HYPERFINE SPLITTING OF THE DRESSED HYDROGEN ATOM 
GROUND STATE IN NON-RELATIVISTIC QED

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ABSTRACT. We consider a spin-\(\frac{1}{2}\) electron and a spin-\(\frac{1}{2}\) nucleus interacting with the quantized electromagnetic field in the standard model of non-relativistic QED. For a fixed total momentum sufficiently small, we study the multiplicity of the ground state of the reduced Hamiltonian. We prove that the coupling between the spins of the charged particles and the electromagnetic field splits the degeneracy of the ground state.

1. Introduction

This paper is concerned with the spectral analysis of the quantum Hamiltonian associated with a free hydrogen atom, in the context of non-relativistic QED. Before describing our result more precisely, we begin with recalling a few well-known facts about the spectrum of Hydrogen in the case where the corrections due to quantum electrodynamics are not taken into account. For more details, we refer the reader to classical textbooks on Quantum Mechanics (see, e.g., [Me, CTDL]). See also [BS, IZ, And].

We consider a neutral hydrogenoid system composed of one electron with spin \(\frac{1}{2}\) and one nucleus with spin \(\frac{1}{2}\). The Pauli Hamiltonian in \(L^2(\mathbb{R}^6; \mathbb{C}^4)\) associated with this system can be written in the following way:

\[
H_{Pa} := \frac{1}{2m_{el}} (p_{el} - \alpha A_n(x_{el}))^2 - \frac{\alpha^2}{2m_{el}} \sigma_{el} \cdot B_n(x_{el}) \\
+ \frac{1}{2m_n} (p_n + \alpha A_{el}(x_n))^2 + \frac{\alpha^2}{2m_n} \sigma^n \cdot B_{el}(x_n) - \frac{\alpha}{|x_{el} - x_n|}.
\]

(1.1)

Here the units are chosen such that \(\hbar = c = 1\), where \(\hbar = h/2\pi\), \(h\) is the Planck constant, and \(c\) is the velocity of light. The notations \(m_{el}, x_{el}\) and \(p_{el} = -i\nabla x_{el}\) (respectively \(m_n, x_n\) and \(p_n = -i\nabla x_n\)) stand for the mass, the position and the momentum of the electron (respectively of the nucleus), and \(\alpha = e^2\) is the fine-structure constant (with \(e\) the charge of the electron). Moreover, \(\sigma_{el} = (\sigma_1^{el}, \sigma_2^{el}, \sigma_3^{el})\) (respectively \(\sigma_n\)) are the Pauli matrices accounting for the spin of the electron (respectively of the nucleus), and \(A_n(x_{el})\) is the vector potential of the electromagnetic field generated by the nucleus at the position of the electron, that is \(A_n(x_{el}) = C \alpha^{1/2} (\sigma^n \wedge (x_{el} - x_n))/(m_n|x_{el} - x_n|^3)\) where \(C\) is a positive constant (and similarly for \(A_{el}(x_n)\)). Finally, \(B_n(x_n) = ip_{el} \wedge A_n(x_{el})\) and \(B_{el}(x_n) = ip_n \wedge A_{el}(x_n)\).

The Hamiltonian \(H_{Pa}\) can be derived from the Dirac equation in the non-relativistic regime. It allows one to justify the so-called hyperfine structure of the ground state of the Hydrogen atom. More precisely, let \(H_{Pa}(0)\) be the Hamiltonian obtained when the total momentum vanishes. Then \(H_{Pa}(0)\) in \(L^2(\mathbb{R}^3; \mathbb{C}^4)\) can be decomposed into a sum of four terms, \(H_{Pa}(0) = H_0 + H_1 + H_2 + H_3\), where \(H_0 = \frac{p^2}{2\mu} - \alpha/|r|\) (here \(\mu\) denotes the reduced mass of the atom

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and $p_r = -i\nabla_r$), $H_1$ is the orbital interaction, $H_2$ is the spin-orbit interaction, and $H_3$ is the spin-spin interaction (see e.g. [And, Chapter 4] and [AA] for details). It is seen that $H_0$ has a 4-fold degenerate ground state. The correction terms, $H_1$, $H_2$, and $H_3$, produce an energy shift. Moreover, under the influence of the spin-spin interaction, the unperturbed ground state eigenvalue splits into two parts: a simple eigenvalue associated with a unique ground state, and a 3-fold degenerate eigenvalue. This phenomenon is referred to as the hyperfine splitting of the hydrogen atom ground state. Let us mention that this splitting explains the famous observed 21-cm Hydrogen line.

In this paper, we investigate the hyperfine structure of the hydrogen atom in the standard model of non-relativistic QED. We aim at establishing that a hyperfine splitting does occur in the framework of non-relativistic QED. The Hamiltonian is still given by the expression (1.1), except that $A_n(x_{el})$ and $A_{el}(x_{el})$ are replaced by the vector potentials of the quantized electromagnetic field in the Coulomb gauge (and likewise for $B_n(x_{el})$ and $B_{el}(x_{el})$, precise definitions will be given in Subsection 2.1 below). Moreover the energy of the free photon field is added. Since both the electron and the nucleus are treated as moving particles, the total Hamiltonian, $H_g$, is translation invariant. Here $g$ denotes a coupling parameter depending on the fine-structure constant $\alpha$. The translation invariance implies that $H_g$ admits a direct integral decomposition, $H_g \sim \int_{\mathbb{R}^3} H_g(P)dP$, with respect to the total momentum $P$ of the system. We set $E_g(P) := \inf \sigma(H_g(P))$.

In [AGG], it is established that, for $g$ and $P$ sufficiently small, $E_g(P)$ is an eigenvalue of $H_g(P)$, that is $H_g(P)$ has a ground state. We also mention [LMS1] where the existence of a ground state for $H_g(P)$ is obtained for any value of $g$, under the assumption that $E_g(0) \leq E_0(P)$. Using a method due to [Hi2], it is proven in [AGG] that the multiplicity of $E_g(P)$ cannot exceed the multiplicity of $E_0(P) := \inf \sigma(H_0(P))$, where $H_0(P) := H_{g=0}(P)$ denotes the non-interacting Hamiltonian. In other words,

$$\dim \ker (H_g(P) - E_g(P)) \leq \dim \ker (H_0(P) - E_0(P)).$$

(1.2)

Our purpose is to determine whether the inequality in (1.2) is strict, or, on the contrary, is an equality.

Of course, the multiplicity of $E_g(P)$ depends on the value of the spins of the charged particles. If the spin of the electron is neglected and the spin of the nucleus is equal to 0, then $E_0(P)$ is simple, and hence, according to (1.2), $E_g(P)$ is also a simple eigenvalue. In particular, (1.2) is an equality.

If the spin of the electron is taken into account, and the spin of the nucleus is equal to 0, then $E_0(P)$ is twice-degenerate. Using Kramer’s degeneracy theorem (see [LMS2]), one can prove that the multiplicity of $E_g(P)$ is even. Therefore, by (1.2), $E_g(P)$ is also twice-degenerate, and hence (1.2) is again an equality. We refer the reader to [HS, Sp, Sa, Hi1, LMS2] for results on the twice-degeneracy of the ground state of various QED models.

Consider now a hydrogen atom composed of a spin-$\frac{1}{2}$ electron and a spin-$\frac{1}{2}$ nucleus (e.g. a proton). In this case, the multiplicity of $E_0(P)$ is equal to 4. Our main result states that

$$\dim \ker (H_g(P) - E_g(P)) < \dim \ker (H_0(P) - E_0(P)) = 4,$$

(1.3)

for $g \neq 0$ small enough. Equation (1.3) can be interpreted as a hyperfine splitting of the ground state of $H_g(P)$. In other words, the Hamiltonian of a freely moving hydrogen atom at a fixed total momentum in non-relativistic QED contains hyperfine interaction terms which split the degeneracy of the ground state, in the same way as for the Pauli Hamiltonian of Quantum Mechanics mentioned above. Pursuing the analogy with the Pauli Hamiltonian...
(1.1), one can conjecture that $E_g(P)$ is simple. Proving this is however beyond the scope of the present paper.

We also mention that non-relativistic QED provides a suitable framework to rigorously justify radiative decay and Bohr’s frequency condition (see [BFS1, BFS2, AFFS, Sig] for the case of atomic systems with an infinitely heavy nucleus). In particular, save for the ground state, all stationary states are expected to turn into metastable states with a finite lifetime. Hence in relation with the 21-cm hydrogen line mentioned above, one can expect that a resonance appears near the ground state energy $E_g(P)$, with a very small imaginary part. Showing this would presumably require the use of complex dilatations together with renormalization techniques as in [BFS1].

The case of a nucleus of spin $\geq 1$ is not considered here (for instance, the nucleus of deuterium, composed of one proton and one neutron, can be treated as a spin-1 particle), but we expect that a similar hyperfine splitting of the ground state occurs in this case also. As for positively charged hydrogenoid ions, the question of the existence of a ground state is more subtle than for the hydrogen atom. Indeed, it is proven in [HH] that the Hamiltonian of a positive ion at a fixed total momentum in non-relativistic QED does not have a ground state in Fock space. This result should be compared with the corresponding one for the model of a freely moving, dressed non-relativistic electron in non-relativistic QED, which has been studied recently by several authors (see, among other papers, [Ch, CF, BCFS2, HH, CFP, LMS2, FP]; see also [AFGG]).

Let us finally mention that the ground state degeneracy of the non-relativistic hydrogen atom confined by its center of mass (see [AF, Fa]) could also be analyzed by the techniques developed here, provided that both the electron and the nucleus have a spin equal to $\frac{1}{2}$.

2. Definition of the model and statement of the main result

2.1. Definition of the model. In the standard model of non-relativistic QED, the Hamiltonian associated with the system we consider acts on the Hilbert space $\mathcal{H} := \mathcal{H}_{at} \otimes \mathcal{H}_{ph}$, where

$$\mathcal{H}_{at} := L^2(\mathbb{R}^3; \mathbb{C}^2) \otimes L^2(\mathbb{R}^3; \mathbb{C}^2) \sim L^2(\mathbb{R}^6; \mathbb{C}^4) \quad (2.1)$$

is the Hilbert space for the charged particles (the electron and the nucleus), and

$$\mathcal{H}_{ph} := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} S_n \left[ L^2(\mathbb{R}^3 \times \{1, 2\})^{\otimes n} \right] \quad (2.2)$$

is the symmetric Fock space for the photons. Here $S_n$ denotes the symmetrization operator.

The Hamiltonian of the system, $H^{SM}$, is formally given by the expression

$$H^{SM} := \frac{1}{2m_{el}} \left( p_{el} - \alpha \frac{1}{2} A(x_{el}) \right)^2 + \frac{1}{2m_n} \left( p_n + \alpha \frac{1}{2} A(x_n) \right)^2 + V(x_{el}, x_n) + H_{ph}$$

$$- \frac{\alpha^2}{2m_{el}} \sigma^{el} \cdot B(x_{el}) + \frac{\alpha^2}{2m_n} \sigma^n \cdot B(x_n), \quad (2.3)$$

where $x_{el}, x_n, p_{el}, p_n$ and $\alpha$ are defined as in (1.1). For $x \in \mathbb{R}^3$, $A(x)$ is defined by

$$A(x) := \frac{1}{2\pi} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\chi_{A}(k)}{|k|^{\frac{1}{2}}} \varepsilon(k) \left[ e^{-ik \cdot x} a^{\dagger}_{\lambda}(k) + e^{ik \cdot x} a_{\lambda}(k) \right] dk, \quad (2.4)$$
and $B(x)$ is given by

$$B(x) := -\frac{i}{2\pi} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k|^\frac{1}{2} \chi_\Lambda(k) \left( \frac{k}{|k|} \wedge \varepsilon^\lambda(k) \right) \left[ e^{-ik\cdot x} a^*_\lambda(k) - e^{ik\cdot x} a_\lambda(k) \right] dk,$$

(2.5)

where the polarization vectors $\varepsilon^1(k)$ and $\varepsilon^2(k)$ are chosen in the following way:

$$\varepsilon^1(k) := \frac{(k_2, -k_1, 0)}{\sqrt{k_1^2 + k_2^2}}, \quad \varepsilon^2(k) := \frac{k}{|k|} \wedge \varepsilon^1(k) = \frac{(-k_1 k_3, -k_2 k_3, k_1^2 + k_2^2)}{\sqrt{k_1^2 + k_2^2} \sqrt{k_1^2 + k_2^2 + k_3^2}}.$$  

(2.6)

In (2.4) and (2.5), $\chi_\Lambda(k)$ denotes an ultraviolet cutoff function which, for the sake of concreteness, we choose as

$$\chi_\Lambda(k) := \mathbb{1}_{|k| \leq \Lambda \alpha^2}(k).$$

(2.7)

Here, $\Lambda$ is supposed to be a given arbitrary (large and) positive parameter. As explained in [BFS2, Sig], the model is physically relevant if we assume that $1 \ll \Lambda \ll \alpha^{-2}$. The reason for introducing $\alpha^2$ into the definition (2.7) will appear below (see (2.18)).

As usual, for any $h \in L^2(\mathbb{R}^3 \times \{1, 2\})$, we set

$$a^*(h) := \sum_{\lambda=1,2} \int_{\mathbb{R}^3} h(k, \lambda) a^*_\lambda(k) dk, \quad a(h) := \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \bar{h}(k, \lambda) a_\lambda(k) dk,$$

(2.8)

and $\Phi(h) := a^*(h) + a(h)$, where the creation and annihilation operators, $a^*_\lambda(k)$ and $a_\lambda(k)$, obey the canonical commutation relations

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

(2.9)

Hence, in particular, for $j \in \{1, 2, 3\}$, we have $A_j(x) = \Phi(h^A_j(x))$ and $B_j(x) = \Phi(h^B_j(x))$, with

$$h^A_j(x, k, \lambda) := \frac{1}{2\pi} \frac{\chi_\Lambda(k)}{|k|^\frac{1}{2}} \varepsilon_j^\lambda(k) e^{-ik\cdot x},$$

(2.10)

$$h^B_j(x, k, \lambda) := -\frac{i}{2\pi} |k|^\frac{1}{2} \chi_\Lambda(k) \left( \frac{k}{|k|} \wedge \varepsilon^\lambda(k) \right)_j e^{-ik\cdot x}.$$  

(2.11)

The Coulomb potential $V(x_{el}, x_n)$ is given by

$$V(x_{el}, x_n) \equiv V(x_{el} - x_n) := -\frac{\alpha}{|x_{el} - x_n|},$$

(2.12)

and $H_{ph}$ is the Hamiltonian of the free photon field, defined by

$$H_{ph} := \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| a^*_\lambda(k) a_\lambda(k) dk.$$

(2.13)

The 3-uples $\sigma^1 = (\sigma^1_1, \sigma^1_2, \sigma^1_3)$ and $\sigma^2 = (\sigma^2_1, \sigma^2_2, \sigma^2_3)$ are the Pauli matrices associated with the spins of the electron and the nucleus respectively. They can be written as $4 \times 4$ matrices in the following way:

$$\sigma^1_1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad \sigma^1_2 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \quad \sigma^1_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix},$$

(2.14)

$$\sigma^2_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \sigma^2_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \quad \sigma^2_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$  

(2.15)
In order to exhibit the perturbative behavior of the interaction between the charged particles and the photon field, we proceed to a change of units. More precisely, let $\mathcal{U} : \mathcal{H} \to \mathcal{H}$ be the unitary operator associated with the scaling

$$(x_{el}, x_n, k_1, \lambda_1, \ldots, k_n, \lambda_n) \mapsto (x_{el}/\alpha, x_n/\alpha, \alpha^2 k_1, \lambda_1, \ldots, \alpha^2 k_n, \lambda_n).$$

(2.16)

We have

$$\frac{1}{\alpha^2} \mathcal{U} H_{\text{SM}} \mathcal{U}^* = \frac{1}{2m_{el}} \left( p_{el} - \frac{\alpha^2}{2} \tilde{A}(\alpha x_{el}) \right)^2 + \frac{1}{2m_n} \left( p_n + \frac{\alpha^2}{2} \tilde{A}(\alpha x_n) \right)^2$$

$$- \frac{1}{|x_{el} - x_n|} + H_{\text{ph}} - \frac{\alpha^2}{2m_{el}} \sigma^{el} \cdot \tilde{B}(\alpha x_{el}) + \frac{\alpha^2}{2m_n} \sigma^n \cdot \tilde{B}(\alpha x_n),$$

(2.17)

where $\tilde{A}$ and $\tilde{B}$ are defined in the same way as $A$ and $B$, except that the ultraviolet cutoff function $\chi_\Lambda(k)$ is replaced by

$$\tilde{\chi}_\Lambda(k) := \chi_\Lambda(\alpha^2 k) = \mathbf{1}_{|k| \leq \Lambda}(k).$$

(2.18)

To simplify the notations, we redefine $\tilde{\chi}_\Lambda = \chi_\Lambda$, $A = \tilde{A}$ and $B = \tilde{B}$. Setting $g := \alpha^2$, we are thus led to study the Hamiltonian

$$H_{g}^{\text{SM}} := \frac{1}{2m_{el}} \left( p_{el} - gA(g^2 x_{el}) \right)^2 + \frac{1}{2m_n} \left( p_n + gA(g^2 x_n) \right)^2$$

$$- \frac{1}{|x_{el} - x_n|} + H_{\text{ph}} - \frac{g}{2m_{el}} \sigma^{el} \cdot B(g^2 x_{el}) + \frac{g}{2m_n} \sigma^n \cdot B(g^2 x_n).$$

(2.19)

Let the total mass, $M$, and the reduced mass, $\mu$, be defined respectively by

$$M := m_{el} + m_n, \quad \frac{1}{\mu} := \frac{1}{m_{el}} + \frac{1}{m_n}.$$  

(2.20)

Let

$$r := x_{el} - x_n, \quad R := \frac{m_{el}}{M} x_{el} + \frac{m_n}{M} x_n, \quad \frac{p_r}{\mu} := \frac{p_{el}}{m_{el}} - \frac{p_n}{m_n}, \quad P_R := p_{el} + p_n.$$  

(2.21)

For $g = 0$, the Hamiltonian $H_{g=0}^{\text{SM}} := H_0^{\text{SM}}$ is given by

$$H_0^{\text{SM}} = \frac{p^2}{2m_{el}} + \frac{p^2}{2m_n} - \frac{1}{|x_{el} - x_n|} + H_{\text{ph}} = H_R + H_r + H_{\text{ph}},$$

(2.22)

where the Schrödinger operators $H_R$ and $H_r$ on $L^2(\mathbb{R}^3)$ are defined by

$$H_R := \frac{P_R^2}{2M}, \quad H_r := \frac{P_r^2}{2\mu} - \frac{1}{|r|}.$$  

(2.23)

Let $e_0 := -\frac{\beta^2}{2}$ be the ground state eigenvalue of $H_r$ and $e_1$ be the first eigenvalue above $e_0$. Note that a normalized eigenstate associated with $e_0$ is given by

$$\phi_0(r) := (\pi^{-1} \mu^3)^{\frac{1}{2}} e^{-\mu |r|}.$$  

(2.24)

To conclude this subsection, we recall the definition of the photon number operator, $N_{\text{ph}}$, which will be used in the sequel:

$$N_{\text{ph}} := \sum_{\lambda=1,2} \int_{\mathbb{R}^3} a^*_\lambda(k) a_\lambda(k) dk.$$  

(2.25)
2.2. Fiber decomposition. The Hamiltonian $H^{SM}_g$ is translation invariant in the sense that $H^{SM}_g$ formally commutes with the total momentum operator $P_{tot} := P_R + P_{ph}$, where $P_{ph}$ denotes the momentum operator of the photon field, given by the expression

$$P_{ph} := \sum_{\lambda=1,2} \int_{\mathbb{R}^3} k a^*_\lambda(k) a_\lambda(k) dk. \quad (2.26)$$

In the same way as in [AGG], it follows that $H^{SM}_g$ can be decomposed into a direct integral, which is expressed in the following proposition.

**Proposition 2.1 ([AGG])**. There exists $g_c > 0$ such that for all $|g| \leq g_c$, the following holds: the Hamiltonian $H^{SM}_g$ given by the formal expression (2.19) identifies with a self-adjoint operator which is unitarily equivalent to the direct integral $\int_{\mathbb{R}^3} H_g(P) dP$. Moreover, for all $P \in \mathbb{R}^3$, $H_g(P)$ is a self-adjoint operator acting on the Hilbert space

$$\mathcal{H}(P) := L^2(\mathbb{R}^3; \mathbb{C}^4) \otimes \mathcal{H}_{ph} \sim \mathbb{C}^4 \otimes L^2(\mathbb{R}^3, dr) \otimes \mathcal{H}_{ph},$$

with domain $D(H_g(P)) = D(H_0(P))$, and $H_g(P)$ is given by the expression:

$$H_g(P) = \frac{1}{2m_{el}} \left( \frac{m_{el}}{M} (P - P_{ph}) + p_r - g A(\frac{m_{el}}{M} g^2 r) \right)^2$$

$$+ \frac{1}{2m_n} \left( \frac{m_n}{M} (P - P_{ph}) - p_r + g A(\frac{m_n}{M} g^2 r) \right)^2$$

$$- \frac{1}{|r|} + H_{ph} - \frac{g}{2m_{el}} \sigma^{el} \cdot B \left( \frac{m_{el}}{M} g^2 r \right) + \frac{g}{2m_n} \sigma^{n} \cdot B \left( -\frac{m_n}{M} g^2 r \right). \quad (2.28)$$

Let us mention that this direct integral decomposition remains true for an arbitrary value of the coupling constant $g$ (see [LMS1]). However, in this paper, we shall only be interested in the small coupling regime.

For $g = 0$, the fiber Hamiltonian $H_0(P) := H_{g=0}(P)$ reduces to the diagonal operator

$$H_0(P) = H_r + \frac{1}{2M} (P - P_{ph})^2 + H_{ph}, \quad (2.29)$$

where $H_r$ is the Schrödinger operator defined in (2.23). Let $\Omega$ denote the photon vacuum in $\mathcal{H}_{ph}$. One can verify that

$$E_0(P) := \inf \sigma(H_0(P)) = e_0 + \frac{p^2}{2M}, \quad (2.30)$$

and that $e_0 + p^2/2M$ is an eigenvalue of multiplicity 4 of $H_0(P)$. Moreover, the associated normalized eigenstates can be written under the form $y \otimes \phi_0 \otimes \Omega$, where $y$ is an arbitrary normalized element in $\mathbb{C}^4$. 
The operator $H_0(P)$ is treated as an unperturbed Hamiltonian, the perturbation $W_g(P) := H_g(P) - H_0(P)$ being given by

\[
W_g(P) = -\frac{g}{m_{el}} \left( \left( \frac{m_{el}}{M} (P - P_{ph}) + p_r \right) \cdot A \left( \frac{m_{el}}{M} g^2 r \right) \right) + \frac{g}{m_n} \left( \left( \frac{m_n}{M} (P - P_{ph}) - p_r \right) \cdot A \left( -\frac{m_n}{M} g^2 r \right) \right) + \frac{g^2}{2m_{el}} A \left( \frac{m_{el}}{M} g^2 r \right)^2 + \frac{g^2}{2m_n} A \left( -\frac{m_n}{M} g^2 r \right)^2 - \frac{g}{2m_{el}} \sigma_{el} \cdot B \left( \frac{m_{el}}{M} g^2 r \right) + \frac{g}{2m_n} \sigma_{el} \cdot B \left( -\frac{m_n}{M} g^2 r \right). \tag{2.31}
\]

Note that, due to the choice of the Coulomb gauge, the operators $A(m_{el}g^{2/3}r/M)$ and $A(-m_ng^{2/3}r/M)$ commute both with $p_r$ and $P_{ph}$.

### 2.3. Main result and organization of the paper

Our main result is stated in the following theorem.

**Theorem 2.2.** There exist $g_c > 0$ and $p_c > 0$ such that, for any $0 < |g| \leq g_c$ and $0 \leq |P| \leq p_c$,

\[
\dim \ker (H_g(P) - E_g(P)) < 4. \tag{2.32}
\]

Our proof of Theorem 2.2 is based on a contradiction argument and the use of the Feshbach-Schur identity. The point is that the assumption $\dim \ker (H_g(P) - E_g(P)) = 4$ will allow us to compute the second order expansion in $g$ of the expression $(E_g(P) - E_0(P))\Pi_0$, where $\Pi_0$ denotes the projection onto the eigenspace associated with the eigenvalue $E_0(P)$ of $H_0(P)$. More precisely, applying in a suitable way the Feshbach-Schur map, we will find that $(E_g(P) - E_0(P))\Pi_0 = \Gamma + O(|g|^{2+\tau})$ for some $\tau > 0$, where $\Gamma$ is an explicitly given $4 \times 4$ matrix. The previous identity implies in particular that all the coefficients of order $g^2$ in the matrix $\Gamma$ must be located on the diagonal, which will lead to a contradiction.

We decompose the proof of Theorem 2.2 into two main steps. In Section 3, we introduce and study some properties of the Feshbach-Schur operator that we consider. Next, in Section 4, we assume that the multiplicity of $E_g(P)$ is equal to 4, and we conclude the proof of Theorem 2.2 by a contradiction argument. In Appendix A, we collect some fairly standard estimates which are used in Sections 3 and 4.

Throughout the paper, $C, C', C''$ will denote positive constants that may differ from one line to another.

### 3. The Feshbach-Schur operator

In this section, we introduced the Feshbach-Schur operator that we consider, and we study some of its properties. They will be used below in Section 4 in order to prove Theorem 2.2.

It is convenient to work with the Hamiltonian $\tilde{H}_g(P)$ obtained from $H_g(P)$ by Wick ordering, that is $\tilde{H}_g(P) = : H_g(P) :$, with the usual notations. It is not difficult to check that $\tilde{H}_g(P) = H_g(P) - g^2C_\Lambda$, where $C_\Lambda$ is a positive constant depending on the ultraviolet cutoff parameter $\Lambda$. Hence it suffices to prove Theorem 2.2 with $\tilde{H}_g(P)$ replacing $H_g(P)$ and $\tilde{E}_g(P) := \inf \sigma(\tilde{H}_g(P))$ replacing $E_g(P)$. To simplify the notations, we redefine $H_g(P) := \tilde{H}_g(P)$ and $E_g(P) := \tilde{E}_g(P)$. Moreover, in what follows, we drop the dependence
Lemma 3.1. There exist \( E \) with the eigenvalue \( \varepsilon \).

Lemma 3.2. There exist \( \Pi_\rho \) in the tensor product \( \mathbb{C}^4 \otimes L^2(\mathbb{R}) \otimes \mathcal{H}_{ph} \) by

\[
\Pi_\rho := 1 \otimes \Pi_{\phi_0} \otimes 1_{\text{H}_{ph} \leq \rho},
\]

where \( \Pi_{\phi_0} \) denotes the projection onto the eigenspace associated with the eigenvalue \( \varepsilon_0 \) of \( H_\varepsilon \). In particular, as above, \( \Pi_0 = 1 \otimes \Pi_{\phi_0} \otimes \Pi_{\Omega} \) is the projection onto the eigenspace associated with the eigenvalue \( \varepsilon_0 \) of \( H_0 \) (here \( \Pi_{\Omega} \) is the projection onto the Fock vacuum).

Lemma 3.1 gives

\[
\| (H_0 - E_g) \Pi_\rho \| = \| (E_0 - E_g) \Pi_\rho + (\frac{P}{M} \cdot P_{ph} + \frac{P_{ph}}{2M} + H_{ph}) \Pi_\rho \| \leq Cg^2 + C^\rho \leq C'' \rho,
\]

since, by assumption, \( \rho \gg g^2 \). Next, by Lemma A.8, we have that

\[
\Pi_\rho W_g \Pi_\rho \| \leq C|g| \rho^{\frac{3}{2}} \leq C' \rho.
\]

Lemma 3.1 gives

\[
\Pi_\rho W_g [H_0 - E_g]^{-1} \Pi_\rho W_g \Pi_\rho = \Pi_\rho W_g [H_0 - E_g]^{-1} \Pi_\rho \sum_{n \geq 0} (-W_g \Pi_\rho [H_0 - E_g]^{-1} \Pi_\rho)^n W_g \Pi_\rho.
\]
Using again Lemma A.8, we obtain that, for all \( n \geq 0 \),
\[
\|\Pi_\rho W_g [H_0 - E_g]^{-1} \Pi_\rho \left( -W_g \Pi_\rho [H_0 - E_g]^{-1} \Pi_\rho \right)^n W_g \Pi_\rho \| \leq C g^2 (C' |g| \rho^{-\frac{1}{2}})^n, \tag{3.11}
\]
which implies
\[
\|\Pi_\rho W_g [\Pi_\rho H_0 \Pi_\rho - E_g]^{-1} \Pi_\rho W_g \Pi_\rho \| \leq C g^2 \leq C' \rho. \tag{3.12}
\]
Equations (3.8), (3.9) and (3.12) give (3.7).  \( \square \)

We now turn to the Feshbach-Schur identity. We refer to [BFS1, BCFS1, GH] for definitions and properties of the (smooth) Feshbach-Schur map, and its use in the context of non-relativistic QED. In our case, the operator \( H_g - E_g + \varepsilon \) is obviously invertible (for \( \varepsilon > 0 \)), so that the following lemma simply follows from usual second order perturbation theory.

**Lemma 3.3.** There exist \( g_c > 0 \) and \( p_c > 0 \) such that, for all \( 0 \leq |g| \leq g_c, 0 \leq |P| \leq p_c, \varepsilon > 0 \) and \( g^2 \ll \rho \ll 1 \), the operators \( H_g - E_g + \varepsilon : D(H_0) \to \mathbb{C}^4 \otimes L^2(\mathbb{R}^3) \otimes \mathcal{H}_{\text{ph}} \) and \( F_\rho(\varepsilon) : \text{Ran}(\Pi_\rho) \to \text{Ran}(\Pi_\rho) \) are invertible and satisfy
\[
\Pi_\rho [H_g - E_g + \varepsilon]^{-1} \Pi_\rho = F_\rho(\varepsilon)^{-1}. \tag{3.13}
\]

**Proof.** Since \( H_g - E_g \geq 0 \), for any \( \varepsilon > 0 \), the operator \( H_g - E_g + \varepsilon \) from \( D(H_0) \) to \( \mathbb{C}^4 \otimes L^2(\mathbb{R}^3, dr) \otimes \mathcal{H}_{\text{ph}} \) is obviously invertible. The identity (3.13) is then easily verified following for instance [BCFS1, Theorem 2.1].  \( \square \)

As a consequence of Lemmata 3.2 and 3.3, we obtain the following lemma.

**Lemma 3.4.** There exist \( g_c > 0 \) and \( p_c > 0 \) such that, for all \( 0 \leq |g| \leq g_c, 0 \leq |P| \leq p_c, \) and \( g^2 \ll \rho \ll 1 \),
\[
F_\rho(0) \Pi_\rho \mathbb{1}_{\{E_g\}}(H_g) \Pi_\rho = 0. \tag{3.14}
\]

**Proof.** We obtain from (3.13) that
\[
F_\rho(\varepsilon) \Pi_\rho [H_g - E_g + \varepsilon]^{-1} \Pi_\rho = \Pi_\rho, \tag{3.15}
\]
for all \( \varepsilon > 0 \). It follows from the functional calculus that
\[
s - \lim_{\varepsilon \to 0^+} \varepsilon [H_g - E_g + \varepsilon]^{-1} = \mathbb{1}_{\{E_g\}}(H_g), \tag{3.16}
\]
where \( s - \lim \) stands for strong limit. Hence, using (3.6), we obtain (3.14) by multiplying (3.15) by \( \varepsilon \) and letting \( \varepsilon \) go to 0.  \( \square \)

The next lemma will be used in the proof of Theorem 2.2.

**Lemma 3.5.** There exist \( g_c > 0 \) and \( p_c > 0 \) such that, for all \( 0 \leq |g| \leq g_c \) and \( 0 \leq |P| \leq p_c \),
\[
\Pi_0 F_\rho(0) \Pi_0 = (E_0 - E_g) \Pi_0 \]
\[ - \sum_{\lambda = 1,2} \int_{\mathbb{R}^3} \Pi_0 \tilde{w}(r, k, \lambda) [H_r + \frac{1}{2M}(P - k)^2 + |k| - E_g]^{-1} w(r, k, \lambda) \Pi_0 dk + O(|g|^{2+\tau}), \tag{3.17}
\]
where \( \rho = |g|^{2-2\tau}, \tau > 0 \) is fixed sufficiently small,
\[
w(r, k, \lambda) := - \frac{g}{m_{\text{el}}} \left( \frac{m_{\text{el}}}{M}(P - P_{\text{ph}}) + p_r \right) \cdot h^{A} \left( \frac{m_{\text{el}}}{M} g^2 r, k, \lambda \right)
\]
\[ + \frac{g}{m_n} \left( \frac{m_n}{M}(P - P_{\text{ph}}) - p_r \right) \cdot h^{A} \left( - \frac{m_n}{M} g^2 r, k, \lambda \right)
\]
\[ - \frac{g}{2m_{\text{el}}} \sigma^{\text{el}} \cdot h^{B} \left( \frac{m_{\text{el}}}{M} g^2 r, k, \lambda \right) + \frac{g}{2m_n} \sigma^{n} \cdot h^{B} \left( - \frac{m_n}{M} g^2 r, k, \lambda \right), \tag{3.18}
\]
and $\hat{w}(r, k, \lambda)$ is given by the same expression as $w(r, k, \lambda)$ except that $h^A$ and $h^B$ are replaced by $\hat{h}^A$ and $\hat{h}^B$ respectively.

Proof. We have that $\Pi_0\Pi_\rho = \Pi_\rho\Pi_0 = \Pi_0$ and $H_0\Pi_0 = E_0\Pi_0$. Introducing (3.3) into (3.5), we thus obtain that

$$\Pi_0 F_\rho(0)\Pi_0 = (E_0 - E_g)\Pi_0 + \Pi_0 W_g\Pi_0 - \Pi_0 W_g[H_0 - E_g]^{-1}\Pi_\rho W_g\Pi_0$$

$$- \sum_{n \geq 1} \Pi_0 W_g[H_0 - E_g]^{-1}(-\Pi_\rho W_g\Pi_\rho[H_0 - E_g]^{-1})^n\Pi_\rho W_g\Pi_0. \quad (3.19)$$

Observe that $\Pi_0 W_g\Pi_0 = 0$ since $W_g$ is Wick ordered. Hence Estimate (3.11) for $n \geq 1$ yields

$$\Pi_0 F_\rho(0)\Pi_0 = (E_0 - E_g)\Pi_0 - \Pi_0 W_g[H_0 - E_g]^{-1}\Pi_\rho W_g\Pi_0 + O(|g|^3\rho^{-\frac{1}{2}}). \quad (3.20)$$

We conclude the proof by applying Lemma A.9 of Appendix A.

4. PROOF OF THEOREM 2.2

From now on we assume that $\dim \ker (H_g - E_g) = 4$, which will lead to a contradiction at the end of this section.

Lemma 4.1. There exist $g_c > 0$ and $p_c > 0$ such that, for all $0 \leq |g| \leq g_c$ and $0 \leq |P| \leq p_c$, the following holds: If $\dim \ker (H_g - E_g) = 4$, then $\Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0$ is invertible on $\text{Ran}(\Pi_0)$ and satisfies

$$\|\Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0^{-1}\| \leq \frac{1}{1 - Cg^2}. \quad (4.1)$$

Proof. In order to prove that $\Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0$ is invertible on $\text{Ran}(\Pi_0)$, it suffices to show that $\|\Pi_0 - \Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0\| < 1$. Observe that $\Pi_0 - \Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0$ is a finite rank and positive operator. We have that

$$\|\Pi_0 - \Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0\| \leq \text{tr}(\Pi_0 - \Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0)$$

$$= \text{tr}(\Pi_0) - \text{tr}(\Pi_0 \mathbb{1}_{\{E_g\}}(H_g))$$

$$= \text{tr}(\Pi_0) - \text{tr}(\mathbb{1}_{\{E_g\}}(H_g)) + \text{tr}(\Pi_0 \mathbb{1}_{\{E_g\}}(H_g))$$

$$= 4 - 4 + \text{tr}(\Pi_0 \mathbb{1}_{\{E_g\}}(H_g)) = \text{tr}(\Pi_0 \mathbb{1}_{\{E_g\}}(H_g)). \quad (4.2)$$

The projection $\Pi_0$ can be decomposed as

$$\Pi_0 = \mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega + \mathbb{1} \otimes \Pi \otimes \Pi_\Omega. \quad (4.3)$$

It follows from Lemma A.7 that

$$\text{tr}((\mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)\mathbb{1}_{\{E_g\}}(H_g)) \leq Cg^2, \quad (4.4)$$

and from Lemma A.5 that

$$\text{tr}((\mathbb{1} \otimes \mathbb{1} \otimes \Pi_\Omega)P_g) \leq \text{tr}(N_{\phi h}P_g) \leq C'g^2. \quad (4.5)$$

Therefore, $\|\Pi_0 - \Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0\| \leq C''g^2$. The invertibility of $\Pi_0 \mathbb{1}_{\{E_g\}}(H_g)\Pi_0$ and Equation (4.1) directly follow from the latter estimate.

As a consequence of Lemma 4.1, we obtain the following lemma.
Lemma 4.2. Let $\Gamma$ denote the operator on $\text{Ran}(\Pi_0)$ defined by

$$\Gamma := \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \Pi_0 \bar{w}(r, k, \lambda) \left[ H_r + \frac{1}{2M} (P - k)^2 + |k| - E_g \right]^{-1} w(r, k, \lambda) \Pi_0 dk,$$

with $w(r, k, \lambda)$ and $\bar{w}(r, k, \lambda)$ as in (3.18). There exist $g_c > 0$ and $p_c > 0$ such that, for all $0 \leq |g| \leq g_c$ and $0 \leq |P| \leq p_c$, the following holds: If $\dim \ker (H_g - E_g) = 4$, then

$$\Gamma = (E_0 - E_g) \Pi_0 + \mathcal{O}(|g|^{2+\tau}),$$

where $\tau > 0$ is fixed sufficiently small.

Proof. Fix $\rho = |g|^{2-2\tau}$ for some sufficiently small $\tau > 0$. Multiplying both sides of Equation (3.14) by $\Pi_0$, we get

$$\Pi_0 F_\rho(0) \Pi_0 \Pi(E_0) (H_g) \Pi_0 = 0.$$

Introducing the decomposition $\mathbb{1} = \Pi_0 + \Pi\Pi_0$ into (4.8), this yields

$$\Pi_0 F_\rho(0) \Pi_0 = -\Pi_0 F_\rho(0) \Pi_0 \Pi(E_0) (H_g) \Pi_0 \Pi_0 \Pi(E_0) (H_g) \Pi_0^{-1}.$$

By Equations (4.3), (4.4) and (4.5), we learn that

$$\left\| \Pi_0 \Pi(E_0) (H_g) \right\| \leq \text{tr}(\Pi_0 \Pi(E_0) (H_g)) \leq C g^2,$$

which, combined with (3.7) and (4.1), implies that

$$\left\| \Pi_0 F_\rho(0) \Pi_0 \Pi(E_0) (H_g) \Pi_0 \Pi_0 \Pi(E_0) (H_g) \Pi_0^{-1} \right\| \leq C g^2 \rho = C|g|^{4-2\tau}.$$

We conclude the proof thanks to Lemma 3.5.

Let us consider the canonical orthonormal basis of $\mathbb{C}^4$ in which the Pauli matrices $\sigma_{ij}^\rho, j \in \{1, 2, 3\}$, are given by (2.14)–(2.15). Obviously, $\Gamma$ identifies with a $4 \times 4$ matrix in this basis. In the next theorem, we determine a non-diagonal coefficient of $\Gamma$ of the form $-C_0 g^2 + o(g^2)$ with $C_0 > 0$.

Theorem 4.3. Let $\Gamma$ be given as in (4.6). There exist $g_c > 0$ and $p_c > 0$ such that, for all $0 \leq |g| \leq g_c$ and $0 \leq |P| \leq p_c$, the coefficient of $\Gamma$ located on the third line and second column, $\Gamma_{32}$, satisfies

$$\Gamma_{32} = -C_0 g^2 + \mathcal{O}(|g|^\frac{3}{2}),$$

where $C_0$ is a strictly positive constant independent of $g$.

Proof. We view $w(r, k, \lambda)$ as a linear combination (some coefficients being given by operators) of the functions $h_j^A(\cdots)$ and $h_j^B(\cdots), j \in \{1, 2, 3\}$. We introduce the corresponding expression into (4.6) and consider each term separately.

Since the coefficients located on the third line and second column of the Pauli matrices expressed in (2.14)–(2.15) vanish, the terms containing at least one factor $h_j^A(\cdots)$ do not contribute to $\Gamma_{32}$. The same holds for the terms containing at least one factor $h_j^B(\cdots)$, since the third Pauli matrices, $\sigma^\rho_3$ and $\sigma^\rho_3$, are diagonal.
Therefore, $\Gamma_{32}$ is equal to the coefficient located on the third line and second column of the matrix $\Gamma'$ given by

$$\Gamma' = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \Pi_0 \sum_{j=1,2} \left( -\frac{g}{2m_{el}} \sigma_{j} \hat{h}_j^{B} \left( \frac{m_{el}}{M} g^{2} r, k, \lambda \right) + \frac{g}{2m_{n}} \sigma_{j}^n \hat{h}_j^{B} \left( \frac{m_{n}}{M} g^{2} r, k, \lambda \right) \right) \left[ H_r + \frac{1}{2M} (P - k)^2 + |k| - E_g \right]^{-1} \sum_{j'=1,2} \left( -\frac{g}{2m_{el}} \sigma_{j'}^e \hat{h}_{j'}^{B} \left( \frac{m_{el}}{M} g^{2} r, k, \lambda \right) + \frac{g}{2m_{n}} \sigma_{j'}^{n} \hat{h}_{j'}^{B} \left( \frac{m_{n}}{M} g^{2} r, k, \lambda \right) \right) \Pi_0 dk. \quad (4.13)$$

It follows from the definition (2.11) of $h_j^{B}$ that

$$|h_j^{B}(r, k, \lambda) - h_j^{B}(0, k, \lambda)| \leq C |k|^2 \chi_\lambda(k) |r|, \quad (4.14)$$

for any $j \in \{1, 2, 3\}$, $\lambda \in \{1, 2\}$, $r \in \mathbb{R}^3$ and $k \in \mathbb{R}^3$. Moreover, the expression (2.24) of $\phi_0$ implies that

$$\| |r| \phi_0(r) \| \leq C. \quad (4.15)$$

Hence, using in addition that, for $|P|$ sufficiently small,

$$\left\| \left[ H_r + \frac{(P - k)^2}{2M} + |k| - E_g \right]^{-1} \right\| \leq \frac{C}{|k|}, \quad (4.16)$$

we obtain from (4.13) and (4.14)–(4.16) that

$$\Gamma' = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \Pi_0 \sum_{j=1,2} \left( -\frac{g}{2m_{el}} \sigma_{j} \hat{h}_j^{B}(0, k, \lambda) + \frac{g}{2m_{n}} \sigma_{j}^n \hat{h}_j^{B}(0, k, \lambda) \right) \left[ \epsilon_0 + \frac{1}{2M} (P - k)^2 + |k| - E_g \right]^{-1} \sum_{j'=1,2} \left( -\frac{g}{2m_{el}} \sigma_{j'}^e \hat{h}_{j'}^{B}(0, k, \lambda) + \frac{g}{2m_{n}} \sigma_{j'}^{n} \hat{h}_{j'}^{B}(0, k, \lambda) \right) \Pi_0 dk + O(|g|^{\frac{8}{5}}). \quad (4.17)$$

Notice now that, for $j, j' \in \{1, 2\}$, the coefficient on the third line and second column of the products $\sigma_{j}^e \sigma_{j'}^{e}$ and $\sigma_{j}^n \sigma_{j'}^{n}$ vanishes. We thus obtain from (4.17) that

$$\Gamma_{32} = \Gamma'_{32} = \gamma_1 + \gamma_2 + O(|g|^{\frac{8}{5}}), \quad (4.18)$$

where

$$\gamma_1 := -\frac{g^2}{4m_{el} m_{n}} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \left( \phi_0, \left[ \hat{h}_1^{B}(0, k, \lambda) + i\hat{h}_2^{B}(0, k, \lambda) \right] \right) \left[ \epsilon_0 + \frac{1}{2M} (P - k)^2 + |k| - E_g \right]^{-1} \left[ \hat{h}_1^{B}(0, k, \lambda) - i\hat{h}_2^{B}(0, k, \lambda) \right] \phi_0 dk, \quad (4.19)$$

and

$$\gamma_2 := -\frac{g^2}{4m_{el} m_{n}} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \left( \phi_0, \left[ \hat{h}_1^{B}(0, k, \lambda) - i\hat{h}_2^{B}(0, k, \lambda) \right] \right) \left[ \epsilon_0 + \frac{1}{2M} (P - k)^2 + |k| - E_g \right]^{-1} \left[ \hat{h}_1^{B}(0, k, \lambda) + i\hat{h}_2^{B}(0, k, \lambda) \right] \phi_0 dk. \quad (4.20)$$
We remark that the cross terms involving $h_B^1(0, k; \lambda)$ and $h_B^2(0, k; \lambda)$ vanish. Thus, we obtain
\[
\Gamma_{32} = -\frac{g^2}{2m_qm_n} \sum_{j=1,2} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \tilde{h}_j^B(0, k, \lambda)
\left[ e_0 + \frac{(P - k)^2}{2M} + |k| - E_g \right]^{-1} h_j^B(0, k, \lambda) dk + \mathcal{O}(|g|^8). \tag{4.21}
\]

The integral in the right-hand-side of (4.21) still depends on $g$ through the ground state energy $E_g$. Nevertheless, one can readily check that
\[
\left| e_0 + \frac{(P - k)^2}{2M} + |k| - E_g \right|^{-1} - \left[ e_0 + \frac{(P - k)^2}{2M} + |k| - E_0 \right]^{-1}
\leq |E_0 - E_g| \frac{C}{|k|^2} \leq \frac{C'}{g^2 |k|^2}, \tag{4.22}
\]
where, in the last inequality, we used Lemma A.6. Therefore, since, for any $j \in \{1, 2\}$ and $\lambda \in \{1, 2\}$, the functions $h_j^B(0, k, \lambda)$ satisfy $|h_j^B(0, k, \lambda)| \leq C |k|^{1/2} \chi_{\Lambda}(k)$, we get
\[
\Gamma_{32} = -\frac{g^2}{2m_qm_n} \sum_{j=1,2} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \tilde{h}_j^B(0, k, \lambda)
\left[ e_0 + \frac{(P - k)^2}{2M} + |k| - E_0 \right]^{-1} h_j^B(0, k, \lambda) dk + \mathcal{O}(|g|^8). \tag{4.23}
\]

Now, the integrals in the right-hand-side of (4.23) can be explicitly computed, which leads to
\[
\Gamma_{32} = -\frac{g^2}{8\pi^2 m_qm_n} \int_{\mathbb{R}^3} |k| |\chi_{\Lambda}(k)|^2 \frac{k^2/2M - k \cdot P/M + |k| (k^2/|k|^2 + 1)}{k^2/|k|^2} dk + \mathcal{O}(|g|^8). \tag{4.24}
\]
The integrand in (4.24) is strictly positive (for $P$ sufficiently small), and hence the integral does not vanish. This concludes the proof of the theorem. \hfill \Box

We are now able to prove Theorem 2.2:

**Proof of Theorem 2.2.** By [AGG], we know that $\dim \ker(H_g - E_g) \leq 4$. Assume by contradiction that $\dim \ker(H_g - E_g) = 4$. By Lemma 4.2, the matrix $\Gamma$ defined in (4.6) satisfies (4.7). In particular, in any basis of $\mathbb{C}^4$, the non-vanishing terms of order $g^2$ of $\Gamma$ are necessarily located on the diagonal. However, according to Theorem 4.3, in the canonical orthonormal basis of $\mathbb{C}^4$ in which the Pauli matrices are given by (2.14)–(2.15), the non-diagonal coefficient $\Gamma_{32}$ contains a non-vanishing term of order $g^2$. Hence we get a contradiction and the theorem is proven. \hfill \Box

### Appendix A

In this appendix, we collect some estimates which were used in Sections 3 and 4. Some of them are standard (see for instance [BFS1, BFS2]). We begin with two lemmata concerning the non-interacting Hamiltonian $H_0$ defined in (2.29).

**Lemma A.1.** There exists $p_c > 0$ such that for all $0 \leq |P| \leq p_c$,
\[
H_{ph} \leq 2(H_0 - E_0). \tag{A.1}
\]
Proof. For \( j \in \{1, 2, 3\} \), one can easily verify that \( |(P_{ph})_j| \leq H_{ph} \). Hence, since \( E_0 = e_0 + P^2/2M \), we have that

\[
H_0 = H_r + \frac{P^2}{2M} - \frac{1}{M} P \cdot P_{ph} + \frac{1}{2M} P^2_{ph} + H_{ph} \geq E_0 + \frac{1}{2} H_{ph}, \tag{A.2}
\]

for \( P \) sufficiently small, which proves the lemma. \( \square \)

**Lemma A.2.** There exists \( p_c > 0 \) such that, for all \( 0 \leq |P| \leq p_c \) and \( \rho \geq 0 \),

\[
\Pi_\rho H_0 \Pi_\rho \geq \left( \frac{P^2}{2M} + \min(e_0 + \frac{\rho}{2}, e_1) \right) \Pi_\rho. \tag{A.3}
\]

**Proof.** Since \( \Pi_\rho = 1 \otimes \Pi_{\phi_0} \otimes 1_{H_{ph} \leq \rho} \) in the tensor product \( C^4 \otimes L^2(\mathbb{R}^3) \otimes \mathcal{H}_{ph} \), we can write \( \Pi_\rho = 1 - \Pi_\rho = 1 \otimes \Pi_{\phi_0} \otimes 1_{H_{ph} \leq \rho} + 1 \otimes 1 \otimes 1_{H_{ph} \geq \rho} \), where \( \Pi_{\phi_0} = 1 - \Pi_{\phi_0} \). Since \( H_r \Pi_{\phi_0} \geq e_1 \Pi_{\phi_0} \), we get that

\[
H_0(1 \otimes \Pi_{\phi_0} \otimes 1_{H_{ph} \leq \rho}) \geq (e_1 + \frac{P^2}{2M})(1 \otimes \Pi_{\phi_0} \otimes 1_{H_{ph} \leq \rho}), \tag{A.4}
\]

for \( P \) small enough. Moreover, by Lemma A.1,

\[
H_0(1 \otimes 1 \otimes 1_{H_{ph} \geq \rho}) \geq (e_0 + \frac{P^2}{2M} + \frac{\rho}{2})(1 \otimes 1 \otimes 1_{H_{ph} \geq \rho}). \tag{A.5}
\]

Hence (A.3) is proven. \( \square \)

The proofs of the next two lemmata being standard, we omit them.

**Lemma A.3.** For any \( f \in L^2(\mathbb{R}^3 \times \{1, 2\}) \), the operators \( a(f)[N_{ph} \Pi_{\Omega}]^{-1/2} \) and \( [N_{ph} \Pi_{\Omega}]^{-1/2} a(f) \) extend to bounded operators on \( \mathcal{H}_{ph} \) satisfying

\[
\|a(f)[N_{ph} \Pi_{\Omega}]^{-1/2}\| \leq \|f\|, \tag{A.6}
\]

\[
\|[N_{ph} \Pi_{\Omega}]^{-1/2} a(f)\| \leq \sqrt{2}\|f\|. \tag{A.7}
\]

**Lemma A.4.** Let \( f \in L^2(\mathbb{R}^3 \times \{1, 2\}) \) be such that \( (k, \lambda) \mapsto |k|^{-1/2} f(k, \lambda) \in L^2(\mathbb{R}^3 \times \{1, 2\}) \). Then, for any \( \rho > 0 \), the operators \( a(f)[H_{ph} + \rho]^{-1/2} \) and \( [H_{ph} + \rho]^{-1/2} a(f) \) extend to bounded operators on \( \mathcal{H}_{ph} \) satisfying

\[
\|a(f)[H_{ph} + \rho]^{-1/2}\| \leq \|f\|, \tag{A.8}
\]

\[
\|[H_{ph} + \rho]^{-1/2} a(f)\| \leq \|f\|. \tag{A.9}
\]

The following lemma is taken from [AGG]. Its proof is based on a “pull-through” formula (see [AGG]).

**Lemma A.5.** There exist \( g_c > 0 \) and \( p_c > 0 \) such that, for all \( 0 \leq |g| \leq g_c \) and \( 0 \leq |P| \leq p_c \), the following holds:

\[
\forall \Phi_g \in \text{Ker}(H_g - E_g), \|\Phi_g\| = 1, \text{ we have } (\Phi_g, N_{ph} \Phi_g) \leq C g^2, \tag{A.10}
\]

where \( C \) is a positive constant independent of \( g \).

In the next lemma, we estimate the difference between the ground state energies \( E_g = \inf \sigma(H_g) \) and \( E_0 = \inf \sigma(H_0) \).
Lemma A.6. There exist \( g_c > 0 \) and \( p_c > 0 \) such that, for all \( 0 \leq |g| \leq g_c \) and \( 0 \leq |P| \leq p_c \),

\[ E_g \leq E_0 \leq E_g + Cg^2, \tag{A.11} \]

where \( C \) is a positive constant independent of \( g \).

Proof. Note that, since the perturbation \( W_g \) is Wick-ordered, we have that \((\mathbf{1} \otimes \mathbf{1} \otimes \Pi_\Omega)W_g(\mathbf{1} \otimes \mathbf{1} \otimes \Pi_\Omega) = 0\), where, recall, \( \Pi_\Omega \) denotes the orthogonal projection onto the vector space spanned by the Fock vacuum \( \Omega \). Hence, by the Rayleigh-Ritz principle,

\[ E_g \leq \left( \left( y \otimes \phi_0 \otimes \Omega \right), H_g \left( y \otimes \phi_0 \otimes \Omega \right) \right) = E_0, \tag{A.12} \]

where, as above, \( y \) denotes an arbitrary normalized element in \( \mathbb{C}^4 \).

In order to prove the second inequality in (A.11), we use Lemmata A.3 and A.5. More precisely, let \( \Phi_g \in \text{Ker}(H_g - E_g), \|\Phi_g\| = 1 \) (\( \Phi_g \) exists by \([AGG]\)). We have that

\[ E_0 - E_g \leq (\Phi_g, (H_0 - H_g)\Phi_g) = -(\Phi_g, W_g\Phi_g). \tag{A.13} \]

Recall that \( W_g \) is given by the Wick-ordered expression obtained from (2.31). We express the latter in terms of operators of creation and annihilation, and estimate each term separately. Consider for instance the term

\[ \frac{g}{m_{el}} \left( \frac{m_{el}}{M} (P - P_{ph}) + p_r \right) \cdot a(h^A \left( \frac{m_{el}}{M} g^2 r \right)). \tag{A.14} \]

It is not difficult to check that

\[ (P - P_{ph})^2 \leq aH_0 + b \quad \text{and} \quad p_r^2 \leq aH_0 + b, \tag{A.15} \]

for some positive constants \( a \) and \( b \) depending on \( \mu \) and \( M \). One easily deduces from (A.15) that

\[ \| \left( \frac{m_{el}}{M} (P - P_{ph}) + p_r \right) \Phi_g \| \leq C. \tag{A.16} \]

Moreover, by Lemmata A.3 and A.5, we have that

\[ \| a(h^A \left( \frac{m_{el}}{M} g^2 r \right))\Phi_g \| \leq C\| N_{ph}^{\frac{3}{2}} \Phi_g \| \leq C|g|. \tag{A.17} \]

Equations (A.16) and (A.17) imply that \(|(\Phi_g, (A.14)\Phi_g)| \leq Cg^2\), and since the other terms in \( W_g \) are estimated similarly, this concludes the proof. \( \square \)

Lemma A.5 gives an estimation of the overlap of the ground state \( \Phi_g \) of \( H_g \) with the Fock vacuum. We also need to estimate the overlap of \( \Phi_g \) with the ground state \( \phi_0 \) of the electronic Hamiltonian \( H_r \) in the sense stated in the following lemma.

Lemma A.7. There exist \( g_c > 0 \) and \( p_c > 0 \) such that, for all \( 0 \leq |g| \leq g_c \) and \( 0 \leq |P| \leq p_c \), the following holds:

\[ \forall \Phi_g \in \text{Ker}(H_g - E_g), \|\Phi_g\| = 1, \text{ we have } (\Phi_g, (\mathbf{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)\Phi_g) \leq Cg^2, \tag{A.18} \]

where \( C \) is a positive constant independent of \( g \).
Proof. Let $\Phi_g$ be a normalized ground state of $H_g$, that is $(H_g - E_g)\Phi_g = 0$, $\|\Phi_g\| = 1$. Since $E_0 - E_g = e_0 + P^2/2M - E_g \geq 0$ by Lemma A.6, we have that

$$0 = |(\Phi_g, (\mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)(H_g - E_g)\Phi_g)|$$

$$= |(\Phi_g, (\mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)(H_r + \frac{p^2}{2M} - E_g + W_g)\Phi_g)|$$

$$\geq (e_1 - e_0)(\Phi_g, (\mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)\Phi_g) - |(\Phi_g, (\mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)W_g\Phi_g)|,$$

(A.19)

and hence

$$(\Phi_g, (\mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)\Phi_g) \leq \frac{1}{e_1 - e_0}|(\Phi_g, (\mathbb{1} \otimes \Pi_{\phi_0} \otimes \Pi_\Omega)W_g\Phi_g)|.$$  

(A.20)

We conclude the proof thanks to Lemmata A.3 and A.5, by arguing in the same way as in the proof of Lemma A.6. \hfill \Box

We now give estimates relating the perturbation $W_g$ to $H_0$.

**Lemma A.8.** There exist $g_c > 0$ and $p_c > 0$ such that, for all $0 \leq |g| \leq g_c$, $0 \leq |P| \leq p_c$, $0 < \rho \ll 1$ and $\varepsilon \geq 0$, the following estimates hold:

$$\|(H_0 - E_g + \varepsilon)^{-\frac{1}{2}}\Pi_\rho W_g\Pi_\rho[H_0 - E_g + \varepsilon]^{-\frac{1}{2}}\| \leq C|g|\rho^{-\frac{1}{2}},$$

(A.21)

$$\|\Pi_\rho W_g\Pi_\rho[H_0 - E_g + \varepsilon]^{-\frac{1}{2}}\| \leq C|g|,$$

(A.22)

$$\|(H_0 - E_g + \varepsilon)^{-\frac{1}{2}}\Pi_\rho W_g\Pi_\rho\| \leq C|g|,$$

(A.23)

$$\|\Pi_\rho W_g\Pi_\rho\| \leq C|g|\rho^{-\frac{1}{2}}.$$

(A.24)

Proof. Let us begin with proving (A.21). As in the proof of Lemma A.6, we express $W_g$ in terms of creation and annihilation operators from the Wick-ordered expression obtained from (2.31), and we estimate each term separately. Let us consider again the term (A.14) as an example. Using (A.15), Lemma A.2, and the fact that $E_0 \geq E_g$, we obtain

$$\|(H_0 - E_g + \varepsilon)^{-\frac{1}{2}}\Pi_\rho \frac{m_{el}}{M} (P - P_{ph}) + p_r)\| \leq C\rho^{-\frac{1}{2}}.$$  

(A.25)

for $j \in \{1, 2, 3\}$. Next, for $j \in \{1, 2, 3\}$, Lemma A.4 gives

$$\|a(h_j^A \frac{m_{el}}{M} g^2 r) [H_{ph} + \rho]^{-1/2}\| \leq C,$$

(A.26)

and it follows from Lemmata A.1 and A.2 that

$$\|(H_{ph} + \rho)^{\frac{1}{2}}\Pi_\rho[H_0 - E_g + \varepsilon]^{-\frac{1}{2}}\| \leq C.$$  

(A.27)

Using (A.25), (A.26) and (A.27), we obtain

$$\|(H_0 - E_g + \varepsilon)^{-\frac{1}{2}}\Pi_\rho (A.14)\Pi_\rho[H_0 - E_g + \varepsilon]^{-\frac{1}{2}}\| \leq C|g|\rho^{-\frac{1}{2}}.$$  

(A.28)

The other terms in $W_g$ are estimated similarly, using in particular Estimate (A.9) (in addition to (A.8)) for the terms quadratic in the annihilation and creation operators. Hence (A.21) is proven. In order to prove (A.22), (A.23) and (A.24), we proceed similarly, using the further following estimates:

$$\|\left(\frac{m_{el}}{M} (P - P_{ph}) + p_r\right)\| \leq C, \quad \|(H_{ph} + \rho)^{\frac{1}{2}}\Pi_\rho\| \leq C\rho^{\frac{1}{2}}.$$  

(A.29)
The first estimate in (A.29) follows from (A.15), while the second is an obvious consequence of the Spectral Theorem.

**Lemma A.9.** There exist \( g_c > 0 \) and \( p_c > 0 \) such that, for all \( 0 \leq |g| \leq g_c, 0 \leq |P| \leq p_c, 0 < \rho \ll 1, \) and \( \varepsilon \geq 0, \) we have

\[
\Pi_0 W_g [H_0 - E_g]^{-1} \Pi_0 W_g \Pi_0 = \sum_{\lambda = 1, 2} \int_{\mathbb{R}^3} \Pi_0 \tilde{w}(r, k, \lambda) [H_r + \frac{1}{2M}(P - k)^2 + |k| - E_g]^{-1} w(r, k, \lambda) \Pi_0 dk
\]

where \( w(r, k, \lambda) \) and \( \tilde{w}(r, k, \lambda) \) are defined in (3.18).

**Proof.** The perturbation \( W_g \) appears twice in \( \Pi_0 W_g [H_0 - E_g]^{-1} \Pi_0 W_g \Pi_0. \) We introduce the expression (2.31) of \( W_g \) into the latter operator, and consider each term separately.

First, the terms containing a creation operator in the “first” \( W_g \) vanish since \( \Pi_0 \) projects onto the Fock vacuum. The same holds for the terms containing an annihilation operator in the “second” \( W_g. \) Next, the terms involving the parts of \( W_g \) quadratic in the creation and annihilation operators are (at least) of order \( \mathcal{O}(|g|^3), \) as follows again from Lemmata A.4 and A.8. Therefore, one can compute

\[
\begin{align*}
\Pi_0 W_g [H_0 - E_g]^{-1} \Pi_0 W_g \Pi_0 &= \sum_{\lambda = 1, 2} \int_{\mathbb{R}^3} \Pi_0 \tilde{w}(r, k, \lambda) [H_r + \frac{1}{2M}(P - k)^2 + |k| - E_g]^{-1} w(r, k, \lambda) \Pi_0 dk \\
&\quad - \sum_{\lambda = 1, 2} \int_{|k| \leq \rho} \Pi_0 \tilde{w}(r, k, \lambda) [\epsilon_0 + \frac{1}{2M}(P - k)^2 + |k| - E_g]^{-1} w(r, k, \lambda) \Pi_0 dk \\
&\quad \times (\mathbb{1} \otimes \Pi_{\phi_0} \otimes \mathbb{1}) |w(r, k, \lambda) \Pi_0 dk + \mathcal{O}(|g|^3). \\
&= (A.31)
\end{align*}
\]

The second term in the right-hand-side of (A.31) is estimated as follows:

\[
\left\| \sum_{\lambda = 1, 2} \int_{|k| \leq \rho} \Pi_0 \tilde{w}(r, k, \lambda) [\epsilon_0 + \frac{1}{2M}(P - k)^2 + |k| - E_g]^{-1} w(r, k, \lambda) \Pi_0 dk \right\| \leq \sum_{\lambda = 1, 2} \int_{|k| \leq \rho} C \frac{1}{|k|^2} dk \leq C' \rho. \quad (A.32)
\]

Hence (A.30) is proven. \( \square \)

**References**


