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Contribution of the spin-Zeeman term to the binding energy for hydrogen in non-relativistic QED.

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Abstract - We show that the spin-Zeeman term contributes at least to the same order as the first radiative correction of the binding energy for hydrogen atom in non relativistic quantum electrodynamics obtained in the spinless case [8].

Key words and phrases : Pauli-Fierz Hamiltonian, binding energy, ground state energy.

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1. Introduction

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

$$\inf \operatorname{spec}(-\Delta) - \inf \operatorname{spec}(-\Delta - \frac{\alpha Z}{|x|}) \;=\; \frac{(Z\alpha)^2}{4}\ ,$$

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 $-\Delta - \alpha Z/|x|$ the photon field energy operator H_f, and an operator $I(\alpha)$ which describes the coupling of the electron to the quantized electromagnetic field, yielding the so-called Pauli-Fierz operator (see details in Section 2).

In this case, the binding energy is given by

$$\Sigma_0 - \Sigma := \inf \operatorname{spec}\big(-\Delta + H_f + I(\alpha)\big) \;-\; \inf \operatorname{spec}\big(-\Delta - \frac{\alpha Z}{|x|} + H_f + I(\alpha)\big) \tag{1.1}$$

The free infraparticle binds a larger quantity of low-energetic photons than the confined particle and thus possesses a larger effective mass. In order for the particle to leave the potential well, an additional energetic effort is therefore necessitated compared to the situation without coupling to the quantized electromagnetic field.

It remains a difficult task, however, to determine the binding energy. There are mainly two difficulties. The first is that the ground state energy is not an isolated eigenvalue of the Hamiltonian, and can not be determined with ordinary perturbation theory. The second is due to the infrared problem in quantum electrodynamics whose origin is in the photon form factor in the quantized electromagnetic vector potential occurring in the interaction term $I(\alpha)$, that contains a critical frequency space singularity.

The systematic study of the Pauli-Fierz operator, in a more general case involving more than one electron, was initiated by Bach, Fröhlich and Sigal [3, 4, 5].

Later on, several rigorous results [15, 18, 16, 12, 14, 6, 17, 2, 7, 8, 10, 19, 11] have been obtained addressing both qualitative and quantitative estimates on the binding energy and the ground state energies Σ_0 and Σ occuring in (1.1).

The case of spinless particle attracted most of the attention since the additional spin-Zeeman term $\sqrt{\alpha}\sigma \cdot B(x)$ in the case of a spin 1/2 particle induces substantial technical difficulties for quantitative estimates. From a rigorous point of view, if one takes into account the spin of the particle, it is not clear of what order the first correction in powers of the fine structure constant α is. This question is sensible since both the self-energy Σ_0 and the ground state energy Σ for Hydrogen atom, up to a normal ordering constant, are of the order α^2 in the case of a spinless particle (see [7, 8, 10, 17] and references therein), whereas in the case of an electron, i.e. a spin 1/2 particle, they are proportional to α (see e.g. [16, 12, 11] and references therein). In the latter case, though, the binding energy is still expected to be proportional to α^2 in the leading order. This fact together with the upper bound on the contribution of the spin-Zeeman term to the binding energy will be proved by the authors in a subsequent paper; see also Remark 2.2.

In the present paper, we prove Theorem 2.1 which gives a lower bound on this contribution.

2. Model and main result

We study an electron, i.e., a spin 1/2 particle, interacting with the quantized electromagnetic field in the Coulomb gauge, and with the electrostatic potential generated by a nucleus.

The Hilbert space accounting for the Schrödinger electron is given by $\mathfrak{H}_{el} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. Here $\mathbb{R}^3$ is the configuration space of the particle, while $\mathbb{C}^2$ accommodates its spin.

The Fock space of photon states is given by

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

where the 0-photon space is $\mathfrak{F}_0 = \mathbb{C}$, and for $n \geq 1$ the n-photon space $\mathfrak{F}_n = \bigotimes_s^n \left(L^2(\mathbb{R}^3) \otimes \mathbb{C}^2\right)$ is the symmetric tensor product of n copies of one-photon Hilbert spaces $L^2(\mathbb{R}^3) \otimes \mathbb{C}^2$. The factor $\mathbb{C}^2$ accounts for the two independent transversal polarizations of the photon.

On $\mathfrak{F}$, we introduce creation and annihilation operators $a_\lambda^*(k)$, $a_\lambda(k)$ satisfying the distributional commutation relations

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

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 atomic 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 has physical value about $1/137$ and will here be considered as a small parameter.

Similarly to the Pauli operator which acts on Hilbert space $L^2(\mathbb{R}^3,\, \mathbb{C}^2)$ and describes the energy of a spin $1/2$ particle interacting with classical external magnetic field, the Pauli-Fierz operator we consider in this paper is the Hamiltonian for a particle interacting with the quantized radiation field (see [3, 4, 5] and references therein). For an atom with nuclear charge $Z = 1$, this operator is defined by

$$:\left(-i\nabla_x \otimes I_f + \sqrt{\alpha}A(x)\right)^2: \;+\; \sqrt{\alpha}\,\sigma\cdot B(x) + V(x)\otimes I_f + I_{el}\otimes H_f\,, \tag{2.1}$$

where V is the electrostatic potential.

The operator that couples a particle to the quantized vector potential is

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

where

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

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

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

The vectors $\varepsilon_\lambda(k) \in \mathbb{R}^3$ ($\lambda = 1, 2$), 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 $\zeta(|k|)$ implements an *ultraviolet cutoff*, independent of α, on the photon momentum k. We assume ζ to be of class C^1 and to have a compact support.

The symbol : ... : denotes normal ordering and is applied to the operator $A(x)^2$. It corresponds here to the subtraction of a constant operator $c_{\mathrm{n.o.}}\,\alpha$, with $c_{\mathrm{n.o.}} = [A^-(x),\, A^+(x)] = (2/\pi)\int_0^\infty r|\zeta(r)|^2 \mathrm{d}r$.

The operator that couples a particle to the magnetic field $B = \mathrm{curl}A$ is given by

$$B(x) = B^-(x) + B^+(x)\,,$$

where

$$B^-(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\zeta(|k|)}{2\pi|k|^{1/2}} k \times i\varepsilon_\lambda(k) e^{ikx} \otimes a_\lambda(k) \mathrm{d}k\,,$$

$$B^+(x) = -\sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\zeta(|k|)}{2\pi|k|^{1/2}} k \times i\varepsilon_\lambda(k) e^{-ikx} \otimes a_\lambda^*(k) \mathrm{d}k\,.$$

In Equation (2.1), $\sigma = (\sigma_1, \sigma_2, \sigma_3)$ is the 3-component vector of Pauli matrices

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

The Coulomb potential is the operator of multiplication by

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

The photon field energy operator H_f is given by

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

In the sequel, instead of the operator (2.1), we shall proceed to a change of variables, and study the unitarily equivalent Hamiltonian

$$H = U\Big(: \big(i\nabla_x \otimes I_f - \sqrt{\alpha} A(x)\big)^2 : + \sqrt{\alpha}\sigma\cdot B(x) \,+\, V(x) \otimes I_f \,+\, I_{el} \otimes H_f \Big) U^*\,, \tag{2.2}$$

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

$$U i\nabla_x U^* = i\nabla_x + P_f\,, \quad U A(x) U^* = A(0)\,, \quad \text{and} \quad U B(x) U^* = B(0)\ .$$

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, and omitting by abuse of notations the operators I_{el} and I_f, the Hamiltonian (2.2) reads

$$H = :\big((i\nabla_x - P_f) - \sqrt{\alpha} A(0)\big)^2 : \ + \sqrt{\alpha}\sigma \cdot B(0) \ - \ \frac{\alpha}{|x|} \ + \ H_f\,, \tag{2.3}$$

where : ... : denotes again the normal ordering.

The Hamiltonian for a free electron, i.e., a free spin 1/2 particle, coupled to the quantized radiation field is given by the self-energy operator T,

$$\begin{aligned} T &= H - \frac{\alpha}{|x|} \\ &= :\big((i\nabla_x - P_f) - \sqrt{\alpha} A(0)\big)^2 : \ + \sqrt{\alpha}\sigma \cdot B(0) \ + \ H_f\,, \end{aligned} \tag{2.4}$$

where we omit again the operators I_{el} and I_f.

This system is translationally invariant, that is, T commutes with the operator of total momentum

$$P_{tot} = p_{el} + P_f,$$

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

Therefore, for fixed value $p \in \mathbb{R}^3$ of the total momentum, the restriction of T to the fibre space $\mathbb{C}^2 \otimes \mathfrak{F}$ is given by (see e.g. [13, 11])

$$T(p) = \ :(p - P_f - \sqrt{\alpha} A(0))^2 : + \sqrt{\alpha}\sigma \cdot B(0) + H_f\,. \tag{2.5}$$

Henceforth, we will write

$$A^\pm = A^\pm(0) \quad \text{and} \quad B^\pm = B^\pm(0).$$

The ground state energies of T and H are respectively denoted by

$$\Sigma_0 = \inf \operatorname{spec}(T) \quad \text{and} \quad \Sigma = \inf \operatorname{spec}(H)\,,$$

and the binding energy is defined by

$$\Sigma_0 \;-\; \Sigma \,.$$

It is proven in [1, 13] that

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

Our main result is the following,

Theorem 2.1. *The binding energy fulfills the following inequality*

$$\Sigma_0 - \Sigma \;\geq\; \frac{1}{4}\alpha^2 \;+\; \left(e^{(1)} + e^{(1)}_{\text{Zeeman}}\right)\alpha^3 \;+\; \mathcal{O}(\alpha^4|\log\alpha|)\,, \tag{2.6}$$

where

$$e^{(1)} = \frac{2}{3\pi}\int_0^\infty \frac{\zeta^2(t)}{1+t}\,\mathrm{d}t \quad \textit{and} \quad e^{(1)}_{\text{Zeeman}} = \frac{2}{3\pi}\int_0^\infty \frac{t^2\,\zeta^2(t)}{(1+t)^3}\,\mathrm{d}t\,.$$

Remark 2.1. We recall that for the spinless Pauli-Fierz model it is known (see [8] and references therein) that the binding energy is

$$\Sigma_0 - \Sigma \;=\; \frac{1}{4}\,\alpha^2 \;+\; e^{(1)}\alpha^3 \;+\; \mathcal{O}(\alpha^4)\,.$$

The above Theorem 2.1 thus shows that the spin-Zeeman term yields an additional contribution of order at least α^3.

Remark 2.2. In a forthcoming paper we will show that this result is optimal, namely that the inequality (2.6) can be turned into an equality, by deriving a sharp upper bound for the binding energy up to the order α^3. This upper bound will coincide with the lower bound of the work at hand and gives the correct coefficient of the order α^3 in the expansion of the binding energy in powers of α. Such an estimate is much more involved than the proof of the lower bound which requires only a construction of a trial function. In addition to the problems encountered in the spinless case, there are several additional difficulties when taking into account the spin-Zeeman term. The degeneracy of the ground state in the spin case (see [21, 20] and references therein) gives rise to technical difficulties. A more severe problem for the proof of the upper bound is that the ground state energy Σ_0 of the self-energy operator T given by (2.4) is of the order α and not of the order α^2 as in the spinless case ([11]). In addition, the photon number bound for a ground state of H, which is a crucial estimate for the proof of the upper bound, is only of the order α, instead of α^2 in the spinless case.

In the remainder, we will need the following notations. For $n \in \mathbb{N}$, let Π_n be the orthogonal projection onto the subspace $\mathfrak{H}_{el} \otimes \mathfrak{F}_n$ of the space $\mathfrak{H}_{el} \otimes \mathfrak{F}$, and $\Pi_{\geq n}$ be the orthogonal projection onto the space $\mathfrak{H}_{el} \otimes \left(\bigoplus_{k \geq n} \mathfrak{F}_k \right)$.

On $\mathfrak{H}_{el} \otimes \mathfrak{F}$, we define the positive bilinear form

$$\langle v,\, w \rangle_* := \langle v,\, (H_f + P_f^2) w \rangle \,,$$

and its associated semi-norm $\|v\|_* = \langle v,\, v \rangle_*$.

Proof. To prove the theorem we will construct a trial function Ψ^{trial} such that holds $\langle \Psi^{\mathrm{trial}},\, H \Psi^{\mathrm{trial}} \rangle / \|\Psi^{\mathrm{trial}}\|^2 \leq \Sigma_0 - \alpha^2/4 - (e^{(1)} + e^{(1)}_{\mathrm{Zeeman}}) \alpha^3 + \mathcal{O}(\alpha^4 |\log \alpha|)$.

Let

$$P := i \nabla_x \,.$$

We denote by θ_{GS} the ground state of $T(0)$ with the normalization condition $\Pi_0 \theta_{\mathrm{GS}} = \Omega_f \uparrow$, where $\uparrow = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is the normalized spin up component (see(A.3)-(A.4) in Theorem A.1 for detailed definiton and properties of θ_{GS}), and let

$$\Theta := u_\alpha \otimes \theta_{\mathrm{GS}}$$

For Γ_1 defined as in (A.1) by

$$\Gamma_1 := \ -(H_f + P_f^2)^{-1} \sigma \cdot B^+ \uparrow \otimes \Omega_f \,,$$

and u_α the normalized ground state of the Schrödinger operator $-\Delta - \alpha/|x|$,

$$u_\alpha = \frac{1}{\sqrt{8\pi}} \alpha^{3/2} \mathrm{e}^{-\alpha |x|/2} \,. \tag{2.7}$$

we set

$$\Phi_\alpha := \ 2\, P \cdot P_f \, (H_f + P_f^2)^{-1} u_\alpha \otimes \Gamma_1 \,, \tag{2.8}$$

and

$$\Upsilon_\alpha := \ 2\, \chi_{(\alpha,\, \infty)}(H_f) (H_f + P_f^2)^{-1} \, P \cdot A^+ u_\alpha \uparrow \otimes \Omega_f \,, \tag{2.9}$$

where $\chi_{(\alpha,\, \infty)}(H_f)$ is an infrared cutoff and $\chi_{(\alpha,\, \infty)}$ is the characteristic function of $(\alpha,\, \infty)$.

Let us define the following trial function

$$\Psi^{\mathrm{trial}} = \Theta + \alpha^{\frac{1}{2}} \Phi_\alpha + \alpha^{\frac{1}{2}} \Upsilon_\alpha \,.$$

The state Ψ^{trial} has only non zero vacuum and one-photon component, i.e.,

$$\Pi_{\geq 2} \Psi^{\mathrm{trial}} = 0 \,.$$

In comparison with the trial function used in the spinless case [8] to recover the estimate up to the order α^3, with error α^4, the function Ψ^{trial} differs in two points. First we pick now the state $\theta_{\rm GS}$ as the ground state of the translation invariant operator $T(0)$ with spin. Second, we have an additional vector Φ_α at the origin of the $e^{(1)}_{\rm Zeeman}\,\alpha^3$ term in (2.6).

From the definition of H, expanding (2.3) and taking into account the normal ordering, we obtain

$$\begin{aligned} H =&(-\Delta - \frac{\alpha}{|x|}) + (H_f + P_f^2) - 2\,P\cdot P_f - 4\alpha^{\frac12}{\rm Re}\,P\cdot A^- \\ &+ 4\alpha^{\frac12} P_f\cdot A^- + 2\alpha A^+\cdot A^- + 2\alpha({\rm Re}\,A^-)^2 + 2\alpha^{\frac12}{\rm Re}\,\sigma\cdot B^- \end{aligned} \tag{2.10}$$

We shall use this expression to estimate all terms occurring in

$$\begin{aligned} &\langle \Psi^{\rm trial},\, H\,\Psi^{\rm trial}\rangle \\ &= \Big\langle \Theta + \alpha^{\frac12}\Phi_\alpha + \alpha^{\frac12}\Upsilon_\alpha\,,\ H\ \Big(\Theta + \alpha^{\frac12}\Phi_\alpha + \alpha^{\frac12}\Upsilon_\alpha\Big)\Big\rangle\,. \end{aligned} \tag{2.11}$$

Step 1. We first compute the direct terms $\langle\Theta, H\Theta\rangle$, $\langle\alpha^{\frac12}\Phi_\alpha, H\alpha^{\frac12}\Phi_\alpha\rangle$ and $\langle\alpha^{\frac12}\Upsilon_\alpha, H\alpha^{\frac12}\Upsilon_\alpha\rangle$.

Since $\theta_{\rm GS}$ is a ground state vector of $T(0)$, and using orthogonality between the components of Pu_α and u_α, we have

$$\begin{aligned} \langle\Theta,\, H\Theta\rangle &= \langle u_\alpha\theta_{\rm GS},\, H\,u_\alpha\theta_{\rm GS}\rangle \\ &= \|u_\alpha\|^2\langle\theta_{\rm GS},\, T(0)\,\theta_{\rm GS}\rangle + \|\theta_{\rm GS}\|^2\langle u_\alpha,\, (-\Delta - \frac{\alpha}{|x|})\,u_\alpha\rangle \\ &= (\Sigma_0 - \frac{\alpha^2}{4})\|\Theta\|^2\,. \end{aligned} \tag{2.12}$$

Using that for $i,\, j,\, k \in \{1,\, 2\,,3\}$, $\partial u_\alpha/\partial x_i$ and $\partial^2 u_\alpha/(\partial x_j\partial x_k)$ are orthogonal, and the fact that non particle conserving operators have mean value zero in the state Φ_α, yields

$$\begin{aligned} &\langle\alpha^{\frac12}\Phi_\alpha, H\alpha^{\frac12}\Phi_\alpha\rangle \\ &= \Big\langle \alpha^{\frac12}\Phi_\alpha, \Big(-\Delta - \frac{\alpha}{|x|}\ +\ (H_f + P_f^2)\ +\ \alpha A^-\cdot A^+\Big)\,\alpha^{\frac12}\Phi_\alpha\Big\rangle \\ &= \alpha\|\Phi_\alpha\|_*^2\ +\ \mathcal{O}(\alpha^4)\,, \end{aligned} \tag{2.13}$$

where the last inequality holds since $\|Pu_\alpha\| = \mathcal{O}(\alpha)$, $\|(-\Delta - \frac{\alpha}{|x|})Pu_\alpha\| = \mathcal{O}(\alpha^3)$.

Using the same arguments as above, and the fact that

$$\|(H_f + P_f^2)^{-1}\chi_{(\alpha,\infty)}(H_f)(A^+)_j{\uparrow}\otimes\Omega_f\| = \mathcal{O}(|\log\alpha|^{\frac12})\,,$$

the last direct term can be estimated as

$$\begin{aligned} &\langle\alpha^{\frac12}\Upsilon_\alpha,\, H\alpha^{\frac12}\Upsilon_\alpha\rangle \\ &= \Big\langle \alpha^{\frac12}\Upsilon_\alpha, \Big(-\Delta - \frac{\alpha}{|x|} + (H_f + P_f^2) + \alpha A^-\cdot A^+\Big)\,\alpha^{\frac12}\Upsilon_\alpha\Big\rangle \\ &= \mathcal{O}(\alpha^5\log\alpha) + \alpha\,\big\langle\Upsilon_\alpha, (H_f + P_f^2)\Upsilon_\alpha\big\rangle + \mathcal{O}(\alpha^4) \\ &= \alpha\|\Upsilon_\alpha\|_*^2\ +\ \mathcal{O}(\alpha^4|\log\alpha|)\,. \end{aligned} \tag{2.14}$$

Step 2. We compute in (2.11) the cross terms with Φ_α and Υ_α. Using as above the estimates $\|(H_f+P_f^2)^{-1}\chi_{(\alpha,\infty)}(H_f)(A^+)_j\Omega_f\!\uparrow\| = \mathcal{O}(|\log\alpha|^{\frac12})$, $\|Pu_\alpha\| = \mathcal{O}(\alpha)$, and $\|(-\Delta - \frac{\alpha}{|x|})Pu_\alpha\| = \mathcal{O}(\alpha^3)$ yields

$$\langle\alpha^{\frac12}\Phi_\alpha, (-\Delta - \frac{\alpha}{|x|})\alpha^{\frac12}\Upsilon_\alpha\rangle + \langle\alpha^{\frac12}\Upsilon_\alpha, (-\Delta - \frac{\alpha}{|x|})\alpha^{\frac12}\Phi_\alpha\rangle = \mathcal{O}(\alpha^5|\log\alpha|^{\frac12})\,. \tag{2.15}$$

Due to Lemma B.1 (see Appendix B) holds

$$\langle\alpha^{\frac12}\Phi_\alpha, (H_f+P_f^2)\alpha^{\frac12}\Upsilon_\alpha\rangle + \langle\alpha^{\frac12}\Upsilon_\alpha, (H_f+P_f^2)\alpha^{\frac12}\Phi_\alpha\rangle = 0\,. \tag{2.16}$$

Furthermore, $\|A^-\Phi_\alpha\| \le c\|\Phi_\alpha\| = \mathcal{O}(\alpha)$ and $\|A^-\Upsilon_\alpha\| \le c\|H_f^{\frac12}\Upsilon_\alpha\| = \mathcal{O}(\alpha)$ implies

$$\begin{aligned} &\langle\alpha^{\frac12}\Phi_\alpha,\, 2\alpha A^+\cdot A^-\alpha^{\frac12}\Upsilon_\alpha\rangle + \langle\alpha^{\frac12}\Upsilon_\alpha,\, 2\alpha A^+\cdot A^-\alpha^{\frac12}\Phi_\alpha\rangle \\ &\le 4\alpha^2\|A^-\Phi_\alpha\|\,\|A^-\ \Upsilon_\alpha\| = \mathcal{O}(\alpha^4)\,. \end{aligned} \tag{2.17}$$

In addition, due either to the symmetry of u_α or the occurrence of non-particle conserving terms, all other cross terms with Φ_α and Υ_α in (2.11) are equal to zero. Therefore, collecting (2.15)-(2.17) we get

$$\langle\alpha^{\frac12}\Phi_\alpha,\, H\,\alpha^{\frac12}\Upsilon_\alpha\rangle + \langle\alpha^{\frac12}\Upsilon_\alpha,\, H\,\alpha^{\frac12}\Phi_\alpha\rangle = \mathcal{O}(\alpha^4)\,. \tag{2.18}$$

Step 3. We estimate in (2.11) the cross terms involving Φ_α and $\Theta = \theta_{\mathrm{GS}}u_\alpha$. Only terms coming from $-2\mathrm{Re}\,P\cdot P_f$ and $-4\mathrm{Re}\,\alpha^{\frac12}P\cdot A^-$ can a priori contribute since other terms are zero due to the symmetry of u_α.

The contribution of $-2\mathrm{Re}\,P\cdot P_f$ is

$$-2\mathrm{Re}\,\langle\Pi_1\Theta,\, P\cdot P_f\Phi_\alpha\rangle - 2\mathrm{Re}\,\langle\Phi_\alpha,\, P\cdot P_f\Pi_1\Theta\rangle\,.$$

We write $\Pi_1\Theta$ as $(\alpha^{\frac12}\gamma_1\Gamma_1 + \Pi_1 R)u_\alpha$, where R and γ_1 are defined by (A.3) and (A.4) in Theorem A.1. This implies

$$\begin{aligned} &-2\mathrm{Re}\,\langle\Pi_1\Theta,\, P\cdot P_f\Phi_\alpha\rangle - 2\mathrm{Re}\,\langle\Phi_\alpha,\, P\cdot P_f\Pi_1\Theta\rangle \\ &= -4\mathrm{Re}\,\Big\langle(\alpha^{\frac12}\gamma_1\Gamma_1 + \Pi_1R)u_\alpha,\, P\cdot P_f 2\alpha^{\frac12}(H_f+P_f^2)^{-1}P\cdot P_f\Gamma_1 u_\alpha\Big\rangle \\ &= -8\alpha\mathrm{Re}\,\gamma_1\langle P\cdot P_f\Gamma_1u_\alpha,\, (H_f+P_f^2)^{-1}P\cdot P_f\Gamma_1u_\alpha\rangle \\ &-8\alpha^{\frac12}\mathrm{Re}\,\langle Pu_\alpha\cdot P_f\Pi_1R,\, Pu_\alpha\cdot(H_f+P_f^2)^{-1}P_f\Gamma_1\rangle \\ &\ge -2\alpha\mathrm{Re}\,\gamma_1\|\Phi_\alpha\|_*^2 - c\alpha\|Pu_\alpha\|^2\|P_f\Pi_1\Gamma_1\| \\ &= -2\alpha\|\Phi_\alpha\|_*^2 + \mathcal{O}(\alpha^4)\,, \end{aligned} \tag{2.19}$$

where in the last equality, we used $\|Pu_\alpha\| = \mathcal{O}(\alpha)$ and from (A.5) of Theorem A.1 that $|\gamma_1 - 1| = \mathcal{O}(\alpha)$ and $\|\Pi_1R\|_* \le \|R\|_* = \mathcal{O}(\alpha^{\frac32})$.

The contribution of $-4\alpha^{\frac{1}{2}}\mathrm{Re}\,P.A^-$ is

$$\begin{aligned}
&-4\alpha^{\frac{1}{2}}\mathrm{Re}\,\left\langle \Pi_0\Theta,\, P\cdot A^-\Phi_\alpha\right\rangle - 4\alpha^{\frac{1}{2}}\mathrm{Re}\,\left\langle \Phi_\alpha,\, P\cdot A^-\Pi_2\Theta\right\rangle\\
&= -4\alpha^{\frac{1}{2}}\mathrm{Re}\,\left\langle P\cdot A^+\Pi_0\Theta,\, \Phi_\alpha\right\rangle\\
&- 4\alpha^{\frac{1}{2}}\mathrm{Re}\,\left\langle 2\alpha^{\frac{1}{2}} P\cdot P_f(H_f+P_f^2)^{-1}\Gamma_1 u_\alpha,\, P\cdot A^-(\alpha\gamma_2\Gamma_2+\Pi_2 R)u_\alpha\right\rangle\\
&= -4\alpha^{\frac{1}{2}}\mathrm{Re}\,\left\langle P\cdot A^+\Omega_f u_\alpha\!\uparrow,\, \Phi_\alpha\right\rangle\\
&- 8\alpha^2\mathrm{Re}\,\overline{\gamma_2}\langle P u_\alpha\cdot P_f(H_f+P_f^2)^{-1}\Gamma_1,\, P u_\alpha\cdot A^-\Gamma_2\rangle\\
&- 8\alpha\mathrm{Re}\,\langle P u_\alpha\cdot P_f(H_f+P_f^2)^{-1}\Gamma_1,\, P u_\alpha\cdot A^-\Pi_2 R\rangle = \mathcal{O}(\alpha^4)\,,
\end{aligned}\tag{2.20}$$

where in the fourth inequality we used $\|Pu_\alpha\| = \mathcal{O}(\alpha)$, $\|A^-\Pi_2 R\| \leq c\|\Pi_2 R\|_* = \mathcal{O}(\alpha^{\frac{3}{2}})$ from (A.5) in Theorem A.1, and $\langle P\cdot A^+ u_\alpha\!\uparrow\otimes\Omega_f,\, \Phi_\alpha\rangle = 0$ from Lemma B.1.

The estimates (2.19) and (2.20) yields

$$\langle \alpha^{\frac{1}{2}}\Phi_\alpha,\, H\Theta\rangle + \langle\Theta,\, H\alpha^{\frac{1}{2}}\Phi_\alpha\rangle = -2\alpha\|\Phi_\alpha\|_*^2 + \mathcal{O}(\alpha^4)\,. \tag{2.21}$$

Step 4. We next estimate in (2.11) the cross terms involving Υ_α and $\Theta = \theta_{\mathrm{GS}} u_\alpha$. As in the previous step, only terms coming from $-2\mathrm{Re}\,P\cdot P_f$ and $-4\mathrm{Re}\,\alpha^{\frac{1}{2}} P\cdot A^-$ can a priori contribute since other terms are zero due to the symmetry of u_α.

The contribution of $-2\mathrm{Re}\,P\cdot P_f$ is

$$\begin{aligned}
&-2\mathrm{Re}\,\langle \Pi_1\Theta,\, P\cdot P_f\alpha^{\frac{1}{2}}\Upsilon_\alpha\rangle - 2\mathrm{Re}\,\langle \alpha^{\frac{1}{2}}\Upsilon_\alpha,\, P\cdot P_f\Theta\rangle\\
&= -4\mathrm{Re}\,\langle (\alpha^{\frac{1}{2}}\gamma_1\Gamma_1+\Pi_1 R)u_\alpha,\, P\cdot P_f\alpha^{\frac{1}{2}}\Upsilon_\alpha\rangle\\
&= -2\alpha\mathrm{Re}\,\gamma_1\langle 2\,P\cdot P_f(H_f+P_f^2)^{-1}\Gamma_1 u_\alpha,\, \Upsilon_\alpha\rangle_* - 4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle P u_\alpha\cdot P_f\Pi_1 R,\, \Upsilon_\alpha\rangle\\
&= \mathcal{O}(\alpha^4)
\end{aligned}\tag{2.22}$$

where we used $\langle 2\,P\cdot P_f(H_f+P_f^2)^{-1}\Gamma_1 u_\alpha,\, \Upsilon_\alpha\rangle_* = \langle\Phi_\alpha,\, \Upsilon_\alpha\rangle_* = 0$ due to Lemma B.1, and $\|Pu_\alpha\| = \mathcal{O}(\alpha)$, $\|\Upsilon_\alpha\| = \mathcal{O}(\alpha)$ and $\|P_f\Pi_1 R\| \leq \|R\|_* = \mathcal{O}(\alpha^{\frac{3}{2}})$ (Theorem A.1).

The contribution of $-4\alpha^{\frac{1}{2}}\mathrm{Re}\,P\cdot A^-$ is

$$\begin{aligned}
&-4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle \Pi_0\Theta,\, P\cdot A^-\alpha^{\frac{1}{2}}\Upsilon_\alpha\rangle - 4\alpha^{\frac{1}{2}}\mathrm{Re}\,\langle \alpha^{\frac{1}{2}}\Upsilon_\alpha,\, P\cdot A^-\Pi_2\Theta\rangle\\
&= -2\alpha\mathrm{Re}\,\langle 2P\cdot A^+ u_\alpha\!\uparrow\otimes\Omega_f,\, \Upsilon_\alpha\rangle - 4\alpha\mathrm{Re}\,\langle\Upsilon_\alpha,\, P\cdot A^-(\alpha\gamma_2\Gamma_2+\Pi_2 R)u_\alpha\rangle\\
&= -2\alpha\|\Upsilon_\alpha\|_*^2 + \mathcal{O}(\alpha^4)\,,
\end{aligned}\tag{2.23}$$

where we applied in the last equality $\|Pu_\alpha\| = \mathcal{O}(\alpha)$, $\|\Upsilon_\alpha\| = \mathcal{O}(\alpha)$ and $\|A^-\Pi_2 R\| \leq c\|R\|_* = \mathcal{O}(\alpha^{\frac{3}{2}})$.

Equations (2.22) and (2.23) implies

$$\langle \alpha^{\frac{1}{2}} \Upsilon_\alpha,\, H\,\Theta\rangle + \langle \Theta,\, H\,\alpha^{\frac{1}{2}} \Upsilon_\alpha\rangle = -2\alpha \|\Upsilon_\alpha\|_*^2 + \mathcal{O}(\alpha^4)\,. \tag{2.24}$$

Step 5. Collecting all above estimates (2.12), (2.13), (2.14), (2.18), (2.21) and (2.24) yields

$$\langle \Psi^{\rm trial},\, H\Psi^{\rm trial}\rangle = (\Sigma_0 - \frac{\alpha^2}{4})\|\Theta\|^2 - \alpha\|\Phi_\alpha\|_*^2 - \alpha\|\Upsilon_\alpha\|_*^2 + \mathcal{O}(\alpha^4) \tag{2.25}$$

To conclude the proof, we need to normalize the above expression. First note that $\langle \Theta,\, \alpha^{\frac{1}{2}}(\Phi_\alpha + \Upsilon_\alpha)\rangle = 0$ due to orthogonality of u_α and $\partial u_\alpha/\partial x_j$ $(j = 1,\, 2,\, 3)$. Therefore

$$\begin{aligned} \|\Psi^{\rm trial}\|^2 &= \|\Theta\|^2 + \alpha\|\Phi_\alpha + \Upsilon_\alpha\|^2 \\ &= \|\Theta\|^2 + \mathcal{O}(\alpha^3|\log\alpha|)\,, \end{aligned}$$

since $\|\Phi_\alpha + \Upsilon_\alpha\| = \mathcal{O}(\alpha|\log\alpha|^{\frac{1}{2}})$.

This yields

$$\begin{aligned} \Sigma &\le \frac{\langle \Psi^{\rm trial},\ H\,\Psi^{\rm trial}\rangle}{\|\Psi^{\rm trial}\|^2} \\ &= \frac{(\Sigma_0 - \frac{\alpha^2}{4})\|\Theta\|^2 - \alpha\|\Phi_\alpha\|_*^2 - \alpha\|\Upsilon_\alpha\|_*^2 + \mathcal{O}(\alpha^4)}{\|\Theta\|^2 + \mathcal{O}(\alpha^3|\log\alpha|)} \\ &= (\Sigma_0 - \frac{\alpha^2}{4}) - \alpha\|\Phi_\alpha\|_*^2 - \alpha\|\Upsilon_\alpha\|_*^2 + \mathcal{O}(\alpha^4|\log\alpha|)\,, \end{aligned} \tag{2.26}$$

where we used $\|\Theta\|^2 = 1 + \mathcal{O}(\alpha)$ (see Theorem A.1), $\Sigma_0 = \mathcal{O}(\alpha)$, $\|\Phi_\alpha\|_* = \mathcal{O}(\alpha)$, and $\|\Upsilon_\alpha\|_* = \mathcal{O}(\alpha)$.

To conclude the proof, it suffices to replace $\|\Phi_\alpha\|_*$ and $\|\Upsilon_\alpha\|_*$ by their expressions in Lemma B.2. □

A. ground state of $T(0)$

To define the trial function $\Psi^{\rm trial}$ in the proof of Theorem 2.1, we need some properties derived in [11] for the ground state of the self-energy operator with total momentum zero $T(0)$. For convenience of the readers, we remind here these properties.

Theorem A.1. *Let*

$$\Gamma_1 := -(H_f + P_f^2)^{-1}\sigma\cdot B^+\!\uparrow \otimes\Omega_f \tag{A.1}$$

and

$$\Gamma_2 = -(H_f + P_f^2)^{-1}\left(\sigma\cdot B^+\Gamma_1 \ +\ 2A^+\cdot P_f\Gamma_1 \ +\ A^+\cdot A^+\!\uparrow \otimes\Omega_f\right)\,. \tag{A.2}$$

We have

$$\begin{aligned}&\inf\operatorname{spec}(T(0))\\&= -\alpha\|\Gamma_1\|_*^2 \;+\; \alpha^2\left(2\|A^-\Gamma_1\|^2 - \|\Gamma_2\|_*^2 + \|\Gamma_1\|_*^2\,\|\Gamma_1\|^2\right) \;+\; \mathcal{O}(\alpha^3)\,.\end{aligned}$$

In addition, let θ_{GS} be the ground state of $T(0)$ such that $\Pi_0\theta_{GS} = \uparrow\otimes\Omega_f$. Taking the $\langle\,.\,,\,.\,\rangle_*$-orthonormal projections of θ_{GS} along the vectors Γ_1 and Γ_2, and denoting by R the component in the $\langle\,.\,,\,.\,\rangle_*$-orthogonal complement of their span, we get

$$\theta_{GS} = \uparrow\otimes\Omega_f + \alpha^{\frac12}\gamma_1\Gamma_1 + \alpha\gamma_2\Gamma_2 + R \tag{A.3}$$

where for $i = 1,2$

$$\langle\Gamma_i,\,R\rangle_* = 0 \quad \text{and} \quad \langle\uparrow\otimes\Omega_f,\,R\rangle = 0\,. \tag{A.4}$$

Then, we have

$$\begin{aligned}&|\gamma_1 - 1| = \mathcal{O}(\alpha)\,,\quad |\gamma_2 - 1| = \mathcal{O}(\alpha^{\frac12})\,,\\&\|R\|_* = \mathcal{O}(\alpha^{\frac32})\quad \text{and} \quad \|R\| = \mathcal{O}(\alpha)\,.\end{aligned} \tag{A.5}$$

B. Technical results

Lemma B.1. *For Φ_α defined by* (2.8) *and Γ_1 defined by* (A.1)*, we have for all $\alpha > 0$*

$$\langle P\cdot A^+ u_\alpha\uparrow\otimes\Omega_f,\,\Phi_\alpha\rangle = 0 \quad \text{and} \quad \langle\Phi_\alpha,\,\Upsilon_\alpha\rangle_* = 0\,.$$

Proof. This is a straightforward computation. □

Lemma B.2. *For Φ_α defined by* (2.8) *and Υ_α defined by* (2.9)*, we have for all $\alpha > 0$*

$$\|\Phi_\alpha\|_*^2 = \frac{2\alpha^2}{3\pi}\int_0^\infty \frac{t^2\,\zeta^2(t)}{(1+t)^3}\,\mathrm{d}t\,, \quad \text{and} \quad \|\Upsilon_\alpha\|_*^2 = \frac{2\alpha^2}{3\pi}\int_0^\infty \frac{\zeta^2(t)}{1+t}\mathrm{d}t \;+\; \mathcal{O}(\alpha^3)\,.$$

Proof. This is a straightforward computation using the definition of Φ_α and Υ_α, and the fact that (see e.g. [9])

$$\sigma\cdot B^+\uparrow\otimes\Omega_f = \frac{-i\,\zeta(|k|)}{2\pi|k|^{\frac12}}\begin{pmatrix}-\sqrt{k_1^2+k_2^2}\\ 0\\ \frac{(k_1+ik_2)k_3}{\sqrt{k_1^2+k_2^2}}\\ \frac{|k|(-k_2+ik_1)}{\sqrt{k_1^2+k_2^2}}\end{pmatrix}\,,$$

and

$$(H_f + P_f^2)^{-1} A^+ \Omega_f = \frac{\zeta(|k|)}{2\pi |k|^{\frac{1}{2}} (|k|^2 + |k|) \sqrt{k_1^2 + k_2^2}} \begin{pmatrix} k_2 + \frac{k_1 k_3}{|k|} \\ -k_1 + \frac{k_2 k_3}{|k|} \\ \frac{-(k_1^2 + k_2^2)}{|k|} \end{pmatrix} .$$

□

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