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The confined hydrogenoid ion in non-relativistic quantum electrodynamics

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Abstract

We consider a system of a nucleus with an electron together with the quantized electromagnetic field. Instead of fixing the nucleus, the system is confined by its center of mass. This model is used in theoretical physics to explain the Lamb-Dicke effect (see [CTDRG]). When an ultraviolet cut-off is imposed we initiate the spectral analysis of the Hamiltonian describing the system and we derive the existence of a ground state. This is achieved without condition on the fine structure constant.

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1 Introduction and statements of results

In this paper we address the problem of the existence of a ground state for the hydrogen atom and more generally for the hydrogenoid ion confined by its center of mass. The fact that the nucleus is confined but not fixed is important since intense rays appearing in the scattering spectrum for dynamical nucleus disappear when the nucleus is fixed (see [CTDRG]). This model is used to explain the Lamb-Dicke effect (see [CTDRG]). Some questions related to this problem have been considered in [Fe].

We consider a system of one nucleus and one electron, together with the electromagnetic field. Here the nucleus is *dynamical* and our Hamiltonian acts on an Hilbert space describing the nucleus, the electron and the photons. The center of mass of the system is confined by an external potential. Let us denote by U (resp. V) the external confining potential (resp. the attractive Coulomb potential). The Hamiltonian of the system is H_U^V and $H_U^V(m)$ is the corresponding operator if we decide that the photons have a positive mass $m > 0$.

The main result is theorem 1.4 below giving the existence of a ground state for H_U^V . In order to establish it we follow the fundamental strategy of [GLL] and [LL] (see also [G]). However we only reproduce here the new aspects of the proofs and often refer to [GLL] and [LL]. Precisely our contributions are essentially the following three points which are not straightforward modifications of [GLL] and [LL], the first point being the main one.

- The proof of the binding condition (theorem 1.3(ii)) (see section 3.2).
- The systematic use of quadratic forms throughout the paper. In particular, with the help of [H1] and the functional integration method we determine $Q(H_U^V)$, $Q(H_U^V(m))$. This allows us to get $Q(H_U^V(m)) = Q(H_U^V) \cap Q(\mathcal{N})$ where \mathcal{N} is the number operator for the photons (see section 2). This appears to be useful in order to obtain rigorous results. In particular, we always consider $q_{H_U^V}(\varphi, \phi)$, $q_{H_U^V(m)}(\varphi, \phi), \dots$ instead of $(\varphi, H_U^V \phi)$, $(\varphi, H_U^V(m) \phi), \dots$
- The proof of the exponential decay for the ground state of $H_U^V(m)$ (without using [G]). To this end we introduce the localizations functions $\phi_{1,T}$, $\bar{\phi}_{1,T}$, $\phi_{2,\frac{T}{2}}$, $\phi_{3,\frac{T}{2}}$, then we follow the standard method (see section 4.2).

Remark 1.1 (i) *The proof of the other binding condition (theorem 1.3(i)) is closer to theorem 2.1 of [GLL] and is given in section 3.1.*

(ii) *The existence of a ground state for $H_U^V(m)$ follows these two binding conditions and [GLL] when the localization functions (for the electrons and the nucleus) have been properly chosen (see section 4.1).*

Let us state precisely our results (theorems 1.1-1.4 below). We first define H_U^V precisely using quadratic forms:

Theorem 1.1 H_U^V defines a self-adjoint operator.

Remark 1.2 *The hypotheses on the confining potential U are stated in section 2.*

For a semi-bounded self-adjoint operator A , let $E(A)$ be the infimum of the spectrum of A . Let us denote by H_U^0 (resp. H_0^V) the operator H_U^V when V (resp. U) is put to zero. We shall prove

Theorem 1.2 *Assume that $E(H_U^V) < \min(E(H_U^0), E(H_0^V))$. Then H_U^V has a ground state.*

The assumptions in theorem 1.2 are the so-called binding conditions.

Here we obtain the existence of the ground state without assuming any conditions on the smallness for the different charges. We follow the strategy of [G], [GLL] and [LL] where the authors consider a similar system (actually more general) but with *fixed* nuclei and succeed to deal with the quantized electromagnetic field in a non perturbative way. The heart of the proof is to specify correctly the *binding conditions*. These conditions need to be properly chosen so that, on one side we are able to prove them and on the other side they imply the existence of a ground state.

The main result of the paper is theorem 1.3(ii).

Theorem 1.3 *The following inequalities are true.*

$$(i) \ E(H_U^V) < E(H_0^V) \quad , \quad (ii) \ E(H_U^V) < E(H_U^0).$$

Theorem 1.2 and 1.3 imply

Theorem 1.4 *H_U^V has a ground state for all value of the fine structure constant.*

The proof of the existence of the ground state once the binding conditions are assumed (theorem 1.2) and the proof of the first binding condition (theorem 1.3(i)) are derived in the same way as in [GLL]. Indeed, H_0^V is a translation invariant operator. The translation invariance is a key point in the proof of theorem 2.1 of [GLL]. The validity of the remaining binding condition (theorem 1.3(ii)) is more difficult because H_U^0 is not translation invariant and its proof borrows ideas of [LL] and still uses tools given in [LL].

For the sake of simplicity the spin of the electron is not taken into account in this work. This and the case of several electrons should be treated in a similar manner.

As it is already mentioned intense rays should appear in the spectrum of H_U^V . This may provide resonances with a very small imaginary part among other resonances. The resonances for H_U^V are studied in [F] following mainly [BFS1][BFS2].

These results have been announced in [AF]. Let us also mention another case of a similar system with a dynamical nucleus: the case of free atoms and ions with quantized electromagnetic field. It is analyzed in [AGG].

The paper is organized as follows. In section 2 we verify theorem 1.1. In section 3, theorem 1.3 is derived. Finally, we prove theorem 1.2 in section 4.

2 Definition of the Hamiltonian

2.1 Fock space, creation and annihilation operators

The Hilbert space in which operate the Hamiltonian considered in this paper is

$$\mathcal{H} := L^2(\mathbb{R}^6) \otimes \mathcal{F}_s \simeq L^2(\mathbb{R}^6; \mathcal{F}_s), \tag{1}$$

where $L^2(\mathbb{R}^6) \simeq L^2(\mathbb{R}^3) \otimes L^2(\mathbb{R}^3)$ is the space of states describing the nucleus together with the electron, and where \mathcal{F}_s is the bosonic Fock space over $L^2(\mathbb{R}^3; \mathbb{C}^2)$. This Fock space describes the states of the polarized radiation field and is defined by

$$\mathcal{F}_s = \mathcal{F}_s(L^2(\mathbb{R}^3)) \otimes \mathcal{F}_s(L^2(\mathbb{R}^3)), \quad (2)$$

where $\mathcal{F}_s(L^2(\mathbb{R}^3)) = \mathbb{C} \oplus \bigoplus_{n \geq 1} S_n L^2(\mathbb{R}^{3n}; \mathbb{C})$, and where $S_n L^2(\mathbb{R}^{3n}; \mathbb{C})$ is the set of all elements $(k_1, \dots, k_n) \mapsto \Phi(k_1, \dots, k_n)$ in $L^2(\mathbb{R}^{3n}; \mathbb{C})$ which are invariant under any permutations of $\{k_1, \dots, k_n\}$. Note that

$$\mathcal{F}_s \simeq \mathbb{C} \oplus \bigoplus_{n \geq 1} S_n \otimes_{k=1}^n L^2(\mathbb{R}^3; \mathbb{C}^2). \quad (3)$$

Moreover $\mathcal{F}_s^0(L^2(\mathbb{R}^3))$ (respectively \mathcal{F}_s^0) is defined as the set of all $\Phi = (\Phi^{(0)}, \Phi^{(1)}, \Phi^{(2)}, \dots)$ in $\mathcal{F}_s(L^2(\mathbb{R}^3))$ (respectively in \mathcal{F}_s) such that $\Phi^{(n)} = 0$ except for a finite number of terms.

For any $f \in L^2(\mathbb{R}^3)$, the creation operator $a^*(f)$ and the annihilation operator $a(f)$ are defined for all $\Phi \in \mathcal{F}_s^0(L^2(\mathbb{R}^3))$ by

$$\begin{aligned} (a^*(f)\Phi)^{(n)}(k_1, \dots, k_n) &:= \frac{1}{\sqrt{n}} \sum_{j=1}^n \widehat{f}(k_j) \Phi^{(n-1)}(k_1, \dots, \widehat{k}_j, \dots, k_n), \\ (a(f)\Phi)^{(n)}(k_1, \dots, k_n) &:= \sqrt{n+1} \int_{\mathbb{R}^3} \overline{\widehat{f}(k)} \Phi^{(n+1)}(k, k_1, \dots, k_n) dk, \end{aligned} \quad (4)$$

where \widehat{k}_j means that the variable k_j is missing in $\Phi^{(n-1)}$, and where \widehat{f} is the Fourier transform of f . These operators are closable on $\mathcal{F}_s^0(L^2(\mathbb{R}^3))$ (their closed extensions are denoted by the same symbols) and they verify on $\mathcal{F}_s^0(L^2(\mathbb{R}^3))$

$$[a(f), a^*(g)] = (f, g), \quad [a(f), a(g)] = [a^*(f), a^*(g)] = 0, \quad (a(f)\Phi, \Psi) = (\Phi, a^*(f)\Psi).$$

Let

$$D_{\mathcal{S}} := \left\{ \Phi \in \mathcal{F}_s^0(L^2(\mathbb{R}^3)), \Phi^{(n)} \in \mathcal{S}(\mathbb{R}^{3n}) \text{ for all } n \right\}, \quad (5)$$

where $\mathcal{S}(\mathbb{R}^{3n})$ denotes the Schwartz space over \mathbb{R}^{3n} , and let

$$\begin{aligned} (\widehat{a}(k)\Phi)^{(n)}(k_1, \dots, k_n) &:= \sqrt{n+1} \Phi^{(n+1)}(k, k_1, \dots, k_n), \\ (\widehat{a}^*(k)\Phi)^{(n)}(k_1, \dots, k_n) &:= \frac{1}{\sqrt{n}} \sum_{l=1}^n \delta(k - k_l) \Phi^{(n-1)}(k_1, \dots, \widehat{k}_l, \dots, k_n) \end{aligned} \quad (6)$$

as quadratic forms on $D_{\mathcal{S}} \times D_{\mathcal{S}}$.

Then in the sense of quadratic forms on $D_{\mathcal{S}} \times D_{\mathcal{S}}$ we have:

$$a^*(f) = \int_{\mathbb{R}^3} \widehat{a}^*(k) \widehat{f}(k) dk, \quad a(f) = \int_{\mathbb{R}^3} \widehat{a}(k) \overline{\widehat{f}(k)} dk. \quad (7)$$

Now for $\lambda = 1, 2$ and $f \in L^2(\mathbb{R}^3)$, $a_{\lambda}^{\#}(f)$ are defined to be the closures in \mathcal{F}_s of

$$a_1^{\#}(f) = a^{\#}(f) \otimes I, \quad a_2^{\#}(f) = I \otimes a^{\#}(f), \quad (8)$$

where $a^\#$ stands for a or a^* .

$\widehat{a}_\lambda^\#(k)$ is defined as a quadratic form on $(D_S \otimes D_S)^2$ similarly.

It follows that on \mathcal{F}_s^0

$$[a_\lambda(f), a_{\lambda'}^*(g)] = \delta_{\lambda\lambda'}(f, g), \quad [a_\lambda(f), a_{\lambda'}(g)] = [a_\lambda^*(f), a_{\lambda'}^*(g)] = 0.$$

If $f \in L^2(\mathbb{R}^3; \mathbb{C}^2)$, we can write $f = (f_1, f_2)$ with f_1 and f_2 in $L^2(\mathbb{R}^3)$, and $a^\#(f)$ is defined by

$$a^\#(f) = \sum_{\lambda=1,2} a_\lambda^\#(f_\lambda). \quad (9)$$

Finally, for $\lambda = 1, 2$, define the creation and annihilation operators acting in the configuration space by

$$a_\lambda^*(y) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \widehat{a}_\lambda^*(k) e^{-ik \cdot y} dk, \quad a_\lambda(y) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \widehat{a}_\lambda(k) e^{ik \cdot y} dk, \quad (10)$$

as quadratic forms on $(D_S \otimes D_S)^2$. Then we have

$$a^*(f) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} a_\lambda^*(y) f_\lambda(y) dy, \quad a(f) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} a_\lambda(y) \overline{f_\lambda(y)} dy, \quad (11)$$

in the sense of quadratic forms.

The number operator \mathcal{N} is defined by

$$(\mathcal{N}\Phi)^{(n)}(k_1, \dots, k_n) = n\Phi(k_1, \dots, k_n) \quad (12)$$

for all $\Phi \in D(\mathcal{N}) = \left\{ \Phi \in \mathcal{F}_s, \sum_{n \geq 1} n \|\Phi^{(n)}\|_{\otimes_{k=1}^n L^2(\mathbb{R}^3; \mathbb{C}^2)} < \infty \right\}$, and it is easy to see that \mathcal{N} is self-adjoint on $D(\mathcal{N})$. In the sense of quadratic forms, \mathcal{N} is given by

$$\mathcal{N} = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \widehat{a}_\lambda^*(k) \widehat{a}_\lambda(k) dk. \quad (13)$$

Moreover $D(\mathcal{N}^{1/2}) = \left\{ \Phi \in \mathcal{F}_s, \sum_{n \geq 1} n^{1/2} \|\Phi^{(n)}\|_{\otimes_{k=1}^n L^2(\mathbb{R}^3; \mathbb{C}^2)} < \infty \right\}$ and we have

$$(\mathcal{N}^{1/2}\Phi)^{(n)}(k_1, \dots, k_n) = n^{1/2}\Phi(k_1, \dots, k_n) \quad (14)$$

for all $\Phi \in D(\mathcal{N}^{1/2})$.

As in [LL] we can decompose an element of \mathcal{F}_s in a suitable basis. Namely if $(f_i)_{i \in \mathbb{N}}$ is an orthonormal basis of $L^2(\mathbb{R}^3; \mathbb{C}^2)$, the vectors of the form

$$|i_1, p_1; \dots; i_n, p_n\rangle_f := \frac{1}{\sqrt{p_1! \dots p_n!}} a^*(f_{i_1})^{p_1} \dots a^*(f_{i_n})^{p_n} \Omega \quad (15)$$

constitute an orthonormal basis of $\mathcal{F}(L^2(\mathbb{R}^3; \mathbb{C}^2))$ (where $\Omega = (1, 0, 0, \dots)$ denotes the vacuum vector in Fock space). Any $\Phi \in \mathcal{F}_s$ can be written as

$$\Phi = \sum_{n \geq 0} \sum_{i_1 < i_2 < \dots < i_n} \sum_{p_1, \dots, p_n} \Phi_{i_1, p_1; \dots; i_n, p_n} |i_1, p_1; \dots; i_n, p_n\rangle_f, \quad (16)$$

where the term for $n = 0$ in the sum is a constant times Ω .

2.2 Definition of the Hamiltonian

We denote by m_1 and q_1 the mass and the charge of the electron respectively, and by m_2 and q_2 the mass and the charge of the nucleus. Moreover x_1 and $p_1 := -i\hbar\nabla_{x_1}$ denote the position and the momentum of the electron, and x_2, p_2 are the position and the momentum of the nucleus. Let

$$M = m_1 + m_2 \quad , \quad \mu = \frac{m_1 m_2}{m_1 + m_2}. \quad (17)$$

Then the variables R, P of the center of mass, and the relative variables r, p are defined by

$$\begin{aligned} R &= \frac{m_1 x_1 + m_2 x_2}{M} \quad , \quad P = p_1 + p_2, \\ r &= x_1 - x_2 \quad , \quad \frac{p}{\mu} = \frac{p_1}{m_1} - \frac{p_2}{m_2}. \end{aligned} \quad (18)$$

We assume that $\hbar = 1$ and $c = 1$ where c is the velocity of light. Thus the Pauli-Fierz Hamiltonian of the system we consider is given as an operator acting in \mathcal{H} by

$$H_U^V := \sum_{j=1,2} \frac{1}{2m_j} (p_j - q_j A_j)^2 + H_f + V(r) + U(R). \quad (19)$$

Here $A_j := (A_j^1, A_j^2, A_j^3)$ is the quantized electromagnetic vector potential in the Coulomb gauge defined for $i = 1, 2, 3$ by

$$A_j^i = \int_{\mathbb{R}^6}^{\oplus} A^i(x_j) dX, \quad (20)$$

where $X = (x_1, x_2)$ and for $x \in \mathbb{R}^3$

$$A^i(x) = a^*(h^i(x - \cdot)) + a(h^i(x - \cdot)), \quad (21)$$

where the coupling function $h^i = (h_1^i, h_2^i)$ is defined for $\lambda = 1, 2$ by

$$h_\lambda^i(y) = \frac{1}{2\pi} \int_{\mathbb{R}^3} \frac{\widehat{\chi}_\Lambda(k)}{\sqrt{|k|}} \varepsilon_\lambda^i(k) e^{-ik \cdot y} dk. \quad (22)$$

The vectors ε_λ used in the last definition are the orthonormal polarization vectors in the Coulomb gauge. They are chosen as

$$\varepsilon_1(k) = \frac{(k_2, -k_1, 0)}{\sqrt{k_1^2 + k_2^2}} \quad , \quad \varepsilon_2(k) = \frac{k}{|k|} \wedge \varepsilon_1(k). \quad (23)$$

Note that $\varepsilon_1(k)$ and $\varepsilon_2(k)$ are well-defined and smooth only on $\mathbb{R}^3 \setminus Oz$ where Oz is the axis $\{(0, 0, k_3), k_3 \in \mathbb{R}\}$. But this singularity is not a problem in this paper.

Finally, Λ is the parameter of the ultraviolet cutoff, and $\widehat{\chi}_\Lambda$ is a real smooth function depending only on $|k|$, which is equal to 1 in the ball $B(0, \Lambda/2)$ and which vanishes outside the ball $B(0, \Lambda)$. It is well known that $A^i(x)$ is essentially self-adjoint on \mathcal{F}_s^0 for all $x \in \mathbb{R}^3$ (see [RS2]), and one can verify that in the sense of quadratic forms acting in the moment space

$$A(x) = \frac{1}{2\pi} \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\widehat{\chi}_\Lambda(k)}{\sqrt{|k|}} \varepsilon_\lambda(k) (\widehat{a}_\lambda^*(k) e^{-ik \cdot x} + \widehat{a}_\lambda(k) e^{ik \cdot x}) dk. \quad (24)$$

The free energy field of the photons, H_f , acts in $\mathcal{F}_s = \mathcal{F}_s(\mathbb{L}^2(\mathbb{R}^3)) \otimes \mathcal{F}_s(\mathbb{L}^2(\mathbb{R}^3))$ and is defined by

$$H_f := d\Gamma(\omega(-i\nabla)) \otimes I + I \otimes d\Gamma(\omega(-i\nabla)), \quad (25)$$

where $w(k) = |k|$, and where $d\Gamma(A)$ denotes the second quantization of the self-adjoint operator A . The massive photon field $H_f(m)$ will be defined by replacing $\omega(k) = |k|$ with $\omega_m(k) = \sqrt{k^2 + m^2}$, $m > 0$, in the definition of H_f . Then the massive Hamiltonian $H_U^V(m)$ is H_U^V with $H_f(m)$ replaced by H_f .

H_f is essentially self-adjoint on $D_S \otimes D_S$ and we have

$$H_f = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} |k| \hat{a}_\lambda^*(k) \hat{a}_\lambda(k) dk \quad (26)$$

as a quadratic form acting in the moment space.

V is the attractive Coulomb potential and is defined by

$$V(r) = -\frac{C}{|r|}, \quad (27)$$

where C is a positive constant.

Finally, U is a confining potential for which we make the following assumptions:

$$(H_0) \left\{ \begin{array}{l} (i) \quad U \in L_{\text{loc}}^1(\mathbb{R}^3), \\ (ii) \quad \inf(U(R)) > -\infty \text{ and } U^- \text{ is compactly supported,} \\ (iii) \quad P^2/2M + U \text{ has a non-degenerate ground state } \phi > 0 \text{ with energy } -e_0 < 0, \\ \text{and there exists } \gamma \text{ such that } |\phi(R)| \leq \gamma e^{-|R|/\gamma}. \end{array} \right.$$

In the next subsection we precise the relations between domains of self-adjointness (or domains of quadratic forms) for the operators that we work with in this paper.

2.3 Self-adjointness and quadratic forms domains

Let q be the quadratic form defined by

$$q(\Phi, \Psi) := \sum_{j=1,2} \frac{1}{2m_j} ((p_j - q_j A_j)\Phi, (p_j - q_j A_j)\Psi) + (H_f^{1/2}\Phi, H_f^{1/2}\Psi). \quad (28)$$

Lemma 2.1 q is closed on $Q(p_1^2 + p_2^2) \cap Q(H_f)$.

Proof First we have to verify that q is well-defined on $Q(p_1^2 + p_2^2) \cap Q(H_f)$. Lemma A.4 of [GLL] shows that

$$(A_j\Phi, A_j\Phi) \leq 32\pi\Lambda \left[(H_f^{1/2}\Phi, H_f^{1/2}\Phi) + \frac{\Lambda}{8}(\Phi, \Phi) \right], \quad (29)$$

for all $\Phi \in C_0^\infty(\mathbb{R}^6) \otimes D_S$.

Since $C_0^\infty(\mathbb{R}^6) \otimes D_S$ is a core for $H_f^{1/2}$, this proves that $Q(H_f) \subset D(A_j)$. Hence q is well-defined.

Next let us show that q is closed on $Q(p_1^2 + p_2^2) \cap Q(H_f)$. By lemma A.5 of [GLL], we have, for all $\Phi \in Q(p_1^2 + p_2^2) \cap Q(H_f)$,

$$(H_f^{1/2}\Phi, H_f^{1/2}\Phi) \leq q(\Phi, \Phi), \quad (30)$$

$$\sum_{j=1,2} (p_j\Phi, p_j\Phi) \leq a.q(\Phi, \Phi) + b(\Phi, \Phi), \quad (31)$$

where a, b are positive real numbers.

If $\Phi_n \in Q(p_1^2 + p_2^2) \cap Q(H_f)$ is such that $\Phi_n \rightarrow \Phi$ and $q(\Phi_n - \Phi_m, \Phi_n - \Phi_m) \rightarrow 0$, then (30) yields $\Phi \in Q(H_f)$ and (31) yields $\Phi \in Q(p_1^2) \cap Q(p_2^2)$. Hence q is closed. \square

In addition, we see that q is positive. Thus, there exists a unique self-adjoint operator, that we call H_0^0 , associated with q . In other words, $q = q_{H_0^0}$ (where q_A denotes the quadratic form associated with the self-adjoint operator A).

Lemma 2.2 *$V - U^-$ is relatively bounded with respect to q in the sense of forms, with relative bound 0.*

Proof According to the assumption (H_0) , U^- is infinitesimally small with respect to P^2 . Moreover the Coulomb potential V is infinitesimally small with respect to p^2 . Thus, $V - U^-$ is infinitesimally small with respect to $p_1^2 + p_2^2$ since we have

$$\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} = \frac{P^2}{2M} + \frac{p^2}{2\mu}. \quad (32)$$

Then $V - U^-$ is infinitesimally form-bounded with respect to $p_1^2 + p_2^2$ (see [RS2, theorem X.18]). We conclude with (31). \square

With the help of this lemma and the KLMN theorem, we define $H_{U^-}^V$ as the self-adjoint operator associated with the closed and semi-bounded quadratic form $q_{H_{U^-}^V}$ defined on $Q(p_1^2 + p_2^2) \cap Q(H_f)$ by $q_{H_{U^-}^V} = q + q_{V-U^-}$. Next, we define the Hamiltonian H_U^V by

$$H_U^V := H_{U^-}^V + U^+, \quad (33)$$

that is to say, H_U^V is the self-adjoint operator associated with the closed and semi-bounded quadratic form $q_{H_U^V}$ defined on $Q(H_{U^-}^V) \cap Q(U^+)$ by $q_{H_U^V} = q_{H_{U^-}^V} + q_{U^+}$.

Remark 2.1 *One could have defined the Hamiltonian of the system using a Schrödinger representation of \mathcal{F}_s , say $L^2(Q, d\mu)$. Namely, it is proved in [H1] that the operator \hat{H}_0 defined on $D(p_1^2 + p_2^2) \cap D(H_f)$ by*

$$\hat{H}_0 := \sum_{j=1,2} \frac{1}{2m_j} (p_j - q_j A_j)^2 + H_f \quad (34)$$

is self-adjoint. This result is obtained thanks to FKN and FKI formulae that lead to the following functional integral representation:

$$(F, e^{-t\hat{H}_0} G) = \int_M (F(X_0), J_t(X)G(X_t))_{L^2(Q)} dX. \quad (35)$$

Here, $M = \mathbb{R}^6 \times P$, where (P, db) is a probability measure space associated with the 6-dimensional Brownian motion $\{b(t)\}_{t \geq 0}$, and $X_t = X + b(t)$ is the Wiener process on M .

Moreover,

$$J_t(X) = \Xi_0^* e^{-i\phi_0(K(t))} \Xi_t, \quad (36)$$

where Ξ_t is the second quantization of $\oplus^3 \xi_t$. The isometry $\xi_t : \oplus^3 L^2(\mathbb{R}^3) \rightarrow \oplus^3 L^2(\mathbb{R}^4)$ is defined by

$$\widehat{\xi_t f}(k, k_0) = \frac{e^{-itk_0}}{\sqrt{\pi}} \sqrt{\frac{\omega(k)}{\omega(k)^2 + |k_0|^2}} \widehat{f}(k). \quad (37)$$

$\phi_0(f)$ is a Gaussian random process indexed by real $f \in \oplus^3 L^2(\mathbb{R}^4)$, on a probability measure space $(Q_0, d\mu_0)$. Finally, $K(t)$ is the stochastic integral

$$K(t) = \oplus_{i=1}^3 q_1 \int_0^t \xi_s \rho(\cdot - X_s) db_i^1(s) + \oplus_{i=1}^3 q_2 \int_0^t \xi_s \rho(\cdot - X_s) db_i^2(s), \quad (38)$$

with $\widehat{\rho}(k) = \widehat{\chi}_\Lambda(k) / (\pi \sqrt{2|k|})$.

Next it is proved that $V - U^-$ is infinitesimally small with respect to \widehat{H}_0 , so that the Kato-Rellich theorem gives a meaning to $\widehat{H}_{U^-}^V := \widehat{H}_0 + V - U^-$.

Finally, \widehat{H}_U^V is defined in the same way as for H_U^V , that is $\widehat{H}_U^V := \widehat{H}_{U^-}^V + U^+$.

Let us show here that the two definitions of the Hamiltonian are the same:

Proposition 2.1 $H_U^V = \widehat{H}_U^V$.

Proof This will follow from two lemmata:

Lemma 2.3 Let A be a semi-bounded self-adjoint operator and let B be a self-adjoint operator that is relatively bounded with respect to A with a relative bound strictly less than 1. Then

$$A + B = A \dot{+} B,$$

that is to say the definitions given by the Kato-Rellich theorem and the KLMN theorem respectively lead to the same operator.

Proof We easily see that q_{A+B} equals $q_{A \dot{+} B}$ on $D(A)$, and since this domain is a form core for each of the two closed quadratic forms, we get $q_{A+B} = q_{A \dot{+} B}$. Moreover, since A is semi-bounded, we can see that the two quadratic forms are semi-bounded. This yields $A + B = A \dot{+} B$. \square

Lemma 2.4 $H_0^0 = \widehat{H}_0$.

Proof Since $q_{H_0^0}$ and $q_{\widehat{H}_0}$ are positive, it is sufficient to show that these two closed quadratic forms are equal on a domain that is a form core for the two of them. According to [H1], $C_0^\infty(\mathbb{R}^6) \otimes D_S$ is a core for \widehat{H}_0 . Thus it is a form core for $q_{\widehat{H}_0}$. Let us show that it is also a form core for $q_{H_0^0}$.

By lemma A.4 of [GLL], we have

$$q_{H_0^0}(\Phi, \Phi) \leq \sum_{j=1,2} \frac{1}{2m_j} \left[(1 + |q_j|)(p_j \Phi, p_j \Phi) + (|q_j| + q_j^2)(32\pi\Lambda(H_f^{1/2}\Phi, H_f^{1/2}\Phi) + 4\pi\Lambda^2(\Phi, \Phi)) \right] + (H_f^{1/2}\Phi, H_f^{1/2}\Phi),$$

for all $\Phi \in C_0^\infty(\mathbb{R}^6) \otimes D_S$.

Now if $\Phi \in Q(p_1^2 + p_2^2) \cap Q(H_f)$, there is a sequence $\Phi_n \in C_0^\infty(\mathbb{R}^6) \otimes D_S$ such that $\Phi_n \rightarrow \Phi$, $p_j \Phi_n \rightarrow p_j \Phi$ for $j = 1, 2$ and $H_f^{1/2} \Phi_n \rightarrow H_f^{1/2} \Phi$. From the last inequality, we get $q_{H_0^V}(\Phi - \Phi_n, \Phi - \Phi_n) \rightarrow 0$. Hence $C_0^\infty(\mathbb{R}^6) \otimes D_S$ is a form core for $q_{H_0^V}$. \square

Now, $H_U^V(m)$ is defined similarly by $H_U^V(m) := H_{U^-}^V(m) \dot{+} U^+$, so that we have

$$Q(H_U^V(m)) = Q(p_1^2 + p_2^2) \cap Q(H_f(m)) \cap Q(U^+). \quad (39)$$

We note that the inequalities $|k| \leq \sqrt{k^2 + m^2} \leq |k| + m$, for all $k \in \mathbb{R}^3$, yield

$$Q(H_f(m)) = Q(H_f) \cap Q(\mathcal{N}) \quad , \quad Q(H_U^V(m)) = Q(H_U^V) \cap Q(\mathcal{N}). \quad (40)$$

2.4 Massive and massless ground state energy

In this subsection we recall (see [GLL, part. 5]) that the ground state energy of the massive Hamiltonian $H_U^V(m)$, $m > 0$, converges to the ground state energy of the massless one as m goes to 0. We will denote by $E(A)$ the infimum of the spectrum of any semi-bounded self-adjoint operator A , so that we have

$$E(A) = \inf_{\phi \in D(A), \|\phi\|=1} (\phi, A\phi) = \inf_{\phi \in Q(A), \|\phi\|=1} q_A(\phi, \phi).$$

Lemma 2.5 $E(H_U^V(m)) \xrightarrow{m \rightarrow 0} E(H_U^V)$.

Proof We sketch the proof (see [GLL, theorem 5.1] for more details). Namely, if $m > m' > 0$, we have $Q(H_U^V(m)) = Q(H_U^V(m')) \subset Q(H_U^V)$ by (40). Then

$$\begin{aligned} E(H_U^V) &= \inf_{\|\Psi\|=1, \Psi \in Q(H_U^V)} q_{H_U^V}(\Psi, \Psi) \leq \inf_{\|\Psi\|=1, \Psi \in Q(H_U^V(m'))} q_{H_U^V}(\Psi, \Psi) \\ &\leq \inf_{\|\Psi\|=1, \Psi \in Q(H_U^V(m'))} q_{H_U^V(m')}(\Psi, \Psi) = E(H_U^V(m')) \leq \dots \leq E(H_U^V(m)). \end{aligned}$$

Thus $E(H_U^V(m))$ converges to a limit E^* that is greater than $E(H_U^V)$ when m goes to 0.

To see that $E^* \leq E(H_U^V)$, let $\varepsilon > 0$ and take $\Psi_0 \in Q(H_U^V)$ such that $\|\Psi_0\| = 1$ and

$$q_{H_U^V}(\Psi_0, \Psi_0) \leq E(H_U^V) + \varepsilon.$$

If Π_n denotes the projector onto $\mathcal{F}_s^{(n)} := \{\Phi \in \mathcal{F}_s, \Phi^{(k)} = 0 \text{ for all } k > n\}$, then we can see as in [GLL] that $q_{H_U^V}(\Pi_n \Psi_0, \Pi_n \Psi_0) \xrightarrow{n \rightarrow \infty} q_{H_U^V}(\Psi_0, \Psi_0)$. We set $\tilde{\Psi}_0 := \Pi_{n_0} \Psi_0$ where n_0 is chosen such that $\left| q_{H_U^V}(\Pi_{n_0} \Psi_0, \Pi_{n_0} \Psi_0) / \|\Pi_{n_0} \Psi_0\|^2 - q_{H_U^V}(\Psi_0, \Psi_0) \right| \leq \varepsilon$. Then we have

$$\tilde{\Psi}_0 \in Q(H_U^V) \cap Q(\mathcal{N}) = Q(H_U^V(m))$$

for all $m > 0$, so that

$$\begin{aligned} E(H_U^V(m)) &= \inf_{\Psi \in Q(H_U^V(m)), \|\Psi\|=1} q_{H_U^V(m)}(\Psi, \Psi) \leq q_{H_U^V(m)}(\tilde{\Psi}_0, \tilde{\Psi}_0) / \|\tilde{\Psi}_0\|^2 \\ &\leq q_{H_U^V}(\tilde{\Psi}_0, \tilde{\Psi}_0) / \|\tilde{\Psi}_0\|^2 + m \cdot q_{\mathcal{N}}(\tilde{\Psi}_0, \tilde{\Psi}_0) / \|\tilde{\Psi}_0\|^2 \\ &\leq q_{H_U^V}(\Psi_0, \Psi_0) + \varepsilon + m \cdot n_0 \leq E(H_U^V) + 2\varepsilon + m \cdot n_0. \end{aligned}$$

Letting $m \rightarrow 0$, next $\varepsilon \rightarrow 0$, we get the stated result. \square

Note that the same result holds when H_U^V is replaced by H_0^V (respectively H_U^0).

3 Binding conditions

As in [GLL], the key step is to define binding conditions under which we are able to prove that a ground state exists for the Hamiltonian H_U^V . We define the binding conditions as:

$$E(H_U^V) < E(H_0^V), \quad (i)$$

$$E(H_U^V) < E(H_U^0). \quad (ii)$$

The proof of the condition (i) follows the one in [GLL, theorem 2.1], whereas the proof of (ii) is more difficult and needs the localization methods used in [LL].

Remark 3.1 *Note that as soon as (i) and (ii) are satisfied, lemma 2.5 yields*

$$\min [E(H_0^V(m)), E(H_U^0(m))] - E(H_U^V(m)) \geq C > 0, \quad (41)$$

for any suitable constant C and any m small enough.

3.1 Proof of condition (i)

Following [GLL, theorem 2.1], we shall show that $E(H_U^V) \leq E(H_0^V) - e_0$. The point is to find a normalized state $\Phi \in Q(H_U^V)$ such that $q_{H_U^V}(\Phi, \Phi) - (\Phi, [E(H_0^V) - e_0 + \varepsilon] \Phi) \leq 0$ (where $\varepsilon > 0$ is fixed).

Let $\varepsilon > 0$ and let $F \in D(H_0^V)$, $\|F\| = 1$ such that $(F, H_0^V F) < E(H_0^V) + \varepsilon$. Define the unitary operator \mathcal{U}_y for all $y \in \mathbb{R}^3$ by

$$\mathcal{U}_y = e^{iy \cdot (p_1 + p_2 + d\Gamma(-i\nabla))}. \quad (42)$$

\mathcal{U}_y acts in \mathcal{H} , and if $\Psi \in \mathcal{H}$, $\Psi := \Psi_{el} \otimes a^*(f_1)^{\alpha_1} \dots a^*(f_n)^{\alpha_n} \Omega$, then we have

$$\mathcal{U}_y \Psi = \Psi_{el}(\cdot + y, \cdot + y) \otimes a^*(f_1(\cdot + y))^{\alpha_1} \dots a^*(f_n(\cdot + y))^{\alpha_n} \Omega. \quad (43)$$

Since $[H_0^V, \mathcal{U}_y] = 0$ on $C_0^\infty(\mathbb{R}^3) \otimes D_S$ and since this domain is a core for H_0^V (see [H1]), then, for all $\Psi \in D(H_0^V)$, $\mathcal{U}_y \Psi \in D(H_0^V)$ and $[H_0^V, \mathcal{U}_y] \Psi = 0$.

Let us note here that, in particular, this translation invariance of H_0^V is due to the fact that V itself is translation invariant. But this becomes false if V is replaced by U , so that we will have to face a difficulty through the proof of condition (ii).

Now, as in [GLL], we would like to choose $\Phi_y := \phi \mathcal{U}_y F$, for a suitable y , as a trial state. First we have to show that $\Phi_y \in Q(H_U^V)$. We know that $\exists \gamma > 0$ such that $\phi(R) \leq \gamma e^{-|R|/\gamma}$ for all $R \in \mathbb{R}^3$. Thus, $\Phi_y \in \mathcal{H}$ for all y . Let $\xi_n(R) = \xi(R/n)$ be a smooth function in $C_0^\infty(\mathbb{R}^3)$ with $0 \leq \xi \leq 1$, $\xi = 1$ in the ball $B(0, 1)$ and $\xi = 0$ outside the ball $B(0, 2)$; let $\phi_n := \xi_n \phi$. Then $\Phi_y^n := \phi_n \mathcal{U}_y F \xrightarrow{n \rightarrow \infty} \Phi_y$ in \mathcal{H} , and $\Phi_y^n \in Q(H_U^V)$ since ϕ_n is a smooth, compactly supported

function. Thus, to be able to conclude that $\Phi_y \in Q(H_U^V)$, we only need to show that $q_{H_U^V}(\Phi_y^n, \Phi_y^n)$ is bounded uniformly in n . Since $q_{H_U^V}$ is semi-bounded from below, we would like to check that $q_{H_U^V}(\Phi_y^n, \Phi_y^n)$ is bounded from above. But

$$q_{H_U^V}(\Phi_y^n, \Phi_y^n) = \sum_{j=1,2} \frac{1}{2m_j} ((p_j - q_j A_j) \Phi_y^n, (p_j - q_j A_j) \Phi_y^n) + (\Phi_y^n, U \Phi_y^n) + (\Phi_y^n, [H_f + V] \Phi_y^n).$$

The last term of this sum is uniformly bounded from above since V is negative, since $\phi_n^2(R) \leq \phi^2(R) \leq \gamma^2 e^{-|R|/2\gamma}$ and since $(\mathcal{U}_y F, H_f \mathcal{U}_y F) < \infty$ (because $\mathcal{U}_y F \in D(H_0^V)$). As for the other terms, following [GLL], we can show

$$\begin{aligned} & \sum_{j=1,2} \frac{1}{2m_j} ((p_j - q_j A_j) \Phi_y^n, (p_j - q_j A_j) \Phi_y^n) + (\Phi_y^n, U \Phi_y^n) \\ &= \int_{\mathbb{R}^6} \phi_n(R) \left[\left(\frac{P^2}{2M} + U \right) \phi_n(R) \right] \langle \mathcal{U}_y F(X), \mathcal{U}_y F(X) \rangle dX \\ & \quad + \sum_{j=1,2} \frac{1}{2m_j} \int_{\mathbb{R}^6} \phi_n(R)^2 \langle (p_j - q_j A(x_j)) \mathcal{U}_y F(X), (p_j - q_j A(x_j)) \mathcal{U}_y F(X) \rangle dX \\ &= -e_0 \int_{\mathbb{R}^6} \phi_n(R)^2 \langle \mathcal{U}_y F(X), \mathcal{U}_y F(X) \rangle dX + \frac{1}{2M} \int_{\mathbb{R}^6} (P^2 \xi_n)(R) \xi_n(R) \phi(R)^2 \langle \mathcal{U}_y F(X), \mathcal{U}_y F(X) \rangle dX \\ & \quad - \frac{1}{M} \int_{\mathbb{R}^6} \phi(R)^2 P[\xi_n(R)(P\xi_n)(R)] \langle \mathcal{U}_y F(X), \mathcal{U}_y F(X) \rangle dX \\ & \quad + \sum_{j=1,2} \frac{1}{2m_j} \int_{\mathbb{R}^6} \phi_n(R)^2 \langle (p_j - q_j A(x_j)) \mathcal{U}_y F(X), (p_j - q_j A(x_j)) \mathcal{U}_y F(X) \rangle dX. \end{aligned}$$

All of the terms in this last sum are bounded from above, which can be seen using again the fact that $\phi(R) \leq \gamma e^{-|R|/\gamma}$ together with $(\xi_n), (P\xi_n), (P^2\xi_n)$ are uniformly bounded, and $\mathcal{U}_y F \in D(H_0^V)$. Therefore $\Phi_y \in Q(H_U^V)$ for all $y \in \mathbb{R}^3$. In addition, we have

$$\begin{aligned} q_{H_U^V}(\Phi_y, \Phi_y) &= -e_0 \int_{\mathbb{R}^6} \phi(R)^2 \langle \mathcal{U}_y F(X), \mathcal{U}_y F(X) \rangle dX + (\Phi_y, [H_f + V] \Phi_y) \\ & \quad + \sum_{j=1,2} \frac{1}{2m_j} \int_{\mathbb{R}^6} \phi(R)^2 \langle (p_j - q_j A(x_j)) \mathcal{U}_y F(X), (p_j - q_j A(x_j)) \mathcal{U}_y F(X) \rangle dX. \end{aligned}$$

The end of the proof is the same as the one in [GLL]. That is we integrate $q_{H_U^V}(\Phi_y, \Phi_y)$ in y over \mathbb{R}^3 and do the changes of variables $x_1 + y \rightarrow x_1, x_2 + y \rightarrow x_2$, which leads to

$$\int_{\mathbb{R}^3} q_{H_U^V}(\Phi_y, \Phi_y) dy = \int_{\mathbb{R}^3} \Phi(u)^2 du [(F, H_0^V F) - e_0(F, F)] = (F, H_0^V F) - e_0,$$

since $\|\phi\|_{L^2(\mathbb{R}^3)} = 1$ and $\|F\|_{\mathcal{H}} = 1$.

But we assumed $(F, H_0^V F) < E(H_0^V) + \varepsilon$ and we have $\|\Phi_y\| = \|\phi\| \|F\| = 1$ so that

$$\int_{\mathbb{R}^3} q_{H_U^V}(\Phi_y, \Phi_y) - [E(H_U^V) - e_0 + \varepsilon] (\Phi_y, \Phi_y) dy < 0.$$

Therefore $\exists y_0 \in \mathbb{R}^3$, and $\Phi_{y_0} \in Q(H_U^V)$, which is necessary $\neq 0$, such that

$$q_{H_U^V}(\Phi_{y_0}, \Phi_{y_0}) - [E(H_U^V) - e_0 + \varepsilon] (\Phi_{y_0}, \Phi_{y_0}) < 0.$$

Then $E(H_U^V) < E(H_0^V) - e_0 + \varepsilon$, and since this inequality is true for all $\varepsilon > 0$, we obtain

$$E(H_U^V) \leq E(H_0^V) - e_0.$$

3.2 Proof of condition (ii)

As stated above, we can not follow the proof of the previous subsection because the Hamiltonian H_U^0 is not translation invariant. Actually, if (F_j) denotes a minimizing sequence for H_U^0 we can consider two possibilities: either a part of the support of F_j lies in a ball with fixed radius, or F_j is supported outside balls with increasing radius. In other words, consider a state "close to" the ground state. Then, the two particles of the system live either not too far from each other, or, on the contrary, as far as we want from each other. In the first case the proof is easy, whereas in the second case it is more difficult.

Namely, we shall localize the electronic particles together with the photons in a similar way as the one used in [LL]. This brings us to pay attention to a new Hamiltonian \tilde{H}_U^0 which operate in $L^2(\mathbb{R}^6) \otimes \mathcal{F}_s \otimes \mathcal{F}_s$, and whose ground state energy is such that

$$E(H_U^0) \geq E(\tilde{H}_U^0) > E(H_U^V),$$

which will give the result.

We begin with the simplest case:

Theorem 3.1 *Let (F_j) be a normalized sequence in $Q(H_U^0)$ such that $q_{H_U^0}(F_j, F_j) \xrightarrow{j \rightarrow \infty} E(H_U^0)$.*

Assume that

$$\exists \rho > 0, \exists a > 0, \forall j, \int_{B(0, \rho)} \int_{\mathbb{R}^3} \|F_j(X)\|^2 dR dr \geq a. \quad (44)$$

Then, $E(H_U^V) \leq E(H_U^0) - Ca/\rho$.

Proof Since $Q(H_U^V) = Q(H_U^0)$, we have $F_j \in Q(H_U^V)$. Hence it suffices to write

$$\begin{aligned} q_{H_U^V}(F_j, F_j) &= q_{H_U^0}(F_j, F_j) + \int_{\mathbb{R}^6} V(X) \|F_j(X)\|^2 dX \\ &\leq q_{H_U^0}(F_j, F_j) - \int_{B(0, \rho)} \int_{\mathbb{R}^3} \frac{C}{\rho} \|F_j(X)\|^2 dX \leq q_{H_U^0}(F_j, F_j) - \frac{C}{\rho} a. \end{aligned}$$

We get the result as $j \rightarrow \infty$. □

Now we have to deal with the second case. As stated above, we need to define a new Hamiltonian acting in $L^2(\mathbb{R}^6) \otimes \mathcal{F}_s \otimes \mathcal{F}_s$. Namely, we define \tilde{H}_U^0 to be the self-adjoint operator associated with the closed and semi-bounded quadratic form $q_{\tilde{H}_U^0}$, with domain $Q(p_1^2 + p_2^2) \cap Q(\tilde{H}_f) \cap Q(U^+)$, such that:

$$\begin{aligned} q_{\tilde{H}_U^0}(\Phi, \Psi) &= \frac{1}{2m_1} ((p_1 - q_1 A_1) \otimes I) \Phi, [(p_1 - q_1 A_1) \otimes I] \Psi \\ &\quad + \frac{1}{2m_2} ([I \otimes (p_2 - q_2 A_2)] \Phi, [I \otimes (p_2 - q_2 A_2)] \Psi) \\ &\quad + (\tilde{H}_f^{1/2} \Phi, \tilde{H}_f^{1/2} \Psi) - ((U^-)^{1/2} \Phi, (U^-)^{1/2} \Psi) + ((U^+)^{1/2} \Phi, (U^+)^{1/2} \Psi), \end{aligned} \quad (45)$$

where we have set $\tilde{H}_f := H_f \otimes I + I \otimes H_f$. Note that in order to show that $q_{\tilde{H}_U^0}$ is closed, one can follow the subsection 2.3. Then we have:

Theorem 3.2 *Let (F_j) be a normalized sequence in $Q(H_U^0)$ such that $q_{H_U^0}(F_j, F_j) \xrightarrow{j \rightarrow \infty} E(H_U^0)$.*

Assume that

$$\forall n \in \mathbb{N}^*, \exists j_n, \int_{B(0,n)} \int_{\mathbb{R}^3} \|F_{j_n}(X)\|^2 dRdr \leq \frac{1}{n}. \quad (46)$$

Then $E(H_U^V) < E(\tilde{H}_U^0) \leq E(H_U^0)$.

Proof Note that in order to prove that $E(H_U^V) < E(\tilde{H}_U^0)$ with the localization method of [LL], we do not need to assume (46). However, we need it to show that $E(\tilde{H}_U^0) \leq E(H_U^0)$.

We begin with the proof of the first inequality. Since the method is quite similar to prove the second one, we shall not write the details.

First step: proof of the inequality $E(H_U^V) < E(\tilde{H}_U^0)$.

To show this inequality, we follow [LL]. Namely, as in theorem 4.3 of [LL], we would like first to find a state Ψ in $Q(\tilde{H}_U^0)$ such that:

- a) the electronic part of Ψ is supported in $B(y_1, R_0) \times B(y_2, R_0)$,
that is to say $\Psi(X) = 0$ as soon as $x_1 \notin B(y_1, R_0)$ or $x_2 \notin B(y_2, R_0)$,
- b) the photonic part of Ψ is supported in $B(y_1, L) \times B(y_2, L)$,
that is to say the photons of the first component of the tensor product $\mathcal{F}_s \otimes \mathcal{F}_s$ live in $B(y_1, L)$, whereas the photons of the second component live in $B(y_2, L)$,
- c) $\frac{q_{\tilde{H}_U^0}(\Psi, \Psi)}{\|\Psi\|^2} \leq E(\tilde{H}_U^0) + \frac{C_1}{R_0^2} + \frac{C_2}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma}\right) (1 + |\ln(\Lambda R_0)|)$,

where $R_0 > 0$ and $L > 2R_0$ are fixed, where C_1 and C_2 are positive constants, and where γ is any real number such that $0 < \gamma < 1$.

We start with localizing the electron and the nucleus in balls of radius R_0 .

Lemma 3.1 *For any fixed $R_0 > 0$, there exists $y_1, y_2 \in \mathbb{R}^3$ and a state $\Psi \in Q(\tilde{H}_U^0)$ such that the electronic part of Ψ is supported in $B(y_1, R_0) \times B(y_2, R_0)$ and*

$$\frac{q_{\tilde{H}_U^0}(\Psi, \Psi)}{\|\Psi\|^2} \leq E(\tilde{H}_U^0) + \frac{C_1}{R_0^2}, \quad (47)$$

where C_1 is a positive constant.

Proof of the lemma

This lemma is proved in [LL, theorem 4.1]. However in [LL], the authors have to deal with the Pauli principle according to which the states in \mathcal{H} have to be antisymmetric under the exchange of the particles labels. Here the electronic particles are distinct so that we do not have to deal with this problem. Then the proof becomes a bit simpler.

Let $\Psi \in D(\tilde{H}_U^0)$, $\|\Psi\| = 1$ be such that

$$(\Psi, \tilde{H}_U^0 \Psi) < E(\tilde{H}_U^0) + \frac{1}{R_0^2}.$$

Let $u \in C_0^\infty(\mathbb{R}^3)$ be such that $0 \leq u \leq 1$, $u = 1$ in the ball $B(0, 1/2)$ and $u = 0$ outside the ball $B(0, 1)$. Let us set

$$u_{1,y}(X) := u\left(\frac{x_1}{R_0} - y\right) \quad , \quad u_{2,y'}(X) := u\left(\frac{x_2}{R_0} - y'\right), \quad (48)$$

and note that

$$\int_{\mathbb{R}^3} u_{1,y}^2(X) dy = \int_{\mathbb{R}^3} u_{2,y'}^2(X) dy' = \int_{\mathbb{R}^3} u^2(z) dz := \beta > 0. \quad (49)$$

Define $\Psi_{y,y'} := \frac{1}{\beta} u_{1,y} u_{2,y'} \Psi$; with the definition of u , we easily see that $\Psi_{y,y'} \in Q(\tilde{H}_U^0)$. Then we have

$$\int_{\mathbb{R}^6} (\Psi_{y,y'}, \Psi_{y,y'}) dy dy' = \frac{1}{\beta^2} \int_{\mathbb{R}^6} \int_{\mathbb{R}^3} u_{1,y}^2(X) dy \int_{\mathbb{R}^3} u_{2,y'}^2(X) dy' < \Psi(X), \Psi(X) > dX = (\Psi, \Psi) = 1,$$

and

$$q_{\tilde{H}_U^0}(\Psi_{y,y'}, \Psi_{y,y'}) = \frac{1}{\beta^2} (\Psi, (|\nabla_{x_1} u_{1,y}|^2 u_{2,y'}^2 + |\nabla_{x_2} u_{2,y'}|^2 u_{1,y}^2) \Psi) + \frac{1}{\beta^2} \text{Re}(u_{1,y}^2 u_{2,y'}^2 \Psi, \tilde{H}_U^0 \Psi)$$

(here $\text{Re}(z)$ denotes the real part of the complex number z).

We compute in one hand

$$\begin{aligned} & \int_{\mathbb{R}^6} (\Psi, (|\nabla_{x_1} u_{1,y}|^2 u_{2,y'}^2 + |\nabla_{x_2} u_{2,y'}|^2 u_{1,y}^2) \Psi) dy dy' \\ &= \beta \int_{\mathbb{R}^6} \int_{\mathbb{R}^3} < \Psi(X), \frac{1}{R_0^2} |(\nabla u)\left(\frac{x_1}{R_0} - y\right)|^2 \Psi(X) > dy dX \\ & \quad + \beta \int_{\mathbb{R}^6} \int_{\mathbb{R}^3} < \Psi(X), \frac{1}{R_0^2} |(\nabla u)\left(\frac{x_2}{R_0} - y'\right)|^2 \Psi(X) > dy' dX = \frac{2\beta C_0}{R_0^2}, \end{aligned}$$

where $C_0 = \int_{\mathbb{R}^3} |\nabla u(z)|^2 dz > 0$, and in the other hand

$$\int_{\mathbb{R}^6} (u_{1,y}^2 u_{2,y'}^2 \Psi, \tilde{H}_U^0 \Psi) dy dy' = \beta^2 (\Psi, \tilde{H}_U^0 \Psi).$$

This leads to

$$\begin{aligned} & \int_{\mathbb{R}^6} \left[q_{\tilde{H}_U^0}(\Psi_{y,y'}, \Psi_{y,y'}) - (\Psi_{y,y'}, \left(\frac{2C_0}{\beta R_0^2} + \frac{1}{R_0^2} + E(\tilde{H}_U^0) \right) \Psi_{y,y'}) \right] dy dy' \\ &= (\Psi, \tilde{H}_U^0 \Psi) - E(\tilde{H}_U^0) - \frac{1}{R_0^2} < 0. \end{aligned}$$

Therefore $\exists (y_1, y_2) \in \mathbb{R}^6$ such that

$$q_{\tilde{H}_U^0}(\Psi_{y_1,y_2}, \Psi_{y_1,y_2}) < \left[E(\tilde{H}_U^0) + \frac{\text{Cste}}{R_0^2} \right] (\Psi_{y_1,y_2}, \Psi_{y_1,y_2}),$$

and in particular, Ψ_{y_1,y_2} is $\neq 0$ (here we have set $\text{Cste} = 1 + 2C_0\beta$). \square

Back to the proof of the inequality $E(H_U^V) < E(\tilde{H}_U^0)$.

Now, we have to localize the photons around the nucleus and the electron. We do not write the details of the proof here but sketch only it; we refer once again to [LL, lemma 4.3].

First, replacing the Laplacian by the Dirichlet Laplacian, \tilde{H}_U^0 is seen as an operator acting in $L^2(B(y_1, R_0) \times B(y_2, R_0); \mathcal{F}_s \otimes \mathcal{F}_s)$. We can show that this operator (that we call $\tilde{H}_{U,D}^0$) has a ground state Φ_D , so that in particular

$$(\Phi_D, \tilde{H}_{U,D}^0 \Phi_D) \leq q_{\tilde{H}_U^0}(\Psi_{y_1, y_2}, \Psi_{y_1, y_2}) \leq E(\tilde{H}_U^0) + \frac{\text{Cste}}{R_0^2},$$

where Ψ_{y_1, y_2} is the (normalized) state given by lemma 3.1, which satisfies the Dirichlet boundary conditions by construction.

Note that the Hamiltonian $\tilde{H}_{U,D}^0$ is defined in the same way as \tilde{H}_U^0 in (45); the only modification is that the domain of the quadratic form associated with $\tilde{H}_{U,D}^0$ is $H_0^1(B(y_1, R_0) \times B(y_2, R_0); \mathcal{F}_s \otimes \mathcal{F}_s) \cap Q(\tilde{H}_f(m)) \cap Q(U^+)$ instead of $H^1(\mathbb{R}^6; \mathcal{F}_s \otimes \mathcal{F}_s) \cap Q(\tilde{H}_f(m)) \cap Q(U^+)$. In particular if we set $\Phi_D(X) = 0$ outside $B(y_1, R_0) \times B(y_2, R_0)$, then $\Phi_D \in Q(\tilde{H}_U^0)$.

Therefore we would like to localize the photons in the state Φ_D .

Recall from section 2.1 that any state $\Psi \in L^2(\mathbb{R}^6; \mathcal{F}_s \otimes \mathcal{F}_s)$ can be written as $\Psi : X \mapsto \Psi(X)$ with

$$\Psi(X) = \sum_{\substack{n \geq 0 \\ n' \geq 0}} \sum_{\substack{i_1 < i_2 < \dots < i_n \\ i'_1 < i'_2 < \dots < i'_{n'}}} \sum_{\substack{p_1, \dots, p_n \\ p'_1, \dots, p'_{n'}}} \Psi_{\substack{i_1, p_1; \dots; i_n, p_n \\ i'_1, p'_1; \dots; i'_{n'}, p'_{n'}}}(X) |i_1, p_1; \dots; i_n, p_n\rangle_f \otimes |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_f,$$

where

$$|i_1, p_1; \dots; i_n, p_n\rangle_f = \frac{1}{\sqrt{p_1! \dots p_n!}} a^*(f_{i_1})^{p_1} \dots a^*(f_{i_n})^{p_n} \Omega,$$

and where (f_i) is an orthonormal basis of $L^2(\mathbb{R}^3; \mathbb{C}^2)$.

Then the operator \mathcal{J}_L will be defined by

$$\begin{aligned} & \mathcal{J}_L(|i_1, p_1; \dots; i_n, p_n\rangle_f \otimes |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_f) \\ &= \frac{1}{\sqrt{p_1! \dots p_n!}} \frac{1}{\sqrt{p'_1! \dots p'_{n'}!}} a^*(h_1 f_{i_1})^{p_1} \dots a^*(h_1 f_{i_n})^{p_n} \Omega \otimes a^*(h_2 f_{i'_1})^{p'_1} \dots a^*(h_2 f_{i'_{n'}})^{p'_{n'}} \Omega, \end{aligned} \quad (50)$$

where the functions $h_1, h_2 \in C_0^\infty(\mathbb{R}^3)$ are defined by

$$\left\{ \begin{array}{l} * \quad 0 \leq h_1 \leq 1 \text{ and } 0 \leq h_2 \leq 1, \\ * \quad h_1 = 1 \text{ in the ball } B(y_1, L/2) \text{ and } h_2 = 1 \text{ in the ball } B(y_2, L/2), \\ * \quad h_1 = 0 \text{ outside the ball } B(y_1, L) \text{ and } h_2 = 0 \text{ outside the ball } B(y_2, L). \end{array} \right.$$

In other words, h_1 localize photons next to the particle x_1 (which lives in $B(y_1, R_0)$) and h_2 localize photons next to the particle x_2 (which lives in $B(y_2, R_0)$).

Next we set $\Psi_0 := \mathcal{J}_L \Phi_D / \|\mathcal{J}_L \Phi_D\|^2$. Since $\Phi_D \in Q(\tilde{H}_U^0)$, we easily see that $\Psi_0 \in Q(\tilde{H}_U^0)$. Following [LL], theorem 4.3, we can show that

$$\frac{q_{\tilde{H}_U^0}(\mathcal{J}_L \Phi_D, \mathcal{J}_L \Phi_D)}{\|\mathcal{J}_L \Phi_D\|^2} \leq E(\tilde{H}_U^0) + \frac{C_1}{R_0^2} + \frac{C_2}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma} \right) (1 + |\ln(\Lambda R_0)|), \quad (51)$$

for any $0 < \gamma < 1$ and where $C_1, C_2 > 0$.

Note that we can use here some invariance of the Hamiltonian \tilde{H}_U^0 to simplify the proof of the last inequality. Namely, if we set

$$\mathcal{I}_t = e^{it \frac{m^2}{M} (p_1 + d\Gamma(-i\nabla))} \otimes e^{-it \frac{m^2}{M} (p_2 + d\Gamma(-i\nabla))}, \quad (52)$$

we can see that for all $t \in \mathbb{R}^3$ and all $\Phi \in Q(\tilde{H}_U^0)$:

$$q_{\tilde{H}_U^0}(\mathcal{T}_t\Phi, \mathcal{T}_t\Phi) = q_{\tilde{H}_U^0}(\Phi, \Phi). \quad (53)$$

In other words, if one translates the electron (with its cloud of photons) and the nucleus (with its cloud of photons) without moving the position of the center of mass, one does not modify the energy of the state under consideration.

We take $t = 3L - (y_1 - y_2)$ and we replace Ψ_0 by $\Psi_0 := \mathcal{T}_t \mathcal{J}_L \Phi_D / \|\mathcal{J}_L \Phi_D\|^2$, so that the new state Ψ_0 has the same properties as the previous one, except that in the new state a distance L separate the two balls where the particles live. Thus we do not have to pay any attention to the fact that the balls may overlap or not (as it is done in [LL, lemma 6.1]).

Finally we would like to find a state $\Xi \in Q(H_U^0)$ whose energy in H_U^0 would be sufficiently close to $q_{\tilde{H}_U^0}(\Psi_0, \Psi_0)$. Then the term $(\Xi, V\Xi)$ would be the main term in $q_{H_U^V}(\Xi, \Xi)$ and we would be able to conclude.

We shall apply formulae of the type (2.24) of [LL], so that it is convenient to replace $A(x_i)^2$ with the normal-ordered $:A(x_i)^2:$ in the definitions of the Hamiltonians H_U^V and \tilde{H}_U^0 . We write the "normal-ordered Hamiltonians" as \tilde{H}_U^0 and H_U^V respectively. We easily see that $E(:\tilde{H}_U^0:) - E(:H_U^V:) = E(\tilde{H}_U^0) - E(H_U^V)$.

Now, let (f_k) be an orthonormal basis of $L^2(B(y_1, L); \mathbb{C}^2)$ and let (g_l) be an orthonormal basis of $L^2(B(y_2, L); \mathbb{C}^2)$. We know that

- $\left\{ |i_1, p_1; \dots; i_n, p_n\rangle_f = \frac{1}{\sqrt{p_1! \dots p_n!}} a^*(f_{i_1})^{p_1} \dots a^*(f_{i_n})^{p_n} \Omega, n \in \mathbb{N}, i_k, p_k \in \mathbb{N} \right\}$ is an orthonormal basis of $\mathcal{F}_s(L^2(B(y_1, L); \mathbb{C}^2))$,
- and $\left\{ |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_g = \frac{1}{\sqrt{p'_1! \dots p'_{n'}!}} a^*(g_{i'_1})^{p'_1} \dots a^*(g_{i'_{n'}})^{p'_{n'}} \Omega, n' \in \mathbb{N}, i'_k, p'_k \in \mathbb{N} \right\}$ is an orthonormal basis of $\mathcal{F}_s(L^2(B(y_2, L); \mathbb{C}^2))$.

So we can write Ψ_0 as

$$\Psi_0(X) = \sum_{\substack{n \geq 0 \\ n' \geq 0}} \sum_{\substack{i_1 < i_2 < \dots < i_n \\ i'_1 < i'_2 < \dots < i'_{n'}}} \sum_{\substack{p_1, \dots, p_n \\ p'_1, \dots, p'_{n'}}} \Psi_{\substack{i_1, p_1; \dots; i_n, p_n \\ i'_1, p'_1; \dots; i'_{n'}, p'_{n'}}}(X) |i_1, p_1; \dots; i_n, p_n\rangle_f \otimes |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_g,$$

where $\Psi_{\substack{i_1, p_1; \dots; i_n, p_n \\ i'_1, p'_1; \dots; i'_{n'}, p'_{n'}}} \in L^2(\mathbb{R}^6)$, and

$$\sum_{\substack{n \geq 0 \\ n' \geq 0}} \sum_{\substack{i_1 < i_2 < \dots < i_n \\ i'_1 < i'_2 < \dots < i'_{n'}}} \sum_{\substack{p_1, \dots, p_n \\ p'_1, \dots, p'_{n'}}} \int_{\mathbb{R}^6} \left| \Psi_{\substack{i_1, p_1; \dots; i_n, p_n \\ i'_1, p'_1; \dots; i'_{n'}, p'_{n'}}}(X) \right|^2 dX = 1.$$

Pick an orthonormal basis $\{e_l\}$ of $L^2(\mathbb{R}^3)$ in $H^2(\mathbb{R}^3)$. Thus, we can also write $\Psi_{\substack{i_1, p_1; \dots; i_n, p_n \\ i'_1, p'_1; \dots; i'_{n'}, p'_{n'}}}$ as

$$\Psi_{\substack{i_1, p_1; \dots; i_n, p_n \\ i'_1, p'_1; \dots; i'_{n'}, p'_{n'}}}(X) = \sum_{\substack{l \geq 0 \\ l' \geq 0}} \Psi_{\substack{i_1, p_1; \dots; i_n, p_n \\ i'_1, p'_1; \dots; i'_{n'}, p'_{n'}}}^{l, l'} e_l(x_1) e_{l'}(x_2).$$

Then we can compute:

$$\begin{aligned}
& q_{;\tilde{H}_U^0}(\Psi_0, \Psi_0) \\
&= \frac{1}{2m_1} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i_1,p_1;\dots;i_n,p_n}^{l,l'}} \Psi_{j_1,q_1;\dots;j_o,q_o}^{m,m'} \delta_{l'm'} \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})(j'_1,q'_1;\dots;j'_{o'},q'_{o'})} \times \\
&\quad \int_{\mathbb{R}^3} \langle e_l(x_1) | i_1, p_1; \dots; i_n, p_n \rangle_f, : (p_1 - q_1 A(x_1))^2 : e_m(x_1) | j_1, q_1; \dots; j_n, q_n \rangle_f \rangle dx_1 \\
&+ \frac{1}{2m_2} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i'_1,p'_1;\dots;i'_{n'},p'_{n'}}^{l,l'}} \Psi_{j'_1,q'_1;\dots;j'_{o'},q'_{o'}}^{m,m'} \delta_{lm} \delta_{(i_1,p_1;\dots;i_n,p_n)(j_1,q_1;\dots;j_o,q_o)} \times \\
&\quad \int_{\mathbb{R}^3} \langle e_{l'}(x_2) | i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g, : (p_2 - q_2 A(x_2))^2 : e_{m'}(x_2) | j'_1, q'_1; \dots; j'_{n'}, q'_{n'} \rangle_g \rangle dx_2 \\
&+ \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i_1,p_1;\dots;i_n,p_n}^{l,l'}} \Psi_{j_1,q_1;\dots;j_o,q_o}^{m,m'} \delta_{lm} \delta_{l'm'} \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})(j'_1,q'_1;\dots;j'_{o'},q'_{o'})} \times \\
&\quad \langle |i_1, p_1; \dots; i_n, p_n \rangle_f, H_f | j_1, q_1; \dots; j_n, q_n \rangle_f \rangle \\
&+ \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i'_1,p'_1;\dots;i'_{n'},p'_{n'}}^{l,l'}} \Psi_{j'_1,q'_1;\dots;j'_{o'},q'_{o'}}^{m,m'} \delta_{lm} \delta_{l'm'} \delta_{(i_1,p_1;\dots;i_n,p_n)(j_1,q_1;\dots;j_o,q_o)} \times \\
&\quad \langle |i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g, H_f | j'_1, q'_1; \dots; j'_{n'}, q'_{n'} \rangle_g \rangle \\
&+ \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i_1,p_1;\dots;i_n,p_n}^{l,l'}} \Psi_{j_1,q_1;\dots;j_o,q_o}^{m,m'} \delta_{(i_1,p_1;\dots;i_n,p_n)(j_1,q_1;\dots;j_o,q_o)} \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})(j'_1,q'_1;\dots;j'_{o'},q'_{o'})} \times \\
&\quad \int_{\mathbb{R}^6} U(R) \overline{e_l(x_1) e_{l'}(x_2)} e_m(x_1) e_{m'}(x_2) dx_1 dx_2.
\end{aligned}$$

Here δ denotes the Kronecker symbol.

Now, we define the state $\Xi \in L^2(\mathbb{R}^6; \mathcal{F}_s)$ as

$$\Xi(X) = \sum_{\substack{n \geq 0 \\ n' \geq 0}} \sum_{\substack{i_1 < i_2 < \dots < i_n \\ i'_1 < i'_2 < \dots < i'_{n'}}} \sum_{\substack{p_1, \dots, p_n \\ p'_1, \dots, p'_{n'}}} \Psi_{i_1,p_1;\dots;i_n,p_n}^{i'_1,p'_1;\dots;i'_{n'},p'_{n'}}(X) |i_1, p_1; \dots; i_n, p_n \rangle_f \hat{\otimes} |i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g,$$

with

$$\begin{aligned}
& |i_1, p_1; \dots; i_n, p_n \rangle_f \hat{\otimes} |i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g \\
&:= \frac{1}{\sqrt{p_1! \dots p_n!} \sqrt{p'_1! \dots p'_{n'}!}} a^*(f_{i_1})^{p_1} \dots a^*(f_{i_n})^{p_n} a^*(g_{i'_1})^{p'_1} \dots a^*(g_{i'_{n'}})^{p'_{n'}} \Omega.
\end{aligned} \tag{54}$$

In particular we can see that $\Xi \in Q(H_U^V)$ and that $\|\Xi\| = \|\Psi_0\| = 1$.

Thus, applying formulae of the type (2.24) of [LL] to the states

$$|i_1, p_1; \dots; i_n, p_n \rangle_f \hat{\otimes} |i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g,$$

we get

$$q_{;H_U^V}(\Xi, \Xi) = [1] + [2] + [3] + [4] + [5],$$

with

$$\begin{aligned}
[1] = & \frac{1}{2m_1} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{l'm'} \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})} (j'_1,q'_1;\dots;j'_{o'},q'_{o'}) \times \\
& \int_{\mathbb{R}^3} \langle e_l(x_1) | i_1, p_1; \dots; i_n, p_n \rangle_f, : (p_1 - q_1 A(x_1))^2 : e_m(x_1) | j_1, q_1; \dots; j_n, q_n \rangle_f \rangle dx_1 \\
& + \frac{1}{2m_2} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{lm} \delta_{(i_1,p_1;\dots;i_n,p_n)} (j_1,q_1;\dots;j_o,q_o) \times \\
& \int_{\mathbb{R}^3} \langle e_{l'}(x_2) | i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g, : (p_2 - q_2 A(x_2))^2 : e_{m'}(x_2) | j'_1, q'_1; \dots; j'_{n'}, q'_{n'} \rangle_g \rangle dx_2 \\
& + \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{lm} \delta_{l'm'} \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})} (j'_1,q'_1;\dots;j'_{o'},q'_{o'}) \times \\
& \langle | i_1, p_1; \dots; i_n, p_n \rangle_f, H_f | j_1, q_1; \dots; j_n, q_n \rangle_f \rangle \\
& + \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{lm} \delta_{l'm'} \delta_{(i_1,p_1;\dots;i_n,p_n)} (j_1,q_1;\dots;j_o,q_o) \times \\
& \langle | i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g, H_f | j'_1, q'_1; \dots; j'_{n'}, q'_{n'} \rangle_g \rangle \\
& + \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{(i_1,p_1;\dots;i_n,p_n)} (j_1,q_1;\dots;j_o,q_o) \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})} (j'_1,q'_1;\dots;j'_{o'},q'_{o'}) \times \\
& \int_{\mathbb{R}^6} U(R) \overline{e_l(x_1) e_{l'}(x_2)} e_m(x_1) e_{m'}(x_2) dx_1 dx_2 \\
& + \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{(i_1,p_1;\dots;i_n,p_n)} (j_1,q_1;\dots;j_o,q_o) \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})} (j'_1,q'_1;\dots;j'_{o'},q'_{o'}) \times \\
& \int_{\mathbb{R}^6} V(r) \overline{e_l(x_1) e_{l'}(x_2)} e_m(x_1) e_{m'}(x_2) dx_1 dx_2,
\end{aligned}$$

$$\begin{aligned}
[2] = & - \frac{q_1}{m_1} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{l'm'} \delta_{(i_1,p_1;\dots;i_n,p_n)} (j_1,q_1;\dots;j_o,q_o) \times \\
& \int_{\mathbb{R}^3} \overline{e_l(x_1)} (p_1 e_m)(x_1) \langle | i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g, A(x_1) | j'_1, q'_1; \dots; j'_{o'}, q'_{o'} \rangle_g \rangle dx_1 \\
& - \frac{q_2}{m_2} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{lm} \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})} (j'_1,q'_1;\dots;j'_{o'},q'_{o'}) \times \\
& \int_{\mathbb{R}^3} \overline{e_{l'}(x_2)} (p_2 e_{m'})(x_2) \langle | i_1, p_1; \dots; i_n, p_n \rangle_f, A(x_2) | j_1, q_1; \dots; j_o, q_o \rangle_f \rangle dx_2,
\end{aligned}$$

$$\begin{aligned}
[3] = & \frac{q_1^2}{2m_1} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{l'm'} \delta_{(i_1,p_1;\dots;i_n,p_n)} (j_1,q_1;\dots;j_o,q_o) \times \\
& \int_{\mathbb{R}^3} \overline{e_l(x_1)} e_m(x_1) \langle | i'_1, p'_1; \dots; i'_{n'}, p'_{n'} \rangle_g, : A(x_1)^2 : | j'_1, q'_1; \dots; j'_{o'}, q'_{o'} \rangle_g \rangle dx_1 \\
& + \frac{q_2^2}{2m_2} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi^{l,l'}_{i_1,p_1;\dots;i_n,p_n} \Psi^{m,m'}_{j_1,q_1;\dots;j_o,q_o}} \delta_{lm} \delta_{(i'_1,p'_1;\dots;i'_{n'},p'_{n'})} (j'_1,q'_1;\dots;j'_{o'},q'_{o'}) \times \\
& \int_{\mathbb{R}^3} \overline{e_{l'}(x_2)} e_{m'}(x_2) \langle | i_1, p_1; \dots; i_n, p_n \rangle_f, : A(x_2)^2 : | j_1, q_1; \dots; j_o, q_o \rangle_f \rangle dx_2,
\end{aligned}$$

$$\begin{aligned}
[4] &= \frac{q_1^2}{m_1} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i_1,p_1;\dots;i_n,p_n}^{l,l'}} \Psi_{j_1,q_1;\dots;j_o,q_o}^{m,m'} \delta_{l'm'} \times \\
&\quad \int_{\mathbb{R}^3} \overline{e_l(x_1)} e_m(x_1) \langle |i_1, p_1; \dots; i_n, p_n\rangle_f, A(x_1) |j_1, q_1; \dots; j_o, q_o\rangle_f \rangle \\
&\quad \times \langle |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_g, A(x_1) |j'_1, q'_1; \dots; j'_{o'}, q'_{o'}\rangle_g \rangle dx_1 \\
&+ \frac{q_2^2}{m_2} \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i_1,p_1;\dots;i_n,p_n}^{l,l'}} \Psi_{j_1,q_1;\dots;j_o,q_o}^{m,m'} \delta_{lm} \times \\
&\quad \int_{\mathbb{R}^3} \overline{e_{l'}(x_2)} e_{m'}(x_2) \langle |i_1, p_1; \dots; i_n, p_n\rangle_f, A(x_2) |j_1, q_1; \dots; j_o, q_o\rangle_f \rangle \\
&\quad \times \langle |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_g, A(x_2) |j'_1, q'_1; \dots; j'_{o'}, q'_{o'}\rangle_g \rangle dx_2, \\
[5] &= \sum_{n,i,p,l} \sum_{o,j,q,m} \overline{\Psi_{i_1,p_1;\dots;i_n,p_n}^{l,l'}} \Psi_{j_1,q_1;\dots;j_o,q_o}^{m,m'} \delta_{lm} \delta_{l'm'} \times \\
&\quad \left[\sum_{\lambda} \int_{\mathbb{R}^3} |k| \langle \widehat{a}_\lambda(k) |i_1, p_1; \dots; i_n, p_n\rangle_f, |j_1, q_1; \dots; j_o, q_o\rangle_f \rangle \right. \\
&\quad \times \langle |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_g, \widehat{a}_\lambda(k) |j'_1, q'_1; \dots; j'_{o'}, q'_{o'}\rangle_g \rangle dk \\
&\quad + \sum_{\lambda} \int_{\mathbb{R}^3} |k| \langle |i_1, p_1; \dots; i_n, p_n\rangle_f, \widehat{a}_\lambda(k) |j_1, q_1; \dots; j_o, q_o\rangle_f \rangle \\
&\quad \times \langle \widehat{a}_\lambda(k) |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_g, |j'_1, q'_1; \dots; j'_{o'}, q'_{o'}\rangle_g \rangle dk \left. \right].
\end{aligned}$$

We see that [1] equals $q_{\widetilde{H}_V^0}(\Psi_0, \Psi_0) - ((-V)^{1/2}\Psi_0, (-V)^{1/2}\Psi_0)$.

Moreover, [3] is less than $\text{Cste}/L^{2\gamma}$ according to [LL, lemma 5.6].

Finally we can assume [2] + [4] + [5] ≤ 0 because if we replace Ξ by $\widetilde{\Xi}$ where

$$\begin{aligned}
\widetilde{\Xi}(X) &= \sum_{\substack{n \geq 0 \\ n' \geq 0}} \sum_{\substack{i_1 < i_2 < \dots < i_n \\ i'_1 < i'_2 < \dots < i'_{n'}}} \sum_{\substack{p_1, \dots, p_n \\ p'_1, \dots, p'_{n'}}} \sum_{\substack{l \geq 0 \\ l' \geq 0}} \Psi_{i_1, p_1; \dots; i_n, p_n}^{l, l'} \times \\
&\quad \overline{e_l(x_1)} e_{l'}(x_2) |i_1, p_1; \dots; i_n, p_n\rangle_f^{(-)} \otimes |i'_1, p'_1; \dots; i'_{n'}, p'_{n'}\rangle_g,
\end{aligned} \tag{55}$$

with

$$|i_1, p_1; \dots; i_n, p_n\rangle_f^{(-)} := \frac{1}{\sqrt{p_1! \dots p_n!}} (-a^*(f_{i_1}))^{p_1} \dots (-a^*(f_{i_n}))^{p_n} \Omega, \tag{56}$$

then [1] and [3] do not change whereas [2], [4] and [5] are replaced by their opposite terms.

Now in the state Ψ_0 (and also in the state Ξ), the particle x_1 is localized in $B(y_1, R_0) \subset B(y_1, L)$, whereas x_2 is localized in $B(y_2, R_0) \subset B(y_2, L)$, and we have chosen y_1, y_2 such that

the distance between the two balls $B(y_1, L)$ and $B(y_2, L)$ is L . Therefore Ψ_0 is supported in $\{|r| \leq 5L\}$, which yields

$$-((-V)^{1/2}\Psi_0, (-V)^{1/2}\Psi_0) \leq -\frac{C}{5L}(\Psi_0, \Psi_0) = -\frac{C}{5L}.$$

Here (53) is crucial because otherwise the balls $B(y_1, L)$ and $B(y_2, L)$ could be far away from each other and we could not estimate $((-V)^{1/2}\Psi_0, (-V)^{1/2}\Psi_0)$.

To conclude, (51) yields

$$q_{H_U^V}(\Xi, \Xi) \leq E(\tilde{H}_U^0) + \frac{C_1}{R_0^2} + \frac{C_2}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma}\right) (1 + |\ln(\Lambda R_0)|) + \frac{C_3}{L^{2\gamma}} - \frac{C}{5L},$$

for all $\gamma < 1$, all $R_0 > 0$ and all $L > 2R_0$.

We choose γ such that $\frac{3}{4} < \gamma < 1$, and $R_0 = L^\alpha$ with $\frac{1}{2} < \alpha < 2\gamma - 1$. Then, for L large enough, C/L becomes the dominant term in the last inequality, that is to say

$$\frac{C_1}{R_0^2} + \frac{C_2}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L^\gamma}\right) (1 + |\ln(\Lambda R_0)|) + \frac{C_3}{L^{2\gamma}} - \frac{C}{5L} < 0.$$

Thus

$$E(H_U^V) < E(\tilde{H}_U^0)$$

and the proof is complete.

Second step: proof of the inequality $E(\tilde{H}_U^0) \leq E(H_U^0)$.

The proof uses again the localization methods of [LL] and we only sketch it. Let us note yet that the localization errors need not to be estimate as precisely as in the previous step. We only need to know that these corrections can be made as small as we want.

Recall that the assumption (46) tells us that there exists a normalized minimizing sequence for H_U^0 , (F_j) , which verifies:

$$\forall n \in \mathbb{N}^*, \exists j_n, \int_{B(0, n)} \int_{\mathbb{R}^3} \|F_{j_n}(X)\|^2 dRdr \leq \frac{1}{n}. \quad (57)$$

Let τ_n and ν_n be functions defined by

$$\left\{ \begin{array}{l} * \quad \tau_n(r) = 1 \text{ if } |r| \leq n - \frac{1}{2} \\ * \quad \nu_n(r) = 1 \text{ if } |r| \geq n \\ * \quad \tau_n(r) = \tau\left(\frac{|r| - (n-1)}{|r|}r\right) \text{ and } \nu_n(r) = \nu\left(\frac{|r| - (n-1)}{|r|}r\right) \text{ if } n - \frac{1}{2} \leq |r| \leq n, \\ \quad \text{where } \tau \text{ and } \nu \text{ are defined on } 1/2 \leq |r| \leq 1 \text{ and are independent on } n \\ * \quad 0 \leq \nu_n \leq 1 \text{ and } 0 \leq \tau_n \leq 1 \\ * \quad \nu_n, \tau_n \in C^\infty(\mathbb{R}^3) \\ * \quad \nu_n^2 + \tau_n^2 = 1. \end{array} \right.$$

Then we have $\tau_n F_{j_n}, \nu_n F_{j_n} \in Q(H_U^0)$ and

$$q_{H_U^0}(F_{j_n}, F_{j_n}) = q_{H_U^0}(\tau_n F_{j_n}, \tau_n F_{j_n}) + q_{H_U^0}(\nu_n F_{j_n}, \nu_n F_{j_n}) - (F_{j_n}, (|\nabla \tau_n|^2 + |\nabla \nu_n|^2) F_{j_n}),$$

with

$$(F_{j_n}, (|\nabla \tau_n|^2 + |\nabla \nu_n|^2) F_{j_n}) = \int_{\{n - \frac{1}{2} \leq |r| \leq n\}} (|\nabla \tau(r)|^2 + |\nabla \nu(r)|^2) \int_{\mathbb{R}^3} \|F_{j_n}(X)\|^2 dRdr \leq \frac{C_{ste}}{n},$$

so that

$$q_{H_U^0}(\nu_n F_{j_n}, \nu_n F_{j_n}) - E(H_U^0)(\nu_n F_{j_n}, \nu_n F_{j_n}) \leq q_{H_U^0}(F_{j_n}, F_{j_n}) - E(H_U^0) + \frac{\text{Cste}}{n}. \quad (58)$$

Since

$$1 \geq \|\nu_n F_{j_n}\|^2 \geq \int_{B(0,n)^c} \int_{\mathbb{R}^3} \|F_{j_n}(X)\|^2 dRdr \geq 1 - \frac{1}{n},$$

this shows that $\nu_n F_{j_n} / \|\nu_n F_{j_n}\|$ is a normalized minimizing sequence for H_U^0 .

Then, we note again $\nu_n F_{j_n} = \nu_n F_{j_n} / \|\nu_n F_{j_n}\|$, and we localize the particles in this state. More precisely, we pick $R_0 > 0$ and $L > 0$ such that $L - 2R_0 > 0$. Then there exists n_0 such that for all $n \geq n_0$, $\nu_n F_{j_n}(X) = 0$ on $\{X, |r| \leq 3L\}$. Next, with the help of [LL], starting with $\nu_n F_{j_n}$ (for n large enough), we can construct a normalized state Ξ_n in $Q(H_U^0)$ such that

- a) the electronic part of Ξ_n is supported in $B(y_1, R_0) \times B(y_2, R_0)$,
- b) the photonic part of Ξ_n is supported in $B(y_1, L) \cup B(y_2, L)$,
- c) $q_{H_U^0}(\Xi_n, \Xi_n) \leq E(H_U^0) + \frac{C_1}{R_0^2} + \frac{C_2}{(L - 2R_0)^\gamma} \left(\frac{R_0}{L}\right)^\gamma (1 + |\ln(\Lambda R_0)|)$,

where C_1 and C_2 are positive constants, and where γ is any real number such that $0 < \gamma < 1$. In addition, the distance between the balls $B(y_1, L)$ and $B(y_2, L)$ is at least L by construction. The proof to get this result is close to the one of the first step, that is we localize first the nucleus and the electron in the state $\nu_n F_{j_n}$. Next, we replace the Laplacian with the Dirichlet Laplacian, which defines a new Hamiltonian that has a ground state. Finally, we localize the photons around the electron and the nucleus in this ground state. Note that the operator \mathcal{J}_L that allows us to localize the photons is defined here by:

$$\mathcal{J}_L a^*(h_{i_1})^{p_1} \dots a^*(h_{i_n})^{p_n} \Omega := a^*(h_{i_1})^{p_1} \dots a^*(h_{i_n})^{p_n} \Omega, \quad (59)$$

where $0 \leq h \leq 1$ is a function in $C_0^\infty(\mathbb{R}^3)$ that is equal to 1 on $B(y_1, L/2) \cup B(y_2, L/2)$ and that is equal to 0 outside $B(y_1, L) \cup B(y_2, L)$.

Thus, we have $h = h|_{B(y_1, L)} + h|_{B(y_2, L)}$, and we can write Ξ_n as

$$\Xi_n(X) = \sum_{\substack{i_1, p_1, \dots, i_k, p_k \\ i'_1, p'_1, \dots, i'_{k'}, p'_{k'}}} \Xi_n^{i_1, p_1, \dots, i_k, p_k, i'_1, p'_1, \dots, i'_{k'}, p'_{k'}}(X) a^*(f_{i_1})^{p_1} \dots a^*(f_{i_k})^{p_k} a^*(g_{i'_1})^{p'_1} \dots a^*(g_{i'_{k'}})^{p'_{k'}} \Omega,$$

where f_{i_j} is supported in $B(y_1, L)$ and $g_{i'_j}$ is supported in $B(y_2, L)$. In other words, all the factors $a^*(h|_{B(y_1, L)} f)$ are put on the left whereas the factors $a^*(h|_{B(y_2, L)} f)$ are put on the right. Now, we can define Ψ_n in $L^2(\mathbb{R}^6; \mathcal{F}_s \otimes \mathcal{F}_s)$ by

$$\Psi_n(X) := \sum_{\substack{i_1, p_1, \dots, i_k, p_k \\ i'_1, p'_1, \dots, i'_{k'}, p'_{k'}}} \Xi_n^{i_1, p_1, \dots, i_k, p_k, i'_1, p'_1, \dots, i'_{k'}, p'_{k'}}(X) a^*(f_{i_1})^{p_1} \dots a^*(f_{i_k})^{p_k} \Omega \otimes a^*(g_{i'_1})^{p'_1} \dots a^*(g_{i'_{k'}})^{p'_{k'}} \Omega.$$

The same computations as the ones of the previous step yield

$$q_{\tilde{H}_U^0}(\Psi_n, \Psi_n) \leq E(H_U^0) + \varepsilon$$

for all n large enough, where ε depends on R_0 , L and γ but can be made as small as we want. Note that, contrary to what we did in (55), it is useless to replace Ψ_n with a state $\tilde{\Psi}_n$ in order to eliminate some terms, since these terms are small when R_0 and L are large.

This shows that $E(\tilde{H}_U^0) \leq E(H_U^0) + \varepsilon$, where ε can be made as small as we want. Thus the proof is complete. \square

4 Existence of a ground state for H_U^V

In this section we shall prove the existence of a ground state for the Hamiltonian H_U^V . The proof follows the one in [GLL]. Namely, the existence of a ground state Φ_m is proved first for the massive Hamiltonian $H_U^V(m)$. Next it is shown that Φ_m decays exponentially in X , so that Theorems 6.1 and 6.3 of [GLL] concerning $\|\widehat{a}_\lambda(k)\Phi_m\|$ and $\|\nabla_k \widehat{a}_\lambda(k)\Phi_m\|$ follow. Finally the Rellich-Kondrachov theorem shows that the weak limit of Φ_m (when $m \rightarrow 0$) is a ground state for H_U^V .

4.1 Existence of a ground state for $H_U^V(m)$

As in [GLL], the proof is divided into two steps: the first step is to find a sufficient condition in order to get the existence of a ground state. Namely, it is sufficient to show that for all normalized sequence $(\Psi^j) \in Q(H_U^V(m))$ which converges weakly to 0 and such that $q_{H_U^V(m)}(\Psi^j, \Psi^j)$ is uniformly bounded, we have

$$\liminf_{j \rightarrow \infty} q_{H_U^V(m)}(\Psi^j, \Psi^j) > E(H_U^V(m)). \quad (60)$$

The second step is to prove that the condition (60) is satisfied. This follows again from the localization methods of [GLL], with some slight modifications.

Theorem 4.1 *For all $m > 0$ small enough, $\exists \Phi_m \in D(H_U^V(m))$ such that $\|\Phi_m\| = 1$ and*

$$H_U^V(m)\Phi_m = E(H_U^V(m))\Phi_m. \quad (61)$$

Proof *First step*

Assume that (60) is satisfied and let us show that a ground state exists for $H_U^V(m)$.

Let $(\Phi^j) \in Q(H_U^V(m))$ be a normalized sequence such that

$$q_{H_U^V(m)}(\Phi^j, \Phi^j) \xrightarrow{j \rightarrow \infty} E(H_U^V(m)).$$

Since (Φ^j) and $([H_U^V(m) - E(H_U^V(m))]^{1/2} \Phi^j)$ are bounded sequences, they converge weakly along some subsequences to limits denoted by Φ_m and Φ'_m respectively. These subsequences are still denoted by (Φ^j) and $([H_U^V(m) - E(H_U^V(m))]^{1/2} \Phi^j)$. Then we have

$$(\phi, [H_U^V(m) - E(H_U^V(m))]^{1/2} \Phi^j) = ([H_U^V(m) - E(H_U^V(m))]^{1/2} \phi, \Phi^j),$$

for all $\phi \in Q(H_U^V(m))$. When $j \rightarrow \infty$, this leads to

$$(\phi, \Phi'_m) = ([H_U^V(m) - E(H_U^V(m))]^{1/2} \phi, \Phi_m).$$

Therefore $\Phi_m \in Q(H_U^V(m))$ (and $[H_U^V(m) - E(H_U^V(m))]^{1/2} \Phi_m = \Phi'_m$).

Then, setting $\Psi^j = \Phi^j - \Phi_m$ as in [GLL], we have $\Psi^j \rightharpoonup 0$ and $[H_U^V(m) - E(H_U^V(m))]^{1/2} \Psi^j \rightharpoonup 0$,

so that

$$\begin{aligned}
0 &= \lim_{j \rightarrow \infty} q_{H_U^V(m)}(\Phi^j, \Phi^j) - E(H_U^V(m))(\Phi^j, \Phi^j) \\
&= \lim_{j \rightarrow \infty} ([H_U^V(m) - E(H_U^V(m))]^{1/2} (\Phi_m + \Psi^j), [H_U^V(m) - E(H_U^V(m))]^{1/2} (\Phi_m + \Psi^j)) \\
&= ([H_U^V(m) - E(H_U^V(m))]^{1/2} \Phi_m, [H_U^V(m) - E(H_U^V(m))]^{1/2} \Phi_m) \\
&\quad + \lim_{j \rightarrow \infty} ([H_U^V(m) - E(H_U^V(m))]^{1/2} \Psi^j, [H_U^V(m) - E(H_U^V(m))]^{1/2} \Psi^j).
\end{aligned}$$

Thus $[H_U^V(m) - E(H_U^V(m))]^{1/2} \Phi_m = 0$ and $\lim_{j \rightarrow \infty} \|[H_U^V(m) - E(H_U^V(m))]^{1/2} \Psi^j\| = 0$. Together with (60), this leads to $\Psi^j \rightarrow 0$ strongly, so that $\|\Phi_m\| = 1$. Finally $\|\Phi_m\| = 1$, $\Phi_m \in D(H_U^V(m))$ and $H_U^V(m)\Phi_m = E(H_U^V(m))\Phi_m$.

Second step

Let $(\Psi^j) \in Q(H_U^V(m))$ be a normalized sequence which converges weakly to 0 and such that $q_{H_U^V(m)}(\Psi^j, \Psi^j)$ is uniformly bounded. Let us show that

$$\liminf_{j \rightarrow \infty} q_{H_U^V(m)}(\Psi^j, \Psi^j) > E(H_U^V(m)).$$

Let $\phi_1, \phi_2, \phi_3 \in C^\infty(\mathbb{R}^6)$ be such that

$$\begin{cases}
* & \phi_1 = 1 \text{ on the set } \{X \in \mathbb{R}^6, |r| \leq 1, |R| \leq 1\}, \\
* & \phi_1 = 0 \text{ on } \{X \in \mathbb{R}^6, |r| \geq 2\} \cup \{X \in \mathbb{R}^6, |R| \geq 2\}, \\
* & 0 \leq \phi_1 \leq 1, \\
* & \phi_2(X) = \phi_2(r), \\
* & \phi_2 = 1 \text{ on } \{X \in \mathbb{R}^6, |r| \geq 2\}, \\
* & \phi_2 = 0 \text{ on } \{X \in \mathbb{R}^6, |r| \leq 1\}, \\
* & 0 \leq \phi_2 \leq 1, \\
* & \phi_3 = 1 \text{ on } \{X \in \mathbb{R}^6, |r| \leq 1, |R| \geq 2\}, \\
* & \phi_3 = 0 \text{ on } \{X \in \mathbb{R}^6, |r| \geq 2\} \cup \{X \in \mathbb{R}^6, |R| \leq 1\}, \\
* & 0 \leq \phi_3 \leq 1,
\end{cases}$$

and $\phi_1^2 + \phi_2^2 + \phi_3^2 = 1$.

Moreover we set $\phi_{i,T}(X) = \phi_i(X/T)$ for all $T > 0$ and $i = 1, 2, 3$. Then, $\phi_{i,T}\Psi^j \in Q(H_U^V(m))$, and we can show

$$q_{H_U^V(m)}(\Psi^j, \Psi^j) = \sum_{i=1,2,3} q_{H_U^V(m)}(\phi_{i,T}\Psi^j, \phi_{i,T}\Psi^j) - \sum_{i=1,2,3} (\Psi^j, |\nabla \phi_{i,T}|^2 \Psi^j), \quad (62)$$

where ∇ is the gradient vector in \mathbb{R}^6 .

Note that $|\nabla \phi_i| \leq C_i$ where C_i is a positive constant. Therefore

$$- \sum_{i=1,2,3} (\Psi^j, |\nabla \phi_{i,T}|^2 \Psi^j) \geq -\frac{\text{Cste}}{T^2}. \quad (63)$$

Now, let us estimate $q_{H_U^V(m)}(\phi_{1,T}\Psi^j, \phi_{1,T}\Psi^j)$. Here, the Hamiltonian $\tilde{H}_U^V(m)$ is defined in the same way as in (45), as an operator acting in $L^2(\mathbb{R}^6; \mathcal{F}_s \otimes \mathcal{F}_s)$, to be the self-adjoint operator associated with the quadratic form with domain $Q(p_1^2 + p_2^2) \cap Q(U^+) \cap Q(\tilde{H}_f(m))$:

$$\begin{aligned} q_{\tilde{H}_U^V(m)}(\Phi, \Psi) &= \frac{1}{2m_1}([(p_1 - q_1 A_1) \otimes I]\Phi, [(p_1 - q_1 A_1) \otimes I]\Psi) \\ &\quad + \frac{1}{2m_2}([(p_2 - q_2 A_2) \otimes I]\Phi, [(p_2 - q_2 A_2) \otimes I]\Psi) \\ &\quad + (\tilde{H}_f(m)^{1/2}\Phi, \tilde{H}_f(m)^{1/2}\Psi) - ((-V)^{1/2}\Phi, (-V)^{1/2}\Psi) \\ &\quad - ((U^-)^{1/2}\Phi, (U^-)^{1/2}\Psi) + ((U^+)^{1/2}\Phi, (U^+)^{1/2}\Psi), \end{aligned}$$

where we have set $\tilde{H}_f(m) := H_f(m) \otimes I + I \otimes H_f(m)$.

Note that, on $C_0^\infty(\mathbb{R}^6) \otimes D_S \otimes D_S$, we have

$$\tilde{H}_U^V(m) = H_U^V(m) \otimes I + I \otimes H_f(m).$$

Since $H_f(m) \geq mI - mP_\Omega$, where P_Ω denotes the projector onto the subspace spanned by Ω , we get

$$q_{\tilde{H}_U^V(m)} \geq E(H_U^V(m)) + m - mI \otimes P_\Omega. \quad (64)$$

In addition, we define the unitary operator \mathcal{U}_P from \mathcal{F}_s into $\mathcal{F}_s \otimes \mathcal{F}_s$ by

$$\mathcal{U}_P a^*(h) \mathcal{U}_P^* := a^*(j_{1,P}h) \otimes I + I \otimes a^*(j_{2,P}h), \quad (65)$$

for all $h \in L^2(\mathbb{R}^3; \mathbb{C}^2)$, and where $j_{1,P}, j_{2,P} \in C_0^\infty(\mathbb{R}^3)$ are such that

$$\left\{ \begin{array}{l} * \quad j_1 = 1 \text{ in the ball } B(0, 1), \\ * \quad j_1 = 0 \text{ outside the ball } B(0, 2), \\ * \quad 0 \leq j_1 \leq 1, \\ * \quad j_1^2 + j_2^2 = 1, \end{array} \right.$$

and $j_{i,P}(k) := j_i(k/P)$ for $i = 1, 2$.

Then, following [GLL, lemma A.1], we can show that

$$q_{H_U^V(m)}(\phi_{1,T}\Psi^j, \phi_{1,T}\Psi^j) = q_{\tilde{H}_U^V(m)}(\mathcal{U}_P\phi_{1,T}\Psi^j, \mathcal{U}_P\phi_{1,T}\Psi^j) + \nu(m, P, T),$$

where $\nu(m, P, T)$ is such that for all fixed m, T , $\nu(m, P, T) \xrightarrow{P \rightarrow \infty} 0$.

Thus (64) leads to

$$\begin{aligned} & q_{H_U^V(m)}(\phi_{1,T}\Psi^j, \phi_{1,T}\Psi^j) \\ & \geq [E(H_U^V(m)) + m](\phi_{1,T}\Psi^j, \phi_{1,T}\Psi^j) + \nu(m, P, T) - m(\mathcal{U}_P\phi_{1,T}\Psi^j, I \otimes P_\Omega\mathcal{U}_P\phi_{1,T}\Psi^j) \\ & = [E(H_U^V(m)) + m](\phi_{1,T}\Psi^j, \phi_{1,T}\Psi^j) + \nu(m, P, T) - \nu'(m, P, T, j), \end{aligned} \quad (66)$$

with $\nu'(m, P, T, j) := m(\mathcal{U}_P\phi_{1,T}\Psi^j, I \otimes P_\Omega\mathcal{U}_P\phi_{1,T}\Psi^j)$.

Lemma A.3 in [GLL] tells us that for all fixed m, P, T , $\liminf_{j \rightarrow \infty} (\nu'(m, P, T, j)) = 0$. The point to get this result is that $\phi_{1,T}$ is compactly supported, so that the operator

$$\phi_{1,T}\Gamma(j_1) \left[1 + \sum_{j=1,2} p_j^2 + H_f(m) \right]^{-1/2}$$

is compact, where $\Gamma(j_1)$ is defined by $\Gamma(j_1)a^*(f_1)\dots a^*(f_n)\Omega := a^*(j_1f_1)\dots a^*(j_1f_n)\Omega$.

Next, let us estimate $q_{H_U^V(m)}(\phi_{2,T}\Psi^j, \phi_{2,T}\Psi^j)$. We have

$$q_{H_U^V(m)}(\phi_{2,T}\Psi^j, \phi_{2,T}\Psi^j) = q_{H_U^0(m)}(\phi_{2,T}\Psi^j, \phi_{2,T}\Psi^j) - ((-V)^{1/2}\phi_{2,T}\Psi^j, (-V)^{1/2}\phi_{2,T}\Psi^j).$$

Since $\phi_{2,T}$ is supported in $\{X \in \mathbb{R}^6, |r| \geq T\}$, we get

$$q_{H_U^V(m)}(\phi_{2,T}\Psi^j, \phi_{2,T}\Psi^j) \geq \left[E(H_U^0(m)) - \frac{C}{T} \right] (\phi_{2,T}\Psi^j, \phi_{2,T}\Psi^j). \quad (67)$$

Finally, let us estimate $q_{H_U^V(m)}(\phi_{3,T}\Psi^j, \phi_{3,T}\Psi^j)$. We have

$$\begin{aligned} q_{H_U^V(m)}(\phi_{3,T}\Psi^j, \phi_{3,T}\Psi^j) &= q_{H_0^V(m)}(\phi_{3,T}\Psi^j, \phi_{3,T}\Psi^j) \\ &+ ((U^+)^{1/2}\phi_{3,T}\Psi^j, (U^+)^{1/2}\phi_{3,T}\Psi^j) - ((U^-)^{1/2}\phi_{3,T}\Psi^j, (U^-)^{1/2}\phi_{3,T}\Psi^j). \end{aligned}$$

But $\phi_{3,T}$ is supported in $\{X \in \mathbb{R}^6, |R| \geq T\}$ and we know by (H_0) that U^- is compactly supported. So $(U^-)^{1/2}\phi_{3,T} = 0$ for any T large enough. Therefore

$$q_{H_U^V(m)}(\phi_{3,T}\Psi^j, \phi_{3,T}\Psi^j) \geq E(H_0^V(m))(\phi_{3,T}\Psi^j, \phi_{3,T}\Psi^j), \quad (68)$$

for any T large enough.

Then, (62) with the inequalities (63), (66), (67), (68) leads to

$$\begin{aligned} q_{H_U^V(m)}(\Psi^j, \Psi^j) &\geq \min [E(H_U^V(m)) + m, E(H_U^0(m)), E(H_0^V(m))] \\ &+ \nu(m, P, T) + \nu'(m, P, T, j) - \frac{C}{T} - \frac{\text{Cste}}{T^2}, \end{aligned}$$

for any T large enough.

Let $\varepsilon > 0$ and pick T_0 large enough such that $-C/T_0 - \text{Cste}/T_0^2 \geq -\varepsilon$. Next, pick P_0 such that $|\nu(m, P_0, T_0)| \leq \varepsilon$. Then $\liminf_{j \rightarrow \infty} (\nu'(m, P_0, T_0, j)) = 0$ for any m small enough, which yields

$$\liminf_{j \rightarrow \infty} \left(q_{H_U^V(m)}(\Psi^j, \Psi^j) \right) \geq \min [E(H_U^V(m)) + m, E(H_U^0(m)), E(H_0^V(m))] - 2\varepsilon,$$

for all $\varepsilon > 0$ and any m small enough. Thus,

$$\begin{aligned} &\liminf_{j \rightarrow \infty} \left(q_{H_U^V(m)}(\Psi^j, \Psi^j) \right) \\ &\geq \min [E(H_U^V(m)) + m, E(H_U^0(m)), E(H_0^V(m))] \\ &= E(H_U^V(m)) + \min [m, E(H_U^0(m)) - E(H_U^V(m)), E(H_0^V(m)) - E(H_U^V(m))] > E(H_U^V(m)), \end{aligned}$$

for any m small enough (see the remark 3.1 above).

Thus the proof is complete. \square

4.2 Exponential decay of the ground state Φ_m

In order to prove the exponential localization of Φ_m , we follow [GLL, lemma 6.2], with some modifications. More precisely, we would like to show that $\|\exp(\beta|X|)\Phi_m\|$ (where β is a suitable constant) is bounded by a constant which does not depend on m . In [GLL], the bound depended on m . Here, the proof is simpler, and we do not need to follow [G].

Lemma 4.1 *Let Φ_m be a normalized ground state for $H_U^V(m)$.*

Then for all $\beta > 0$ such that $0 < \beta^2 < \min(E(H_0^V) - E(H_U^V), E(H_U^0) - E(H_U^V))$, we have

$$\left\| e^{\beta|X|}\Phi_m \right\|_{\mathcal{H}}^2 \leq C_0, \quad (69)$$

for any m small enough. Here, C_0 is a positive constant which does not depend on m .

Proof For $i = 1, 2, 3$, $\phi_{i,T}$ denotes the function defined in the previous subsection. Moreover, we set

$$\bar{\phi}_{1,T} = \sqrt{\phi_{2,T}^2 + \phi_{3,T}^2}, \quad (70)$$

that is $\bar{\phi}_{1,T}^2 = 1 - \phi_{1,T}^2$.

We have

$$\left\| e^{\beta|X|}\Phi_m \right\|^2 = \left\| \phi_{1,T}e^{\beta|X|}\Phi_m \right\|^2 + \left\| \bar{\phi}_{1,T}e^{\beta|X|}\Phi_m \right\|^2,$$

and since $\phi_{1,T}$ is compactly supported, the first of this two terms is bounded by a positive constant C_1 that does not depend on m .

We set $G_T := \bar{\phi}_{1,T} \exp(f_\varepsilon)$ where f_ε is defined for all $\varepsilon > 0$ by

$$f_\varepsilon(X) := \frac{\beta|X|}{1 + \varepsilon|X|}. \quad (71)$$

Note that f_ε and $|\nabla f_\varepsilon|$ are bounded functions. Thus, $G_T\Phi_m \in Q(H_U^V(m))$, and using the fact that Φ_m is a ground state for $H_U^V(m)$, we can show

$$q_{H_U^V(m)}(G_T\Phi_m, G_T\Phi_m) - E(H_U^V(m))\|G_T\Phi_m\|^2 = (\Phi_m, |\nabla G_T|^2\Phi_m).$$

But we can compute

$$|\nabla G_T|^2 = |\nabla \bar{\phi}_{1,T}|^2 e^{2f_\varepsilon} + 2(\nabla \bar{\phi}_{1,T} \cdot \nabla f_\varepsilon) e^{f_\varepsilon} G_T + |\nabla f_\varepsilon|^2 G_T^2.$$

Therefore

$$\begin{aligned} & q_{H_U^V(m)}(G_T\Phi_m, G_T\Phi_m) - E(H_U^V(m))\|G_T\Phi_m\|^2 - (G_T\Phi_m, |\nabla f_\varepsilon|^2 G_T\Phi_m) \\ &= (\Phi_m, [|\nabla \bar{\phi}_{1,T}|^2 e^{2f_\varepsilon} + 2(\nabla \bar{\phi}_{1,T} \cdot \nabla f_\varepsilon) e^{f_\varepsilon} G_T] \Phi_m) \\ &\leq C_2, \end{aligned} \quad (72)$$

where C_2 is a positive constant which depends on T but not on m or ε . Here, we used the fact that $\nabla \bar{\phi}_{1,T}$ is compactly supported.

In addition, we note that $\phi_{1,T/2} \cdot \bar{\phi}_{1,T} = 0$. Thus

$$\begin{aligned} q_{H_U^V(m)}(G_T\Phi_m, G_T\Phi_m) &= \sum_{i=2,3} q_{H_U^V(m)}(G_T\Phi_m, \phi_{i,T/2}^2 G_T\Phi_m) \\ &= \sum_{i=2,3} q_{H_U^V(m)}(\phi_{i,T/2} G_T\Phi_m, \phi_{i,T/2} G_T\Phi_m) - \sum_{i=2,3} (G_T\Phi_m, |\nabla \phi_{i,T/2}|^2 G_T\Phi_m). \end{aligned}$$

Now, as in the previous subsection we have

$$q_{H_U^V(m)}(\phi_{2,T/2}G_T\Phi_m, \phi_{2,T/2}G_T\Phi_m) \geq \left[E(H_0^V(m)) - \frac{2C}{T} \right] \|\phi_{2,T/2}G_T\Phi_m\|^2,$$

and

$$q_{H_U^V(m)}(\phi_{3,T/2}G_T\Phi_m, \phi_{3,T/2}G_T\Phi_m) \geq E(H_U^0(m))\|\phi_{3,T/2}G_T\Phi_m\|^2,$$

for any T large enough. This leads to

$$q_{H_U^V(m)}(G_T\Phi_m, G_T\Phi_m) \geq \min [E(H_0^V(m)), E(H_U^0(m))] \|G_T\Phi_m\|^2 - \left(\frac{2C}{T} + \frac{C_{\text{ste}}}{T^2} \right) \|G_T\Phi_m\|^2,$$

for any T large enough. Since $|\nabla f_\varepsilon| \leq \beta$, we get

$$\begin{aligned} & q_{H_U^V(m)}(G_T\Phi_m, G_T\Phi_m) - E(H_U^V(m))\|G_T\Phi_m\|^2 - (G_T\Phi_m, |\nabla f_\varepsilon|^2 G_T\Phi_m) \\ & \geq \min [E(H_0^V(m)) - E(H_U^V(m)), E(H_U^0(m)) - E(H_U^V(m))] \|G_T\Phi_m\|^2 - \beta^2 \|G_T\Phi_m\|^2 \\ & \quad - \left(\frac{2C}{T} + \frac{C_{\text{ste}}}{T^2} \right) \|G_T\Phi_m\|^2. \end{aligned}$$

Thus, remark 3.1 leads to

$$\begin{aligned} & q_{H_U^V(m)}(G_T\Phi_m, G_T\Phi_m) - E(H_U^V(m))\|G_T\Phi_m\|^2 - (G_T\Phi_m, |\nabla f_\varepsilon|^2 G_T\Phi_m) \\ & \geq \frac{1}{2} [\min [E(H_0^V) - E(H_U^V), E(H_U^0) - E(H_U^V)] - \beta^2] \|G_T\Phi_m\|^2 - \left(\frac{2C}{T} + \frac{C_{\text{ste}}}{T^2} \right) \|G_T\Phi_m\|^2, \end{aligned}$$

for any m small enough.

Therefore, we can choose T_0 such that

$$\begin{aligned} & q_{H_U^V(m)}(G_{T_0}\Phi_m, G_{T_0}\Phi_m) - E(H_U^V(m))\|G_{T_0}\Phi_m\|^2 - (G_{T_0}\Phi_m, |\nabla f_\varepsilon|^2 G_{T_0}\Phi_m) \\ & \geq \frac{1}{4} [\min [E(H_0^V) - E(H_U^V), E(H_U^0) - E(H_U^V)] - \beta^2] \|G_{T_0}\Phi_m\|^2, \end{aligned} \tag{73}$$

for any m small enough.

(72) and (73) yield

$$\|G_{T_0}\Phi_m\|^2 \leq \frac{4C_2}{\min [E(H_0^V) - E(H_U^V), E(H_U^0) - E(H_U^V)] - \beta^2} := C_3,$$

for any m small enough and any $\varepsilon > 0$. Thus, as $\varepsilon \rightarrow 0$, we get

$$\left\| \bar{\phi}_{1,T_0} e^{\beta|X|} \Phi_m \right\|^2 \leq C_3,$$

for any m small enough. So the proof is complete with $C_0 := C_1 + C_3$. \square

4.3 Convergence of the ground state Φ_m when $m \rightarrow 0$

The end of the proof of the existence of a ground state for H_U^V follows step by step the one in [GLL]. Namely, it is shown that $\|\hat{a}_\lambda(k)\Phi_m\|$ and $\|\nabla_k \hat{a}_\lambda(k)\Phi_m\|$ are bounded for almost every k , with bounds that do not depend on m . Next the Rellich-Kondrachov theorem leads to the conclusion. We only give the results.

Theorem 4.2 *Let Φ_m be a normalized ground state for $H_U^V(m)$, where $m > 0$ is small. Then, for almost every $k \in \mathbb{R}^3$, we have*

$$\|\widehat{a}_\lambda(k)\Phi_m\| \leq C_\Lambda (|q_1| + |q_2|) \frac{\widehat{\chi}_\Lambda(k)}{|k|^{1/2}} \| |X| \Phi_m \|. \quad (74)$$

Moreover, for almost every $k \in \mathbb{R}^3$ such that $|k| < \Lambda/2$ and $(k_1, k_2) \neq (0, 0)$, we have

$$\|\nabla_k \widehat{a}_\lambda(k)\Phi_m\| \leq C'_\Lambda (|q_1| + |q_2|) \frac{1}{|k|^{1/2} \sqrt{k_1^2 + k_2^2}} \| |X| \Phi_m \|. \quad (75)$$

Here C_Λ and C'_Λ are constants that depend on Λ , m_1 , m_2 , but not on m .

Remark 4.1

1. Note that $\Phi_m \in Q(\mathcal{N})$ by (40). Then (74) means

$$q_{\mathcal{N}}(\Phi_m, \Phi_m) \leq C_\Lambda^2 (|q_1| + |q_2|)^2 \int_{\mathbb{R}^3} \frac{\widehat{\chi}_\Lambda^2(k)}{|k|} dk \| |X| \Phi_m \|^2. \quad (76)$$

The meaning of (75) is given in the appendix B of [GLL].

2. A key step to obtain (74) and (75) is to use the following gauge transformation: the unitary operator \mathcal{T} is defined by

$$\mathcal{T} = \int_{\mathbb{R}^6}^\oplus \mathcal{T}(X) dX \quad \text{with} \quad \mathcal{T}(X) = e^{-i \sum_{j=1,2} q_j x_j \cdot A(0)}. \quad (77)$$

Then we have $\widehat{b}_\lambda(k, X) := \mathcal{T}(X) \widehat{a}_\lambda(k) \mathcal{T}^*(X) = \widehat{a}_\lambda(k) - i w_\lambda(k, X)$, with

$$w_\lambda(k, X) = \frac{1}{2\pi} \frac{\widehat{\chi}_\Lambda(k)}{|k|^{1/2}} \varepsilon_\lambda(k) \sum_{j=1,2} q_j x_j. \quad (78)$$

Hence the transformed Hamiltonian is

$$\widetilde{H}_U^V(m) := \mathcal{T} H_U^V(m) \mathcal{T}^* = \sum_{j=1,2} \frac{1}{2m_j} (p_j - q_j \widetilde{A}_j)^2 + \widetilde{H}_f(m) + U + V, \quad (79)$$

with $\widetilde{A}_j = \int_{\mathbb{R}^6}^\oplus \widetilde{A}_j(X) dX$, $\widetilde{H}_f(m) = \int_{\mathbb{R}^6}^\oplus \widetilde{H}_f(m)(X) dX$, and

$$\widetilde{A}_j(X) = A(x_j) - A(0) \quad , \quad \widetilde{H}_f(m)(X) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \omega_m(k) \widehat{b}_\lambda^*(k, X) \widehat{b}_\lambda(k, X) dk. \quad (80)$$

3. Theorem 4.2 together with lemma 4.1 show that $\|\widehat{a}_\lambda(k)\Phi_m\|$ and $\|\nabla_k \widehat{a}_\lambda(k)\Phi_m\|$ are uniformly bounded for small m .

Now let (m_j) be a sequence that decays to 0 and such that (74) and (75) are satisfied for all j . We can suppose that Φ_{m_j} converges weakly to a limit Φ when j goes to ∞ . Let us show that $\Phi \in D(H_U^V)$.

Since, for all j , $Q(H_U^V(m_j)) \subset Q(H_U^V)$ by (40), we can write

$$\begin{aligned} & \left\| [H_U^V - E(H_U^V)]^{1/2} \Phi_{m_j} \right\|^2 = q_{H_U^V}(\Phi_{m_j}, \Phi_{m_j}) - E(H_U^V) \\ & \leq q_{H_U^V(m_j)}(\phi_{m_j}, \phi_{m_j}) - E(H_U^V) = E(H_U^V(m_j)) - E(H_U^V) \xrightarrow{j \rightarrow \infty} 0. \end{aligned}$$

Thus, for all $\psi \in Q(H_U^V)$, we have

$$\begin{aligned} ([H_U^V - E(H_U^V)]^{1/2} \psi, \Phi) &= \lim_{j \rightarrow \infty} ([H_U^V - E(H_U^V)]^{1/2} \psi, \Phi_{m_j}) \\ &= \lim_{j \rightarrow \infty} (\psi, [H_U^V - E(H_U^V)]^{1/2} \Phi_{m_j}) = 0. \end{aligned}$$

Therefore, $\Phi \in Q(H_U^V)$ and $[H_U^V - E(H_U^V)]^{1/2} \Phi = 0$. This yields

$$\Phi \in D(H_U^V) \quad \text{and} \quad H_U^V \Phi = E(H_U^V) \Phi. \quad (81)$$

Then, in the same way as in theorem 7.1 of [GLL], (81), lemma 4.1 and theorem 4.2 lead to

Theorem 4.3 Φ_{m_j} converges strongly to Φ , so that $\|\Phi\| = 1$ and Φ is a ground state for H_U^V .

Remark 4.2 *With the help of the functional integral representation of remark 2.1, we can prove that the ground state of H_U^V is non-degenerate. Indeed, it is shown in [H2] that $\nu^{-1} e^{-tH_U^V} \nu$ is positivity improving as an operator acting on $L^2(\mathbb{R}^6 \times Q)$, where $L^2(Q)$ denotes a Schrödinger representation of \mathcal{F} , and where ν is a unitary operator from $L^2(Q)$ to \mathcal{F} .*

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