Infrared-Finite Algorithms in QED I. The Groundstate of an Atom Interacting with the Quantized Radiation Field

Volker Bach

FB Mathematik; Universität Mainz; D-55099 Mainz;
Germany (vbach@mathematik.uni-mainz.de)

Jürg Fröhlich*

Inst. f. Theoretische Physik; ETH Hönggerberg;
CH-8093 Zürich; Switzerland (juerg@itp.phys.ethz.ch)

Alessandro Pizzo

Dept. de Math.; Univ. Paris-Sud; F-91405 Orsay Cedex;
France (pizzo@itp.phys.ethz.ch)

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Abstract

In this first of a series of papers, the groundstate of a nonrelativistic atom, minimally coupled to the quantized radiation field, and its groundstate energy are constructed by an iteration scheme inspired by [8]. This scheme successively removes an infrared cutoff in momentum space and yields a convergent algorithm enabling us to calculate the groundstate and the groundstate energy, to arbitrary order in the feinstructure constant $\alpha \sim 1/137$.

*also at IHES, Bures-sur-Yvette

I Description of the Problem and Summary of Main Results

The purpose of this paper is to develop an infrared-finite algorithm for the construction of the groundstate of a nonrelativistic atom interacting with the quantized radiation field. Using a scheme that goes back to Pizzo [8], we derive a convergent expansion for the groundstate and the groundstate energy, assuming the feinstructure constant $\alpha \sim 1/137$ to be a sufficiently small positive number.

This is the first in a series of papers devoted to the construction of the groundstate and related quantities and their explicit representation as finite sums of contributions computable in terms of finitely many convergent integrals and an error term bounded above by const $\cdot\, \alpha^N$, for any given $N > 0$. In further papers in this series, we will use the result of the present one to derive an infrared-finite algorithm yielding an explicit representation for the groundstate and a scheme for the calculation of the groundstate energy and of scattering amplitudes for Rayleigh scattering of light at an atom. As a corollary, we will present a mathematically precise justification of Bohr's frequency condition.

In this paper, an atom is described as a quantum-mechanical bound state consisting of a static, positively charged pointlike nucleus surrounded by electrons. The electrons are described as nonrelativistic, pointlike quantum-mechanical particles with electric charge $-e$ and spin $\frac{1}{2}$, as originally proposed by Pauli. They are bound to the nucleus by the electrostatic Coulomb field and interact with the soft modes of the quantized electromagnetic field.

To keep our exposition as simple as possible, we consider a hydrogen atom consisting of a single, static proton of charge e surrounded by only one electron. The spin of the electron then turns out to be an inessential complication, and, for simplicity, we neglect the Zeeman coupling of the magnetic moment of the electron to the quantized magnetic field. It would, however, not be difficult to include the Zeeman term in our analysis.

The Hilbert space of pure state vectors of the system just described is given by

$$\mathcal{H} \;:=\; \mathcal{H}_{el} \otimes \mathcal{F}\,, \tag{I.1}$$

where $\mathcal{H}_{el} = L^2(\mathbb{R}^3)$ is the Hilbert space appropriate for the description of a single electron, disregarding its spin, and $\mathcal{F}$ is the Fock space used to describe the states of the transverse modes of the quantized electromagnetic field, i.e., the *photons*. More explicitly,

$$\mathcal{F} \;:=\; \bigoplus_{N=0}^{\infty} \mathcal{F}^{(N)}\,, \qquad \mathcal{F}^{(0)} = \mathbb{C}\,\Omega\,, \tag{I.2}$$

where Ω is the vacuum vector, i.e., the state of the electromagnetic field without any excited modes, and

$$\mathcal{F}^{(N)} \ := \ \mathcal{S}_N \bigotimes_{j=1}^{N} \mathfrak{h} \,, \qquad N \geq 1 \,, \tag{I.3}$$

where the Hilbert space $\mathfrak{h}$ of state vectors of a single photon is

$$\mathfrak{h} \ := \ L^2[\mathbb{R}^3 \times \mathbb{Z}_2] \,, \tag{I.4}$$

with photon momentum space given by $\mathbb{R}^3$, and $\mathbb{Z}_2$ is accounting for the two independent transverse polarizations, or helicities, of a photon. In Eq. (I.3), $\mathcal{S}_N$ denotes the orthogonal projection onto the subspace of $\bigotimes_{j=1}^N \mathfrak{h}$ of totally symmetric N-photon wave functions, in accordance with the fact that photons satisfy Bose-Einstein statistics. Thus, $\mathcal{F}^{(N)}$ is the subspace of $\mathcal{F}$ of state vectors for configurations of exactly N photons. It is convenient to represent the Hilbert space $\mathcal{H}$ as the space of square-integrable wave functions on the electron position space $\mathbb{R}^3$ with values in the photon Fock space $\mathcal{F}$, i.e.,

$$\mathcal{H} \ \cong \ L^2\Big[\mathbb{R}^3 \, ; \, \mathcal{F}\Big] \,. \tag{I.5}$$

The dynamics of the system is generated by the Hamiltonian

$$H \ := \ \Big(- i\vec{\nabla}_{\vec{x}} - \alpha^{3/2} \vec{A}(\alpha\vec{x}) \Big)^2 \ - \ V(x) \ + \ \check{H} \,. \tag{I.6}$$

In Eq. (I.6), $\vec{\nabla}_{\vec{x}}$ denotes the gradient with respect to the electron position $\vec{x} \in \mathbb{R}^3$, $\alpha \cong 1/137$ is the feinstructure constant, $\vec{A}(\vec{x})$ denotes the vector potential of the transverse modes of the quantized electromagnetic field in the *Coulomb gauge*,

$$\vec{\nabla}_{\vec{x}} \cdot \vec{A}(\vec{x}) \ = \ 0 \,, \tag{I.7}$$

V is the Coulomb potential of electrostatic attraction of the electron to the nucleus, and $\check{H}$ is the Hamiltonian of the quantized, free electromagnetic field.

Throughout this paper, we work with dimensionless quantities: If $\vec{X}$ is the dimensionful position vector of the electron, we set

$$\vec{x} \ := \ \frac{2}{r_{\mathrm{Bohr}}} \vec{X} \,, \tag{I.8}$$

where the Bohr radius $r_{\mathrm{Bohr}} = \frac{\hbar^2}{me^2} = \frac{1}{m\alpha}$, in units where Planck's constant $\hbar = 1$, and the velocity of light $c = 1$. Here, m denotes the electron's mass.

Then the components of the momentum vector, $\vec{K}$, of a single photon have dimension (length)$^{-1}$, and we set

$$\vec{k} \;:=\; \frac{r_{\text{Bohr}}}{2\,\alpha}\,\vec{K}\,. \tag{I.9}$$

The variables $\vec{x}$ and $\vec{k}$ are *dimensionless*. We choose units for the energy such that

$$2\,m\,\alpha^2 \;=\; 4\,\text{Rydberg} \;=\; 1\,. \tag{I.10}$$

With these conventions

$$\vec{K}\cdot\vec{X} \;=\; \alpha\,\vec{k}\cdot\vec{x}\,, \quad \text{and} \quad V(x) \;=\; \frac{1}{|\vec{x}|}\,. \tag{I.11}$$

Furthermore,

$$\check{H} \;:=\; \sum_{\lambda=\pm}\int d^3k\; a^*(\vec{k},\lambda)\,|\vec{k}|\,a(\vec{k},\lambda)\,, \tag{I.12}$$

where $a^*(\vec{k},\lambda)$ and $a(\vec{k},\lambda)$ are the usual photon creation- and annihilation operators, which satisfy the canonical commutation relations

$$[a^*(\vec{k},\lambda)\,,\,a^*(\vec{k}',\lambda')] \;=\; [a(\vec{k},\lambda)\,,\,a(\vec{k}',\lambda')] \;=\; 0\,, \tag{I.13}$$

$$[a(\vec{k},\lambda)\,,\,a^*(\vec{k}',\lambda')] \;=\; \delta_{\lambda\lambda'}\,\delta(\vec{k}-\vec{k}')\,, \tag{I.14}$$

$$a(\vec{k},\lambda)\,\Omega \;=\; 0\,, \tag{I.15}$$

for all $\vec{k},\vec{k}' \in \mathbb{R}^3$ and $\lambda,\lambda' \in \mathbb{Z}_2 \equiv \{\pm\}$.

The vector potential, $\vec{A}(\vec{x})$, in the Coulomb gauge is given by

$$\vec{A}(\vec{x}) \;:= \tag{I.16}$$

$$\frac{1}{(2\pi)^{3/2}}\sum_{\lambda=\pm}\int\frac{d^3k}{\sqrt{2\,|\vec{k}|}}\,\Lambda(\vec{k})\left\{\vec{\varepsilon}(\vec{k},\lambda)e^{-i\vec{k}\cdot\vec{x}}a^*(\vec{k},\lambda) \;+\; \vec{\varepsilon}(\vec{k},\lambda)^*e^{i\vec{k}\cdot\vec{x}}a(\vec{k},\lambda)\right\},$$

where $\Lambda(\vec{k})$ is the characteristic function of the ball $\{\vec{k}\in\mathbb{R}^3 \mid |\vec{k}| \le \kappa\}$ (or a nonnegative, smooth approximation thereof), and $\vec{\varepsilon}(\vec{k},+)$, $\vec{\varepsilon}(\vec{k},-)$ are photon polarization vectors, i.e., two unit vectors in $\mathbb{C}\otimes\mathbb{R}^3$ satisfying

$$\vec{\varepsilon}(\vec{k},\lambda)^*\cdot\vec{\varepsilon}(\vec{k},\mu) \;=\; \delta_{\lambda\mu}\,, \qquad \vec{k}\cdot\vec{\varepsilon}(\vec{k},\lambda) \;=\; 0\,, \tag{I.17}$$

for $\lambda,\mu=\pm$. The identity $\vec{k}\cdot\vec{\varepsilon}(\vec{k},\lambda)=0$ implies the Coulomb gauge condition. We note that, by a famous theorem due to Hopf, the vectors $\vec{\varepsilon}(\vec{k},\pm)$ cannot be chosen to be continuous functions of $\vec{k}/|\vec{k}|$; but this is of no concern for us.

The function $\Lambda(\vec{k})$ insures that modes of the electromagnetic field corresponding to wave vectors $\vec{k}$ with $|\vec{k}| \geq \kappa$ do not interact with the electron; i.e., Λ represents an *ultraviolet cutoff* that will be kept fixed throughout our analysis. The vector potential defined in (I.16) is thus cut off in the ultraviolet - the true vector potential of the electromagnetic field corresponds to the choice $\Lambda \equiv 1$. In our analysis of groundstates of *light* atoms and of low-energy Rayleigh scattereing, an ultraviolet cutoff with $5 \leq \kappa \leq 10$ can be expected to yield reliable results. For convenience, we shall henceforth assume that $\kappa \geq 1$. Of course, it would be desirable to carry out a mathematically precise analysis of ultraviolet renormalization (renormalization of the chemical potential and of the mass of an electron) and to construct the limiting dynamics, as $\kappa \to \infty$. But this problem is outside the scope of our paper.

In the following, we simplify our notations by setting

$$k \;:=\; (\vec{k}, \lambda)\,, \quad \omega(k) \;\equiv\; |k| \;:=\; |\vec{k}|\,, \quad \text{and} \quad \int f(k)\, dk \;:=\; \sum_{\lambda = \pm} \int f(\vec{k}, \lambda)\, d^3k\,, \tag{I.18}$$

for any integrable (possibly vector-valued) function f.

Next, we summarize the main results of this paper.

In Sect. II, we prove that the Hamiltonian H introduced in Eq. (I.6) is selfadjoint on the domain of the operator $-\Delta_x + \check{H}$, provided the feinstructure constant α, which we consider a perturbation parameter, is small, depending on the value of the ultraviolet cutoff κ. (Actually, it is not difficult to construct a canonical selfadjoint extension of H, for *arbitrary* values of κ and α, using Brownian motion and a Feynman-Kac formula for $\exp[-tH]$; see, e.g., [5].) If $\sigma(H)$ denotes the spectrum of H, we prove that

$$E_{\rm gs} \;:=\; \inf \sigma(H) \;>\; -\infty \tag{I.19}$$

is a *simple eigenvalue* of H corresponding to a *groundstate eigenvector* $\phi_{\rm gs} \in \mathcal{H}$ of H, provided α is sufficiently small (depending on κ). Furthermore,

$$\sigma(H) \;=\; [E_{\rm gs}\,,\, \infty)\,, \tag{I.20}$$

in fact, $E_{\rm gs}$ is a threshold for continuous spectrum of H of infinite multiplicity. Stated without more precision, these results are not new. The first result of this type for a slightly simplified model appeared in [1] and for the model described above in [3]; a stronger result valid for *arbitrary values* of α and κ was proven in [4, 7]. The point of our analysis is that we present an *explicit inductive construction* of $(E_{\rm gs}, \phi_{\rm gs})$, based on a decomposition of the terms in the Hamiltonian H that describe the interactions between the electron and the photons into a sum of terms with the property that at least one photon creation- or annihilation operator is localized in a shell

$$\Big\{ k \;\Big|\; \kappa\beta^{n+1} \leq |k| \leq \kappa\beta^{n} \Big\} \,, \quad \kappa \geq 1 \,, \quad 0 < \beta < \kappa^{-1} \,, \quad n \in \mathbb{N}_0 = \{0, 1, 2, \dots\} \,, \tag{I.21}$$

of photon momentum space. Our inductive construction yields a sequence $(E_n, \phi_n)_{n=0}^{\infty}$ of approximate groundstate energies and groundstates constructed from Hamiltonians H_n with an infrared cutoff at $|k| = \kappa\beta^n$. We prove that

$$\lim_{n\to\infty} E_n = E_{\rm gs} \,, \qquad \lim_{n\to\infty} \phi_n = \phi_{\rm gs} \,. \tag{I.22}$$

Our construction is inspired by and similar to one used by Pizzo [8] in an analysis of Nelson's model. The main new challenge we are coping with is that, while the interaction term in H superficially seems to be *marginal* (in the sense of power counting) in the *infrared*, it is actually *irrelevant* in the infrared on the subspace of all those states where the electron is localized near the nucleus in position space. This will be made precise with the help of the identity

$$i\,[H\,,\,\vec{x}] \;=\; 2\,\vec{v}\,, \tag{I.23}$$

where $\vec{v} := -i\vec{\nabla}_{\vec{x}} - \alpha^{3/2}\vec{A}(\alpha\vec{x})$ is the electron velocity operator, the virial theorem, and using the result that, in the groundstate, the electron is (exponentially well) localized near the nucleus in position space.

In a further paper we will explore a rather remarkable consequence of the insight that, in a study of groundstates of atoms - and, for that matter, of low-energy Rayleigh scattering - the interaction term in the Hamiltonian H behaves as if it were *irrelevant* in the *infrared*: If the constant β in (I.21) is chosen to depend on the feinstructure constant α in such a way that $\lim_{\alpha\to 0}\beta = 0$, e.g., $\alpha \leq \beta \leq \sqrt{\alpha}$, for $\alpha \ll 1$, then

$$|E_n - E_{\rm gs}| \;\leq\; \mathcal{O}(\alpha^N)\,, \tag{I.24}$$

$$\|\phi_n - \phi_{\rm gs}\| \;\leq\; \mathcal{O}(\alpha^N)\,, \tag{I.25}$$

for any finite $N > 0$, provided $n \geq \text{const}\, N$.

We plan to use these estimates to prove that, for $\beta := \alpha$, $E_{\rm gs} \equiv E_{\rm gs}(\alpha)$ and $\phi_{\rm gs} \equiv \phi_{\rm gs}(\alpha)$ have expansions of the form

$$E_{\rm gs}(\alpha) \;=\; \sum_{k=1}^{N}\sum_{\ell=k}^{N} \varepsilon_{k,\ell}\,(\ln[1/\alpha])^k\,\alpha^\ell \;+\; o(\alpha^N)\,, \tag{I.26}$$

$$\phi_{\rm gs}(\alpha) \;=\; \sum_{k=1}^{2N}\sum_{\ell=k}^{2N} \varphi_{k,\ell}\,(\ln[1/\alpha])^k\,\alpha^{\ell/2} \;+\; o(\alpha^N)\,, \tag{I.27}$$

for arbitrary $N = 1, 2, 3, \ldots$. The point of the expansions (I.26) and (I.27) is that $\varepsilon_\ell(\alpha)$ and $\varphi_\ell(\alpha)$ are computable in terms of finitely many convergent integrals, for any $0 \leq k \leq \ell < \infty$. We expect that the appearance of powers of $\ln[1/\alpha]$ ("infrared logarithms") on the right side of (I.26) and (I.27) is not an artefact of our algorithm, but is an expression of infrared divergences in naive perturbation theory: The quantities $E_{\rm gs}(\alpha)$ and $\phi_{\rm gs}(\alpha)$ are not analytic nor even smooth at $\alpha = 0$, but their derivatives of sufficiently high order diverge, as $\alpha \to 0$.

II Construction of the Ground State

In this section we prove our first main result. We show that the infimum E_{gs} of the spectrum of H, defined in (I.6), is an eigenvalue of multiplicity one with a corresponding eigenvector ϕ_{gs}. Our proof does not use the explicit form of $V(x) = |\vec{x}|^{-1}$ but only requires that V is an infinitesimal perturbation of $-\Delta$, i.e., that the domain of V includes the domain of $-\Delta$ and that, for any $\varepsilon > 0$, there exists a constant $b_\varepsilon < \infty$, such that

$$\pm V \;\leq\; \varepsilon\,(-\Delta) \,+\, b_\varepsilon \cdot \mathbf{1}\,. \tag{II.1}$$

This is a standard assumption which ensures the self-adjointness and semi-boundedness of $H_{el} = -\Delta - V(x)$ (see [6, 10]). Moreover, we suppose that $\lim_{|x|\to\infty} V(x) = 0$, and that

$$\begin{gathered} e_{el} := \inf \sigma(H_{el}) < 0 \text{ is an isolated eigenvalue of multiplicity} \\ \text{one with corresponding normalized eigenvector } \varphi_{el} \in \mathcal{H}_{el}. \end{gathered} \tag{II.2}$$

Note that if H_{el} possesses a groundstate with $e_{el} < 0$ then it is automatically unique, by the Perron-Frobenius theorem (see, e.g., [9]).

We define $\Delta e_{el} := \inf[\sigma(H_{el} - e_{el}) \setminus \{0\}]$ to be the distance of the atomic ground state energy e_{el} to the first excited atomic energy level or the continuum treshold. We remark that Assumption (II.2) is fulfilled for $H_{el} = -\Delta - 1/|x|$ - the degeneracy of the groundstate of the hydrogen atom is due to the spin of the electron.

Theorem II.1. *Assume Hypothesis H-1 and $g^{(1)}_{\alpha,\beta} = C_1 \alpha^{3/2} \beta^{1/2} \leq 1/8$. Then the groundstate energy $E_{\mathrm{gs}} = \inf \sigma(H)$ is a simple eigenvalue of H corresponding to a ground state eigenvector $\phi_{\mathrm{gs}} \in \mathcal{H}$ of H. Moreover, there exists a constant $C < \infty$ such that, for all $n \in \mathbb{N}$,*

$$1 - |\langle \phi_{\mathrm{gs}} | \phi_n \otimes \Omega^n_\infty \rangle|^2 \;\leq\; C\,\alpha\,\beta^n\,. \tag{II.3}$$

Theorem II.1 is restated in Corollary II.13 in Sect. II.5.

II.1 Notations

We introduce some more notation useful in the proof of Theorem II.1. Given an operator-valued function $F : \mathbb{R}^3 \times \mathbb{Z}_2 \to \mathcal{B}(\mathcal{H}_{el})$, we write $a^*(F) := \int F(k) \otimes a^*(k)\, dk$ and $a(F) := \int F(k)^* \otimes a(k)\, dk$. This allows us to write the velocity operator $\vec{v}$ as

$$\vec{v} \;:=\; -i\vec{\nabla}_x \,+\, a^*(\vec{G}) \,+\, a(\vec{G})\,, \tag{II.4}$$

where $\vec{G} : \mathbb{R}^3 \times \mathbb{Z}_2 \to \mathcal{B}(\mathcal{H}_{el})^3$ are the multiplication operators defined by

$$\vec{G}(k) \; := \; -\frac{\alpha^{3/2}}{(2\pi)^{3/2}} \, \frac{\Lambda(k)}{\sqrt{2\,|k|}} \, e^{-i\alpha \vec{k}\cdot\vec{x}} \, \vec{\varepsilon}(k) \, . \tag{II.5}$$

In terms of the velocity operator, the Hamiltonian assumes the simple form

$$H \; = \; \vec{v}^{\,2} \, - \, V(x) \, + \, \check{H} \, , \tag{II.6}$$

Its significance for our construction of a ground state of H lies in the fact that (formally, at this point)

$$2\,\vec{v} \; = \; i\,[H\,,\,\vec{x}] \, . \tag{II.7}$$

Our construction of a groundstate of H is inductive, as in [8]. Given a constant $\beta > 0$, with $\beta < \kappa^{-1}$, where $\kappa \geq 1$ is the UV-cutoff parameter in Eq. (I.16), we define a decreasing sequence $(\sigma_n)_{n=0}^{\infty}$ of energy scales by setting

$$\sigma_n \; := \; \kappa\,\beta^n \, . \tag{II.8}$$

Note, in passing, that, for all $n \in \mathbb{N}_0$, we have that $\sigma_{n+1} \leq \kappa\beta \leq 1$. To cut the interaction into slices at ever lower energy scales, we introduce

$$\vec{G}_n(k) \; := \; \mathbf{1}\Big(\sigma_n \leq |k|\Big)\, \vec{G}(k) \, , \quad \text{and} \quad \vec{G}_n^m(k) \; := \; \mathbf{1}\Big(\sigma_n \leq |k| < \sigma_m\Big)\, \vec{G}(k) \, , \tag{II.9}$$

for all $k \in \mathbb{R}^3 \times \mathbb{Z}_2$ and $m, n \in \mathbb{N}_0$, with $m < n$. Note that $\vec{G} = \sum_{n=0}^{\infty} \vec{G}_{n+1}^n$ and that $\vec{G}_n$ is the coupling function of the interaction, regularized in the infrared region. We also decompose the Fock space $\mathcal{F} = \mathcal{F}(\mathfrak{h})$ into energy scales by introducing

$$\mathfrak{h}_n \; := \; L^2\Big[\mathcal{K}_n\Big] \quad \text{and} \quad \mathfrak{h}_n^m \; := \; L^2\Big[\mathcal{K}_n^m\Big] \, , \tag{II.10}$$

where

$$\text{for } 0 \leq n \leq \infty\text{:} \quad \mathcal{K}_n \; := \; \Big\{ (\vec{k}, \tau) \in \mathbb{R}^3 \times \mathbb{Z}_2 \; \Big| \; \sigma_n \leq \omega(\vec{k}) \Big\} \, , \tag{II.11}$$

$$\text{for } 0 \leq m < n \leq \infty\text{:} \quad \mathcal{K}_n^m \; := \; \Big\{ (\vec{k}, \tau) \in \mathbb{R}^3 \times \mathbb{Z}_2 \; \Big| \; \sigma_n \leq \omega(\vec{k}) < \sigma_m \Big\} \tag{II.12}$$

Note that $\mathcal{K}_n^0 \subset \mathcal{K}_n$ is a proper subset. For integers $1 \leq m < n < \ell \leq \infty$, we have the disjoint decomposition $\mathcal{K}_\ell = \mathcal{K}_m \cup \mathcal{K}_n^m \cup \mathcal{K}_\ell^n$ and hence the orthogonal sum

$$\mathfrak{h}_\ell \; \cong \; \mathfrak{h}_m \oplus \mathfrak{h}_n^m \oplus \mathfrak{h}_\ell^n \, , \tag{II.13}$$

which gives rise to the isomorphism

$$\mathcal{F}_\ell \;\cong\; \mathcal{F}_m \otimes \mathcal{F}_n^m \otimes \mathcal{F}_\ell^n \,, \tag{II.14}$$

with $\mathcal{F}_n := \mathcal{F}(\mathfrak{h}_n)$ and $\mathcal{F}_n^m := \mathcal{F}(\mathfrak{h}_n^m)$. In particular, for any $n \in \mathbb{N}$,

$$\mathcal{F} \;=\; \mathcal{F}_\infty \;\cong\; \mathcal{F}_n \otimes \mathcal{F}_{n+1}^n \otimes \mathcal{F}_\infty^{n+1} \,. \tag{II.15}$$

Setting

$$\mathcal{H}_n \;:=\; \mathcal{H}_{el} \otimes \mathcal{F}_n \quad \text{and} \quad \mathcal{H}_n^m \;:=\; \mathcal{H}_{el} \otimes \mathcal{F}_n^m \,, \tag{II.16}$$

and given energy scale indices $m, n \in \mathbb{N}_0$, $m < n$, we define the velocity operator $\vec{v}_n$, the field energy operators $\check{H}_n$, $\check{H}_n^m$, and the Hamiltonian H_n at those scales by

$$\vec{v}_n \;:=\; -i\vec{\nabla}_x \,+\, a^*(\vec{G}_n) \,+\, a(\vec{G}_n) \,, \tag{II.17}$$

$$\check{H}_n \;:=\; \int \mathbf{1}(\sigma_n \leq |k|)\, \omega(k)\, a^*(k)a(k)\, dk \,, \tag{II.18}$$

$$\check{H}_n^m \;:=\; \int \mathbf{1}(\sigma_n \leq |k| < \sigma_m)\, \omega(k)\, a^*(k)a(k)\, dk \,, \tag{II.19}$$

$$H_n \;:=\; \vec{v}_n^{\,2} \,-\, V(x) \,+\, \check{H}_n \,, \tag{II.20}$$

as operators on $\mathcal{H}_n$ and $\mathcal{H}_n^m$, respectively. We introduce the groundstate energy at scales n and their differences for different scales $m < n$ by

$$E_n \;:=\; \inf \sigma(H_n) \quad \text{and} \quad E_n^m \;:=\; E_m - E_n \,. \tag{II.21}$$

To compare Hamiltonians H_n and H_{n+1} at successive energy scales, it is convenient to define the positive operators H_n^+ and $\widetilde{H}_n^+$ on $\mathcal{H}_n$ and $\mathcal{H}_{n+1}$, respectively, by

$$H_n^+ \;:=\; H_n \,-\, E_n \,, \tag{II.22}$$

$$\widetilde{H}_n^+ \;:=\; H_n^+ \otimes \mathbf{1}_{n+1}^n \,+\, \mathbf{1}_n \otimes \check{H}_{n+1}^n \,, \tag{II.23}$$

where we denote the identity operator on $\mathcal{H}_n$ and $\mathcal{F}_n^m$ by $\mathbf{1}_n$ and $\mathbf{1}_n^m$, respectively. One resolvent on $\mathcal{H}_{n+1}$ that we use in estimates over and over again is the following one,

$$\widetilde{R}_n \;:=\; \Big(\widetilde{H}_n^+ \,+\, \sigma_{n+1} \Big)^{-1} \,. \tag{II.24}$$

Note that $0 \leq \widetilde{R}_n \leq \sigma_{n+1}^{-1}$. We identify $\vec{v}_n$ with $\vec{v}_n \otimes \mathbf{1}_{n+1}^n$, which is acting on $\mathcal{H}_{n+1}$. Note that, for $n \in \mathbb{N}_0$,

$$\vec{v}_{n+1} \;=\; \vec{v}_n \,+\, a^*(\vec{G}_{n+1}^n) \,+\, a(\vec{G}_{n+1}^n) \,. \tag{II.25}$$

Similarly, given $\psi_n \in \mathcal{H}_n$, we define a vector

$$\tilde{\psi}_n \;:=\; \psi_n \otimes \Omega_{n+1}^n \;\in\; \mathcal{H}_{n+1}\,, \tag{II.26}$$

where Ω_n and Ω_n^m denote the vacuum vectors in $\mathcal{F}_n$ and $\mathcal{F}_n^m$, respectively. With these notations, we have that

$$\begin{aligned} H_{n+1}^+ \;&=\; \widetilde{H}_n^+ \,+\, W_{n+1}^n \,+\, E_{n+1}^n\,, &\text{(II.27)}\\ W_{n+1}^n \;&:=\; (\vec{v}_{n+1})^2 \,-\, (\vec{v}_n)^2 &\text{(II.28)}\\ &=\; 2\,a^*(\vec{G}_{n+1}^n)\cdot\vec{v}_n \,+\, 2\,\vec{v}_n\cdot a(\vec{G}_{n+1}^n) \,+\, \Big(a^*(\vec{G}_{n+1}^n) + a(\vec{G}_{n+1}^n)\Big)^2 \\ &=\; 2\,a^*(\vec{G}_{n+1}^n)\cdot\vec{v}_n \,+\, 2\,\vec{v}_n\cdot a(\vec{G}_{n+1}^n) \,+\, a^*(\vec{G}_{n+1}^n)\cdot a^*(\vec{G}_{n+1}^n) \\ &\quad + a(\vec{G}_{n+1}^n)\cdot a(\vec{G}_{n+1}^n) \,+\, 2\,a^*(\vec{G}_{n+1}^n)\cdot a(\vec{G}_{n+1}^n) \,+\, \Big\|\vec{G}_{n+1}^n\Big\|^2\,, \end{aligned}$$

where $\Big\|\vec{G}_{n+1}^n\Big\|^2 := \int |\vec{G}_{n+1}^n(k)|^2\,dk$. In Eq. (II.28), we make use of the Coulomb gauge condition $\vec{\nabla}\cdot\vec{A}(x) = 0$, which implies that

$$a^*(\vec{G}_{n+1}^n)\cdot\vec{v}_n \;=\; \vec{v}_n\cdot a^*(\vec{G}_{n+1}^n) \quad\text{and}\quad a(\vec{G}_{n+1}^n)\cdot\vec{v}_n \;=\; \vec{v}_n\cdot a(\vec{G}_{n+1}^n)\,. \tag{II.29}$$

Finally, it is convenient to collect the various assumptions which enter the derivations of the estimates, below, in the following Hypothesis.

Hypothesis 1. *Assume that $\kappa \geq 1$ and that $\pm V \leq \varepsilon(-\Delta) + b_\varepsilon$, for $\varepsilon > 0$, and set*

$$C_1 \;:=\; 8(\kappa + b_{1/8}) \;\geq\; 8\,. \tag{II.30}$$

Assume furthermore that

$$0 \;\leq\; \alpha \;\leq\; \beta \;\leq\; \beta_1 \;:=\; \min\left\{\frac{1}{2}\,,\ \kappa^{-1}\,,\ \Delta e_{el}\,\kappa^{-1}\right\}, \tag{II.31}$$

and set

$$g_{\alpha,\beta}^{(1)} \;:=\; \frac{C_1\,\alpha^{3/2}}{\beta^{1/2}}\,. \tag{II.32}$$

II.2 Some Basic Estimates

We make use of the notation

$$\|b\|^2 \;:=\; \int \|b(k)\|^2_{\mathcal{B}(\mathcal{H}_{el})}\,dk\,, \tag{II.33}$$

for $b \in L^2[\mathbb{R}^3 \times \mathbb{Z}_2; \mathcal{B}(\mathcal{H}_{el})]$. Moreover, for $\vec{b} \in L^2[\mathbb{R}^3 \times \mathbb{Z}_2; \mathcal{B}(\mathcal{H}_{el})^3]$, we set

$$\|\vec{b}(k)\|^2_{\mathcal{B}(\mathcal{H}_{el})} := \sum_{\nu=1}^3 \|b_\nu(k)\|^2_{\mathcal{B}(\mathcal{H}_{el})} \quad\text{and}\quad \|\vec{b}\|^2 := \sum_{\nu=1}^3 \|b_\nu\|^2\,. \tag{II.34}$$

Using this notation, we have, for all $n \in \mathbb{N}_0$ and all $k \in \mathbb{R}^3 \times \mathbb{Z}_2$,

$$\|\vec{G}^n_{n+1}(k)\|^2_{\mathcal{B}(\mathcal{H}_{el})} \;\leq\; \frac{3\,\alpha^3}{(2\pi)^3\,2\,|k|}\,\mathbf{1}\Big(\sigma_{n+1} \leq \omega(k) < \sigma_n\Big) \tag{II.35}$$

and

$$\Big\|\vec{G}^n_{n+1}\Big\|^2 \;\leq\; \tfrac{3\,\alpha^3}{2\,\pi^2}\int_0^{\sigma_n} k\,dk \;\leq\; \tfrac{1}{5}\,\sigma_n^2\,\alpha^3\,, \tag{II.36}$$

$$\Big\|\omega^{-1/2}\,\vec{G}^n_{n+1}\Big\|^2 \;\leq\; \tfrac{3\,\alpha^3}{2\,\pi^2}\int_0^{\sigma_n} dk \;\leq\; \tfrac{1}{5}\,\sigma_n\,\alpha^3\,. \tag{II.37}$$

Lemma II.2. *Let $f, g \in L^2[\mathbb{R}^3 \times \mathbb{Z}_2; \mathcal{B}(\mathcal{H}_{el})]$ be operator-valued functions obeying $\|(1+\omega^{-1})^{1/2} f\|, \|(1+\omega^{-1})^{1/2} g\| < \infty$. Then, for any $\rho > 0$*

$$\Big\|a(f)\,(\check{H}+\rho)^{-1/2}\Big\| \;\leq\; \|\omega^{-1/2} f\| \tag{II.38}$$

$$\Big\|(\check{H}+\rho)^{-1/2}\,a(f)\Big\| \;\leq\; \|(\rho^{-1}+\omega^{-1})^{1/2} f\|\,, \tag{II.39}$$

$$\Big\|a(f)\,a(g)\,(\check{H}+\rho)^{-1}\Big\| \;\leq\; \|\omega^{-1/2} f\|\,\|\omega^{-1/2} g\|\,, \tag{II.40}$$

$$\Big\|(\check{H}+\rho)^{-1}\,a(g)\,a(f)\Big\| \;\leq\; \|(\rho^{-1}+\omega^{-1})^{1/2} f\|\,\|(\rho^{-1}+\omega^{-1})^{1/2} g\|\,. \tag{II.41}$$

The proof of Lemma II.2 can be found in many texts, e.g., in [1, 2]. We remark that the relative bounds asserted in Lemma II.2 and (II.1) are the basic input to prove the selfadjointness of $H = \vec{v}^2 - V(x) + \check{H}$ on the domain of $-\Delta + \check{H}$, provided α is not too large.

Lemma II.3. *For all $0 \leq \alpha \leq \kappa^{-1/3}$, all $n \in \mathbb{N}_0$, and any $\rho \in (0, \sigma_n]$,*

$$\Big\|(H_n^+ + \rho)^{-1/2}\,(\vec{v}_n)^2\,(H_n^+ + \rho)^{-1/2}\Big\|_{\mathcal{H}_n} \;\leq\; C_1\,\rho^{-1}\,, \tag{II.42}$$

$$\Big\|\widetilde{R}_n^{1/2}\,(\vec{v}_n)^2\,\widetilde{R}_n^{1/2}\Big\|_{\mathcal{H}_{n+1}} \;\leq\; C_1\,\sigma_{n+1}^{-1}\,, \tag{II.43}$$

where C_1 is defined in (II.30).

The proof of Lemma II.3 is given in Appendix A. In the next lemma, we derive a quadratic form bound on the interaction W^n_{n+1} relative to the energy scale σ_{n+1} which proves that W^n_{n+1} is a small perturbation of $\widetilde{H}_n^+$, provided $g^{(1)}_{\alpha,\beta} := C_1 \alpha^{3/2} \beta^{1/2}$ is sufficiently small.

Lemma II.4. *Assume Hypothesis H-1. Then, for all $n \in \mathbb{N}_0$,*

$$\Big\|\widetilde{R}_n^{1/2}\,W^n_{n+1}\,\widetilde{R}_n^{1/2}\Big\|_{\mathcal{H}_{n+1}} \;\leq\; g^{(1)}_{\alpha,\beta}\,. \tag{II.44}$$

Proof. By Eq. (II.28) and Lemmata II.2 and II.3, we have

$$\begin{aligned}
&\Big\| \widetilde{R}_n^{1/2}\, W_{n+1}^n\, \widetilde{R}_n^{1/2} \Big\|_{\mathcal{H}_{n+1}} \\
&\leq \; 4 \Big\| \widetilde{R}_n^{1/2} \vec{v}_n \Big\|_{\mathcal{H}_{n+1}} \cdot \Big\| a(\vec{G}_{n+1}^n)\, \widetilde{R}_n^{1/2} \Big\|_{\mathcal{H}_{n+1}} \\
&\qquad + \Big\| \Big(a^*(\vec{G}_{n+1}^n) + a(\vec{G}_{n+1}^n) \Big)\, \widetilde{R}_n^{1/2} \Big\|_{\mathcal{H}_{n+1}}^2 \\
&\leq \; \frac{4\, C_1^{1/2}}{\sigma_{n+1}^{1/2}} \, \|\omega^{-1/2} \vec{G}_{n+1}^n\| \; + \; 4\, \|(\sigma_{n+1}^{-1} + \omega^{-1})^{1/2}\, \vec{G}_{n+1}^n\|^2 \\
&\leq \; \frac{4\, C_1^{1/2}\, \alpha^{3/2}\, \sigma_n^{1/2}}{\sqrt{5}\, \sigma_{n+1}^{1/2}} \; + \; \frac{8\, \alpha^3\, \sigma_n^2}{5\, \sigma_{n+1}} \;\; \leq \;\; \left(\frac{4\, C_1^{1/2}}{\sqrt{5}} + \frac{8\, \kappa}{5} \right) \frac{\alpha^{3/2}}{\beta^{1/2}} \\
&\leq \; \left(\frac{4}{\sqrt{5 C_1}} + \frac{1}{5} \right) \frac{C_1\, \alpha^{3/2}}{\beta^{1/2}} \;\; \leq \;\; \frac{C_1\, \alpha^{3/2}}{\beta^{1/2}} \, ,
\end{aligned} \tag{II.45}$$

where we use Estimates (II.36) and (II.37), $\kappa\beta \leq 1$, and $C_1 \geq 8\kappa \geq 8$. $\square$

Corollary II.5. *Assume Hypothesis H-1 and $g_{\alpha,\beta}^{(1)} = C_1 \alpha^{3/2} \beta^{1/2} \leq 1$. Then, for all $n \in \mathbb{N}_0$,*

$$H_{n+1} \;\geq\; E_n \;-\; g_{\alpha,\beta}^{(1)}\, \sigma_{n+1} \;+\; [1 - g_{\alpha,\beta}^{(1)}]\, \widetilde{H}_n^+ \, , \tag{II.46}$$

where $g_{\alpha,\beta}^{(1)} \geq 0$ is defined in (II.44).

Proof. The assertion follows directly from Lemma II.4:

$$\begin{aligned}
H_{n+1} \;&=\; E_n \;+\; \widetilde{H}_n^+ \;+\; W_{n+1}^n \\
&=\; E_n \;-\; \sigma_{n+1} \;+\; (\widetilde{H}_n^+ + \sigma_{n+1})^{1/2} \Big[\mathbf{1} \;+\; \widetilde{R}_n^{1/2} W_{n+1}^n \widetilde{R}_n^{1/2} \Big] (\widetilde{H}_n^+ + \sigma_{n+1})^{1/2} \\
&\geq\; E_n \;-\; \sigma_{n+1} \;+\; [1 - g_{\alpha,\beta}^{(1)}]\, (\widetilde{H}_n^+ + \sigma_{n+1}) \\
&=\; E_n \;-\; g_{\alpha,\beta}^{(1)}\, \sigma_{n+1} \;+\; [1 - g_{\alpha,\beta}^{(1)}]\, \widetilde{H}_n^+ \, .
\end{aligned} \tag{II.47}$$

$\square$

II.3 Energy Shifts and Gaps

In this subsection we estimate the differences $E_{n+1}^n = E_n - E_{n+1}$ of the groundstate energies at scales n and $n+1$, see (II.21). We inductively prove that $E_n = \inf \sigma(H_n)$ is an isolated eigenvalue of multiplicity one and derive a lower bound on the size of the gaps

$$\mathrm{gap}_n \ := \ \inf \Big[\sigma(H_n^+) \setminus \{0\} \Big] \quad \text{and} \quad \widetilde{\mathrm{gap}}_n \ := \ \inf \Big[\sigma(\widetilde{H}_n^+) \setminus \{0\} \Big] \tag{II.48}$$

of H_n^+ and $\widetilde{H}_n^+$ above their lowest spectral value 0.

We first derive a simple estimate on the difference E_{n+1}^n of the ground state energies of H_n and H_{n+1}.

Lemma II.6. *Assume Hypothesis H-1 and $g_{\alpha,\beta}^{(1)} = C_1 \alpha^{3/2} \beta^{1/2} \leq 1$. Then, for all $n \in \mathbb{N}_0$,*

$$|E_{n+1}^n| \ \leq \ g_{\alpha,\beta}^{(1)} \, \sigma_{n+1} \, , \tag{II.49}$$

where $g_{\alpha,\beta}^{(1)} \geq 0$ is defined in (II.44).

Proof. Given $\varepsilon > 0$, suppose that $\psi_n \in \mathcal{H}_n$ is an ε-approximate groundstate of H_n, i.e., $\langle \psi_n | H_n \, \psi_n \rangle \leq E_n + \varepsilon$. The variational principle yields the upper bound

$$\begin{aligned} E_{n+1} \ &\leq \ \langle \tilde{\psi}_n \mid H_{n+1} \, \tilde{\psi}_n \rangle \ = \ E_n \ + \varepsilon \ + \ \langle \tilde{\psi}_n \mid W_{n+1}^n \, \tilde{\psi}_n \rangle \\ &= \ E_n \ + \varepsilon \ + \ \|\vec{G}_{n+1}^n\|^2 \ \leq \ E_n \ + \varepsilon \ + \ \frac{1}{5} \, \alpha^3 \, \sigma_n^2 \ \leq \ E_n \ + \varepsilon \ + \ \Big(g_{\alpha,\beta}^{(1)} \Big)^2 \, , \end{aligned} \tag{II.50}$$

where we use that $C_1 \geq \kappa$, $\beta^n \leq 1$, and $\alpha^3 \leq \beta$ to derive the last inequality. In the limit $\varepsilon \to 0$, we obtain $E_{n+1} \leq E_n + (g_{\alpha,\beta}^{(1)})^2$ from (II.50). Conversely, Eq. (II.46) and $\widetilde{H}_n^+ \geq 0$ imply that

$$E_{n+1} \ \geq \ E_n \ - \ g_{\alpha,\beta}^{(1)} \, \sigma_{n+1} \, . \tag{II.51}$$

□

In the next lemma, we prove that $E_n = \inf \sigma(H_n)$ is an isolated eigenvalue of multiplicity one and derive a lower bound on the size of the spectral gap above E_n. We use a variational argument which would not apply in the degenerate case. That could not be expected, either, because the interaction with the quantized radiation field could lift the degeneracy at any energy scale, and there is, a priori, no control on the resulting splitting.

Lemma II.7. *Assume Hypothesis H-1 and $g_{\alpha,\beta}^{(1)} = C_1 \alpha^{3/2} \beta^{1/2} \leq 1/6$. Then, for all $n \in \mathbb{N}_0$, the groundstate energy $E_n = \inf \sigma(H_n)$ is a simple, isolated eigenvalue of H_n, with corresponding normalized eigenvector $\phi_n \in \mathcal{H}_n$, and*

$$\mathrm{gap}_0 \ = \ \min\{ \Delta e_{el} \ , \ \kappa \} \, , \tag{II.52}$$

$$\mathrm{gap}_{n+1} \ \geq \ [1 - 3 g_{\alpha,\beta}^{(1)}] \, \sigma_{n+1} \, , \tag{II.53}$$

$$\widetilde{\mathrm{gap}}_n \ = \ \sigma_{n+1} \, . \tag{II.54}$$

Proof. We proceed by induction in $n \in \mathbb{N}_0$. Since $H_0 = H_{el} \otimes \mathbf{1}_0 + \mathbf{1}_{el} \otimes \check{H}_0$, we have that

$$\begin{aligned} \sigma(H_0) &= \sigma(H_{el}) + \sigma(\check{H}_0) = \sigma(H_{el}) + \Big(\{0\} \cup [\kappa, \infty) \Big) \\ &\subseteq e_{el} + \Big(\{0\} \cup [\min\{\Delta e_{el}, \kappa\} \ , \ \infty) \Big) , \end{aligned} \tag{II.55}$$

which implies (II.52), as a variational argument shows that $\sigma(H_0) \ni e_{el} + \min\{\Delta e_{el}, \kappa\}$. Clearly, $E_0 = e_{el}$ is an eigenvalue of H_0 of multiplicity one, the corresponding normalized eigenvector being $\phi_0 = \varphi_{el} \otimes \Omega$.

A similar argument is used to demonstrate (II.53). Namely, due to (II.23), we have that

$$\sigma(\widetilde{H}_n^+) = \sigma(H_n^+) + \sigma(\check{H}_{n+1}^n) \subseteq \{0\} \cup [\mathrm{gap}_n, \infty) \cup [\sigma_{n+1}, \infty) , \tag{II.56}$$

which implies that $\widetilde{\mathrm{gap}}_n \geq \min\{\mathrm{gap}_n, \sigma_{n+1}\}$. Since $\sigma(\widetilde{H}_n^+) \ni \min\{\mathrm{gap}_n, \sigma_{n+1}\}$, we even conclude that

$$\widetilde{\mathrm{gap}}_n = \min\Big\{ \mathrm{gap}_n \ , \ \sigma_{n+1} \Big\} , \tag{II.57}$$

for all $n \in \mathbb{N}_0$. Since Hypothesis H-1 implies that $\mathrm{gap}_0 = \min\{\Delta e_{el}, \kappa\} \geq \kappa\beta_1 \geq \kappa\beta = \sigma_1$, we have that $\widetilde{\mathrm{gap}}_0 = \sigma_1$.

Let us now suppose that $n \geq 1$ and $\mathrm{gap}_n \geq [1 - 3g_{\alpha,\beta}^{(1)}]\sigma_n$. Since $3g_{\alpha,\beta}^{(1)} = 3C_1\alpha^{3/2}\beta^{-1/2} \leq 1/2$ and $\beta \leq \beta_1 \leq 1/2$, we have that $\mathrm{gap}_n \geq \sigma_{n+1}$, so $\widetilde{\mathrm{gap}}_n = \sigma_{n+1}$, which establishes (II.54).

To perform the induction step, we assume that E_n is a simple, isolated eigenvalue of H_n, with corresponding normalized eigenvector $\phi_n \in \mathcal{H}_n$, and that $\widetilde{\mathrm{gap}}_n = \sigma_{n+1}$. It remains to prove that E_{n+1} is an eigenvalue of H_{n+1} of multiplicity one and that the gap above E_{n+1}, denoted by gap_{n+1}, obeys (II.53). We observe that due to (II.46) and (II.49),

$$\begin{aligned} X_{n+1} &:= \sup_{\psi_0 \in \mathcal{H}_{n+1} \setminus \{0\}} \ \inf_{\phi \perp \psi_0, \, \|\phi\|=1} \Big\langle \phi \ \Big| \ H_{n+1}^+ \, \phi \Big\rangle \\ &\geq \inf_{\phi \perp \tilde{\phi}_n, \, \|\phi\|=1} \Big\langle \phi \ \Big| \ H_{n+1}^+ \, \phi \Big\rangle \\ &\geq E_{n+1}^n - g_{\alpha,\beta}^{(1)} \, \sigma_{n+1} + [1 - g_{\alpha,\beta}^{(1)}] \, \widetilde{\mathrm{gap}}_n \ \geq \ [1 - 3g_{\alpha,\beta}^{(1)}] \, \sigma_{n+1} \end{aligned} \tag{II.58}$$

holds true. Since $X_{n+1} > 0$, the min-max principle implies that E_{n+1} is an isolated point in the spectrum of H_{n+1} of multiplicity at most one. The multiplicity of E_{n+1} is at least one, however, since E_{n+1} is, by definition, in the spectrum of H_{n+1}. Thus, E_{n+1} is an eigenvalue of H_{n+1} of multiplicity one, and $\mathrm{gap}_{n+1} = X_{n+1}$. □

II.4 Ground State Projections

Lemma II.7 enables us to write the projection $P_n = |\phi_n\rangle\langle\phi_n|$ onto the ground-state ϕ_n of H_n as a contour integral

$$P_n \;=\; \frac{-1}{2\pi i}\int_{\Gamma_n} \frac{dz_n}{H_n^+ - z_n}\,, \tag{II.59}$$

where $\Gamma_n := \{\frac{1}{4}\sigma_n e^{i\vartheta} \in \mathbb{C} | \vartheta \in [0, 2\pi)\}$ and provided that $\frac{1}{4} < 1 - 3g^{(1)}_{\alpha,\beta}$, for $n \in \mathbb{N}$, and $\frac{1}{4} < \min\{\Delta e_{el}/\kappa, 1\}$, for $n = 0$, as these inequalities insure that $|z_n| < \mathrm{gap}_n$. For $\frac{1}{4} < 1 - 3g^{(1)}_{\alpha,\beta}$ and $z_{n+1} \in \Gamma_{n+1}$, we also observe that $|z_{n+1}| < \widetilde{\mathrm{gap}}_n$ and thus

$$\widetilde{P}_n \;=\; \frac{-1}{2\pi i}\int_{\Gamma_{n+1}} \frac{dz_{n+1}}{\widetilde{H}_n^+ - z_{n+1}}\,, \tag{II.60}$$

where $\widetilde{P}_n := |\tilde{\phi}_n\rangle\langle\tilde{\phi}_n| = P_n \otimes P_{\Omega^n_{n+1}}$ is the projection onto $\tilde{\phi}_n$. Note that, for $n \in \mathbb{N}_0$, we have that

$$\mathrm{gap}_{n+1} - |z_{n+1}| - |E^n_{n+1}| \;\geq\; \left(1 - 4g^{(1)}_{\alpha,\beta} - \frac{1}{4}\right)\sigma_{n+1}\,. \tag{II.61}$$

Thus, if $g^{(1)}_{\alpha,\beta} < 1/6$ then $g^{(1)}_{\alpha,\beta} < \frac{1}{4} < [1 - 4g^{(1)}_{\alpha,\beta}]$, and we have that

$$P_{n+1} \;=\; \frac{-1}{2\pi i}\int_{\Gamma_{n+1}} \frac{dz_{n+1}}{H_{n+1} - E_{n+1} - z_{n+1}} \;=\; \frac{-1}{2\pi i}\int_{\Gamma_{n+1}} \frac{dz_{n+1}}{H_{n+1} - E_n - z_{n+1}}\,, \tag{II.62}$$

for all $n \in \mathbb{N}_0$, because in both integrals in (II.62) the only spectral point of H_{n+1} encircled by the integration contours is E_{n+1}.

Lemma II.8. *Assume Hypothesis H-1 and $g^{(1)}_{\alpha,\beta} = C_1\alpha^{3/2}\beta^{1/2} \leq 1/6$. For all $n \in \mathbb{N}_0$, we have that*

$$\sup_{z\in\Gamma_{n+1}} \left\| \frac{\widetilde{H}_n^+ + \sigma_{n+1}}{\widetilde{H}_n^+ - z} \right\| \;\leq\; 4\,. \tag{II.63}$$

Proof. Eq. (II.63) follows directly from the spectral theorem and $\widetilde{\mathrm{gap}}_n = \sigma_{n+1}$, namely

$$\begin{aligned} \left\| \frac{\widetilde{H}_n^+ + \sigma_{n+1}}{\widetilde{H}_n^+ - z} \right\| \;&\leq\; \max\left\{4\,,\; \sup_{r>0}\left| \frac{r + \widetilde{\mathrm{gap}}_n + \sigma_{n+1}}{r + \widetilde{\mathrm{gap}}_n - z} \right| \right\} \\ &\leq\; \max\left\{4\,,\; \sup_{r>0}\left(\frac{r + 2\sigma_{n+1}}{r + \frac{3}{4}\sigma_{n+1}} \right) \right\} \;=\; 4\,. \end{aligned} \tag{II.64}$$

□

Lemma II.9. *Assume Hypothesis H-1 and* $g_{\alpha,\beta}^{(1)} = C_1 \alpha^{3/2} \beta^{1/2} \leq 1/8$. *Then, for all* $n \in \mathbb{N}_0$, *the series expansion*

$$\begin{aligned} P_{n+1} &= \frac{-1}{2\pi i} \sum_{\nu=0}^{\infty} \int_{\Gamma_{n+1}} (-1)^\nu \, Y_{n+1}^{(\nu)}(z_{n+1}) \, dz_{n+1} \, , && \text{(II.65)} \\ Y_{n+1}^{(\nu)}(z) &:= \frac{1}{\widetilde{H}_n^+ - z} \Big(W_{n+1}^n \, \frac{1}{\widetilde{H}_n^+ - z} \Big)^\nu , && \text{(II.66)} \end{aligned}$$

is norm-convergent, with

$$\sup_{|z|=\sigma_{n+1}} \Big\| Y_{n+1}^{(\nu)}(z) \Big\| \;\leq\; \frac{4}{\sigma_{n+1}} \Big(4 \, g_{\alpha,\beta}^{(1)} \Big)^\nu \;\leq\; \frac{(1/2)^\nu}{\sigma_{n+1}} \, , \qquad \text{(II.67)}$$

for all $\nu \in \mathbb{N}_0$.

Proof. We rewrite $Y_{n+1}^{(\nu)}(z)$ as

$$Y_{n+1}^{(\nu)}(z) \;=\; \widetilde{R}_n^{1/2} \, \frac{\widetilde{H}_n^+ + \sigma_{n+1}}{\widetilde{H}_n^+ - z} \left(\widetilde{R}_n^{1/2} \, W_{n+1}^n \, \widetilde{R}_n^{1/2} \, \frac{\widetilde{H}_n^+ + \sigma_{n+1}}{\widetilde{H}_n^+ - z} \right)^\nu \widetilde{R}_n^{1/2} \qquad \text{(II.68)}$$

and obtain the claim from Lemmata II.4 and II.8. ☐

We remark that, by (II.60), the 0^{th}-order term in the series expansion for P_{n+1} equals $\widetilde{P}_n$, so that

$$P_{n+1} - \widetilde{P}_n \;=\; \frac{-1}{2\pi i} \sum_{\nu=1}^{\infty} \int_{\Gamma_{n+1}} (-1)^\nu \, Y_{n+1}^{(\nu)}(z_{n+1}) \, dz_{n+1} \, , \qquad \text{(II.69)}$$

and hence

$$\|P_{n+1} - \widetilde{P}_n\| \;\leq\; 2 \sum_{\nu=1}^{\infty} \Big(4 \, g_{\alpha,\beta}^{(1)} \Big)^\nu \;\leq\; 4 g_{\alpha,\beta}^{(1)} \;\leq\; 4 \, C_1 \, \frac{\alpha^{3/2}}{\beta^{1/2}} \, , \qquad \text{(II.70)}$$

which is of order $\alpha^{3/2}\beta^{-1/2}$. This yields an alternative proof for the fact that if P_n has rank one, so do $\widetilde{P}_n$ and hence also P_{n+1}, provided $\alpha^{3/2}\beta^{-1/2} \geq 0$ is sufficiently small. Eq. (II.70) is not sufficient, however, to prove that the sequence $(P_n)_{n=0}^\infty$ of projections converge. Indeed, this cannot be expected, in general, because the perturbation W is marginal, in the sense of power counting. To prove convergence of $(P_n)_{n=0}^\infty$, we therefore need refined estimates that take the particularities of the model into account - mere power counting cannot achieve this goal.

II.5 Convergence of the Ground State Projections

Our proof of the convergence of $(P_n)_{n=0}^{\infty}$ is based on a virial argument that exploits Identity (II.7) and uses the boundedness of $\langle \phi_n | (x^2 \otimes \mathbf{1}) \phi_n \rangle$ uniformly in n.

Theorem II.10. *Assume Hypothesis H-1. Then $\vec{x}\phi_n \in \mathrm{dom}(H_n)$, for all $n \in \mathbb{N}$,*

$$2\, \vec{v}_n\, \phi_n \;=\; i\, H_n^+\, \vec{x}\, \phi_n \,, \tag{II.71}$$

and there exists a universal constant $C_2 < \infty$, depending only on V, such that

$$\sup_{n \in \mathbb{N}_0} \left\| \vec{x}\, \phi_n \right\|_{\mathcal{H}_n} \;\le\; C_2 \,. \tag{II.72}$$

We remark that actually a much stronger estimate holds. Namely, from a Combes-Thomas argument, or Agmon estimate, it follows that $e^{\gamma|\vec{x}|}\phi_n$ is universally bounded in norm, for some $\gamma > 0$. For our purpose, however, Theorem II.10 is sufficient. Its proof is given in Appendix A.

In the proof of convergence of the sequence $(P_n)_{n=0}^{\infty}$ of projections onto the ground state, we make use of the following lemma.

Lemma II.11. *Let $a, b \in \mathcal{H}$ be two normalized vectors in a Hilbert space $\mathcal{H}$, and denote the corresponding rank-one projections by $P_a := |a\rangle\langle a|$ and $P_b := |b\rangle\langle b|$. Then*

$$\|P_a - P_b\| \;=\; \sqrt{1 - |\langle a|b\rangle|^2} \;=\; \sqrt{\langle a\,|(P_a - P_b)\,a\rangle} \,. \tag{II.73}$$

Proof. We may assume $\{a, b\}$ to be linearly independent. $P_a - P_b$ is a rank-2 operator with matrix representation

$$M \;=\; \begin{pmatrix} 1 & \langle a|b\rangle \\ -\langle b|a\rangle & -1 \end{pmatrix} \tag{II.74}$$

in the basis $\{a, b\}$. Since M is traceless, it has eigenvalues $\pm\lambda$, for some $\lambda > 0$. Hence, (II.73) follows from $\|M\| = |\lambda| = \sqrt{-\det[M]}$. □

Theorem II.12. *Assume Hypothesis H-1 and $g^{(1)}_{\alpha,\beta} = C_1 \alpha^{3/2}\beta^{1/2} \le 1/8$. Then, for all $n \in \mathbb{N}_0$,*

$$\|\widetilde{P}_n - P_{n+1}\| \;\le\; C_3\, g^{(1)}_{\alpha,\beta}\, \beta^{n/2} \,, \tag{II.75}$$

where $C_3 = \kappa^{1/2}\,(C_2 + 1)$.

By Theorem II.12, the sequence $(\phi_n \otimes \Omega_\infty^n)_{n=0}^\infty$ converges to the ground state $\phi_{\rm gs}$.

Corollary II.13. *Assume Hypothesis H-1 and* $g_{\alpha,\beta}^{(1)} = C_1 \alpha^{3/2}\beta^{1/2} \leq 1/8$. *Then the groundstate energy* $E_{\rm gs} = \inf \sigma(H)$ *is a simple eigenvalue of* H *corresponding to a ground state eigenvector* $\phi_{\rm gs} \in \mathcal{H}$ *of* H. *Moreover,*

$$1 - |\langle \phi_{\rm gs} | \phi_n \otimes \Omega_\infty^n \rangle|^2 \;\leq\; 4\, C_3^2 \left(g_{\alpha,\beta}^{(1)} \right)^2 \beta^n \,, \tag{II.76}$$

for all $n \in \mathbb{N}$.

Proof of Theorem II.12. In view of Lemma II.11, we compute

$$\begin{aligned} & \langle \tilde\phi_n \,| (\widetilde P_n - P_{n+1})\, \tilde\phi_n \rangle \\ & = \frac{-1}{2\pi i} \int_{\Gamma_{n+1}} \left\langle \tilde\phi_n \,\middle|\, \left\{ \frac{1}{\widetilde H_n^+ - z_{n+1}} - \frac{1}{H_{n+1} - E_n - z_{n+1}} \right\} \tilde\phi_n \right\rangle dz_{n+1} \\ & = \frac{1}{2\pi i} \int_{\Gamma_{n+1}} \frac{dz_{n+1}}{z_{n+1}} \left\langle \tilde\phi_n \,\middle|\, \frac{1}{H_{n+1} - E_n - z_{n+1}}\, W_{n+1}^n\, \tilde\phi_n \right\rangle \\ & = \frac{-1}{2\pi i} \int_{\Gamma_{n+1}} \frac{dz_{n+1}}{z_{n+1}^2} \left\langle \tilde\phi_n \,\middle|\, W_{n+1}^n\, \tilde\phi_n \right\rangle + \\ & \quad \frac{1}{2\pi i} \int_{\Gamma_{n+1}} \frac{dz_{n+1}}{z_{n+1}^2} \left\langle W_{n+1}^n\, \tilde\phi_n \,\middle|\, \frac{1}{H_{n+1} - E_n - z_{n+1}}\, W_{n+1}^n\, \tilde\phi_n \right\rangle \\ & = \frac{1}{2\pi i} \int_{\Gamma_{n+1}} \frac{dz_{n+1}}{z_{n+1}^2} \left\langle W_{n+1}^n\, \tilde\phi_n \,\middle|\, \frac{1}{H_{n+1} - E_n - z_{n+1}}\, W_{n+1}^n\, \tilde\phi_n \right\rangle , \end{aligned} \tag{II.77}$$

using (II.62), the second resolvent equation, and the fact that the contour integral $\int_{\Gamma_{n+1}} z^{-2}\, dz = 0$ vanishes.

Thus, with $\widetilde Q_n := \widetilde R_n^{-1} = \widetilde H_n^+ + \sigma_{n+1}$, we have

$$\begin{aligned} & |\langle \tilde\phi_n \,| (\widetilde P_n - P_{n+1})\, \tilde\phi_n \rangle| \\ & \leq \sigma_{n+1}^{-1} \left\| \widetilde R_n^{1/2}\, W_{n+1}^n\, \tilde\phi_n \right\|^2 \sup_{z_{n+1} \in \Gamma_{n+1}} \left\| \widetilde Q_n^{1/2} \left(H_{n+1} - E_n - z_{n+1} \right)^{-1} \widetilde Q_n^{1/2} \right\| , \end{aligned} \tag{II.78}$$

and using a Neumann series expansion,

$$\begin{aligned} & \widetilde Q_n^{1/2} \left(H_{n+1} - E_n - z_{n+1} \right)^{-1} \widetilde Q_n^{1/2} \\ & = \sum_{k=0}^\infty \left(\frac{\widetilde H_n^+ + \sigma_{n+1}}{\widetilde H_n^+ - z_{n+1}} \right) \left[\widetilde R_n^{1/2}\, W_{n+1}^n\, \widetilde R_n^{1/2} \left(\frac{\widetilde H_n^+ + \sigma_{n+1}}{\widetilde H_n^+ - z_{n+1}} \right) \right]^k , \end{aligned} \tag{II.79}$$

in connection with Lemmata II.4 and II.8, we obtain the norm bound

$$\left\| \widetilde Q_n^{1/2} \left(H_{n+1} - E_n - z_{n+1} \right)^{-1} \widetilde Q_n^{1/2} \right\| \;\leq\; 4 \sum_{k=0}^\infty \left(4\, g_{\alpha,\beta}^{(1)} \right)^k \;\leq\; 4 \sum_{k=0}^\infty \left(\frac{2}{3} \right)^k \;=\; 12 \,. \tag{II.80}$$

Combining Lemma II.11, Eq. (II.77), and Eq. (II.80), we obtain the bound

$$\|\widetilde{P}_n - P_{n+1}\| \;\le\; \frac{\sqrt{12}}{\sigma_{n+1}^{1/2}} \left\| \widetilde{R}_n^{1/2} \, W_{n+1}^n \, \tilde{\phi}_n \right\| . \tag{II.81}$$

Appealing to (II.28), we write $\widetilde{R}_n^{1/2} \, W_{n+1}^n \tilde{\phi}_n = \psi^{(1)} + \psi^{(2)} + 2\psi^{(3)} + 2\psi^{(4)}$, with

$$\begin{aligned}
\psi^{(1)} &:= \sigma_{n+1}^{-1/2} \left\| \vec{G}_{n+1}^n \right\|^2 \tilde{\phi}_n \,, && \text{(II.82)}\\
\psi^{(2)} &:= \widetilde{R}_n^{1/2} \, a^*(\vec{G}_{n+1}^n) \cdot a^*(\vec{G}_{n+1}^n) \, \tilde{\phi}_n \,, && \text{(II.83)}\\
\psi^{(3)} &:= \widetilde{R}_n^{1/2} \, a^*(\Delta \vec{G}_{n+1}^n) \cdot \vec{v}_n \, \tilde{\phi}_n && \text{(II.84)}\\
&= \widetilde{R}_n^{1/2} \, \vec{v}_n \cdot a^*(\Delta \vec{G}_{n+1}^n) \, \tilde{\phi}_n \,, && \text{(II.85)}\\
\psi^{(4)} &:= \widetilde{R}_n^{1/2} \, a^*(\vec{G}_{\vec{0},n+1}^n) \cdot \vec{v}_n \, \tilde{\phi}_n \,, && \text{(II.86)}
\end{aligned}$$

where $\Delta \vec{G}_{n+1}^n := \vec{G}_{n+1}^n - \vec{G}_{\vec{0},n+1}^n$ and

$$\vec{G}_{\vec{0},n+1}^n(k) \;:=\; \vec{G}_{n+1}^n(k) \Big|_{\vec{x}=\vec{0}} \;=\; -\alpha^{3/2} \sqrt{\frac{2}{\pi}} \, \frac{\mathbf{1}(|k| < \kappa)}{\omega(k)^{1/2}} \, \vec{\varepsilon}(k) \,. \tag{II.87}$$

Eq. (II.85) derives from the transversality of the photon polarization.

The contributions $\psi^{(1)}$ and $\psi^{(2)}$ can easily be estimated by

$$\begin{aligned}
\|\psi^{(1)}\| &\le \sigma_{n+1}^{-1/2} \left\| \vec{G}_{n+1}^n \right\|^2 \le \frac{1}{5} \, \alpha^3 \, \sigma_n^2 \, \sigma_{n+1}^{-1/2} \,, && \text{(II.88)}\\
\|\psi^{(2)}\| &= \sigma_{n+1}^{-1/2} \left\| a^*(\vec{G}_{n+1}^n) \cdot a^*(\vec{G}_{n+1}^n) \, \Omega_{n+1}^n \right\| \le 2 \, \sigma_{n+1}^{-1/2} \left\| \vec{G}_{n+1}^n \right\|^2 \\
&\le \frac{2}{5} \, \alpha^3 \, \sigma_n^2 \, \sigma_{n+1}^{-1/2} \,. && \text{(II.89)}
\end{aligned}$$

To estimate $\psi^{(3)}$, we recall from (II.12) the definition of $\mathcal{K}_{n+1}^n := \{k \in \mathbb{R}^3 \times \mathbb{Z}_2 | \sigma_{n+1} \le \omega(k) < \sigma_n\}$. We observe that, for $k \in \mathcal{K}_{n+1}^n$ and any $\psi \in \mathcal{H}_n$,

$$\begin{aligned}
&\widetilde{R}_n^{1/2} \, \psi \otimes a^*(k) \Omega_{n+1}^n \\
&= \Big[H_n^+ \otimes \mathbf{1} + \mathbf{1} \otimes (\check{H}_{n+1}^n + \sigma_{n+1}) \Big]^{-1/2} \psi \otimes a^*(k) \Omega_{n+1}^n \\
&= \Big(H_n^+ + \omega(k) + \sigma_{n+1} \Big)^{-1/2} \psi \otimes a^*(k) \, \Omega_{n+1}^n \,. && \text{(II.90)}
\end{aligned}$$

Writing $\psi^{(3)}$ as an $\mathcal{F}_{n+1}$-valued function of the electron coordinate and using

(II.90), we hence have

$$\begin{aligned}\left\|\psi^{(3)}(x)\right\|^2_{\mathcal{F}_{n+1}} &= \left\| \int dk\ \widetilde{R}_n^{1/2}\,[\vec{v}_n \cdot \Delta\vec{G}^n_{n+1}(k)\,\phi_n](x) \otimes a^*(k)\Omega^n_{n+1} \right\|^2_{\mathcal{F}_{n+1}} \\ &= \int dk \left\| \Big[\Big(H_n^+ + \omega(k) + \sigma_{n+1}\Big)^{-1/2} \vec{v}_n \cdot \Delta\vec{G}^n_{n+1}(k)\,\phi_n\Big](x)\right\|^2_{\mathcal{F}_n} \\ &\leq C_1 \int \frac{dk}{\omega(k)} \left\| \Big[\Delta\vec{G}^n_{n+1}(k)\,\phi_n\Big](x)\right\|^2_{\mathcal{F}_n}, \end{aligned} \tag{II.91}$$

where the last inequality follows from (II.42). Next, we use that, as a function of the two variables $\vec{x} \in \mathbb{R}^3$ and $k \in \mathbb{R}^3 \times \mathbb{Z}_2$,

$$\left|\Delta\vec{G}^n_{n+1}(k)\right| = \sqrt{\frac{2\,\alpha^3}{\pi\,\omega(k)}}\left|1 - e^{-i\vec{k}\cdot\vec{x}}\right| \leq \sqrt{\frac{2\,\alpha^3\,\omega(k)}{\pi}}\,|\vec{x}| = \omega(k)\left|\vec{G}^n_{n+1}(k)\right|\,|\vec{x}|. \tag{II.92}$$

Therefore,

$$\left\|\psi^{(3)}\right\|_{\mathcal{H}_{n+1}} \leq C_1^{1/2}\left\|\omega^{1/2}\vec{G}^n_{n+1}\right\|\,\left\|\vec{x}\,\phi_n\right\| \leq \frac{1}{2}\,C_1^{1/2}\,C_2\,\alpha^{3/2}\,\sigma_n^{3/2}, \tag{II.93}$$

where C_2 is the universal constant in (II.72).

It remains to estimate $\psi^{(4)}$, our key estimate. We use that $\vec{G}^n_{\vec{0},n+1}(k)$, as an operator on $\mathcal{H}_{el}$, is a multiple of the identity, for each $k \in \mathcal{K}^n_{n+1}$. Thus, by (II.90), we have

$$\psi^{(4)} = \int dk\ \vec{G}^n_{\vec{0},n+1}(k)\cdot\Big(H_n^+ + \omega(k) + \sigma_{n+1}\Big)^{-1/2}\vec{v}_n\,\phi_n \otimes a^*(k)\,\Omega^n_{n+1} \tag{II.94}$$

and then

$$\begin{aligned}\left\|\psi^{(4)}\right\|^2_{\mathcal{H}_{n+1}} &\leq \int dk\left\|\vec{G}^n_{n+1}(k)\right\|^2\left\|\Big(H_n^+ + \omega(k) + \sigma_{n+1}\Big)^{-1/2}\vec{v}_n\,\phi_n\right\|^2_{\mathcal{H}_n} \\ &\leq \int dk\left\|\vec{G}^n_{n+1}(k)\right\|^2\left\|\vec{v}_n\,\phi_n\right\|\left\|\Big(H_n^+ + \omega(k) + \sigma_{n+1}\Big)^{-1}\vec{v}_n\,\phi_n\right\|, \end{aligned} \tag{II.95}$$

where the last estimate follows from Schwarz' inequality. We observe that, by (II.71),

$$\left\|\Big(H_n^+ + \omega(k) + \sigma_{n+1}\Big)^{-1}\vec{v}_n\,\phi_n\right\| \leq \left\|\frac{H_n^+}{H_n^+ + \omega(k) + \sigma_{n+1}}\right\|\left\|\vec{x}\,\phi_n\right\| \leq C_2, \tag{II.96}$$

with C_2 being the universal constant in (II.72). Inserting Estimate (II.96) and using that $\|\vec{v}_n\,\phi_n\| \leq \sigma_{n+1}^{1/2}\|\vec{v}_n\,\widetilde{R}_n^{1/2}\| \leq \sqrt{C_1}$, we arrive at

$$\left\|\psi^{(4)}\right\| \leq C_1^{1/4}\,C_2^{1/2}\left\|\vec{G}^n_{n+1}(k)\right\| \leq \frac{1}{2}\,C_1^{1/4}\,C_2^{1/2}\,\alpha^{3/2}\,\sigma_n\,. \tag{II.97}$$

Adding up the estimates (II.88), (II.89), (II.93), and (II.97), we obtain

$$\begin{aligned}
\|\widetilde{P}_n - P_{n+1}\| \;&\le\; \frac{\sqrt{12}}{\sigma_{n+1}^{1/2}}\Big[\frac{3}{5}\,\frac{\alpha^3\,\sigma_n^2}{\sigma_{n+1}^{1/2}} + \frac{C_1^{1/2}C_2}{2}\,\alpha^{3/2}\,\sigma_n^{3/2} + \frac{C_1^{1/4}C_2^{1/2}}{2}\,\alpha^{3/2}\,\sigma_n\Big] \\
&\le\; \frac{3\sqrt{12}}{5}\Big[\frac{\alpha^3\,\sigma_n}{\beta} + \frac{C_1^{1/2}\,C_2\,\alpha^{3/2}\,\sigma_n}{\beta^{1/2}} + \frac{C_1^{1/4}\,C_2^{1/2}\,\alpha^{3/2}\,\sigma_n^{1/2}}{\beta^{1/2}}\Big] \\
&\le\; \frac{3\sqrt{12}}{5}\,\frac{\alpha^{3/2}\,\sigma_n^{1/2}}{\beta^{1/2}}\Big(1 + C_1^{1/4}C_2^{1/2} + C_1^{1/2}C_2\Big) \\
&\le\; 3\,(C_2+1)\,\frac{C_1\,\alpha^{3/2}}{\beta^{1/2}}\,\beta^{n/2}\,, \qquad \text{(II.98)}
\end{aligned}$$

where we make use of $C_1 \ge 8\kappa \ge 8$ to derive the last inequality. This yields (II.75). $\square$

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A Proofs of Lemma II.3 and Theorem II.10

Proof of Lemma II.3. We first note that (II.43) follows from (II.42) with $\rho := \sigma_{n+1}$. To prove (II.42), we observe that Lemma II.2 implies the quadratic form estimate

$$\Big(a^*(\vec{G}_n) + a(\vec{G}_n)\Big)^2 \;\le\; 4\Big\|(\kappa^{-1}+\omega^{-1})^{1/2}\vec{G}_n\Big\|^2\,(\check{H}_n+\kappa) \;\le\; 8\kappa\,\alpha^3\,(\check{H}_n+\kappa)\,. \qquad \text{(A.1)}$$

This implies that

$$-\Delta \;\le\; 2\,(\vec{v}_n)^2 + 2\Big(a^*(\vec{G}_n)+a(\vec{G}_n)\Big)^2 \;\le\; 2\,(\vec{v}_n)^2 \,+\, 16\kappa\,\alpha^3\,(\check{H}_n+\kappa)\,. \qquad \text{(A.2)}$$

Since V is a small perturbation relative to $-\Delta$, we have that

$$V \;\le\; 2\varepsilon(\vec{v}_n)^2 \,+\, 16\kappa\varepsilon\alpha^3\,(\check{H}_n+\kappa) \,+\, b_\varepsilon\,, \qquad \text{(A.3)}$$

for any $\varepsilon > 0$. As a consequence, we have, for any $\varepsilon, \mu > 0$,

$$(\vec{v}_n)^2 \;\le\; (1+2\varepsilon\mu)(\vec{v}_n)^2 \,-\, \mu V \,+\, 16\kappa\varepsilon\mu\alpha^3\,(\check{H}_n+\kappa) \,+\, \mu b_\varepsilon\,. \qquad \text{(A.4)}$$

We choose $\varepsilon := 1/8$, $\mu := 2$ and observe that then $16\kappa\varepsilon\mu\alpha^3 = 4\kappa\alpha^3 \le 4$, since $\alpha \le \kappa^{-1/3}$, which yields

$$\begin{aligned}
(\vec{v}_n)^2 \;&\le\; 4\Big[(\vec{v}_n)^2 - V + \check{H}_n + \kappa + b_{1/8}\Big] \;\le\; 4[H_n + \kappa + b_{1/8}] \\
&\le\; \frac{C_1'}{\rho}(H_n - E_n + \rho)\,, \qquad \text{(A.5)}
\end{aligned}$$

where the constant C_1' is given by

$$C_1' \;:=\; 4\,\rho\,\sup_{r\geq 0}\Big\{\frac{r+E_n+\kappa+b_{1/8}}{r+\rho}\Big\} \;=\; 4\,\max\Big\{E_n+\kappa+b_{1/8}\;,\;\rho\Big\}\,. \quad \text{(A.6)}$$

Since the groundstate energy e_{el} of H_{el} is strictly negative, $e_{el} < 0$, the variational principle with trial vector $\varphi_{el}\otimes\Omega_n$, where $\varphi_{el}\in\mathcal{H}_{el}$ is the atomic groundstate, $H_{el}\varphi_{el} = e_{el}\varphi_{el}$, yields

$$E_n \;\leq\; \langle\varphi_{el}\otimes\Omega_n \,|\, H_n\,(\varphi_{el}\otimes\Omega_n)\rangle \;=\; e_{el}+\|\vec{G}_n\|^2 \;\leq\; e_{el}+\frac{1}{5}\kappa^2\alpha^3 \;\leq\; \kappa. \quad \text{(A.7)}$$

Moreover, $\rho\leq\sigma_n\leq\kappa$, and thus $C_1'\leq C_1 = 8(\kappa+b_{1/8})$. □

Proof of Theorem II.10. Fix $n\in\mathbb{N}_0$. We first observe that, for any $f\in C_0^\infty(\mathbb{R}^3;\mathbb{R})$, the vector $f(\vec{x})\phi_n$ lies in the domain of H_n, and we have

$$H_n^+\,f(\vec{x})\,\phi_n \;=\; [H_n\,,\,f(\vec{x})]\,\phi_n \;=\; \Big(-\Delta f(\vec{x}) - 2i\vec{\nabla}f(\vec{x})\cdot\vec{v}_n\Big)\,\phi_n\,. \quad \text{(A.8)}$$

By Lemma II.3, $\|\vec{v}_n\,\phi_n\|$ is bounded by C_1, uniformly in $n\in\mathbb{N}$. Thus,

$$\Big\|H_n^+\,f(\vec{x})\,\phi_n\Big\| \;\leq\; \Big(\|\Delta f\|_\infty + \|\vec{\nabla}f\|_\infty\Big)\,(2C_1+1)\,. \quad \text{(A.9)}$$

We choose a smooth characteristic function $\chi\in C_0^\infty(\mathbb{R}^3;[0,1])$ of the unit ball in $\mathbb{R}^3$, i.e., $\chi(\vec{x})=1$, for $|\vec{x}|\leq 1$, and $\chi(\vec{x})=0$, for $|\vec{x}|\geq 2$, and define

$$\vec{F}_{r,R}(\vec{x}) \;:=\; \vec{x}\,\Big[1-\chi\Big(\frac{\vec{x}}{r}\Big)\Big]\,\chi\Big(\frac{\vec{x}}{R}\Big)\,, \quad \text{(A.10)}$$

where $r\geq 1$ is chosen sufficiently large such that $\sup_{|\vec{x}|\geq r/2}|V(\vec{x})|\leq -e_{el}/3$, and $R>r$. One easily checks that

$$\sup_{R>r>1}\sum_{j=1}^{3}\Big\{\|\Delta F_{r,R;j}\|_\infty + \|\vec{\nabla}F_{r,R;j}\|_\infty\Big\} \;\leq\; C_2'\,, \quad \text{(A.11)}$$

where $C_2'<\infty$ depends only on χ and its derivatives up to second order, and $\vec{F}_{r,R} =: (F_{r,R;1}, F_{r,R;2}, F_{r,R;3})$. Note that $\vec{F}_{r,R}\neq 0$ implies $|\vec{x}|\geq r/2$. Hence

$$\begin{aligned}\Big\langle\vec{F}_{r,R}\phi_n\Big|\,H_n^+\,\vec{F}_{r,R}\phi_n\Big\rangle \;&\geq\; \Big\langle\vec{F}_{r,R}\phi_n\Big|\,[V(\vec{x})-e_{el}-2\|\vec{G}_n\|^2]\,\vec{F}_{r,R}\phi_n\Big\rangle \\ &\geq\; \frac{|e_{el}|}{3}\Big\|\vec{F}_{r,R}\phi_n\Big\|^2\,, \end{aligned} \quad \text{(A.12)}$$

where $\vec{F}_{r,R}\phi_n := \vec{F}_{r,R}(\vec{x})\phi_n$, using that $\|\vec{G}_n\|^2 \leq |e_{el}|/6$. The Cauchy-Schwarz inequality, (A.9), and (A.11) thus yield

$$\|\vec{F}_{r,R}\phi_n\| \;\leq\; \frac{3}{|e_{el}|}\,\|(H_n - E_n)\,\vec{F}_{r,R}\phi_n\| \;\leq\; \frac{3\,(2C_1+1)\,C_2'}{|e_{el}|}\,. \tag{A.13}$$

We have $\vec{x}\phi_n(\vec{x}) = \vec{x}\chi(\vec{x}/r)\phi_n(\vec{x}) + \lim_{R\to\infty}\vec{F}_{r,R}(\vec{x})\phi_n(\vec{x})$, for a. e. $\vec{x} \in \mathbb{R}^3$, by Lebesgue's monotone convergence theorem, and we obtain the bound

$$\|\vec{x}\,\phi_n\| \;\leq\; \|\chi(\vec{x}/r)\,\vec{x}\,\phi_n\| + \|[1-\chi(\vec{x}/r)]\,\vec{x}\,\phi_n\| \;\leq\; 2\,r + 3\,(2C_1+1)\,C_2'\,|e_{el}|^{-1}\,. \tag{A.14}$$

Moreover, the closedness of H_n in combination with the limit $R \to \infty$ implies that $\vec{x}\,\phi_n$ belongs to its domain. □

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