}\|\nabla u_\alpha\|^2\sum_i|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2.
\end{aligned} \tag{84}$$

which gives

$$\kappa_{2,i} = \mathcal{O}(1) \quad \text{and} \quad |\kappa_2|\,\|\Gamma^0\Psi_1^\perp\| = \mathcal{O}(\alpha).$$

The last two estimates are consequences of (69). □

To derive the lower bound on the quadratic form of $\langle H(u_\alpha\Psi^{u_\alpha}+g), u_\alpha\Psi^{u_\alpha}+\Psi^\perp\rangle$, we will follow the same strategy as in Section 5, the only difference being that now we have better a priori estimates on Ψ^{u_α} and $\Psi^\perp$.

Proposition 6.1. *We have*

$$
\begin{aligned}
&2\mathrm{Re}\,\langle H\Psi^\perp, u_\alpha\Psi^{u_\alpha}\rangle \geq -\frac{1}{3}\alpha^4\mathrm{Re}\sum_{i=1}^{3}\overline{\kappa_{2,i}}\langle (H_f+P_f^2)^{-1}P_f^i\Phi_*^2, W_i\rangle\\
&-4\alpha\mathrm{Re}\,\langle\nabla u_\alpha.P_f\Phi_*^2,\Gamma^2\Psi_2^\perp\rangle - 2\mathrm{Re}\,\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha}\|\Phi_\sharp^{u_\alpha}\|_\sharp^2\\
&-\frac{2}{3}\alpha^4\mathrm{Re}\sum_{i=1}^{3}\langle\,(H_f+P_f^2)^{-\frac12}(A^-)^i\Phi_*^2,(H_f+P_f^2)^{-\frac12}(A^+)^i\Omega_f\rangle\\
&-\epsilon\alpha^2\|(\Psi_1^\perp)^a\|^2-\frac{5}{8}M[\Psi_2^\perp]-\epsilon\alpha^5\log\alpha^{-1}-\epsilon\alpha^5|\kappa_3|^2-|\kappa_1-1|c\alpha^4+\mathcal{O}(\alpha^5).
\end{aligned}
\tag{85}
$$

The proof of this Proposition is detailed in Subsection 6.2

Proposition 6.2.

$$
\begin{aligned}
&\langle H\Psi^\perp,\Psi^\perp\rangle \geq (\Sigma_0-e_0)\|\Psi^\perp\|^2-4\alpha\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp PA^-\Phi_*^{u_\alpha}\|^2\\
&+|\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+2\alpha\|A^-\Phi_*^{u_\alpha}\|^2+\frac{\alpha^4}{12}\sum_{i=1}^{3}|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2\\
&+\frac{2}{3}\alpha^4\mathrm{Re}\sum_{i=1}^{3}\kappa_{2,i}\langle P_f.A^-(H_f+P_f^2)^{-1}W_i,(H_f+P_f^2)^{-1}(A^+)^i\Omega_f\rangle\\
&+4\alpha^{\frac12}\mathrm{Re}\,\langle\Gamma^2\Psi_2^\perp,A^+.P_f\Phi_*^{u_\alpha}\rangle+M_1[\Psi^\perp],
\end{aligned}
\tag{86}
$$

where

$$
\begin{aligned}
M_1[\Psi^\perp] =&(1-c_0\alpha)\|(h_\alpha+e_0)^{\frac12}\Gamma^0(\Psi_1^\perp)^a\|^2+\frac{|\kappa_3+1|^2}{2}\alpha^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2\\
&-|\kappa_1-1|c\alpha^4+\frac{3}{4}M[\Psi_2^\perp]+o(\alpha^5\log\alpha^{-1})\ ,
\end{aligned}
\tag{87}
$$

and $Q_\alpha^\perp$ *is the projection onto the orthogonal complement to the ground state* u_α *of the Schrödinger operator* $h_\alpha=-\Delta-\frac{\alpha}{|x|}$

The proof of this Proposition is detailed in Subsection 6.3.

6.1. **Proof of Theorem 6.1 on the upper bound up to the order** $\alpha^5\log\alpha^{-1}$**.** We have

$$
\langle H\Psi^{\mathrm{GS}},\Psi^{\mathrm{GS}}\rangle=(\Sigma_0-e_0)\|\Psi^{u_\alpha}\|^2+2\mathrm{Re}\,\langle H\Psi^\perp,u_\alpha\Psi^{u_\alpha}\rangle+\langle H\Psi^\perp,\Psi^\perp\rangle.
\tag{88}
$$

The estimates for the last two terms are given in Propositions 6.1 and 6.2. We will minimize this expression with respect to the parameters κ_1, $\kappa_{2,i}$, and κ_3.

• We first estimate the second term on the right hand side of (85) together with the seventh term on the right hand side of (86). We have

$$
\begin{aligned}
&-4\alpha\mathrm{Re}\,\langle\nabla u_\alpha.P_f\Phi_*^2,\Gamma^2\Psi_2^\perp\rangle+4\alpha^{\frac12}\mathrm{Re}\,\langle\Gamma^2\Psi_2^\perp,A^+.P_f\Phi_*^{u_\alpha}\rangle\\
&=-4\alpha\mathrm{Re}\,\langle\Gamma^2\Psi_2^\perp,(\sum_{i=1}^{3}P_f^i\Phi_*^2-2A^+.P_f(H_f+P_f^2)^{-1}(A^+)^i\Omega_f)\frac{\partial u_\alpha}{\partial x_i}\rangle\\
&=-4\alpha\sum_{i=1}^{3}\mathrm{Re}\,\langle\Gamma^2\Psi_2^\perp,(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\rangle_*.
\end{aligned}
\tag{89}
$$

Using the $\langle\,\cdot\,,\,\cdot\,\rangle_\sharp$-orthogonality of $\Gamma^2\Psi_2^\perp$ and $(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}$, the last expression can be estimated as

$$-4\alpha\sum_{i=1}^{3}\mathrm{Re}\,\langle\Gamma^2\Psi_2^\perp,(h_\alpha+e_0)(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\rangle. \tag{90}$$

By the Schwarz inequality, this term is bounded below by

$$-\epsilon\alpha^2\|\Gamma^2\Psi_2^\perp\|^2-c\sum_{i=1}^{3}\|(h_\alpha+e_0)\frac{\partial u_\alpha}{\partial x_i}\|^2=-\epsilon\alpha^2\|\Gamma^2\Psi_2^\perp\|^2-\mathcal{O}(\alpha^6). \tag{91}$$

- Next, we collect all the terms involving κ_1 in (85) and (86). This yields

$$\begin{aligned}&-2\mathrm{Re}\,\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha}\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+|\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2-|\kappa_1-1|c\alpha^4\\&\geq-|\Gamma^0\Psi^{u_\alpha}|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+|\kappa_1-\Gamma^0\Psi^{u_\alpha}|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2-|\kappa_1-1|c\alpha^4\end{aligned} \tag{92}$$

Notice that from Theorem 5.2 we have $|\Gamma^0\Psi^{u_\alpha}|^2=1+\mathcal{O}(\alpha^2)$; moreover, we have $|\Gamma^0\Psi^{u_\alpha}|=1+\mathcal{O}(\alpha^2)$. This yields

$$\begin{aligned}&-2\mathrm{Re}\,\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha}\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+|\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2-|\kappa_1-1|c\alpha^4\\&\geq-\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+|\kappa_1-1|^2c'\alpha^3-|\kappa_1-1|c\alpha^4+\mathcal{O}(\alpha^5)=-\|\Phi_\sharp^{u_\alpha}\|_\sharp^2+\mathcal{O}(\alpha^5).\end{aligned} \tag{93}$$

- We now collect and estimates the terms in (85) and (86) involving $\kappa_{2,i}$. We get

(94)

$$\begin{aligned}&-\frac{1}{3}\alpha^4\mathrm{Re}\sum_{i=1}^{3}\kappa_{2,i}\langle(H_f+P_f^2)^{-1}W_i,P_f^i\Phi_*^2\rangle+\frac{\alpha^4}{12}\sum_{i=1}^{3}|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2\\&+\frac{2}{3}\alpha^4\mathrm{Re}\sum_{i=1}^{3}\kappa_{2,i}\langle(H_f+P_f^2)^{-1}W_i,P_f.A^+(H_f+P_f^2)^{-1}(A^+)^i\Omega_f\rangle\\&=-\frac{1}{3}\alpha^4\mathrm{Re}\sum_{i=1}^{3}\kappa_{2,i}\|(H_f+P_f^2)^{-1}W_i\|_*^2+\frac{\alpha^4}{12}\sum_{i=1}^{3}|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2\\&\geq-\frac{\alpha^4}{3}\sum_{i=1}^{3}\|(H_f+P_f^2)^{-1}W_i\|_*^2\end{aligned}$$

- Collecting in (85) and (86) the terms containing κ_3 yields

(95)

$$\frac{|\kappa_3+1|^2}{2}\alpha^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2-\epsilon\alpha^5|\kappa_3|^2\geq c_1\alpha^5\log\alpha^{-1}|\kappa_3+1|^2-\epsilon\alpha^5|\kappa_3|^2\geq-c_2\alpha^5,$$

where c_1 and c_2 are positive constants.

- The fifth term on the right hand side of (85) and the first term on the right hand side of (87) are estimated, for α small enough, as

$$(1-c_0\alpha)\|(h_\alpha+e_0)^{\frac{1}{2}}\Gamma^0(\Psi_1^\perp)^a\|^2-\epsilon\alpha^2\|(\Psi_1^\perp)^a\|^2\geq(\frac{\delta}{2}-\epsilon\alpha^2)\|(\Psi_1^\perp)^a\|^2\geq0, \tag{96}$$

with $\delta=\frac{3}{32}\alpha^2$, and where we used that $(\Psi_1^\perp)^a$ is orthogonal to u_α.

• Substituting the above estimates in (88)

(97)
$$
\begin{aligned}
&\langle H\Psi^{\rm GS},\Psi^{\rm GS}\rangle\\
&\geq (\Sigma_0-e_0)\|\Psi^{u_\alpha}\|^2+(\Sigma_0-e_0)\|\Psi^\perp\|^2-\|\Phi_\sharp^{u_\alpha}\|_\sharp^2-\alpha^4\sum_{i=1}^3\|(H_f+P_f^2)^{-1}W_i\|_*^2\\
&-\frac{2}{3}\alpha^4{\rm Re}\sum_{i=1}^3\langle\,(H_f+P_f^2)^{-\frac12}(A^-)^i\Phi_*^2,(H_f+P_f^2)^{-\frac12}(A^+)^i\Omega_f\rangle\\
&-4\alpha\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp PA^-\Phi_*^{u_\alpha}\|^2+2\alpha\|A^-\Phi_*^{u_\alpha}\|^2+o(\alpha^5\log\alpha^{-1})\ ,
\end{aligned}
$$

where $Q_\alpha^\perp$ is the projection onto the orthogonal complement to the ground state u_α of the Schrödinger operator $h_\alpha=-\Delta-\frac{\alpha}{|x|}$.

To complete the proof of Theorem 6.1 we first note that

$$\|\Psi^{u_\alpha}\|^2+\|\Psi^\perp\|^2=\|\Psi^{\rm GS}\|^2. \tag{98}$$

Moreover, according to Lemma A.4

$$-\|\Phi_\sharp^{u_\alpha}\|_\sharp^2=-\|\Phi_*^{u_\alpha}\|_*^2+\frac{1}{3\pi}\|(h_1+\frac14)^{\frac12}\nabla u_1\|^2\alpha^5\log\alpha^{-1}+o(\alpha^5\log\alpha^{-1}), \tag{99}$$

and

$$\|\Phi_*^{u_\alpha}\|_*^2=\frac{\alpha^3}{2\pi}\int_0^\infty\frac{\chi_\Lambda(t)}{1+t}{\rm d}t=e^{(1)}\alpha^3. \tag{100}$$

In addition, we have the following identities ($i=1,2,3$)

$$
\begin{aligned}
&\|(H_f+P_f^2)^{-1}W_i\|_*^2=\\
&\|(H_f+P_f^2)^{-\frac12}\Big(2A^+.P_f(H_f+P_f^2)^{-1}(A^+)^i-P_f^i(H_f+P_f^2)^{-1}A^+.A^+\Big)\Omega_f\|^2,
\end{aligned}
\tag{101}
$$

and

$$
\begin{aligned}
&-\frac{2}{3}\alpha^4{\rm Re}\sum_{i=1}^3\langle\,(H_f+P_f^2)^{-\frac12}A^-\Phi_*^2,(H_f+P_f^2)^{-\frac12}(A^+)^i\Omega_f\rangle\\
&=-\frac{2}{3}\alpha^4{\rm Re}\sum_{i=1}^3\langle A^-(H_f+P_f^2)^{-1}A^+.A^+\Omega_f,(H_f+P_f^2)^{-1}(A^+)^i\Omega_f\rangle\ .
\end{aligned}
\tag{102}
$$

We also have

$$-4\alpha\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp PA^-\Phi_*^{u_\alpha}\|^2=-4\alpha^4a_0^2\|(-\Delta-\frac{1}{|x|}+\frac14)^{-\frac12}Q_1^\perp\Delta u_1\|^2, \tag{103}$$

with

$$a_0=\int\frac{k_1^2+k_2^2}{4\pi^2|k|^3}\frac{2}{|k|^2+|k|}\chi_\Lambda(|k|)\,{\rm d}k_1{\rm d}k_2{\rm d}k_3,$$

and

$$2\alpha\|A^-\Phi_*^{u_\alpha}\|^2=\frac{2}{3}\alpha^4\sum_{i=1}^3\|A^-(H_f+P_f^2)^{-1}(A^+)^i\Omega_f\|^2. \tag{104}$$

Substituting (98)-(104) into (97) finishes the proof of Theorem 6.1.

6.2. **Proof of Proposition 6.1.**

Lemma 6.2. *The following holds*

(105)
$$
\begin{aligned}
&-4\mathrm{Re}\,\langle P.P_f u_\alpha \Psi^{u_\alpha}, \Psi^\perp\rangle \geq -\frac{4}{3}\alpha^2 \mathrm{Re} \sum_{i=1}^{3} \overline{\kappa_{2,i}}\,\|\nabla u_\alpha\|^2\, \langle (H_f+P_f^2)^{-1} P_f^i \Phi_*^2, W_i\rangle \\
&-4\alpha \mathrm{Re}\,\langle \nabla u_\alpha . P_f \Phi_*^2, \Gamma^2 \Psi_2^\perp\rangle - \epsilon \|H_f^{\frac12} \Psi_2^\perp\|^2 - \epsilon\alpha^5 |\kappa_3|^2 + \mathcal{O}(\alpha^5)
\end{aligned}
$$

Proof. For $n \neq 2,3$, with the estimates from the proof of Lemma 5.2 and using that due to Theorem 5.2 we have

$$\|H_f^{\frac12}\Delta_*^{u_\alpha}\|^2 = \mathcal{O}(\alpha^4),\ |\eta_1| = \mathcal{O}(1),\ \text{and } |\kappa_1| = \mathcal{O}(1),$$

and since $\Gamma^1 \Delta_\sharp^\perp = \Gamma^1 \Psi_2^\perp$ and $\Gamma^{n\geq 4}\Delta_\sharp^\perp = \Gamma^{n\geq 4}\Psi_2^\perp$, we obtain

$$\sum_{n\neq 2,3} -4\mathrm{Re}\,\langle P.P_f u_\alpha \Gamma^n \Psi^{u_\alpha}, \Gamma^n \Psi^\perp\rangle \geq -\epsilon \|H_f^{\frac12}\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5). \tag{106}$$

For $n = 2$,

(107)
$$
\begin{aligned}
&-4\mathrm{Re}\,\langle \nabla u_\alpha . (\alpha\eta_2 P_f \Phi_*^2 + P_f \Gamma^2 \Delta_*^{u_\alpha}), \Gamma^2 \Psi^\perp\rangle \geq -4\mathrm{Re}\,\langle \nabla u_\alpha . \alpha\eta_2 P_f \Phi_*^2, \Gamma^2 \Psi_1^\perp\rangle \\
&-4\mathrm{Re}\,\langle \nabla u_\alpha . \alpha\eta_2 P_f \Phi_*^2, \Gamma^2 \Psi_2^\perp\rangle - c\alpha \|H_f^{\frac12}\Gamma^2\Delta_*^{u_\alpha}\|^2 - c\alpha\|H_f^{\frac12}\Gamma^2\Psi^\perp\|^2.
\end{aligned}
$$

Using Theorem 5.2, the last two terms on the right hand side of (107) can be estimated by $\mathcal{O}(\alpha^5)$. For the first term on the right hand side of (107), using from Lemma A.1 that $\langle P_f^i \Phi_*^2, \Phi_*^2\rangle = 0$, from Theorem 5.2 that $\eta_2 = 1 + \mathcal{O}(\alpha)$, and from Lemma 6.1 that $\kappa_{2,i} = \mathcal{O}(1)$, holds

$$
\begin{aligned}
&-4\alpha \mathrm{Re}\,\langle \nabla u_\alpha . \eta_2 P_f \Phi_*^2, \Gamma^2 \Psi_1^\perp\rangle \\
&= -4\mathrm{Re}\,\alpha \langle \nabla u_\alpha . \eta_2 P_f \Phi_*^2, \alpha\kappa_2 \Phi_*^2 \Gamma^0 \Psi^\perp\rangle \\
&-4\mathrm{Re}\,\alpha\langle \nabla u_\alpha . \eta_2 P_f \Phi_*^2, \sum_i \alpha\kappa_{2,i}(H_f+P_f^2)^{-1} W_i \frac{\partial u_\alpha}{\partial x_i}\rangle \\
&= -\frac{4}{3}\mathrm{Re}\,\alpha^2 \|\nabla u_\alpha\|^2 \sum_i \overline{\kappa_{2,i}} \langle (H_f+P_f^2)^{-1} P_f^i \Phi_*^2, W_i\rangle \\
&= -\frac{1}{3}\alpha^4 \mathrm{Re} \sum_{i=1}^{3} \overline{\kappa_{2,i}} \langle (H_f+P_f^2)^{-1} P_f^i \Phi_*^2, W_i\rangle.
\end{aligned}
\tag{108}
$$

We also used that $\langle \frac{\partial u_\alpha}{\partial x_i}, \frac{\partial u_\alpha}{\partial x_j}\rangle = 0$ for $i \neq j$ and $\|\frac{\partial u_\alpha}{\partial x_i}\| = \|\frac{\partial u_\alpha}{\partial x_j}\|$ for all i and j.

Finally, the second term on the right hand side of (107) gives the second term on the right hand side of (105) plus $\mathcal{O}(\alpha^5)$, using from Theorem 5.2 that $|\eta_2 - 1|^2 = \mathcal{O}(\alpha^2)$ and $\|H_f^{\frac12}\Gamma^2\Psi_2^\perp\| = \mathcal{O}(\alpha^2)$.

To complete the proof, we shall estimate now the term for $n = 3$,

$$
\begin{aligned}
&4\mathrm{Re}\,\langle P.P_f u_\alpha \Gamma^3 \Psi^{u_\alpha}, \Gamma^3 \Psi^\perp\rangle = 4\mathrm{Re}\,\alpha^{\frac32} 2\eta_3 \langle P.P_f u_\alpha \Phi_*^3, \Gamma^3 \Psi_1^\perp\rangle \\
&+ 4\mathrm{Re}\,\alpha^{\frac32} 2\eta_3 \langle P.P_f u_\alpha \Phi_*^3, \Gamma^3 \Psi_2^\perp\rangle + 4\mathrm{Re}\,\langle P.P_f u_\alpha \Gamma^3 \Delta_*^{u_\alpha}, \Gamma^3 \Psi^\perp\rangle.
\end{aligned}
\tag{109}
$$

The inequalities $\|H_f^{\frac12}\Delta_*^{u_\alpha}\| \leq c\alpha^2$ and $\|H_f^{\frac12}\Gamma^3\Psi^\perp\| \leq c\alpha^2$ (see Theorem 5.2) imply that the last term on the right hand side of (109) is $\mathcal{O}(\alpha^5)$. For the second term on the right hand side of (109) holds

$$\mathrm{Re}\,\alpha^{\frac{3}{2}}\eta_3\langle P.P_f u_\alpha \Phi_*^3, \Gamma^3\Psi_2^\perp\rangle \geq -\epsilon\|H_f^{\frac{1}{2}}\Gamma^3\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5), \tag{110}$$

since from Theorem 5.2 we have $\eta_3 = \mathcal{O}(1)$.

Finally to estimate the first term on the right hand side of (109), we note that

$$|k_1|^{-\frac{1}{6}}|k_2|^{-\frac{1}{6}}|k_3|^{-\frac{1}{6}}\Phi_*^3(k_1,k_2,k_3) \in L^2(\mathbb{R}^9,\mathbb{C}^6)\ ,$$

and from Lemma A.5,

$$\|\,|k_1|^{\frac{1}{6}}|k_2|^{\frac{1}{6}}|k_3|^{\frac{1}{6}}(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|^2 = \mathcal{O}(\alpha^3).$$

This implies, using again $|\eta_3| = \mathcal{O}(1)$, and the explicit expression of $\Gamma^3\Psi_1^\perp$

$$|\alpha^{\frac{3}{2}}2\eta_3\langle P.P_f u_\alpha\Phi_*^3, \Gamma^3\Psi_1^\perp\rangle| \leq c\alpha^{\frac{5}{2}}|\kappa_3|\alpha^{\frac{3}{2}}|\eta_3|\,\|Pu_\alpha\| \leq \epsilon\alpha^5|\kappa_3|^2 + \mathcal{O}(\alpha^5). \tag{111}$$

Collecting (106)-(111) concludes the proof. □

Lemma 6.3. *The following estimate holds*

$$\begin{aligned} &-4\sqrt{\alpha}\mathrm{Re}\,\langle P.A^+u_\alpha\Psi^{u_\alpha},\Psi^\perp\rangle \\ &= -2\mathrm{Re}\,\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha}\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 - \frac{1}{4}M[\Psi_2^\perp] - \alpha^5|\kappa_3|^2 + \mathcal{O}(\alpha^5), \end{aligned} \tag{112}$$

Proof. Obviously

$$\begin{aligned} &-4\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+u_\alpha\Psi^{u_\alpha},\Psi^\perp\rangle \\ &= -4\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+u_\alpha(\Gamma^0\Psi^{u_\alpha} + 2\eta_1\alpha^{\frac{3}{2}}\Phi_*^1 + \eta_2\alpha\Phi_*^2 + 2\eta_3\alpha^{\frac{3}{2}}\Phi_*^3 + \Delta_*^{u_\alpha}),\Psi^\perp\rangle. \end{aligned} \tag{113}$$

⋄ *Step 1* From (113), let us first estimate the term

$$-4\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+u_\alpha\Delta_*^{u_\alpha},\Psi^\perp\rangle = -4\alpha^{\frac{1}{2}}\mathrm{Re}\sum_{n=0}^\infty\langle P.A^+\Gamma^n u_\alpha\Delta_*^{u_\alpha},\Gamma^{n+1}\Psi^\perp\rangle. \tag{114}$$

For $n=0$, the corresponding term vanishes since $\Gamma^0\Delta_*^{u_\alpha} = 0$.

For $n>2$, we can use (50) where the term $\mathcal{O}(\alpha^5\log\alpha^{-1})$ can be replaced with $\mathcal{O}(\alpha^5)$ because we know from Theorem 5.2 that $\|\Delta_*^{u_\alpha}\|^2 = \mathcal{O}(\alpha^{\frac{33}{16}})$.

For $n=1$, we have

$$\begin{aligned} &|4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P.A^+\Gamma^1u_\alpha\Delta_*^{u_\alpha},\Gamma^2\Psi_1^\perp+\Gamma^2\Psi_2^\perp\rangle| \leq c\alpha^3\|\Gamma^1\Delta_*^{u_\alpha}\|^2 + \epsilon\|H_f^{\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2 \\ &+ |4\alpha^{\frac{1}{2}}\langle\nabla u_\alpha\Gamma^1\Delta_*^{u_\alpha}, A^-\left(\alpha\kappa_2\Phi_*^2\Gamma^0\Psi_1^\perp + \alpha\sum_{i=1}^3\kappa_{2,i}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\right)\rangle|. \end{aligned} \tag{115}$$

To estimate the last term on the right hand side we note that $H_f^{-\frac{1}{2}}A^-\Phi_*^2 \in L^2$ and $H_f^{-\frac{1}{2}}A^-(H_f+P_f^2)^{-1}W_i \in L^2$ which thus gives for this term the bound

$$c\alpha\|H_f^{\frac{1}{2}}\Delta_*^{u_\alpha}\|^2 + \epsilon\alpha^4|\kappa_2|^2\|\Gamma^0\Psi_1^\perp\|^2 + \epsilon\alpha^6\sum_i|\kappa_{2,i}|^2 = \mathcal{O}(\alpha^5), \tag{116}$$

using Theorem 5.2 and Lemma 6.1. The inequalities (115) and (116) imply

$$|\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+\Gamma^1u_\alpha\Delta_*^{u_\alpha},\Gamma^2\Psi_1^\perp+\Gamma^2\Psi_2^\perp\rangle| \leq \epsilon\|H_f^{\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5). \tag{117}$$

To complete the estimate of the term $4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P.A^+ u_\alpha \Delta_*^{u_\alpha}, \Psi^\perp\rangle$ we have to estimate the term for $n=2$ in (114), namely $4\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+ u_\alpha \Gamma^2\Delta_*^{u_\alpha}, \Gamma^3\Psi_1^\perp + \Gamma^3\Psi_2^\perp\rangle$. Obviously,

$$|\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+ u_\alpha \Gamma^2\Delta_*^{u_\alpha}, \Gamma^3\Psi_2^\perp\rangle| \le \epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5). \tag{118}$$

For the term involving $\Gamma^3\Psi_1^\perp$ we have

$$\begin{aligned} &|\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P u_\alpha \Gamma^2\Delta_*^{u_\alpha}, \alpha\kappa_3 A^-(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\rangle| \\ &\le c\alpha^{3-\frac{1}{16}}\|\Gamma^2\Delta_*^{u_\alpha}\|^2 + \epsilon|\kappa_3|^2\alpha^{2+\frac{1}{16}}\|\Phi_\sharp^{u_\alpha}\|^2 = |\kappa_3|^2\alpha^5 + \mathcal{O}(\alpha^5), \end{aligned} \tag{119}$$

using Theorem 5.2 and Lemma A.5. Collecting (114)-(119) yields

$$|\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+ u_\alpha \Delta_*^{u_\alpha}, g\rangle| \le \epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 + \alpha^5|\kappa_3|^2 + \mathcal{O}(\alpha^5). \tag{120}$$

$\diamond$ *Step 2* We next estimate in (113) the term $-4\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+ u_\alpha(\Gamma^0\Psi^{u_\alpha} + \alpha^{\frac{3}{2}}2\eta_1\Phi_*^1 + \alpha\eta_2\Phi_*^2 + \alpha^{\frac{3}{2}}2\eta_3\Phi_*^3), \Psi^\perp\rangle$. First using (50) yields

$$-4\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+ u_\alpha \Gamma^0\Psi^{u_\alpha}, \Psi^\perp\rangle = -2\mathrm{Re}\,(\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha})\|\Phi_\sharp^{u_\alpha}\|_\sharp^2. \tag{121}$$

We also have, using Theorem 5.2

$$\begin{aligned} &|\alpha^{\frac{1}{2}}\langle P u_\alpha(\alpha^{\frac{3}{2}}2\eta_1\Phi_*^1 + \alpha^{\frac{3}{2}}2\eta_3\Phi_*^3), A^-\Psi^\perp\rangle| \\ &\le \alpha\|H_f^{\frac{1}{2}}\Gamma^2\Psi^\perp\|^2 + \alpha\|H_f^{\frac{1}{2}}\Gamma^4\Psi^\perp\|^2 + \mathcal{O}(\alpha^5) = \mathcal{O}(\alpha^5), \end{aligned} \tag{122}$$

and

$$\begin{aligned} &|\alpha^{\frac{1}{2}}\langle P u_\alpha \alpha\eta_2\Phi_*^2, A^-(\Gamma^3\Psi_1^\perp + \Gamma^3\Psi_2^\perp)\rangle| \\ &\le \epsilon\|H_f^{\frac{1}{2}}\Gamma^3\Psi_2^\perp\|^2 + |\alpha^{\frac{3}{2}}\langle P u_\alpha\eta_2|k_1|^{-\frac{1}{4}}|k_2|^{-\frac{1}{4}}\Phi_*^2, |k_1|^{\frac{1}{4}}|k_2|^{\frac{1}{4}}A^-\Gamma^3\Psi_1^\perp\rangle| + \mathcal{O}(\alpha^5) \\ &\le \epsilon\|H_f^{\frac{1}{2}}\Gamma^3\Psi_2^\perp\|^2 + \epsilon|\kappa_3|^2\alpha^5 + \mathcal{O}(\alpha^5). \end{aligned} \tag{123}$$

Here we used $|k_1|^{-\frac{1}{4}}|k_2|^{-\frac{1}{4}}\Phi_*^2 \in L^2$ and $\||k_1|^{\frac{1}{4}}|k_2|^{\frac{1}{4}}A^-(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|^2 = \mathcal{O}(\alpha^3)$ (see Lemma A.5).

Collecting (120)-(123) yields

$$-4\mathrm{Re}\,\alpha^{\frac{1}{2}}\langle P.A^+ u_\alpha\Psi^{u_\alpha}, \Psi^\perp\rangle \ge -2\mathrm{Re}\,\overline{\kappa_1}\Gamma^0\Psi^{u_\alpha}\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 - \epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 - \epsilon\alpha^5|\kappa_3|^2 + \mathcal{O}(\alpha^5). \tag{124}$$

□

Lemma 6.4.

$$\begin{aligned} &-4\sqrt{\alpha}\mathrm{Re}\,\langle P.A^- u_\alpha\Psi^{u_\alpha}, \Psi^\perp\rangle \ge \\ &-\frac{2}{3}\alpha^4\mathrm{Re}\sum_{i=1}^3\langle\, (H_f+P_f^2)^{-\frac{1}{2}}(A^-)^i\Phi_*^2, (H_f+P_f^2)^{-\frac{1}{2}}(A^+)^i\Omega_f\rangle \\ &-\frac{1}{4}M[\Psi_2^\perp] - \epsilon\alpha^2\|(\Psi_1^\perp)^a\|^2 - \epsilon\alpha^5\log\alpha^{-1}(\alpha|\kappa_3|^2+1) - |\kappa_1-1|c\alpha^4 + \mathcal{O}(\alpha^5)\ , \end{aligned} \tag{125}$$

where $(\Psi_1^\perp)^a(x) := (\Gamma^0\Psi_1^\perp(x) - \Gamma^0\Psi_1^\perp(-x))/2$ *is the odd part of* $\Gamma^0\Psi_1^\perp$.

Proof. Since from Lemma A.1 we have $\nabla u_\alpha . A^- \Phi_*^1 = 0$, we have

$$
\begin{aligned}
& 4\mathrm{Re}\,\alpha^{\frac{1}{2}} \langle P.A^- u_\alpha \Psi^{u_\alpha}, \Psi^\perp \rangle = 4\alpha^{\frac{3}{2}} \mathrm{Re}\,\eta_2 \langle A^- \Phi_*^2 . P u_\alpha, \Gamma^1 \Psi^\perp \rangle \\
& + 4\alpha^2 \mathrm{Re}\, 2\eta_3 \langle A^- \Phi_*^3 . P u_\alpha, \Gamma^2 \Psi^\perp \rangle + 4\alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} . P u_\alpha, \Psi^\perp \rangle.
\end{aligned} \tag{126}
$$

For the first term on the right hand side of (126) we have

$$
\begin{aligned}
& 4\alpha^{\frac{3}{2}} \mathrm{Re}\,\eta_2 \langle A^- \Phi_*^2 . P u_\alpha, \Gamma^1 \Psi_2^\perp + \kappa_1 \Phi_\sharp^{u_\alpha} \rangle \\
& = 4\alpha^{\frac{3}{2}} \mathrm{Re}\,\eta_2 \langle H_f^{-\frac{1}{2}} A^- \Phi_*^2 . P u_\alpha, H_f^{\frac{1}{2}} \Gamma^1 \Psi_2^\perp \rangle + 4\alpha^{\frac{3}{2}} \mathrm{Re}\,\eta_2 \langle A^- \Phi_*^2 . P u_\alpha, \kappa_1 \Phi_\sharp^{u_\alpha} \rangle.
\end{aligned} \tag{127}
$$

The first term on the right hand side of (127) is bounded from below by $-\epsilon \| H_f^{\frac{1}{2}} \Gamma^1 \Psi_2^\perp \|^2 + \mathcal{O}(\alpha^5)$.

Applying Lemma A.4, we can replace $\Phi_\sharp^{u_\alpha}$ in the second term of the right hand side of (127) by $\Phi_*^{u_\alpha}$, at the expense of $\mathcal{O}(\alpha^5)$. More precisely

$$
\begin{aligned}
& |\alpha^{\frac{3}{2}} \langle \eta_2 A^- \Phi_*^2 . P u_\alpha, \kappa_1 (\Phi_\sharp^{u_\alpha} - \Phi_*^{u_\alpha}) \rangle | \\
& \leq c\alpha^5 |\eta_2|^2 \| (H_f + P_f^2)^{-\frac{1}{2}} A^- \Phi_*^2 \|^2 + |\kappa_1|^2 \| \Phi_\sharp^{u_\alpha} - \Phi_*^{u_\alpha} \|_*^2 = \mathcal{O}(\alpha^5).
\end{aligned}
$$

Moreover

$$
\begin{aligned}
& 4\alpha^{\frac{3}{2}} \mathrm{Re}\,\eta_2 \overline{\kappa_1} \langle A^- \Phi_*^2 . P u_\alpha, \Phi_*^{u_\alpha} \rangle \\
& = \frac{8}{3} \alpha^2 \| \nabla u_\alpha \|^2 \mathrm{Re}\,\eta_2 \overline{\kappa_1} \sum_{i=1}^3 \langle (A^-)^i \Phi_*^2, (H_f + P_f^2)^{-1} (A^+)^i \Omega_f \rangle \\
& = \frac{2}{3} \alpha^4 \mathrm{Re}\,\eta_2 \overline{\kappa_1} \sum_{i=1}^3 \langle (A^-)^i \Phi_*^2, (H_f + P_f^2)^{-1} (A^+)^i \Omega_f \rangle \\
& \geq \frac{2}{3} \alpha^4 \mathrm{Re} \sum_{i=1}^3 \langle (A^-)^i \Phi_*^2, (H_f + P_f^2)^{-1} (A^+)^i \Omega_f \rangle - |\kappa_1 - 1| c\alpha^4,
\end{aligned} \tag{128}
$$

where we used $\kappa_1 = \mathcal{O}(1)$ (Lemma 6.1) and $\eta_2 = 1 + \mathcal{O}(\alpha)$ (Theorem 5.2). Note that the right hand side of (128) is well defined since $(H_f + P_f^2)^{-\frac{1}{2}} A^+ \Omega_f \in \mathfrak{F}$ and $(H_f + P_f^2)^{-\frac{1}{2}} A^- \Phi_*^2 \in \mathfrak{F}$.

Collecting the estimates for the first and the second term in the right hand side of (127), we arrive at

$$
\begin{aligned}
& - 4\alpha^{\frac{3}{2}} \mathrm{Re}\,\eta_2 \langle A^- \Phi_*^2 . P u_\alpha, \Gamma^1 \Psi^\perp \rangle \\
& \geq -\frac{8}{3} \alpha^2 \| \nabla u_\alpha \|^2 \mathrm{Re}\, \overline{\kappa_1} \langle (A^-)^i \Phi_*^2, (H_f + P_f^2)^{-1} A^+ \Omega_f \rangle - \epsilon \| H_f^{\frac{1}{2}} \Gamma^1 \Psi_2^\perp \|^2 + \mathcal{O}(\alpha^5).
\end{aligned} \tag{129}
$$

Here we used also $\eta_2 = 1 + \mathcal{O}(\alpha)$.

As the next step, we return to (126) and estimate the second term on the right hand side as

$$
4\alpha^2 \mathrm{Re}\, 2\eta_3 \langle A^- \Phi_*^3 . P u_\alpha, \Gamma^2 \Psi^\perp \rangle = 8\alpha^2 \mathrm{Re}\,\eta_3 \langle H_f^{-\frac{1}{2}} A^- \Phi_*^3 . P u_\alpha, H_f^{\frac{1}{2}} \Gamma^2 \Psi^\perp \rangle = \mathcal{O}(\alpha^5), \tag{130}
$$

where we used $H_f^{-\frac{1}{2}} A^- \Phi_*^3 \in L^2$ and $\|\Gamma^2 H_f^{\frac{1}{2}} \Delta_\sharp^\perp\|^2 = \|\Gamma^2 H_f^{\frac{1}{2}} \Psi^\perp\|^2 = \mathcal{O}(\alpha^4)$ from Theorem 5.2. For the last term on the right hand side of (126), we have

$$
\begin{aligned}
&4\alpha^{\frac{1}{2}} \mathrm{Re}\, \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Psi^\perp \rangle \\
&= 4\alpha^{\frac{1}{2}} \mathrm{Re}\, \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Gamma^0 \Psi_1^\perp \rangle + 4\alpha^{\frac{1}{2}} \mathrm{Re}\, \overline{\kappa_1} \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Phi_\sharp^{u_\alpha} \rangle \\
&+ 4\alpha^{\frac{1}{2}} \mathrm{Re}\, \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Gamma^1 \Psi_2^\perp \rangle + 4\alpha^{\frac{1}{2}} \mathrm{Re}\, \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Gamma^2 \Psi^\perp \rangle \\
&+ 4\alpha^{\frac{1}{2}} \mathrm{Re}\, \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Gamma^3 \Psi^\perp \rangle + 4\alpha^{\frac{1}{2}} \mathrm{Re}\, \langle A^- \Delta_*^{u_\alpha} . \nabla u_\alpha, \Gamma^{n \geq 4} \Psi^\perp \rangle .
\end{aligned}
\tag{131}
$$

We write the function $\Gamma^0 \Psi_1^\perp = (\Psi_1^\perp)^s + (\Psi_1^\perp)^a$ where $(\Psi_1^\perp)^s$ (respectively $(\Psi_1^\perp)^a$) denotes the even (respectively odd) part of $\Gamma^0 \Psi_1^\perp$. Obviously, we have

$$
|\alpha^{\frac{1}{2}} \mathrm{Re}\, \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Gamma^0 \Psi_1^\perp \rangle| \leq c\alpha \|H_f^{\frac{1}{2}} R\|^2 + \epsilon \alpha^2 \|(\Psi_1^\perp)^a\|^2 = \epsilon \alpha^2 \|(\Psi_1^\perp)^a\|^2 + \mathcal{O}(\alpha^5).
\tag{132}
$$

The constant ϵ can be chosen small for large c.

For the second term on the right hand side of (131), we have

$$
|\alpha^{\frac{1}{2}} \overline{\kappa_1} \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Phi_\sharp^{u_\alpha} \rangle| \leq \epsilon \alpha^5 \log \alpha^{-1} |\kappa_1|^2 + c\alpha \|H_f^{\frac{1}{2}} \Delta_*^{u_\alpha}\|^2 = \epsilon \alpha^5 \log \alpha^{-1} + \mathcal{O}(\alpha^5).
\tag{133}
$$

For the third term on the right hand side of (131), we have, since $\delta = \frac{3}{32}\alpha^2$

$$
|4\alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Gamma^1 \Psi_2^\perp \rangle| \leq \frac{\delta}{8} \|\Gamma^1 \Psi_2^\perp\|^2 + c\alpha \|H_f^{\frac{1}{2}} \Delta_*^{u_\alpha}\|^2 = \frac{\delta}{8} \|\Gamma^1 \Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5).
\tag{134}
$$

Similarly

$$
|4\alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} \cdot \nabla u_\alpha, \Gamma^{n\geq 4} \Psi^\perp \rangle| \leq \frac{\delta}{8} \|\Gamma^{n \geq 4} \Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5).
\tag{135}
$$

To complete the estimate of the last term in (131), we have to estimate two terms: $-4\mathrm{Re}\, \alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} . P u_\alpha, \Gamma^2 \Psi^\perp \rangle$ and $-4\mathrm{Re}\, \alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} . P u_\alpha, \Gamma^3 \Psi^\perp \rangle$. For the first one we have

$$
\begin{aligned}
&|\mathrm{Re}\, \alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} . P u_\alpha, \Gamma^2 \Psi^\perp \rangle| \leq c\alpha \|H_f^{\frac{1}{2}} \Delta_*^{u_\alpha}\|^2 + \epsilon \alpha^2 \|\Gamma^2 \Psi_2^\perp\|^2 + \epsilon \alpha^4 |\kappa_2|^2 \|\Gamma^0 \Psi^\perp\|^2 \\
&+ \epsilon \alpha^6 \sum_{i=1}^{3} |\kappa_{2,i}|^2 = \epsilon \alpha^2 \|\Gamma^2 \Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5).
\end{aligned}
$$

Similarly,

$$
|\mathrm{Re}\, \alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} . P u_\alpha, \Gamma^3 \Psi^\perp \rangle| \leq c\alpha \|H_f^{\frac{1}{2}} \Delta_*^{u_\alpha}\|^2 + \epsilon \alpha^2 \|\Gamma^3 \Psi_2^\perp\|^2 + \epsilon \alpha^6 \log \alpha^{-1} |\kappa_3|^2 + \mathcal{O}(\alpha^5).
\tag{136}
$$

Collecting the estimates (131)-(136) yields

$$
|4\mathrm{Re}\, \alpha^{\frac{1}{2}} \langle A^- \Delta_*^{u_\alpha} . P u_\alpha, \Psi^\perp \rangle| \leq \frac{\delta}{8} \|\Psi_2^\perp\|^2 + \epsilon \|H_f^{\frac{1}{2}} \Psi_2^\perp\|^2 + \epsilon \alpha^5 \log \alpha^{-1} (1 + \alpha |\kappa_3|^2) + \mathcal{O}(\alpha^5).
\tag{137}
$$

Collecting (120), (124), (129), (130) and (137) concludes the proof. □

We can now prove the estimate of $\mathrm{Re}\, \langle Hg,\, u_\alpha \Psi^{u_\alpha} \rangle$ of Proposition 6.1.

Proof of the Proposition 6.1. Using the orthogonality (39) of u_α and $\Psi^\perp$, yields

$$
2\mathrm{Re}\, \langle H \Psi^\perp, \Psi^{u_\alpha} \rangle = -4\mathrm{Re}\, \langle P.P_f u_\alpha \Psi^{u_\alpha}, \Psi^\perp \rangle - 4\sqrt{\alpha} \mathrm{Re}\, \langle P.A(0) u_\alpha \Psi^{u_\alpha}, \Psi^\perp \rangle .
$$

Together with Lemmata 6.2-6.4, this concludes the proof of Proposition 6.1. □

6.3. **Proof of Proposition 6.2.** We have the estimate

Proposition 6.3. *We have*

$$
\begin{aligned}
&\langle H\Psi^{\perp},\Psi^{\perp}\rangle\\
&\geq \langle H\Psi_1^{\perp},\Psi_1^{\perp}\rangle + \langle H\Psi_2^{\perp},\Psi_2^{\perp}\rangle + 2\alpha\left(\|A^-\Psi^{\perp}\|^2 - \|A^-\Psi_1^{\perp}\|^2 - \|A^-\Psi_2^{\perp}\|^2\right)\\
&- 4\mathrm{Re}\,\langle P.P_f\Psi_2^{\perp},\Psi_1^{\perp}\rangle - 4\alpha^{\frac12}\mathrm{Re}\,\langle P.A(0)\Psi_2^{\perp},\Psi_1^{\perp}\rangle + 4\mathrm{Re}\,\langle P_f.A(0)\Psi_2^{\perp},\Psi_1^{\perp}\rangle\\
&- \epsilon M[\Psi_2^{\perp}] - c\alpha^6\log\alpha^{-1}|\kappa_3|^2 - c_0\alpha\|(h_\alpha+e_0)^{\frac12}\Gamma^0\Psi_1^{\perp}\|^2 + \mathcal{O}(\alpha^5).
\end{aligned}
\tag{138}
$$

Proof. Recall that

$$
H = P^2 - \frac{\alpha}{|x|} + T(0) - 2\mathrm{Re}\,P.\left(P_f + \alpha^{\frac12}A(0)\right),
\tag{139}
$$

and

$$
T(0) =: (P_f + \alpha^{\frac12}A(0))^2 : + H_f.
\tag{140}
$$

Due to the orthogonality

$$
\langle \Gamma^n\Psi_1^{\perp},\Gamma^n\Psi_2^{\perp}\rangle_\sharp = 0,\quad n=0,1,\dots\ ,
$$

and (139), (140), we obtain

$$
\begin{aligned}
&\langle (H+e_0)\Psi^{\perp},\Psi^{\perp}\rangle\\
&= \langle (H+e_0)\Psi_2^{\perp},\Psi_2^{\perp}\rangle + \langle (H+e_0)\Psi_1^{\perp},\Psi_1^{\perp}\rangle + \sum_{n=0}^{3} 2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^{n+2}\Psi_2^{\perp},\Gamma^n\Psi_1^{\perp}\rangle\\
&+ 2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^3\Psi_1^{\perp},\Gamma^1\Psi_2^{\perp}\rangle + 2\alpha(\|A^-\Psi^{\perp}\|^2 - \|A^-\Psi_1^{\perp}\|^2 - \|A^-\Psi_2^{\perp}\|^2)\\
&- 4\mathrm{Re}\,\langle P.P_f\Psi_2^{\perp},\Psi_1^{\perp}\rangle - 4\alpha^{\frac12}\mathrm{Re}\,\langle P.A(0)\Psi_2^{\perp},\Psi_1^{\perp}\rangle + 4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A(0)\Psi_2^{\perp},\Psi_1^{\perp}\rangle.
\end{aligned}
\tag{141}
$$

We have

$$
\begin{aligned}
&2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^5\Psi_2^{\perp},\Gamma^3\Psi_1^{\perp}\rangle \geq -\epsilon\|H_f^{\frac12}\Gamma^5\Psi_2^{\perp}\|^2 - c\alpha^2\|\Gamma^3\Psi_1^{\perp}\|^2\\
&\geq -\epsilon\|H_f^{\frac12}\Gamma^5\Psi_2^{\perp}\|^2 - c\alpha^7\log\alpha^{-1}|\kappa_3|^2.
\end{aligned}
\tag{142}
$$

Similarly,

$$
\begin{aligned}
&2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^4\Psi_2^{\perp},\Gamma^2\Psi_1^{\perp}\rangle\\
&\geq -\epsilon\|H_f^{\frac12}\Gamma^4\Psi_2^{\perp}\|^2 - c\alpha^4|\kappa_2|^2\|\Gamma^0\Psi_1^{\perp}\|^2 - \sum_{i=1}^{3} c\alpha^6|\kappa_{2,i}|^2\\
&\geq -\epsilon\|H_f^{\frac12}\Gamma^4\Psi_2^{\perp}\|^2 + \mathcal{O}(\alpha^5).
\end{aligned}
$$

To estimate the term $2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^3\Psi_2^{\perp},\Gamma^1\Psi_1^{\perp}\rangle$ we rewrite it as $2\alpha\mathrm{Re}\,\langle \Gamma^3\Psi_2^{\perp},A^+.A^+\kappa_1\Phi_\sharp^{u_\alpha}\rangle$ and use that $\langle \Gamma^3\Psi_2^{\perp},(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\rangle_\sharp = 0$. This yields, using Lemma A.5

$$
\begin{aligned}
\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^3\Psi_2^{\perp},\Gamma^1\Psi_1^{\perp}\rangle &= -\alpha\mathrm{Re}\,\langle \Gamma^3\Psi_2^{\perp},(h_\alpha+e_0)(H_f+P_f^2)^{-1}A^+.A^+\kappa_1\Phi_\sharp^{u_\alpha}\rangle\\
&\geq -\epsilon\alpha^2\|\Gamma^3\Psi_2^{\perp}\|^2 + c\alpha^7\log\alpha^{-1}.
\end{aligned}
\tag{143}
$$

Similarly, if $\|\Gamma^0\Psi_1^\perp\| > \alpha^{\frac{3}{2}}$,

(144)

$$2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^2\Psi_2^\perp, \Gamma^0\Psi_1^\perp\rangle = -2\alpha\mathrm{Re}\,\langle \Gamma^2\Psi_2^\perp, (h_\alpha+e_0)(H_f+P_f^2)^{-1}A^+.A^+\Gamma^0\Psi_1^\perp\rangle$$
$$\geq -c\alpha\|(h_\alpha+e_0)^{\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2 - c\alpha\|(h_\alpha+e_0)^{\frac{1}{2}}(H_f+P_f^2)^{-1}A^+.A^+\Gamma^0\Psi_1^\perp\|^2$$
$$\geq -c\alpha\|P\Gamma^2\Psi_2^\perp\|^2 + c\alpha\||x|^{-\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2 - c\alpha e_0\|\Gamma^2\Psi_2^\perp\|^2 - c_0\alpha\|(h_\alpha+e_0)^{\frac{1}{2}}\Gamma^0\Psi_1^\perp\|^2$$
$$\geq -c\alpha\|P\Gamma^2\Psi_2^\perp\|^2 - \epsilon\alpha^2\|\Gamma^2\Psi_2^\perp\|^2 - c_0\alpha\|(h_\alpha+e_0)^{\frac{1}{2}}\Gamma^0\Psi_1^\perp\|^2\ .$$

If $\|\Gamma^0\Psi_1^\perp\| \leq \alpha^{\frac{3}{2}}$, we have instead

$$(145)\qquad \begin{aligned} 2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^2\Psi_2^\perp, \Gamma^0\Psi_1^\perp\rangle &\geq -\epsilon\|H_f^{\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2 - c\alpha^2\|\Gamma^0\Psi_1^\perp\|^2 \\ &\geq -\epsilon\|H_f^{\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5). \end{aligned}$$

Finally, using Lemma A.6 yields

$$(146)\qquad 2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^3\Psi_1^\perp, \Gamma^1\Psi_2^\perp\rangle \geq -\epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5).$$

Collecting (141)-(146) concludes the proof of the proposition. □

In the rest of this subsection, we estimate further terms in (138).

6.3.1. *Estimate of crossed terms involving $\Psi_1^\perp$ and $\Psi_2^\perp$.*

Lemma 6.5.

$$(147)\qquad 2\alpha(\|A^-\Psi^\perp\|^2 - \|A^-\Psi_1^\perp\|^2 - \|A^-\Psi_2^\perp\|^2) \geq -\epsilon M[\Psi_2^\perp] + \mathcal{O}(\alpha^5).$$

Proof. Obviously, the left hand side of (147) is equal to

(148)

$$4\alpha\mathrm{Re}\,\langle A^-\Psi_1^\perp, A^-\Psi_2^\perp\rangle \geq -c\alpha\sum_n \|H_f^{\frac{1}{2}}\Gamma^n\Psi_1^\perp\|\,\|H_f^{\frac{1}{2}}\Gamma^n\Psi_2^\perp\|$$
$$\geq -\epsilon\|H_f^{\frac{1}{2}}\Gamma^1\Psi_2^\perp\|^2 - c\alpha^2|\kappa_1|^2\|H_f^{\frac{1}{2}}\Phi_\sharp^{u_\alpha}\|^2 - \sum_{n\neq 1} c\alpha\left(3\|H_f^{\frac{1}{2}}\Gamma^n\Psi_2^\perp\|^2 + 2\|H_f^{\frac{1}{2}}\Gamma^n\Psi^\perp\|^2\right)$$
$$\geq -\epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5),$$

where in the last inequality we used (210) of Lemma A.3, and (69) of Theorem 5.2. □

Lemma 6.6.

$$|\langle P.P_f\Psi_2^\perp, \Psi_1^\perp\rangle| \leq \epsilon M[\Psi_2^\perp] + c\alpha^7\log\alpha^{-1}|\kappa_3|^2 + \mathcal{O}(\alpha^5)$$

Proof. We have

(149)

$$\langle P.P_f\Psi_2^\perp, \Psi_1^\perp\rangle = \langle P_f\Gamma^1\Psi_2^\perp, P\Gamma^1\Psi_1^\perp\rangle + \langle P_f\Gamma^2\Psi_2^\perp, P\Gamma^2\Psi_1^\perp\rangle + \langle P_f\Gamma^3\Psi_2^\perp, P\Gamma^3\Psi_1^\perp\rangle.$$

Obviously, using Lemma A.3 and the equality $\kappa_1 = \mathcal{O}(1)$ from Lemma 6.1, yields

(150)

$$\langle P_f\Gamma^1\Psi_2^\perp, P\Gamma^1\Psi_1^\perp\rangle| \leq \epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 + |\kappa_1|^2\|P|P_f|^{\frac{1}{2}}\Phi_\sharp^{u_\alpha}\|^2 \leq \epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5).$$

We also have, by definition of $\Gamma^2\Psi_1^\perp$ and using the estimates $\kappa_{2,i} = \mathcal{O}(1)$ from Lemma 6.1,

$$(151)\qquad \langle P_f\Gamma^2\Psi_2^\perp, P\Gamma^2\Psi_1^\perp\rangle| \leq \epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2 + c|\kappa_2|^2\alpha^2\|P\Gamma^0\Psi_1^\perp\|^2 + \mathcal{O}(\alpha^6).$$

We next bound the second term on the right hand side of (151). Notice that by definition of κ_2, this term is nonzero only if $\|\Gamma^0\Psi_1^\perp\|^2 > \alpha^3$, which implies, with Lemma 6.1, that $\|P\Gamma^0\Psi_1^\perp\|^2 \le c\alpha\|\Gamma^0\Psi_1^\perp\|^2$. The inequality (151) can thus be rewritten as

(152)
$$|\langle P.P_f\Gamma^2\Psi_2^\perp, \Gamma^2\Psi_1^\perp\rangle| \le \epsilon\|H_f^{\frac12}\Psi_2^\perp\|^2 + c|\kappa_2|^2\alpha^3\|\Gamma^0\Psi_1^\perp\|^2 + \mathcal{O}(\alpha^6) \le \epsilon\|H_f^{\frac12}\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5),$$

using in the last inequality that $|\kappa_2|\,\|\Gamma^0\Psi_1^\perp\| = \mathcal{O}(\alpha)$ (see Lemma 6.1).

For the second term on the right hand side of (149), using (212) from Lemma A.3 yields

$$\langle\Gamma^3 P_f\Psi_2^\perp, \Gamma^3 P\Psi_1^\perp\rangle \le \epsilon\|\Gamma^3 H_f^{\frac12}\Psi_2^\perp\|^2 + c\alpha^7\log\alpha^{-1}|\kappa_3|^2. \tag{153}$$

The inequalities (149), (152) and (153) prove the lemma. □

Lemma 6.7.

$$-4\alpha^{\frac12}\,\mathrm{Re}\,\langle P.A^+\Psi_2^\perp, \Psi_1^\perp\rangle \ge -\epsilon M[\Psi_2^\perp] + \mathcal{O}(\alpha^5).$$

Proof. Since $\Gamma^{n>3}\Psi_1^\perp = 0$, $\Gamma^0\Psi_2^\perp = 0$ and

$$\|H_f^{\frac12}\Gamma^{n\neq1}\Psi_1^\perp\|^2 \le 2\|H_f^{\frac12}\Gamma^{n\neq1}\Psi^\perp\|^2 + 2\|H_f^{\frac12}\Gamma^{n\neq1}\Psi_2^\perp\|^2 \le cM[\Psi_2^\perp] + \mathcal{O}(\alpha^4),$$

(see (69) of Theorem 5.2) we obtain

$$4\alpha^{\frac12}\,\mathrm{Re}\,\langle P.A^+\Psi_2^\perp, \Psi_1^\perp\rangle \le \epsilon\|\Gamma^{n\le2}P\Psi_2^\perp\|^2 + c\alpha\|\Gamma^{n\ge2}H_f^{\frac12}\Psi_1^\perp\|^2 \le \epsilon M[\Psi_2^\perp] + \mathcal{O}(\alpha^5)\ .$$

□

Lemma 6.8.

$$-4\alpha^{\frac12}\,\mathrm{Re}\,\langle P.A^-\Psi_2^\perp, \Psi_1^\perp\rangle \ge -\epsilon M[\Psi_2^\perp] + \mathcal{O}(\alpha^5).$$

Proof.

$$\begin{aligned}
&-4\alpha^{\frac12}\,\mathrm{Re}\,\langle P.A^-\Psi_2^\perp, \Psi_1^\perp\rangle \ge -\epsilon\|H_f^{\frac12}\Psi_2^\perp\|^2 - c\alpha\|P\Psi_1^\perp\|^2\\
&\ge -\epsilon\|H_f^{\frac12}\Psi_2^\perp\|^2 - c\alpha\left(\|\Gamma^{n=0,2,3,4}P\Psi^\perp\|^2 + \|\Gamma^{n=0,2,3,4}P\Psi_2^\perp\|^2\right) - c\alpha|\kappa_1|^2\|P\Phi_\sharp^{u_\alpha}\|^2\\
&\ge -\epsilon\|H_f^{\frac12}\Psi_2^\perp\|^2 - \epsilon\|\Gamma^{n\le4}P\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^6\log\alpha^{-1}) \ge -\epsilon M[\Psi_2^\perp] + \mathcal{O}(\alpha^6\log\alpha^{-1}),
\end{aligned}$$

using (212) of Lemma A.3. □

Lemma 6.9.

$$4\alpha^{\frac12}\,\mathrm{Re}\,\langle P_f.A(0)\Psi_2^\perp, \Psi_1^\perp\rangle \ge 4\alpha^{\frac12}\,\mathrm{Re}\,\langle\Gamma^2\Psi_2^\perp, P_f.A^+\Phi_*^{u_\alpha}\rangle - \epsilon M[\Psi_2^\perp] + \mathcal{O}(\alpha^5).$$

Proof. We have

$$\begin{aligned}
&4\alpha^{\frac12}\,\mathrm{Re}\,\langle P_f.A^-\Psi_2^\perp, \Psi_1^\perp\rangle\\
&\ge -\epsilon\|H_f^{\frac12}\Psi_2^\perp\|^2 - c\alpha\|\Gamma^{n\ge2}P_f\Psi_1^\perp\|^2 + 4\alpha^{\frac12}\,\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_2^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle\\
&\ge -\epsilon\|H_f^{\frac12}\Psi_2^\perp\|^2 - c\alpha\|\Gamma^{n=2,3}H_f^{\frac12}\Psi^\perp\|^2 + 4\alpha^{\frac12}\,\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_2^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle\\
&\ge -\epsilon M[\Psi_2^\perp] + 4\alpha^{\frac12}\,\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_2^\perp, \kappa_1\Phi_\sharp^{u_\alpha}\rangle + \mathcal{O}(\alpha^5).
\end{aligned}$$

We estimate the second term on the right hand side as follows,

$$\begin{aligned}&4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_2^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle\\&\geq 4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_2^\perp,\Phi_\sharp^{u_\alpha}\rangle-\epsilon\|H_f^{\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2-c\alpha|\kappa-1|^2\|P_f\Phi_\sharp^{u_\alpha}\|^2\\&\geq 4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_2^\perp,\Phi_*^{u_\alpha}\rangle-\epsilon\|H_f^{\frac{1}{2}}\Gamma^2\Psi_2^\perp\|^2+\mathcal{O}(\alpha^5),\end{aligned}$$

where we used $|\kappa_1-1|^2=\mathcal{O}(\alpha)$ from Lemma 6.1, $\|\Phi_\sharp^{u_\alpha}\|_*^2=\mathcal{O}(\alpha^3)$ from Lemma A.3, and $\|P_f(\Phi_\sharp^{u_\alpha}-\Phi_*^{u_\alpha})\|^2=\mathcal{O}(\alpha^4)$ from Lemma A.4.

We also have, using $P_f.A^+=A^+.P_f$,

$$\begin{aligned}&4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P_f.A^+\Psi_2^\perp,\Psi_1^\perp\rangle=4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle\Gamma^{n\leq 2}P_f\Psi_2^\perp,A^-\Gamma^{n\geq 2}\Psi_1^\perp\rangle\\&\geq-\epsilon\|H_f^{\frac{1}{2}}\Psi_2^\perp\|^2-c\alpha\|H_f^{\frac{1}{2}}\Gamma^{n\geq 2}\Psi_1^\perp\|^2\geq-\epsilon M[\Psi_2^\perp]+\mathcal{O}(\alpha^5),\end{aligned}$$

where $\|H_f^{\frac{1}{2}}\Gamma^{n\geq 2}\Psi_1^\perp\|$ has been estimated as $\|P\Psi_1^\perp\|$ in the proof of Lemma 6.8. □

6.3.2. *Estimates of the term* $\langle(H+e_0)\Psi_1^\perp,\Psi_1^\perp\rangle$.

Due to (139) and (140), one finds

$$\begin{aligned}&\langle(H+e_0)\Psi_1^\perp,\Psi_1^\perp\rangle=\langle\Psi_1^\perp,\Psi_1^\perp\rangle_\sharp-2\mathrm{Re}\,\langle P.(P_f+\alpha^{\frac{1}{2}}A(0))\Psi_1^\perp,\Psi_1^\perp\rangle\\&+2\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P_f.A(0)\Psi_1^\perp,\Psi_1^\perp\rangle+2\alpha\|A^-\Psi_1^\perp\|^2+2\alpha\mathrm{Re}\,\langle A^-.A^-\Psi_1^\perp,\Psi_1^\perp\rangle\end{aligned}\tag{154}$$

We estimate the terms in (154) below.

Lemma 6.10. *We have*

$$\begin{aligned}&-2\mathrm{Re}\,\langle P.(P_f+\alpha^{\frac{1}{2}}A(0))\Psi_1^\perp,\Psi_1^\perp\rangle\\&\geq-4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle A^-\Phi_\sharp^{u_\alpha},P\Gamma^0(\Psi_1^\perp)^s\rangle-\epsilon M[\Psi_2^\perp]-|\kappa_1-1|c\alpha^4+\mathcal{O}(\alpha^5),\end{aligned}$$

where $\Gamma^0(\Psi_1^\perp)^s=\Gamma^0\Psi_1^\perp-\Gamma^0(\Psi_1^\perp)^a$ *is the even part of* $\Gamma^0\Psi_1^\perp$.

Proof. Using $\langle\Phi_*^2,P_f^i\Phi_*^2\rangle=0$ (see Lemma A.1), the symmetry of u_α, and $\langle P.P_f\Phi_\sharp^{u_\alpha},\Phi_\sharp^{u_\alpha}\rangle=0$, we obtain

$$\begin{aligned}&|2\langle P.P_f\Psi_1^\perp,\Psi_1^\perp\rangle|=|2\langle P_f\alpha\kappa_2\Phi_*^2\Gamma^0\Psi_1^\perp,P\alpha\sum_{i=1}^3\kappa_{2,i}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\rangle|\\&\leq c\alpha^3|\kappa_2|^2\|\Gamma^0\Psi_1^\perp\|^2+c\alpha^5\sum_{i=1}^3|\kappa_{2,i}|^2=\mathcal{O}(\alpha^5),\end{aligned}\tag{155}$$

where in the last inequality we used Lemma 6.1.

We also have, using again the symmetry of u_α,

$$
\begin{aligned}
&-2\alpha^{\frac12}\mathrm{Re}\,\langle P.A(0)\Psi_1^\perp,\Psi_1^\perp\rangle = -4\alpha^{\frac12}\mathrm{Re}\,\langle P.A^-\Psi_1^\perp,\Psi_1^\perp\rangle\\
&= -4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\kappa_1\Phi_\sharp^{u_\alpha}, P\Gamma^0(\Psi_1^\perp)^s\rangle - 4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\kappa_2\alpha\Phi_*^2\Gamma^0\Psi_1^\perp, P\kappa_1\Phi_\sharp^{u_\alpha}\rangle\\
&-4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\Gamma^3\Psi_1^\perp, P\alpha\kappa_2\Phi_*^2\Gamma^0\Psi_1^\perp\rangle\\
&\geq -4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\kappa_1\Phi_\sharp^{u_\alpha}, P\Gamma^0(\Psi_1^\perp)^s\rangle - c\alpha\|H_f^{\frac12}\Gamma^3\Psi_1^\perp\|^2 - c\alpha^2\|P\Gamma^0\Psi_1^\perp\|^2|\kappa_2|^2\\
&-4\alpha^{\frac12}\mathrm{Re}\,\langle |k|^{-\frac16}A^-\kappa_2\alpha\Phi_*^2\Gamma^0\Psi_1^\perp, |k|^{\frac16}\kappa_1 P\Phi_\sharp^{u_\alpha}\rangle\\
&\geq -4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\kappa_1\Phi_\sharp^{u_\alpha}, P\Gamma^0(\Psi_1^\perp)^s\rangle - c\alpha\|H_f^{\frac12}\Gamma^3\Psi^\perp\|^2 - c\alpha\|H_f^{\frac12}\Gamma^3\Psi_2^\perp\|^2\\
&-c\alpha^5 - c\alpha^{\frac32}|\kappa_2|\,\|\Gamma^0\Psi_1^\perp\|\,\|\,|k|^{\frac16}P\Phi_\sharp^{u_\alpha}\|\\
&\geq -4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\kappa_1\Phi_\sharp^{u_\alpha}, P\Gamma^0(\Psi_1^\perp)^s\rangle - \epsilon M[\Psi_2^\perp] - c\alpha^5,
\end{aligned}
\tag{156}
$$

where we used Theorem 5.2 and Lemma A.3.

Moreover, because $\|A^-\Phi_*^{u_\alpha}\| = \mathcal{O}(\alpha^{\frac32})$ and $\|P\Gamma^0\Psi_1^\perp\| = \mathcal{O}(\alpha^2)$, we obtain

$$
-4\mathrm{Re}\,\alpha^{\frac12}\mathrm{Re}\,\langle A^-\kappa_1\Phi_\sharp^{u_\alpha}, P\Gamma^0(\Psi_1^\perp)^s\rangle \geq -4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\Phi_\sharp^{u_\alpha}, P\Gamma^0(\Psi_1^\perp)^s\rangle - |\kappa_1-1|c\alpha^4.
\tag{157}
$$

This estimate, together with (155) and (156), proves the lemma. □

Lemma 6.11. *We have*

$$
\begin{aligned}
&2\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A(0)\Psi_1^\perp,\Psi_1^\perp\rangle\\
&\geq \frac23\alpha^4\mathrm{Re}\sum_i \kappa_{2,i}\langle P_f.A^-(H_f+P_f^2)^{-1}W_i, (H_f+P_f^2)^{-1}(A^+)^i\Omega_f\rangle\\
&-|\kappa_1-1|c\alpha^4 + \mathcal{O}(\alpha^5).
\end{aligned}
$$

Proof. The following holds

$$
\begin{aligned}
&2\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A(0)\Psi_1^\perp,\Psi_1^\perp\rangle = 4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A^-\Gamma^3\Psi_1^\perp,\Gamma^2\Psi_1^\perp\rangle + 4\alpha\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle\\
&= 4\alpha^{\frac32}\mathrm{Re}\sum_{i=1}^3\overline{\kappa_{2,i}}\langle |k_1|^{\frac16}|k_2|^{\frac16}A^-\Gamma^3\Psi_1^\perp, P_f|k_1|^{-\frac16}|k_2|^{-\frac16}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\rangle\\
&+4\alpha^{\frac32}\mathrm{Re}\,\kappa_2\langle |k_1|^{\frac16}|k_2|^{\frac16}A^-\Gamma^3\Psi_1^\perp, |k_1|^{-\frac16}|k_2|^{-\frac16}P_f\Phi_*^2\Gamma^0\Psi_1^\perp\rangle\\
&+4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle.
\end{aligned}
\tag{158}
$$

Applying the Schwarz inequality and the estimates $\||k_1|^{\frac16}|k_2|^{\frac16}A^-\Gamma^3\Psi_1^\perp\|^2 = \mathcal{O}(\alpha^5)$ (Lemma A.5), $\kappa_{2,i} = \mathcal{O}(1)$ (Lemma 6.1), and $\|\nabla u_\alpha\|^2 = \mathcal{O}(\alpha^2)$, we see that the first term on the right hand side of (158) is $\mathcal{O}(\alpha^5)$. Applying also the estimate $|\kappa_2|\,\|\Gamma^0\Psi_1^\perp\| = \mathcal{O}(\alpha)$ (Lemma 6.1), we obtain that the second term on the right hand side of (158) is also $\mathcal{O}(\alpha^5)$.

Finally, we estimate $4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle$. The following inequality holds,

$$
4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle| \geq 4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp,\Phi_\sharp^{u_\alpha}\rangle - |\kappa_1-1|c\alpha^4,
\tag{159}
$$

whose proof is similar to the one of (157). Next we get

$$
\begin{aligned}
&|4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp,\Phi_\sharp^{u_\alpha}\rangle - 4\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp,\Phi_*^{u_\alpha}\rangle|\\
&\leq \alpha^{\frac12}\|H_f^{\frac12}\Gamma^2\Psi_1^\perp\|\,\|P_f(\Phi_\sharp^{u_\alpha}-\Phi_*^{u_\alpha})\| = \mathcal{O}(\alpha^6|\log\alpha|^{\frac12}),
\end{aligned}
\tag{160}
$$

using $\|P_f(\Phi_\sharp^{u_\alpha} - \Phi_*^{u_\alpha})\| = \mathcal{O}(\alpha^{\frac{7}{2}}|\log\alpha|^{\frac{1}{2}})$ (see Lemma A.4) and $\|H_f^{\frac{1}{2}}\Gamma^2\Psi_1^\perp\| = \mathcal{O}(\alpha^2)$. Moreover,

$$\begin{aligned}
&4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P_f.A^-\Gamma^2\Psi_1^\perp, \Phi_*^{u_\alpha}\rangle \\
&= 4\alpha^{\frac{3}{2}}\mathrm{Re}\,\langle P_f.A^-(\kappa_2\Phi_*^2\Gamma^0\Psi_1^\perp + \sum_i \kappa_{2,i}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}), \Phi_*^{u_\alpha}\rangle \\
&= 4\alpha^{\frac{3}{2}}\mathrm{Re}\,\langle P_f.A^-\sum_i \kappa_{2,i}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}, \Phi_*^{u_\alpha}\rangle \\
&= \frac{2}{3}\alpha^4\mathrm{Re}\sum_i \kappa_{2,i}\langle P_f.A^-(H_f+P_f^2)^{-1}W_i, (H_f+P_f^2)^{-1}(A^+)^i\Omega_f\rangle
\end{aligned} \tag{161}$$

where we used (207) of Lemma A.1 in the third equality.

Collecting (158)-(181) concludes the proof. □

Lemma 6.12. *We have*

$$\begin{aligned}
&\langle\Psi_1^\perp,\Psi_1^\perp\rangle_\sharp + 2\alpha\mathrm{Re}\,\langle A^-.A^-\Psi_1^\perp,\Psi_1^\perp\rangle \geq \Sigma_0\left(\|\Gamma^0\Psi_1^\perp\|^2 + \|\Gamma^1\Psi_1^\perp\|^2\right) \\
&+ \frac{\alpha^4}{12}\sum_{i=1}^3 |\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2 + \alpha^2|\kappa_3+1|^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2 \\
&+ \|\Gamma^1\Psi_1^\perp\|_\sharp^2 + \|\Gamma^0\Psi_1^\perp\|_\sharp^2 + o(\alpha^5\log\alpha^{-1}).
\end{aligned}$$

Proof. Obviously we have

$$\langle\Psi_1^\perp,\Psi_1^\perp\rangle_\sharp = \sum_{i=0}^3\langle\Gamma^i\Psi_1^\perp,\Gamma^i\Psi_1^\perp\rangle_\sharp, \tag{162}$$

and using Lemma A.1

$$\langle\Gamma^2\Psi_1^\perp,\Gamma^2\Psi_1^\perp\rangle_\sharp = \alpha^2|\kappa_2|^2\|\Phi_*^2\Gamma^0\Psi_1^\perp\|_\sharp^2 + \alpha^2\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\|_\sharp^2, \tag{163}$$

Moreover, from the inequality $\|\Phi_*^2\Gamma^0\Psi_1^\perp\|_\sharp^2 > \|\Phi_*^2\|_*^2\|\Gamma^0\Psi_1^\perp\|^2$ we obtain,

$$\begin{aligned}
&\alpha^2|\kappa_2|^2\|\Phi_*^2\Gamma^0\Psi_1^\perp\|_\sharp^2 + 2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^2\Psi_1^\perp,\Gamma^0\Psi_1^\perp\rangle \\
&\geq \alpha^2|\kappa_2|^2\|\Phi_*^2\|_*^2\|\Gamma^0\Psi_1^\perp\|^2 + 2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^2\Psi_1^\perp,\Gamma^0\Psi_1^\perp\rangle \\
&= \alpha^2|\kappa_2|^2\|\Phi_*^2\|_*^2\|\Gamma^0\Psi_1^\perp\|^2 - 2\alpha^2\mathrm{Re}\,\kappa_2\|\Phi_*^2\|_*^2\|\Gamma^0\Psi_1^\perp\|^2 \\
&+ 2\alpha\mathrm{Re}\sum_{i=1}^3\alpha\langle A^-.A^-\kappa_{2,i}(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i},\Gamma^0\Psi_1^\perp\rangle \\
&\geq \Sigma_0\|\Gamma^0\Psi_1^\perp\|^2 + |\kappa_2-1|^2c\alpha^2\|\Gamma^0\Psi_1^\perp\|^2 + \mathcal{O}(\alpha^5) \geq \Sigma_0\|\Gamma^0\Psi_1^\perp\|^2 + \mathcal{O}(\alpha^5).
\end{aligned} \tag{164}$$

where we used $\Sigma_0 = -\alpha^2\|\Phi_*^2\|_*^2 + \mathcal{O}(\alpha^3)$ and $\langle A^-.A^-(H_f+P_f^2)^{-1}W_i,\Gamma^0\Psi_1^\perp\rangle = -\overline{\Gamma^0\Psi_1^\perp}\langle W_i,\Phi_*^2\rangle = 0$.

Similarly $\|\Gamma^3\Psi_1^\perp\|_\sharp > \|\Gamma^3\Psi_1^\perp\|_*$ yields

(165)
$$\begin{aligned}&\|\Gamma^3\Psi_1^\perp\|_\sharp^2 + 2\alpha\mathrm{Re}\,\langle A^-.A^-\Gamma^3\Psi_1^\perp, \Gamma^1\Psi_1^\perp\rangle \geq \alpha^2|\kappa_3|^2\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|_*^2\\&+2\mathrm{Re}\,\alpha^2\kappa_3\langle A^-.A^-(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}, \kappa_1\Phi_\sharp^{u_\alpha}\rangle\\&\geq -\alpha^2\|(H_f+P_f^2)^{-1}A^+.A^+\kappa_1\Phi_\sharp^{u_\alpha}\|_*^2 + |\kappa_3+1|^2\alpha^2\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|_*^2\\&\geq \Sigma_0\|\Gamma^1\Psi_1^\perp\|^2 + \alpha^2|\kappa_3+1|^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2 + o(\alpha^5\log\alpha^{-1}),\end{aligned}$$

where in the last inequality, we used (222) from Lemma A.5, $\kappa_1 = 1+\mathcal{O}(\alpha^{\frac12})$ from Lemma 6.1, $\|\Phi_\sharp^{u_\alpha}\|^2 = \mathcal{O}(\alpha^3\log\alpha^{-1})$ from Lemma A.3 and $-\alpha^2\|\Phi_*^2\|_*^2 = \Sigma_0 + \mathcal{O}(\alpha^3)$.

The second term on the right hand side of (163) is estimated as

(166)
$$\begin{aligned}&\alpha^2\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\|_\sharp^2 \geq \alpha^2\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\|_*^2\\&=\alpha^2\frac13\|\nabla u_\alpha\|^2\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2 = \frac{\alpha^4}{12}\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2.\end{aligned}$$

Collecting (162)-(166) conclude the proof. □

Proposition 6.4. *We have*

$$\begin{aligned}&\langle(H+e_0)\Psi_1^\perp,\Psi_1^\perp\rangle\\&\geq -4\alpha\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2 + \|(h_\alpha+e_0)^{\frac12}\Gamma^0(\Psi_1^\perp)^a\|^2\\&+c_0\alpha\|(h_\alpha+e_0)^{\frac12}\Gamma^0(\Psi_1^\perp)^s\|^2 + \Sigma_0(\|\Gamma^0\Psi_1^\perp\|^2+\|\Gamma^1\Psi_1^\perp\|^2)\\&+\frac{\alpha^4}{12}\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2 + 4\alpha^{\frac12}\mathrm{Re}\,\langle\Gamma^2\Psi_1^\perp, A^+.P_f\Phi_\sharp^{u_\alpha}\rangle\\&+\|\kappa_1\Phi_\sharp^{u_\alpha}\|_\sharp^2 + 2\alpha\|A^-\Phi_*^{u_\alpha}\|^2 + \alpha^2|\kappa_3+1|^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2\\&-\epsilon M[\Psi_2^\perp] - |\kappa_1-1|c\alpha^4 + o(\alpha^5\log\alpha^{-1}),\end{aligned}\tag{167}$$

where $Q_\alpha^\perp$ *is the orthogonal projection onto* $\mathrm{Span}(u_\alpha)^\perp$*,* $(\Psi_1^\perp)^a$ *is the odd part of* $\Gamma^0\Psi_1^\perp$*, and* c_0 *is the same positive constant as in Proposition 6.3.*

Proof. Collecting Lemmata 6.10, 6.11, and 6.12 yields

(168)
$$\begin{aligned}&\langle(H+e_0)\Psi_1^\perp,\Psi_1^\perp\rangle \geq -4\alpha^{\frac12}\mathrm{Re}\,\langle A^-\Phi_\sharp^{u_\alpha}, P\Gamma^0(\Psi_1^\perp)^s\rangle + 4\alpha\mathrm{Re}\,\langle\Gamma^2\Psi_1^\perp, A^+.P_f\Phi_\sharp^{u_\alpha}\rangle\\&+\Sigma_0(\|\Gamma^0\Psi_1^\perp\|^2+\|\Gamma^1\Psi_1^\perp\|^2) + \alpha^2|\kappa_3+1|^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2\\&+\|(h_\alpha+e_0)^{\frac12}\Gamma^0\Psi_1^\perp\|^2 + \|\Gamma^1\Psi_1^\perp\|_\sharp^2 + 2\alpha\|A^-\kappa_1\Phi_\sharp^{u_\alpha}\|^2 - |\kappa_1-1|c\alpha^4\\&+\frac{\alpha^4}{12}\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2 - \epsilon M[\Psi_2^\perp] + o(\alpha^5\log\alpha^{-1}).\end{aligned}$$

Obviously,

$$\|(h_\alpha+e_0)^{\frac12}\Gamma^0\Psi_1^\perp\|^2 = \|(h_\alpha+e_0)^{\frac12}\Gamma^0(\Psi_1^\perp)^s\|^2 + \|(h_\alpha+e_0)^{\frac12}\Gamma^0(\Psi_1^\perp)^a\|^2.\tag{169}$$

As before, we write $\Gamma^0\Psi_1^\perp$ as the sum of its odd part $(\Psi_1^\perp)^a$ and its even part $(\Psi_1^\perp)^s$. Since $\Gamma^0\Psi_1^\perp$ is orthogonal to u_α by definition of $\Psi^\perp$, and $(\Psi_1^\perp)^a$ is orthogonal to u_α by symmetry of u_α, we also have $(\Psi_1^\perp)^s$ orthogonal to u_α. Therefore, one can replace $\Gamma^0(\Psi_1^\perp)^s$ by $Q_\alpha^\perp\Gamma^0(\Psi_1^\perp)^s$ in (168) and (169). Thus, as the next step, given a constant $c_0 > 0$, we minimize

$$(170)\quad \begin{aligned}&(1-c_0\alpha)\|(h_\alpha+e_0)^{\frac12}Q_\alpha^\perp\Gamma^0(\Psi_1^\perp)^s\|^2 - 4\alpha^{\frac12}\mathrm{Re}\,\langle Q_\alpha^\perp P.A^-\Phi_\sharp^{u_\alpha}, Q_\alpha^\perp\Gamma^0(\Psi_1^\perp)^s\rangle\\ &\geq -\frac{4\alpha}{1-c_0\alpha}\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_\sharp^{u_\alpha}\|^2.\end{aligned}$$

Obviously,

$$(171)\quad \begin{aligned}&-\frac{4\alpha}{1-c_0\alpha}\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_\sharp^{u_\alpha}\|^2\\ &\geq -\frac{4(1+\alpha)\alpha}{1-c_0\alpha}\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2\\ &\quad -\frac{4(1+\alpha^{-1})\alpha}{1-c_0\alpha}\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-(\Phi_\sharp^{u_\alpha}-\Phi_*^{u_\alpha})\|^2.\end{aligned}$$

There exist γ_1 and γ_2 positive, independent of α, such that

$$Q_\alpha^\perp(h_\alpha+e_0)^{-1}Q_\alpha^\perp \leq (\gamma_1 P^2+\gamma_2\alpha^2)^{-1},$$

and thus $PQ_\alpha^\perp(h_\alpha+e_0)^{-1}Q_\alpha^\perp P$ is a bounded operator. In addition, since $\|A^-(\Phi_\sharp^{u_\alpha} - \Phi_*^{u_\alpha})\|^2 = \mathcal{O}(\alpha^7\log\alpha^{-1})$ (Lemma A.3), this shows that

$$(172)\quad \frac{4(1+\alpha^{-1})\alpha}{1-c_0\alpha}\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-(\Phi_\sharp^{u_\alpha}-\Phi_*^{u_\alpha})\|^2 = \mathcal{O}(\alpha^6\log\alpha^{-1}).$$

In addition, using $\|A^-\Phi_*^{u_\alpha}\| \leq \|A^-(\Phi_*^{u_\alpha}-\Phi_\sharp^{u_\alpha})\| + \|A^-\Phi_\sharp^{u_\alpha}\| \leq c\alpha^{\frac32}$ (Lemma A.3 and Lemma A.4), and the fact that $PQ_\alpha^\perp(h_\alpha+e_0)^{-1}Q_\alpha^\perp P$ is bounded, yields

$$(173)\quad \begin{aligned}&-\frac{(1+\alpha)\alpha}{1-c_0\alpha}\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2\\ &= -4\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2 + \mathcal{O}(\alpha^5).\end{aligned}$$

Collecting (171)-(173), one gets

$$(174)\quad -\frac{4\alpha}{1-c_0\alpha}\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_\sharp^{u_\alpha}\|^2 \geq -4\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2 + \mathcal{O}(\alpha^5).$$

Finally, using $\|A^-\Phi_*^{u_\alpha}\|^2 = \mathcal{O}(\alpha^3)$, we obtain

$$(175)\quad 2\alpha|\kappa_1|^2\|A^-\Phi_*^{u_\alpha}\|^2 \geq 2\alpha\|A^-\Phi_*^{u_\alpha}\|^2 - c|\kappa_1-1|\alpha^4.$$

Substituting (169), (170), (174) and (175) into (168) concludes the proof. □

We can now write the proof of Proposition 6.2

Proof of Proposition 6.2 Collecting the results of Proposition 6.3, Lemmata 6.5-6.9 and Proposition 6.4 yields directly the following bound,

(176)
$$\langle H\Psi^\perp,\Psi^\perp\rangle \geq \langle H\Psi_2^\perp,\Psi_2^\perp\rangle - \epsilon M[\Psi_2^\perp] - c|\kappa_2|^2\alpha^4\|\Gamma^0\Psi_1^\perp\|^2 - c\alpha^6\log\alpha^{-1}|\kappa_3|^2 - e_0\|\Psi_1^\perp\|^2$$
$$- 4\alpha\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2 + (1-c_0\alpha)\|(h_\alpha+e_0)^{\frac12}\Gamma^0(\Psi_1^\perp)^a\|^2$$
$$+ \Sigma_0(\|\Gamma^0\Psi_1^\perp\|^2 + \|\Gamma^1\Psi_1^\perp\|^2) + \frac{\alpha^4}{12}\sum_{i=1}^3|\kappa_{2,i}|^2\|(H_f+P_f^2)^{-1}W_i\|_*^2$$
$$+ 4\alpha^{\frac12}\mathrm{Re}\,\langle\Gamma^2\Psi_2^\perp, A^+.P_f\Phi_*^{u_\alpha}\rangle + 4\alpha^{\frac12}\mathrm{Re}\,\langle\Gamma^2\Psi_1^\perp, A^+.P_f\Phi_\sharp^{u_\alpha}\rangle + |\kappa_1|^2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 + 2\alpha\|A^-\Phi_*^{u_\alpha}\|^2$$
$$+ \alpha^2|\kappa_3+1|^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2 - |\kappa_1-1|c\alpha^4 + o(\alpha^5\log\alpha^{-1}).$$

Comparing this expression with the statement of the Proposition we see that it suffices to show that

(177)
$$- \epsilon M[\Psi_2^\perp] - c|\kappa_2|^2\alpha^4\|\Gamma^0\Psi_1^\perp\|^2 - c\alpha^6\log\alpha^{-1}|\kappa_3|^2 - e_0\|\Psi_1^\perp\|^2 + \langle H\Psi_2^\perp,\Psi_2^\perp\rangle$$
$$+ \Sigma_0(\|\Gamma^0\Psi_1^\perp\|^2 + \|\Gamma^1\Psi_1^\perp\|^2) + \alpha^2|\kappa_3+1|^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2$$
$$\geq (\Sigma_0-e_0)\|\Psi^\perp\|^2 + (1-\epsilon)M[\Psi_2^\perp] + \frac{|\kappa_3+1|^2}{2}\alpha^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2 + \mathcal{O}(\alpha^5).$$

Using from Corollary 4.2 that $\langle H\Psi_2^\perp,\Psi_2^\perp\rangle \geq (\Sigma_0-e_0)\|\Psi_2^\perp\|^2 + M[\Psi_2^\perp]$, we first estimate the following terms in (177),

$$\begin{aligned}&\Sigma_0\left(\|\Gamma^0\Psi_1^\perp\|^2 + \|\Gamma^1\Psi_1^\perp\|^2\right) - e_0\|\Psi_1^\perp\|^2 + \langle H\Psi_2^\perp,\Psi_2^\perp\rangle - \epsilon M[\Psi_2^\perp]\\ &\geq (1-\epsilon)M[\Psi_2^\perp] + (\Sigma_0-e_0)(\|\Psi_1^\perp\|^2 + \|\Psi_2^\perp\|^2) - \Sigma_0\|\Gamma^{n\geq 2}\Psi_1^\perp\|^2\\ &\geq (1-\epsilon)M[\Psi_2^\perp] + (\Sigma_0-e_0)\|\Psi^\perp\|^2\\ &- (\Sigma_0-e_0)(\|\Psi^\perp\|^2 - \|\Psi_1^\perp\|^2 - \|\Psi_2^\perp\|^2) - \Sigma_0\|\Gamma^{n\geq 2}\Psi_1^\perp\|^2.\end{aligned} \tag{178}$$

We have obviously

(179)
$$\|\Psi^\perp\|^2 - \|\Psi_1^\perp\|^2 - \|\Psi_2^\perp\|^2 = 2\mathrm{Re}\,(\langle\Gamma^1\Psi_1^\perp,\Gamma^1\Psi_2^\perp\rangle + \langle\Gamma^2\Psi_1^\perp,\Gamma^2\Psi_2^\perp\rangle + \langle\Gamma^3\Psi_1^\perp,\Gamma^3\Psi_2^\perp\rangle).$$

Since $|\Sigma_0-e_0|\leq c\alpha^2$, by definition of $\Gamma^3\Psi_1^\perp$ and Lemma A.5, we obtain

(180)
$$|(\Sigma_0-e_0)2\mathrm{Re}\,\langle\Gamma^3\Psi_1^\perp,\Gamma^3\Psi_2^\perp\rangle| \leq \epsilon\alpha^2\|\Gamma^3\Psi_2^\perp\|^2 + c\alpha^4|\kappa_3|^2\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|^2$$
$$\leq \epsilon\alpha^2\|\Gamma^3\Psi_2^\perp\|^2 + c|\kappa_3|^2\alpha^7\log\alpha^{-1}.$$

Similarly, for the two-photon sector, we find

(181)
$$|(\Sigma_0-e_0)\langle\Gamma^2\Psi_1^\perp,\Gamma^2\Psi_2^\perp\rangle| \leq \epsilon\alpha^2\|\Gamma^2\Psi_2^\perp\|^2 + c\alpha^4|\kappa_2|^2\|\Gamma^0\Psi_1^\perp\|^2 + c\sum_{i=1}^3|\kappa_{2,i}|^2\alpha^6$$
$$= \epsilon\alpha^2\|\Gamma^2\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^6),$$

where we used Lemma 6.1. For the term $\langle\Gamma^1\Psi_1^\perp,\Gamma^1\Psi_2^\perp\rangle$, one gets

$$\begin{aligned}&|(\Sigma_0-e_0)\langle\Gamma^1\Psi_2^\perp,\kappa_1\Phi_\sharp^{u_\alpha}\rangle| = |(\Sigma_0-e_0)(|k|^{\frac12}\Gamma^1\Psi_2^\perp, |k|^{-\frac12}\kappa_1\Phi_\sharp^{u_\alpha}\rangle|\\ &\leq \epsilon\|H_f^{\frac12}\Gamma^1\Psi_2^\perp\|^2 + c\alpha^4|\kappa_1|^2\|\,|k|^{-\frac12}\Phi_\sharp^{u_\alpha}\|^2 \leq \epsilon\|H_f^{\frac12}\Gamma^1\Psi_2^\perp\|^2 + \mathcal{O}(\alpha^5),\end{aligned} \tag{182}$$

since $\| \, |k|^{-\frac{1}{2}} \Phi_\sharp^{u_\alpha} \|^2 = \mathcal{O}(\alpha)$ (Lemma A.3) and $\kappa_1 = \mathcal{O}(1)$ (Lemma 6.1).

Collecting (179), (180), (181) and (182) yields

$$|\Sigma_0 - e_0| \, \left| \, \|\Psi^\perp\|^2 - \|\Psi_1^\perp\|^2 - \|\Psi_2^\perp\|^2 \right| \le \epsilon M[\Psi_2^\perp] + c|\kappa_3|^2 \alpha^7 \log \alpha^{-1} + \mathcal{O}(\alpha^5). \tag{183}$$

Therefore, together with (178), one finds

(184)

$$\begin{aligned} &\Sigma_0 \left(\|\Gamma^0 \Psi_1^\perp\|^2 + \|\Gamma^1 \Psi_1^\perp\|^2 \right) - e_0 \|\Psi_1^\perp\|^2 + \langle H\Psi_2^\perp, \Psi_2^\perp \rangle - \epsilon M[\Psi_2^\perp] \\ &\ge (1 - 2\epsilon) M[\Psi_2^\perp] + (\Sigma_0 - e_0)\|\Psi^\perp\|^2 - c|\kappa_3|^2 \alpha^7 \log \alpha^{-1} - \Sigma_0 \|\Gamma^{n \ge 2} \Psi_1^\perp\|^2 + \mathcal{O}(\alpha^5), \end{aligned}$$

By definition of $\Psi_1^\perp$ and using $\Sigma_0 = \mathcal{O}(\alpha^2)$, $|\kappa_2| \|\Gamma^0 \Psi_1^\perp\| = \mathcal{O}(\alpha)$ (Lemma 6.1) and Inequality (223) of Lemma A.5, we straightforwardly obtain

$$\Sigma_0 \|\Gamma^{n \ge 2} \Psi_1^\perp\|^2 \le c\alpha^6 + c|\kappa_3|^2 \alpha^7 \log \alpha^{-1}.$$

Substituting this in (184) yields

$$\begin{aligned} &\Sigma_0 \left(\|\Gamma^0 \Psi_1^\perp\|^2 + \|\Gamma^1 \Psi_1^\perp\|^2 \right) - e_0 \|\Psi_1^\perp\|^2 + \langle H\Psi_2^\perp, \Psi_2^\perp \rangle - \epsilon M[\Psi_2^\perp] \\ &\ge (1 - 2\epsilon) M[\Psi_2^\perp] + (\Sigma_0 - e_0)\|\Psi^\perp\|^2 - 2c|\kappa_3|^2 \alpha^7 \log \alpha^{-1} + \mathcal{O}(\alpha^5). \end{aligned} \tag{185}$$

To conclude the proof of (177), and thus of the Proposition, we first note that according to Lemma 6.1,

$$-c|\kappa_2|^2 \alpha^4 \|\Gamma^0 \Psi_1^\perp\|^2 = \mathcal{O}(\alpha^6). \tag{186}$$

Similarly, taking into account that $\|\Phi_\sharp^{u_\alpha}\|^2 = c\alpha^3 \log \alpha^{-1}$ (see (209) in Lemma A.3), we get for some $c_2 > 0$,

(187)

$$\alpha^2 \frac{|\kappa_3 + 1|^2}{2} \|\Phi_*^2\|_*^2 \|\Phi_\sharp^{u_\alpha}\|^2 - c\alpha^6 \log \alpha^{-1} |\kappa_3|^2 - 2c\alpha^7 \log \alpha^{-1} |\kappa_3|^2 \ge -c_2 \alpha^6 \log \alpha^{-1}.$$

Collecting (185), (186) and (187) yields the bound (177), and thus concludes the proof of the Proposition 6.2. □

6.4. **Lower bound up to the order $\alpha^5 \log \alpha^{-1}$ for the binding energy.** To get a lower bound for $\Sigma_0 - \Sigma$ in Theorem 2.1 which coincides with the upper bound given in (97), it suffices to compute

$$\frac{\langle (H - \Sigma_0 + e_0) \widetilde{\Phi}^{\mathrm{trial}}, \ \widetilde{\Phi}^{\mathrm{trial}} \rangle}{\|\widetilde{\Phi}^{\mathrm{trial}}\|^2},$$

with the following trial function

$$\widetilde{\Phi}^{\mathrm{trial}} = u_\alpha \Psi_0 + \widetilde{\Psi}_0^\perp,$$

where Ψ_0 is ground state of the operator $T(0)$ with the normalization $\Gamma^0 \Psi_0 = \Omega_f$, u_α is the normalized ground state of $h_\alpha = -\Delta - \frac{\alpha}{|x|}$, and $\widetilde{\Psi}_0^\perp$ is defined by

$$\begin{aligned} &\Gamma^0 \widetilde{\Psi}_0^\perp = 2\alpha^{\frac{1}{2}} (h_\alpha + e_0)^{-1} Q_\alpha^\perp P.A^- \Phi_*^{u_\alpha}, \ \Gamma^1 \widetilde{\Psi}_0^\perp = \Phi_\sharp^{u_\alpha}, \\ &\Gamma^2 \widetilde{\Psi}_0^\perp = \alpha \Phi_*^2 \Gamma^0 \widetilde{\Psi}_0^\perp + \sum_{i=1}^3 2\alpha (H_f + P_f^2)^{-1} W_i \frac{\partial u_\alpha}{\partial x_i}, \\ &\Gamma^3 \widetilde{\Psi}_0^\perp = -\alpha (H_f + P_f^2)^{-1} A^+ . A^+ \Phi_\sharp^{u_\alpha}. \end{aligned} \tag{188}$$

Where $\Phi_*^{u_\alpha}$, $\Phi_\sharp^{u_\alpha}$, Φ_*^2 and W_i are defined as in Sections 5 and 6.

We compute

$$\langle H\widetilde{\Phi}^{\mathrm{trial}},\widetilde{\Phi}^{\mathrm{trial}}\rangle = \langle Hu_\alpha\Psi_0, u_\alpha\Psi_0\rangle + 2\mathrm{Re}\,\langle Hu_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle + \langle H\widetilde{\Psi}_0^\perp,\widetilde{\Psi}_0^\perp\rangle, \tag{189}$$

and we recall

$$H = h_\alpha + (H_f+P_f^2) - 2\mathrm{Re}\,P.P_f - 2\alpha^{\frac12}P.A(0) + 2\alpha^{\frac12}P_f.A(0) + 2\alpha A^+.A^- + 2\alpha(A^-)^2. \tag{190}$$

• For the first term in (189), a straightforward computation shows

$$\langle Hu_\alpha\Psi_0, u_\alpha\Psi_0\rangle = (\Sigma_0 - e_0)\|u_\alpha\|^2\|\Psi_0\|^2. \tag{191}$$

• We estimate the second term on the right hand side of (189) by computing each term that occurs in the decomposition (190).

⋄ Using the symmetry of u_α, the only non zero terms in $2\mathrm{Re}\,\langle Hu_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle$ are given by

$$2\mathrm{Re}\,\langle Hu_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle = -4\mathrm{Re}\,\langle P.P_f u_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle - 4\mathrm{Re}\,\langle P.A^+u_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle - 4\mathrm{Re}\,\langle P.A^-u_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle. \tag{192}$$

⋄ The first term on the right hand side of (192) is estimated with similar arguments as in Lemma 5.2, and using $\|\Delta_*^{u_\alpha}\|^2 = \mathcal{O}(\alpha^3)$ (Lemma A.7) and $\|\Delta_*^{u_\alpha}\|_*^2 = \mathcal{O}(\alpha^4)$ ([4, Theorem 3.2]). We obtain

$$-4\mathrm{Re}\,\langle P.P_f u_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle = -\frac{2}{3}\alpha^4\sum_{i=1}^3\langle P_f^i\Phi_*^2,(H_f+P_f^2)W_i\rangle + \mathcal{O}(\alpha^5\sqrt{\log\alpha^{-1}}). \tag{193}$$

⋄ The second and third terms on the right hand side of (192) are estimated as in Lemma 5.3, and using again $\|\Delta_*^{u_\alpha}\|^2 = \mathcal{O}(\alpha^2)$ and $\|\Delta_*^{u_\alpha}\|_*^2 = \mathcal{O}(\alpha^4)$. This yields

$$-4\mathrm{Re}\,\langle P.A^+u_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle = -2\|\Phi_\sharp^{u_\alpha}\|_\sharp^2 + o(\alpha^5\log\alpha^{-1}), \tag{194}$$

and

$$\begin{aligned} &-4\mathrm{Re}\,\langle P.A^-u_\alpha\Psi_0,\widetilde{\Psi}_0^\perp\rangle \\ &= -\frac{2}{3}\alpha^4\sum_{i=1}^3\langle (A^-)^i\Phi_*^2,(H_f+P_f^2)^{-1}(A^+)^i\Omega_f\rangle + \mathcal{O}(\alpha^5\sqrt{\log\alpha^{-1}}). \end{aligned} \tag{195}$$

• Next, we estimate the third term on the right hand side of (189). For that sake, we also use the decomposition (190) for H.

⋄ For the term involving h_α, using $\|(h_\alpha+e_0)\Gamma^0\widetilde{\Psi}_0^\perp\| = \mathcal{O}(\alpha^3)$ (since $\|P.A^-\Phi_*^{u_\alpha}\| = \mathcal{O}(\alpha^{\frac52})$), and $\|(h_\alpha+e_0)\frac{\partial u_\alpha}{\partial x_i}\| = \mathcal{O}(\alpha^3)$, we directly obtain

$$\begin{aligned} &\langle h_\alpha\widetilde{\Psi}_0^\perp,\widetilde{\Psi}_0^\perp\rangle = \langle (h_\alpha+e_0)\widetilde{\Psi}_0^\perp,\widetilde{\Psi}_0^\perp\rangle - e_0\|\widetilde{\Psi}_0^\perp\|^2 \\ &= 4\alpha\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2 + \langle (h_\alpha+e_0)\Phi_\sharp^{u_\alpha},\Phi_\sharp^{u_\alpha}\rangle - e_0\|\widetilde{\Psi}_0^\perp\|^2 + \mathcal{O}(\alpha^5). \end{aligned} \tag{196}$$

⋄ For the term with $H_f + P_f^2$, we use the estimate (222) of Lemma A.5, and the $\langle\,\cdot\,,\,\cdot\,\rangle_*$-orthogonality (see (206) of Lemma A.1) of the two vectors $\alpha\Phi_*^2\Gamma^0 g$ and $\sum_{i=1}^3 2\alpha(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}$ that occur in $\Gamma^2\widetilde{\Psi}_0^\perp$. We therefore obtain

$$\begin{aligned} &\langle (H_f+P_f^2)\widetilde{\Psi}_0^\perp,\widetilde{\Psi}_0^\perp\rangle = \langle (H_f+P_f^2)\Phi_\sharp^{u_\alpha},\Phi_\sharp^{u_\alpha}\rangle + \alpha^2\|\Phi_*^2\Gamma^0\widetilde{\Psi}_0^\perp\|_*^2 \\ &+ \|\sum_{i=1}^3 2\alpha(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\|_*^2 + \|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2 + o(\alpha^5\log\alpha^{-1}). \end{aligned} \tag{197}$$

⋄ Using the symmetry of u_α, all terms in $\mathrm{Re}\,\langle P.P_f\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle$ are zero, except the expression $\mathrm{Re}\,\langle P.P_f\Gamma^2 g, \Gamma^2\widetilde{\Psi}_0^\perp\rangle$, which is estimated as follows

$$\mathrm{Re}\,\langle P.P_f\Gamma^2\widetilde{\Psi}_0^\perp, \Gamma^2\widetilde{\Psi}_0^\perp\rangle = 2\mathrm{Re}\,\langle P.P_f\alpha\Phi_*^2\Gamma^0\widetilde{\Psi}_0^\perp, \sum_{i=1}^3 2\alpha(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\rangle = \mathcal{O}(\alpha^5),$$

where we used Lemma A.1 in the third equality to prove that only the crossed term remains. Therefore, we obtain

$$-2\mathrm{Re}\,\langle P.P_f\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle = \mathcal{O}(\alpha^5). \tag{198}$$

⋄ The terms involving $-2\alpha^{\frac12}\mathrm{Re}\,\langle P.A(0)\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle$ is estimated as in the proof of Lemma 6.10. This yields

$$\begin{aligned} &-2\alpha^{\frac12}\langle P.A(0)\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle = -4\mathrm{Re}\,\alpha^{\frac12}\langle P.A^+\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle \\ &= -4\mathrm{Re}\,\langle P.A^+\Gamma^0\widetilde{\Psi}_0^\perp, \Gamma^1\widetilde{\Psi}_0^\perp\rangle + \mathcal{O}(\alpha^5\sqrt{\log\alpha^{-1}}) \\ &= -8\alpha\|(h_\alpha+e_0)^{-\frac12}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2 + \mathcal{O}(\alpha^5\sqrt{\log\alpha^{-1}}). \end{aligned} \tag{199}$$

⋄ For $2\alpha^{\frac12}\mathrm{Re}\,\langle P_f.A(0)\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle$, we proceed as in the proof of Lemma 6.11, and obtain

$$\begin{aligned} &2\alpha^{\frac12}\langle P_f.A(0)\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle = 4\mathrm{Re}\,\alpha^{\frac12}\langle P_f.A^-\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle \\ &= 4\alpha^{\frac12}\langle P_f.A^-\alpha\sum_{i=1}^3 2(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}, \Phi_*^{u_\alpha}\rangle + \mathcal{O}(\alpha^5\sqrt{\log\alpha^{-1}}). \end{aligned} \tag{200}$$

⋄ Using the symmetry of u_α and $\Gamma^0 g$, the term $2\alpha\mathrm{Re}\,\langle A^-.A^-\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle$ is estimated as follows,

$$\begin{aligned} &2\alpha\mathrm{Re}\,\langle A^-.A^-\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle \\ &= 2\alpha\mathrm{Re}\,\langle A^-.A^-(\alpha\Phi_*^2\Gamma^0\widetilde{\Psi}_0^\perp + \sum_{i=1}^3 2\alpha(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}), \Gamma^0\widetilde{\Psi}_0^\perp\rangle \\ &+ 2\alpha\mathrm{Re}\,\langle A^-.A^-(-\alpha(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}), \Phi_\sharp^{u_\alpha}\rangle \\ &= -2\alpha^2\|\Gamma^0\widetilde{\Psi}_0^\perp\|^2\|\Phi_*^2\|_*^2 - 2\alpha^2\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|^2 \\ &= -2\alpha^2\|\Gamma^0\widetilde{\Psi}_0^\perp\|^2\|\Phi_*^2\|_*^2 - 2\alpha^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2 + o(\alpha^5\log\alpha^{-1}), \end{aligned} \tag{201}$$

where in the last inequality we used (222) of Lemma A.5.

⋄ Finally, a straightforward computation yields

$$2\alpha\mathrm{Re}\,\langle A^-.A^+\widetilde{\Psi}_0^\perp, \widetilde{\Psi}_0^\perp\rangle = 2\alpha\|A^-\Phi_\sharp^{u_\alpha}\|^2 + \mathcal{O}(\alpha^5) = 2\alpha\|A^-\Phi_*^{u_\alpha}\|^2 + \mathcal{O}(\alpha^5), \tag{202}$$

where in the last equality, we used Lemma A.4.

• Before collecting (192)-(202), we show that gathering some terms yields simpler expressions. Namely, we have

$$\begin{aligned} &-\frac23\alpha^4\sum_{i=1}^3\langle P_f^i\Phi_*^2, (H_f+P_f^2)W_i\rangle + 4\alpha^{\frac12}\langle P_f.A^-\alpha\sum_{i=1}^3 2(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}, \Phi_*^{u_\alpha}\rangle \\ &+\|\sum_{i=1}^3 2\alpha(H_f+P_f^2)^{-1}W_i\frac{\partial u_\alpha}{\partial x_i}\|_*^2 = -\frac13\alpha^4\sum_{i=1}^3\|(H_f+P_f^2)^{-1}W_i\|_*^2. \end{aligned} \tag{203}$$

We also have, using $-\alpha^2\|\Phi_*^2\|_*^2 = \Sigma_0 + \mathcal{O}(\alpha^3)$ (see e.g. [4])

$$\begin{aligned}(\Sigma_0 - e_0)\|\Psi_0\|^2 - e_0\|\widetilde{\Psi}_0^\perp\|^2 - \alpha^2\|\Phi_*^2\|_*^2\|\Gamma^0\widetilde{\Psi}_0^\perp\|^2 - \alpha^2\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2 \\ = (\Sigma_0 - e_0)(\|\Psi_0\|^2 + \|\widetilde{\Psi}_0^\perp\|^2) + \mathcal{O}(\alpha^5).\end{aligned} \tag{204}$$

Therefore, collecting (192)-(202), and using the two equalities (203)-(204), we obtain

$$\begin{aligned}&\langle H(u_\alpha\Psi_0 + g), u_\alpha\Psi_0 + \widetilde{\Psi}_0^\perp\rangle = (\Sigma_0 - e_0)(\|\Psi_0\|^2 + \|\widetilde{\Psi}_0^\perp\|^2) - \frac{1}{3}\alpha^4\sum_{i=1}^3\|(H_f + P_f^2)^{-1}W_i\|_*^2 \\ &- \frac{2}{3}\alpha^4\sum_{i=1}^3\langle (A^-)^i\Phi_*^2, (H_f + P_f^2)^{-1}(A^+)^i\Omega_f\rangle - \|\Phi_\sharp^{u_\alpha}\|_\sharp^2 - 4\alpha\|(h_\alpha + e_0)^{-\frac{1}{2}}Q_\alpha^\perp P.A^-\Phi_*^{u_\alpha}\|^2 \\ &+ 2\alpha\|A^-\Phi_*^{u_\alpha}\|^2 + o(\alpha^5\log\alpha^{-1}).\end{aligned}$$

With the definition $e^{(1)}$, $e^{(2)}$, and $e^{(3)}$, of Theorem 2.1 this expression can be rewritten as

$$\langle (H - \Sigma_0 + e_0)\widetilde{\Phi}^{\mathrm{trial}},\ \widetilde{\Phi}^{\mathrm{trial}}\rangle = e^{(1)}\alpha^3 + e^{(2)}\alpha^4 + e^{(3)}\alpha^5\log\alpha^{-1} + o(\alpha^5\log\alpha^{-1}). \tag{205}$$

Using Lemma A.7 yields $\|\Psi_0\|^2 = 1+\mathcal{O}(\alpha^2)$, which implies, due to the orthogonality of $\widetilde{\Psi}_0^\perp$ and u_α in $L^2(\mathbb{R}^3, \mathrm{d}x)$,

$$\|\widetilde{\Phi}^{\mathrm{trial}}\|^2 = \|u_\alpha\|^2\|\Psi_0\|^2 + \|\widetilde{\Psi}_0^\perp\|^2 = 1 + \mathcal{O}(\alpha^2).$$

Therefore, together with (205), this gives

$$\frac{\langle (H - \Sigma_0 + e_0)\widetilde{\Phi}^{\mathrm{trial}},\ \widetilde{\Phi}^{\mathrm{trial}}\rangle}{\|\widetilde{\Phi}^{\mathrm{trial}}\|^2} = e^{(1)}\alpha^3 + e^{(2)}\alpha^4 + e^{(3)}\alpha^5\log\alpha^{-1} + o(\alpha^5\log\alpha^{-1}).$$

which concludes the proof of the lower bound in Theorem 2.1.

Appendix A

Lemma A.1. *We have*

$$P.A^-u_\alpha\Phi_*^1 = 0,$$

and

$$\langle\Phi_*^2, \zeta(H_f, P_f^2)P_f^i\Phi_*^2\rangle = 0\ ,\ \textit{and}\ \langle\Phi_*^2, \zeta(H_f, P_f^2)W_i\rangle = 0\ , \tag{206}$$

for any function ζ for which the scalar products are defined. Similarly, we have

$$\langle\Phi_*^2\Gamma^0\Psi_1^\perp, A^+.P_f\Phi_*^{u_\alpha}\rangle = 0. \tag{207}$$

Proof. Straightforward computations using the symmetries of $A^-\Phi_*^1$ and Φ_*^2. □

Lemma A.2. *We have*

$$P.A^-\Phi_*^{u_\alpha} = \sqrt{\alpha}a_0\Delta u_\alpha,$$

where

$$a_0 = \int\frac{k_1^2 + k_2^2}{4\pi^2|k|^3}\frac{2}{|k|^2 + |k|}\chi_\Lambda(|k|)\,\mathrm{d}k_1\mathrm{d}k_2\mathrm{d}k_3.$$

Proof. Straightforward computations using the symmetries of $A^-\Phi_*^{u_\alpha}$. □

Lemma A.3.

$$\forall \varphi \in \mathfrak{F},\ \langle P.P_f \Gamma^1 \varphi u_\alpha, \Phi_\sharp^{u_\alpha}\rangle = 0 \ , \tag{208}$$

$$\|\Phi_\sharp^{u_\alpha}\|^2 = \mathcal{O}(\alpha^3 \log \alpha^{-1}) \ , \tag{209}$$

$$\|\Phi_\sharp^{u_\alpha}\|_*^2 = \mathcal{O}(\alpha^3) \ , \tag{210}$$

$$\| \, |k|^{-\frac12} \Phi_\sharp^{u_\alpha} \, \|^2 = \mathcal{O}(\alpha) \ . \tag{211}$$

$$\|P\Phi_\sharp^{u_\alpha}\|^2 = \mathcal{O}(\alpha^5 \log \alpha^{-1}) \ , \tag{212}$$

$$\|P\Phi_\sharp^{u_\alpha}\|_*^2 = \mathcal{O}(\alpha^5) \ , \tag{213}$$

$$\| \, |k|^{\frac16} P\Phi_\sharp^{u_\alpha}\|^2 = \mathcal{O}(\alpha^5) \ . \tag{214}$$

Proof. The proof of (208) is as follows

$$\begin{aligned} &\langle P.P_f \Gamma^1 \varphi u_\alpha, \Phi_\sharp^{u_\alpha}\rangle \\ &= \int \sum_{i=1}^3 k^i \frac{\partial u_\alpha}{\partial x_i} \varphi(k) \frac{1}{k^2 + |k| + h_\alpha + e_0} \sum_{j=1}^3 \sum_{\lambda=1,2} \frac{\epsilon_\lambda^j(k) \chi_\Lambda(|k|)}{2\pi |k|^{\frac12}} \overline{\frac{\partial u_\alpha}{\partial x_j}} \mathrm{d}x \mathrm{d}k \\ &= \sum_{i=1}^3 \int \mathrm{d}k \left(\int \mathrm{d}x \frac{\partial u_\alpha}{\partial x_i} \frac{1}{k^2 + |k| + h_\alpha + e_0} \overline{\frac{\partial u_\alpha}{\partial x_i}} \right) \sum_{\lambda=1,2} \frac{k^i \epsilon_\lambda^i(k) \chi_\Lambda(|k|)}{2\pi |k|^{\frac12}} \varphi(k) \mathrm{d}k = 0, \end{aligned} \tag{215}$$

using that the integral over x is independent of the value of i, and since $k.\epsilon_\lambda(k) = 0$.

To prove (211), we note that

$$\begin{aligned} \| \, |k|^{-\frac12} \Phi_\sharp^{u_\alpha} \|^2 &\leq c\alpha \int \left| \frac{\chi_\Lambda(|k|)}{|k| \, (|k| + k^2 + h_\alpha + e_0)} \nabla u_\alpha \right|^2 \mathrm{d}k \mathrm{d}x \\ &\leq c\alpha^3 \int \frac{\chi_\Lambda(|k|)^2}{|k|^2 (|k| + \frac{3}{16}\alpha^2)^2} \mathrm{d}k = \mathcal{O}(\alpha). \end{aligned}$$

The proofs of (209) and (210) are similar, but simpler.

We next prove (212).

$$\|P\Phi_\sharp^{u_\alpha}\|^2 = c\alpha \sum_{i=1}^3 \int \|P \frac{\chi_\Lambda(|k|)}{|k|^{\frac12} (|k| + k^2 + h_\alpha + e_0)} \frac{\partial u_\alpha}{\partial x_i} \|_{L^2(\mathbb{R}^3)}^2 \mathrm{d}k. \tag{216}$$

The function $\partial u_\alpha / \partial x_i$ is odd. On the subspace of antisymmetric functions on $L^2(\mathbb{R}^3)$, one has that $-(1-\gamma_0)\Delta - \frac{\alpha}{|x|} > -e_0$ for some $\gamma_0 > 0$, which implies on this subspace that $h_\alpha + e_0 > \gamma_0 P^2$, and thus,

$$P^2 < \gamma_0^{-1} (h_\alpha + e_0). \tag{217}$$

The relation (217) yields, for all k

$$\begin{aligned} &\|P \frac{\chi_\Lambda(|k|)}{|k|^{\frac12} (|k| + k^2 + h_\alpha + e_0)} \frac{\partial u_\alpha}{\partial x_i} \|^2 \\ &\leq \gamma_0^{-1} \| \frac{\chi_\Lambda(|k|)}{|k|^{\frac12} (|k| + k^2 + h_\alpha + e_0)} (h_\alpha + e_0)^{\frac12} \frac{\partial u_\alpha}{\partial x_i} \|^2 \\ &\leq \gamma_0^{-1} c\alpha^4 \left(\frac{\chi_\Lambda(|k|)}{|k|^{\frac12} (|k| + k^2 + \frac{3}{16}\alpha^2)} \right)^2 . \end{aligned} \tag{218}$$

Substituting (218) into (216) and integrating over k proves (212).

The proof of (214) is similar. □

Lemma A.4. *We have*

$$\|\Phi_*^{u_\alpha}\|_*^2 - \|\Phi_\sharp^{u_\alpha}\|_\sharp^2 = \frac{1}{3\pi}\|(h_1+\frac{1}{4})^{\frac12}\nabla u_1\|^2\alpha^5\log\alpha^{-1} + o(\alpha^5\log\alpha^{-1}) \ ,$$
$$\|\Phi_*^{u_\alpha} - \Phi_\sharp^{u_\alpha}\|_*^2 = \mathcal{O}(\alpha^5) \ ,$$
$$\|A^-(\Phi_\sharp^{u_\alpha} - \Phi_*^{u_\alpha})\|^2 = \mathcal{O}(\alpha^7\log\alpha^{-1}).$$

Proof. We have

$$\begin{aligned}&\|\Phi_*^{u_\alpha}\|_*^2 - \|\Phi_\sharp^{u_\alpha}\|_\sharp^2\\ &= \frac{\alpha^5}{(2\pi)^2}\frac{4}{3}\left\|\frac{\chi_\Lambda(|k|)}{|k|^{\frac12}(|k|+k^2)^{\frac12}(|k|+k^2+\alpha^2(h_1+\frac14))^{\frac12}}(h_1+\frac{1}{4})^{\frac12}\nabla u_1\right\|^2\end{aligned} \tag{219}$$

Since $(h_1+\frac14)\nabla u_1 \in L^2$, it implies that for sufficiently large $c>0$ independent of α,

$$\|\chi(h_1>c)(h_1+\frac{1}{4})^{\frac12}\nabla u_1\|^2 < \epsilon,$$

and

$$\begin{aligned}&\left\|\frac{\chi_\Lambda(|k|)}{|k|^{\frac12}(|k|+k^2)^{\frac12}(|k|+k^2+\alpha^2(h_1+\frac14))^{\frac12}}\chi(h_1>c)(h_1+\frac{1}{4})^{\frac12}\nabla u_1\right\|^2\\ &\le \epsilon\int_0^\infty \frac{\chi_\Lambda^2(t)}{t+c\alpha^2}\mathrm{d}t = \epsilon\log\alpha^{-1} + \mathcal{O}(1).\end{aligned} \tag{220}$$

For the contribution of $\chi(h_1\le c)(h_1+\frac14)^{\frac12}\nabla u_1$ in (219), the following inequalities hold,

$$\begin{aligned}&(\frac{1}{\pi}\log\alpha^{-1}+\mathcal{O}(1))\frac{1}{3}\|\chi(h_1<c)(h_1+\frac{1}{4})^{\frac12}\nabla u_1\|^2\\ &= \frac{1}{(2\pi)^2}\frac{1}{3}\left\|\frac{\chi_\Lambda(|k|)}{|k|^{\frac12}(|k|+k^2)^{\frac12}(|k|+k^2+(c+\frac14)\alpha^2))^{\frac12}}\chi(h_1<c)(h_1+\frac{1}{4})^{\frac12}\nabla u_1\right\|^2\\ &\le \frac{1}{(2\pi)^2}\frac{1}{3}\left\|\frac{\chi_\Lambda(|k|)}{|k|^{\frac12}(|k|+k^2)^{\frac12}(|k|+k^2+(h_1+\frac14)\alpha^2))^{\frac12}}\chi(h_1<c)(h_1+\frac{1}{4})^{\frac12}\nabla u_1\right\|^2\\ &\le \frac{1}{(2\pi)^2}\frac{1}{3}\left\|\frac{\chi_\Lambda(|k|)}{|k|^{\frac12}(|k|+k^2)^{\frac12}(|k|+k^2+\frac{3}{16}\alpha^2))^{\frac12}}\chi(h_1<c)(h_1+\frac{1}{4})^{\frac12}\nabla u_1\right\|^2\\ &\le (\frac{1}{\pi}\log\alpha^{-1}+\mathcal{O}(1))\frac{1}{3}\|\chi(h_1<c)(h_1+\frac{1}{4})^{\frac12}\nabla u_1\|^2.\end{aligned} \tag{221}$$

The inequalities (220) and (221) prove the first equality of the Lemma.

The proofs of the last two equalities are similar but simpler. □

Lemma A.5.

$$\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|_*^2-\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2=o(\alpha^3\log\alpha^{-1}), \tag{222}$$

$$\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|^2=\mathcal{O}(\alpha^3\log\alpha^{-1}) \tag{223}$$

$$\|\,|k_1|^{\frac16}|k_2|^{\frac16}|k_3|^{\frac16}(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|^2=\mathcal{O}(\alpha^3) \tag{224}$$

$$\|(h_\alpha+e_0)(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|^2=\mathcal{O}(\alpha^7\log\alpha^{-1}). \tag{225}$$

Proof. Denoting by σ_n the set of all permutations of $\{1,2,...,n\}$, we have

$$\begin{aligned}&\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|_*^2\\&=\frac{4\alpha}{(2\pi)^3}\Big\|\frac{1}{\sqrt6}\sum_{(i,j,n)\in\sigma_n}\frac{\sum_{\lambda=1,2}\varepsilon_\lambda(k_i).\sum_{\nu=1,2}\varepsilon_\nu(k_j)}{\Big(\sum_{p=1}^3|k_p|+(\sum_{p=1}^3k_p)^2\Big)^{\frac12}}\\&\times\frac{\sum_{\kappa=1,2}\varepsilon_\kappa(k_n)\chi_\Lambda(|k_1|)\chi_\Lambda(|k_2|)\chi_\Lambda(|k_3|)}{|k_i|^{\frac12}|k_j|^{\frac12}|k_n|^{\frac12}(|k_n|+k_n^2+(h_\alpha+e_0))}\nabla u_\alpha\Big\|^2\end{aligned}$$

If we pick two triples (i,j,n) and (i',j',n'), such that $n\neq n'$, then we get a product which is integrable at $k_1=k_2=k_3=0$, even without the term $(h_\alpha+e_0)$. The contribution of such terms is $c\alpha\|\nabla u_\alpha\|^2=\mathcal{O}(\alpha^3)$. Moreover, using the symmetry in k_1, k_2, k_3, the twelve remaining terms give the same contribution. This yields

(226)

$$\begin{aligned}&\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|_*^2\\&=\frac{8\alpha}{(2\pi)^3}\Big\|\frac{\sum_\lambda\varepsilon_\lambda(k_3).\sum_\nu\varepsilon_\nu(k_2)\sum_\kappa\varepsilon_\kappa(k_1)\chi_\Lambda(|k_1|)\chi_\Lambda(|k_2|)\chi_\Lambda(|k_3|)}{\Big(\sum_{i=1}^3|k_i|+(\sum_{i=1}^3k_i)^2\Big)^{\frac12}|k_3|^{\frac12}|k_2|^{\frac12}|k_1|^{\frac12}(|k_1|+k_1^2+(h_\alpha+e_0))}.\nabla u_\alpha\Big\|^2\\&+\mathcal{O}(\alpha^3).\end{aligned}$$

On the other hand, we have

$$\begin{aligned}&\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2\\&=\frac{8\alpha}{(2\pi)^3}\Big\|\frac{\sum_\lambda\varepsilon_\lambda(k_3).\sum_\nu\varepsilon_\nu(k_2)\sum_\kappa\varepsilon_\kappa(k_1)\chi_\Lambda(|k_1|)\chi_\Lambda(|k_2|)\chi_\Lambda(|k_3|)}{(|k_2|+|k_3|+(k_2+k_3)^2)^{\frac12}|k_3|^{\frac12}|k_2|^{\frac12}|k_1|^{\frac12}(|k_1|+k_1^2+(h_\alpha+e_0))}.\nabla u_\alpha\Big\|^2.\end{aligned}$$

Therefore, we obtain

(227)

$$\begin{aligned}&\|(H_f+P_f^2)^{-1}A^+.A^+\Phi_\sharp^{u_\alpha}\|_*^2-\|\Phi_*^2\|_*^2\|\Phi_\sharp^{u_\alpha}\|^2\\&=-\frac{8\alpha}{(2\pi)^3}\int\Bigg(\frac{(|k_1|^2+2|k_1|\,|k_3|+2|k_1|\,|k_2|)}{|k_2|\,|k_3|\,(|k_1|+|k_2|+|k_3|+|k_1+k_2+k_3|^2)(|k_2|+|k_3|+|k_2+k_3|^2)}\\&\times\sum_\lambda\varepsilon_\lambda(k_3).\sum_\nu\varepsilon_\nu(k_2)\chi_\Lambda(|k_1|)\chi_\Lambda(|k_2|)^2\chi_\Lambda(|k_3|)^2|u(k_1,x)|^2\mathrm{d}k_1\mathrm{d}k_2\mathrm{d}k_3\mathrm{d}x\Bigg)\,,\end{aligned}$$

where

$$u(k_1,x)=\frac{\sum_\kappa\varepsilon_\kappa(k_1)\chi_\Lambda(|k_1|)^{\frac12}}{|k_1|^{\frac12}(|k_1|+k_1^2+(h_\alpha+e_0))}.\nabla u_\alpha\ .$$

For fixed δ, we first compute the integral in (227) over the regions $|k_1|>\delta$. This yields a term $c_\delta\alpha^3$, where c_δ is independent on α.

Next, integrating (227) over the regions $|k_1| \leq \delta$ yields a bound $\mathcal{O}(\delta)\alpha^3 \log \alpha$, with $\mathcal{O}(\delta)$ independent of α.

This concludes the proof of (222).

The proof of (223) is a straightforward computation showing

$$\begin{aligned}
&\|(H_f + P_f^2)^{-1} A^+ . A^+ \Phi_\sharp^{u_\alpha}\|^2 \\
&= \frac{8\alpha}{(2\pi)^3} \Big\| \frac{\sum_\lambda \varepsilon_\lambda(k_3). \sum_\nu \varepsilon_\nu(k_2) \sum_\kappa \varepsilon_\kappa(k_1) \chi_\Lambda(|k_1|)\chi_\Lambda(|k_2|)\chi_\Lambda(|k_3|)}{\left(\sum_{i=1}^3 |k_i| + (\sum_{i=1}^3 k_i)^2\right) |k_3|^{\frac12}|k_2|^{\frac12}|k_1|^{\frac12}(|k_1| + k_1^2 + (h_\alpha + e_0))} . \nabla u_\alpha \Big\|^2 \\
&= \mathcal{O}(\alpha^3 \log \alpha^{-1}) \ .
\end{aligned}$$

The proofs of (224) and (225) are similar to the above. □

Lemma A.6. *For $\Psi_1^\perp$ and $\Psi_2^\perp$ given in Definition 6.1, we have*

$$|2\alpha \mathrm{Re}\, \langle A^- . A^- \Gamma^3 \Psi_1^\perp, \Gamma^1 \Psi_2^\perp \rangle| \leq c\alpha^5 + \epsilon \|H_f^{\frac12} \Psi_2^\perp\|^2 \ . \tag{228}$$

Proof. Using $2\alpha \mathrm{Re}\, \langle A^- . A^- \Gamma^3 \Psi_1^\perp, \Gamma^1 \Psi_2^\perp\rangle = 2\alpha \mathrm{Re}\, \langle \Gamma^3 \Psi_1^\perp, A^+ . A^+ \Gamma^1 \Psi_2^\perp\rangle$, we obtain that $2\alpha \mathrm{Re}\, \langle A^- . A^- \Gamma^3 \Psi_1^\perp, \Gamma^1 \Psi_2^\perp\rangle$ can be rewritten as a linear combination of the following two integrals I_1 and I_2

$$\begin{aligned}
I_1 &= \alpha^{\frac52} \int \frac{\mathrm{d}k\, \mathrm{d}k'\, \mathrm{d}k''\, \mathrm{d}x}{|k|+|k'|+|k''| + |k+k'+k''|^2} \sum_{\kappa,\nu} \frac{\epsilon_\kappa(k') . \epsilon_\nu(k'')}{|k'|^{\frac12}\, |k''|^{\frac12}} \\
&\times \Big(\frac{1}{|k|+|k|^2 + (h_\alpha + e_0)} \sum_\lambda \frac{\epsilon_\lambda(k)}{|k|^{\frac12}} \nabla u_\alpha \Big) \sum_{\kappa,\eta} \frac{\epsilon_\kappa(k') . \epsilon_\eta(k'')}{|k'|^{\frac12}\, |k''|^{\frac12}} \overline{(\Gamma^1 \Psi_2^\perp)(k,x)},
\end{aligned} \tag{229}$$

and I_2 is defined as I_1, except that in the last sum, we reverse the role of k and k'', namely

$$\begin{aligned}
I_2 &= \alpha^{\frac52} \int \frac{\mathrm{d}k\, \mathrm{d}k'\, \mathrm{d}k''\, \mathrm{d}x \chi_\Lambda(|k|)\chi_\Lambda(|k'|)\chi_\Lambda(|k''|)}{|k|+|k'|+|k''| + |k+k'+k''|^2} \sum_{\kappa,\nu} \frac{\epsilon_\kappa(k') . \epsilon_\nu(k'')}{|k'|^{\frac12}\, |k''|^{\frac12}} \\
&\times \Big(\frac{1}{|k|+|k|^2 + (h_\alpha + e_0)} \sum_\lambda \frac{\epsilon_\lambda(k)}{|k|^{\frac12}} \nabla u_\alpha \Big) \sum_{\kappa,\eta} \frac{\epsilon_\kappa(k') . \epsilon_\eta(k)}{|k'|^{\frac12}\, |k|^{\frac12}} \overline{(\Gamma^1 \Psi_2^\perp)(k'',x)}.
\end{aligned} \tag{230}$$

To bound I_2, we use the Schwarz inequality, $|ab| \leq \frac{1}{2\epsilon} a^2 + \frac{\epsilon}{2} b^2$. This yields

$$\begin{aligned}
|I_2| &\leq \alpha^{\frac52} \Big(\int \frac{\mathrm{d}k\, \mathrm{d}k'\, \mathrm{d}k''\, \mathrm{d}x \chi_\Lambda^2(|k|)\chi_\Lambda^2(|k'|)\chi_\Lambda^2(|k''|)}{(|k|+|k'|+|k''| + |k+k'+k''|^2)^2} \frac{2}{|k'|\,|k''|} \\
&\times \Big| \frac{1}{|k|+|k|^2 + (h_\alpha + e_0)} \frac{1}{|k|^{\frac12}} \nabla u_\alpha \Big|^2 |k|^{2-\epsilon} |k'|^{2-\epsilon} \frac{1}{|k''|} \Big)^{\frac12} \\
&\times \Big(2 \int \frac{\mathrm{d}k\, \mathrm{d}k'\, \mathrm{d}k''\, \mathrm{d}x}{|k'||k|} |(\Gamma^1 \Psi_2^\perp)(k'',x)|^2 |k''| \frac{\chi_\Lambda^2(|k|)\chi_\Lambda^2(|k'|)\chi_\Lambda^2(|k''|)}{|k|^{2-\epsilon}|k'|^{2-\epsilon}} \Big)^{\frac12} \\
&\leq c\alpha^7 + \epsilon \|H_f^{\frac12} \Psi_2^\perp\|^2,
\end{aligned}$$

Similarly, we bound I_1 as follows,

$$
\begin{aligned}
|I_1| &\le \alpha^{\frac{5}{2}} \Big(\int \frac{\mathrm{d}k\,\mathrm{d}k'\,\mathrm{d}k''\,\mathrm{d}x}{(|k|+|k'|+|k''|+|k+k'+k''|^2)^2} \frac{2}{|k'|\,|k''|} \\
&\times \Big| \frac{1}{|k|+|k|^2+(h_\alpha+e_0)} \frac{1}{|k|^{\frac{1}{2}}} \nabla u_\alpha \Big|^2 |k'|^{2-\epsilon} |k''|^{2-\epsilon} \frac{\chi_\Lambda^2(|k|)\chi_\Lambda^2(|k'|)\chi_\Lambda^2(|k''|)}{|k|} \Big)^{\frac{1}{2}} \\
&\times \Big(2 \int \frac{\mathrm{d}k\,\mathrm{d}k'\,\mathrm{d}k''\,\mathrm{d}x}{|k'||k''|} |(\Gamma^1 \Psi_{\frac{1}{2}})(k,x)|^2 |k| \frac{\chi_\Lambda^2(|k|)\chi_\Lambda^2(|k'|)\chi_\Lambda^2(|k''|)}{|k'|^{2-\epsilon}|k''|^{2-\epsilon}} \Big)^{\frac{1}{2}} \\
&\le c\alpha^5 \int \mathrm{d}k'\,\mathrm{d}k'' |k'|^{-\epsilon} |k''|^{-\epsilon} \chi_\Lambda^2(|k'|)\chi_\Lambda^2(|k''|) \int \mathrm{d}k \, \frac{1}{|k|^2} \frac{\chi_\Lambda^2(|k|)}{(|k|+\frac{1}{16}\alpha^2)^2} \|\nabla u_\alpha\|^2 \\
&+ \epsilon \|H_f^{\frac{1}{2}} \Gamma^1 \Psi_{\frac{1}{2}}\|^2 \le c\alpha^5 + \epsilon \|H_f^{\frac{1}{2}} \Psi_{\frac{1}{2}}\|^2,
\end{aligned}
$$

where we took into account that $\frac{\partial u_\alpha}{\partial x_i}$ is orthogonal to u_α, and on the subspace of such functions we have $(h-\alpha+e_0) \ge \frac{1}{16}\alpha^2$.

□

Lemma A.7. *Let Ψ_0 be the ground state of $T(0)$, with $|\Gamma^0 \Psi_0| = 1$. Then we have*

$$
\begin{aligned}
&\Psi_0 = \Omega_f + 2\eta_1 \alpha^{\frac{3}{2}} \Phi_*^1 + \eta_2 \alpha \Phi_*^2 + 2\eta_3 \alpha^{\frac{3}{2}} \Phi_*^3 + \Delta_*^0, \\
&\textit{with } \langle \Delta_*^0, \Phi_*^i \rangle_* = 0 \ (i=1,2,3), \Gamma^0 \Delta_*^0 = 0
\end{aligned}
$$

and

$$\|\Delta_*^0\|^2 = \mathcal{O}(\alpha^3).$$

Proof. It follows from a similar argument as in [7, Proposition 5.1] that

$$\|a_\lambda(k) \Delta_*^0\| \le \frac{c\alpha}{|k|}.$$

This yields

$$
\begin{aligned}
\|\Delta_*^0\|^2 &\le \int \|a_\lambda(k)\Delta_*^0\|^2 \mathrm{d}k \le \int_{|k|\le\alpha} \frac{c^2\alpha^2}{|k|^2} \mathrm{d}k + \int_{|k|>\alpha} \frac{|k|\,\|a_\lambda(k)\Delta_*^0\|^2 \chi_\Lambda(|k|)}{|k|} \mathrm{d}k \\
&\le c^2\alpha^3 + c'\alpha^{-1} \|H_f^{\frac{1}{2}} \Delta_*^0\|^2 = \mathcal{O}(\alpha^3) \ ,
\end{aligned}
$$

where in the last equality we used the estimate $\|\Delta_*^0\|_*^2 = \|(H_f + P_f^2)^{\frac{1}{2}} \Delta_*^0\|^2 = \mathcal{O}(\alpha^4)$ proved in [4, Theorem 3.2]. □

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