Mathematical Theory of Non-Relativistic Matter and Radiation

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Abstract

We consider a system of finitely many non-relativistic electrons bound in an atom or molecule which are coupled to the electromagnetic field via minimal coupling or the dipole approximation. Among a variety of results, we give sufficient conditions for the existence of a ground state (an eigenvalue at the bottom of the spectrum) and resonances (eigenvalues of a complex dilated Hamiltonian) of such a system. We give a brief outline of the proofs of these statements which will appear in full length in [3].

Dedicated to the memory of J. Schwinger, whose understanding of Quantum Electrodynamics was profound.

1 Introduction

In this note we describe some recent mathematical results concerning physical phenomena that stood at the origin of quantum theory: those of emission and absorption of electromagnetic radiation by systems of non-relativistic, quantum-mechanical matter, such as atoms and molecules.

The key point of our analysis is not that it changes the conventional picture of atoms and molecules interacting with the quantized radiation field provided by low-order quantum-mechanical perturbation theory, but that it supplies *non-perturbative* results supporting this picture and adding mathematical precision to it. In particular, our results concerning the structure of resonances in the fully interacting theory corresponding to excited energy levels of an atom or molecule decoupled from the radiation field are not entirely part of the conventional wisdom in this field and complement the perturbative analysis, due to Bethe [5], of the Lamb shift in a rather significant way.

The starting point of our analysis is the following standard model of non-relativistic, quantum mechanical matter and radiation. The system consists of a finite number of nuclei, in the following treated as static, and of electrons treated as non-relativistic, quantum-mechanical point particles coupled to the quantized radiation field. The Hilbert space of the system is given by

$$\mathcal{H} \;=\; \mathcal{H}_{el} \;\otimes\; \mathcal{H}_f, \tag{1}$$

where

$$\mathcal{H}_{el} \;:=\; \left(L^2\left(\mathbb{R}^3, d^3x\right) \;\otimes\; \mathbb{C}^2\right)^{\otimes_a N}, \tag{2}$$

and

$$\mathcal{H}_f \;\equiv\; \mathcal{F} \;:=\; \bigoplus_{n=0}^{\infty} \left(L^2\left(\mathbb{R}^3, d^3k\right) \;\otimes\; \mathbb{C}^2\right)^{\otimes_s n}. \tag{3}$$

In these formulae, N denotes the total number of electrons (which is conserved), the factor $\mathbb{C}^2$ on the r.s. of (2) accounts for the spin of electrons, and $\otimes_a$ denotes an anti-symmetric tensor product, in accordance with the Pauli principle. The space $\mathcal{H}_f = \mathcal{F}$ is the Fock space of photons ("f" stands for "(electromagnetic) field"). The factor $\mathbb{C}^2$ on the r.s. of (3) accounts for the two possible polarizations of photons, and $\otimes_s$ denotes a symmetric tensor product appropriate for Bose-Einstein statistics.

The transverse modes of the quantized electromagnetic field are described in terms of the vector potential, $\vec{A}$, in the Coulomb gauge: At time $t = 0$, $\vec{A}$ is given by

$$\vec{A}(\vec{x}) := \sum_{\lambda=1,2} \frac{1}{\pi} \int \frac{d^3k}{\sqrt{2\omega(\vec{k})}} \left[\vec{\varepsilon}_\lambda(\vec{k})\, e^{-i\,\vec{k}\cdot\vec{x}}\, a^\dagger_\lambda(\vec{k}) \;+\; \vec{\varepsilon}_\lambda(\vec{k})^*\, e^{i\,\vec{k}\cdot\vec{x}}\, a_\lambda(\vec{k})\right], \tag{4}$$

where $\omega(\vec{k}) = |\vec{k}|$ is the energy of a photon of momentum $\vec{k}$; $\vec{\varepsilon}_\lambda(\vec{k})$, $\lambda = 1, 2$, are polarization vectors satisfying

$$\vec{\varepsilon}_\lambda(\vec{k})^* \cdot \vec{\varepsilon}_\mu(\vec{k}) = \delta_{\lambda\mu}, \quad \vec{k} \cdot \varepsilon_\lambda(\vec{k}) = 0, \quad \lambda, \mu \;=\; 1, 2;$$

and $a^\dagger_\lambda(\vec{k})$, $a_\lambda(\vec{k})$ are the usual creation- and annihilation operators on $\mathcal{F}$ obeying the canonical commutation relations

$$[a^\#_\lambda(\vec{k}_1),\ a^\#_\mu(\vec{k}_2)] = 0, \quad [a_\lambda(\vec{k}_1),\ a^\dagger_\mu(\vec{k}_2)] \;=\; \delta_{\lambda\mu}\, \delta(\vec{k}_1 - \vec{k}_2), \tag{5}$$

where $a^\# = a$ or $a^\dagger$. The vector potential $\vec{A}$ and the creation- and annihilation operators are unbounded operator-valued distributions on $\mathcal{F}$.

The free time-evolution of the radiation field is generated by the Hamiltonian

$$H_f \;:=\; \sum_{\lambda=1,2} \int d^3k\; \omega(k)\; a^\dagger_\lambda(\vec{k})\; a_\lambda(\vec{k}). \tag{6}$$

Setting

$$\vec{A}(\vec{x}, t) \;=\; e^{i\,t\,H_f}\; \vec{A}(\vec{x})\; e^{-i\,t\,H_f},$$

the *free* electric and magnetic fields are given by

$$\vec{E}(\vec{x}, t) \;=\; \frac{\partial}{\partial t}\, \vec{A}(\vec{x}, t), \quad \vec{B}(\vec{x}, t) \;=\; \vec{\nabla} \wedge \vec{A}(\vec{x}, t).$$

Here we temporarily use units such that $\hbar = c = 1$. Although customary, this choice of units is not natural in the present context and we will change it below.

The Hamiltonian generating the time evolution of the total system composed of the photon field and N electrons moving in the additional electrostatic potential generated by M fixed nuclei of charges $Z_l e$ at positions $\vec{R}_l$, $l = 1, \ldots, M$ is given by

$$H' \;=\; H'_{el} \;+\; \mathbf{1} \otimes H_f, \tag{7}$$

with

$$\begin{aligned} H'_{el} \;&=\; \sum_{j=1}^{N} \frac{1}{2m} \left[\vec{\sigma}_j \cdot \;(-i\, \vec{\nabla}_j - e\vec{A}_\kappa(\vec{x}_j))\right]^2 \\ &+\; \left\{ \sum_{j=1}^{N} \sum_{l=1}^{M} \frac{-Z_l \alpha}{|\,\vec{x}_j - \vec{R}_l\,|} + \sum_{1 \le i < j \le N} \frac{\alpha}{|\,\vec{x}_i - \vec{x}_j\,|} \right\} \;\otimes\; \mathbf{1}, \end{aligned} \tag{8}$$

where $2\pi m^{-1}$ is the Compton wave length of an electron, σ_j^x, σ_j^y and σ_j^z are the three Pauli matrices acting on spin space of the j^{th} electron, $\alpha = \frac{e^2}{4\pi} \approx (137)^{-1}$ is the fein-structure constant, $\vec{A}_\kappa(\vec{x}) = \int d^3y\, \check{\kappa}(\vec{x}-\vec{y})\vec{A}(\vec{y})$ is the regularized vector potential, where $\check{\kappa}$ is the Fourier transform of a smooth function, κ, with support contained in the ball $\{\vec{k} \; : \; |\; \vec{k}\; | \leq m^{-1}\}$, $\sum_{l=1}^M Z_l \alpha |\vec{x} - \vec{R}_l|^{-1}$ is the electrostatic potential corresponding to the charge distribution of the nuclei, and $\frac{\alpha}{|\vec{x}_i - \vec{x}_j|}$ is the repulsive Coulomb potential between the i^{th} and the j^{th} electron. We impose the UV-cutoff κ to make focussing on the infrared regime $\vec{k} \approx 0$ as easy as possible. By completing a square, one sees that H' is bounded from below by some constant $-C \cdot N$, where C depends on N, Z_j, $\vec{R}_j$, α, and m, and that H' has a unique self-adjoint extension on a domain $\mathcal{D}$ dense in $\mathcal{H}$. The question of stability, i.e., whether C can be chosen independent of N has recently been discussed in [9], while aspects of semiboundedness and stability for the corresponding model with unregularized, but classical electromagnetic field are discussed in [11, 21, 22].

To exhibit the perturbative character of the present spectral problem we change our units. To this end, we dilate the electron coordinates and photon momenta independently, $(\vec{x}_j, \vec{k}) \mapsto (\eta \vec{x}_j, \mu \vec{k})$, employing a suitable unitary, U_1, on $\mathcal{H}$. It is easily checked that

$$\begin{aligned} \mu H \;&:=\; U_1 H' U_1^\dagger = \sum_{j=1}^N \frac{1}{2m\eta^2} \left[\vec{\sigma}_j \cdot \left(-i\, \vec{\nabla}_j - \eta\mu e \vec{A}_\kappa(\eta\mu\vec{x}_j) \right) \right]^2 \\ &+\; \frac{\alpha}{\eta} \Big\{ \sum_{j=1}^N \sum_{l=1}^M \frac{-Z_l}{|\; \vec{x}_j - \eta^{-1}\vec{R}_l \;|} + \sum_{1 \leq i < j \leq N} \frac{1}{|\; \vec{x}_i - \vec{x}_j \;|} \Big\} \otimes \mathbf{1} \;+\; \mu \mathbf{1} \otimes H_f \,. \end{aligned} \tag{9}$$

Upon making the choice $\frac{1}{2m\eta^2} = \frac{\alpha}{\eta} = \mu$, we obtain $\eta = \frac{1}{2m\alpha}$, $\mu = 2m\alpha^2$, $\eta\mu = \alpha$ and $\mu\eta e = \alpha e = 2\pi^{1/2}\alpha^{3/2}$. This yields

$$\begin{aligned} H \;&=\; \sum_{j=1}^N [\vec{\sigma}_j \cdot \; (-i\, \vec{\nabla}_j - 2\pi^{1/2}\alpha^{3/2}\vec{A}_\kappa(\alpha\vec{x}_j))]^2 \\ &+\; \Big\{ \sum_{j=1}^N \sum_{l=1}^M \frac{-Z_l}{|\; \vec{x}_j - \eta^{-1}\vec{R}_l \;|} + \sum_{1 \leq i < j \leq N} \frac{1}{|\; \vec{x}_i - \vec{x}_j \;|} \Big\} \otimes \mathbf{1} \;+\; \mathbf{1} \otimes H_f \,. \end{aligned} \tag{10}$$

Our concern, in this note, is to describe properties of the spectrum of H, for small values of α, that yield information on the processes of absorption and emission of photons by the electrons. Interpreting η in (10) as a parameter independent of α and setting $\alpha = 0$, the Hamiltonian H reduces to

$$H_{\alpha=0} \;=\; H_{el}^0 \otimes \mathbf{1} \;+\; \mathbf{1} \otimes H_f,$$

where

$$H^0_{el} \;=\; \sum_{j=1}^{N} \Big\{ - \triangle_j + \sum_{l=1}^{M} \frac{-Z_l}{\mid \vec{x}_j - \eta^{-1}\vec{R}_l \mid} \Big\} \;+\; \sum_{1\le i<j\le N} \frac{1}{\mid \vec{x}_i - \vec{x}_j \mid} \tag{11}$$

is the usual Hamiltonian of non-relativistic Schrödinger quantum mechanics. We shall choose the configuration of nuclei and the number of electrons such that the total system has bound states; more precisely that the spectrum, $\sigma(H^0_{el})$, of H^0_{el} has the following structure:

$$\sigma(H^0_{el}) \;=\; \sigma_{pp}(H^0_{el}) \;\cup\; \sigma_{ac}(H^0_{el}), \tag{12}$$

where

$$\begin{aligned} \sigma_{pp}(H^0_{el}) \;&=\; \{E_j\}_{j=0}^{\infty}\,, \quad \text{with} \\ E_0 \;<\; E_1 \;<\; E_2 \;&<\; \cdots \;<\; \Sigma \;\le\; 0, \end{aligned} \tag{13}$$

and

$$\sigma_{ac}(H^0_{el}) \;=\; [\Sigma, \infty).$$

Note that our new choice of units guarantees for H^0_{el} the typical eigenvalue spacing for $E_{j+1} - E_j$, as well as the ionization energy $\Sigma - E_0$ to be of order $min_l Z_l^2 \ge 1$ uniformly in $\eta > 0$.

We are interested in understanding the fate of the eigenvalues $E_j, j = 0, 1, 2, \cdots$, of H^0_{el} when α is increased from 0 to 1/137. We expect the following picture to emerge: Let $0 < \alpha$ be sufficiently small. Then

(a) The Hamiltonian $H = H(\alpha)$, defined in eqs. (10), (4), and (6), has a *ground state* corresponding to an eigenvalue $E_0(\alpha)$, with $E_0(\alpha) \to E_0$, as $\alpha \to 0$.

(b) $E_0(\alpha)$ is the *only* eigenvalue of H, i.e., all excited states of H^0_{el} become *unstable*. The spectrum of H above $E_0(\alpha)$ is purely absolutely continuous.

(c) There are complex numbers $\{E_{j,l}(\alpha)\}_{j\ge1}$, $l = 1, 2, \cdots, l_j$, where l_j is the multiplicity of E_j, such that $E_{j,l}(\alpha) \to E_j$, as $\alpha \to 0$, for $l = 1, 2, \cdots, l_j$; to second order in $\alpha^{3/2}$, *Re* $E_{j,l}(\alpha)$ is given by a Bethe-type formula [5], and *Im* $E_{j,l}(\alpha)$ is given by Fermi's golden rule [6]. Physically, the numbers $E_{j,l}(\alpha)$ are the complex energies of resoncances.

There is a domain $\mathcal{D}$ of compactly supported functions which is dense in the Hilbert space $\mathcal{H}$ (defined in eqs. (1)–(3)) such that, for ψ_1 and ψ_2 in $\mathcal{D}$, $\langle\psi_1, (z - H)^{-1}\psi_2\rangle$

has an analytic continuation in the variable z from the upper to the complement of the shaded regions in the lower half-plane depicted in Fig. 1, below.

Fig. 1

The angle of inclination of the shaded regions emanating from $E_{j,l}(\alpha)$, $l = 1, \cdots, l_j$, $j = 1, 2, \cdots$ is related to the choice of projection of the Riemann surface on which $\langle \psi_1, (z-H)^{-1}\psi_2 \rangle$ is defined onto the complex energy plane. (Of course, one does not expect to be able to control the analytic properties of $\langle \psi_1, (z-H)^{-1}\psi_2 \rangle$, for a small, but fixed value of α, in a small neighbourhood of the threshold $\sum$; in fact, $\sum$ is usually an accumulation point of eigenvalues of H^0_{el}.)

The picture described in **(c)**, in particular the analytic structure of the functions $r(z) := \langle \psi_1, (z-H)^{-1}\psi_2 \rangle$, is not, to our knowledge, part of the conventional lore about radiation theory, although some of its consequences are: The properties of $r(z)$ described in **(c)** are important to derive bounds on the life-time of resonances corresponding to excited states of H^0_{el} [16] and to partially justify the Bohr-Einstein frequency condition.

In the course of the past several years, we have proven mathematical results that corroborate the picture described in **(a)**–**(c)**, above, to a large extent. Precise statements of our results and proofs will appear in [3]. For earlier results on related, but simpler systems see [2, 10, 14, 19, 24, 30].

2 Description of a simplified model

In order to formulate precise results and convey some key ideas about our methods, it is useful to consider a simplified model that, however, retains the basic difficulties encountered in the analysis of the Hamiltonian H introduced in eqs. (10),(4),(6). The choice of a simplified model is primarily motivated by the desire to describe our ideas and results in a transparent context, but most of our results apply to the physical model described in the introduction [3].

First, assuming that the charge distribution of the nuclei is concentrated around the origin in $\mathbb{R}^3$, we unitarily transform the Hamiltonian H in (10) by $U_2 := \exp[-i\tau \vec{A}_\kappa(\vec{0}) \cdot (\sum_{j=1}^N \vec{x}_j)]$ which leaves all terms in H unchanged except for

$$U_2(-i\,\vec{\nabla}_j)U_2^* = -i\,\vec{\nabla}_j + \tau \vec{A}_\kappa(\vec{0})$$

and

$$U_2\, a_\lambda^\dagger(\vec{k})\, U_2^* = a_\lambda^\dagger(\vec{k}) + i\tau \vec{\varepsilon}_\lambda(\vec{k}) \cdot (\sum_{j=1}^N \vec{\varepsilon}_\lambda(\vec{k}) \cdot \vec{x}_j) \frac{\kappa(\vec{k})}{\pi\sqrt{2\omega(\vec{k})}}.$$

Thus, choosing $\tau := 2\pi^{1/2}\alpha^{3/2}$, H is unitarily equivalent to

$$\begin{aligned} H'' \;&:=\; U_2 H U_2^* \qquad (14)\\ &=\; H_{el}^0 \otimes \mathbb{1} + \mathbb{1} \otimes H_f + 2\pi^{1/2}\alpha^{3/2}\vec{E}_\kappa(0)\cdot(\sum_{j=1}^N \vec{x}_j) + c_\kappa \alpha^3 (\sum_{j=1}^N \vec{x}_j)^2 \otimes \mathbb{1}\\ &\quad + \sum_{j=1}^N \{ i4\pi^{1/2}\alpha^{3/2}\,\vec{\nabla}_j \cdot [\vec{A}_\kappa(\alpha\vec{x}_j) - \vec{A}_\kappa(\vec{0})] \;+\; 4\pi\alpha^3[\vec{A}_\kappa(\alpha\vec{x}_j) - \vec{A}_\kappa(\vec{0})]^2\\ &\quad - 2\pi^{1/2}\alpha^{5/2}\vec{\sigma}_j \cdot \vec{B}(\alpha\vec{x}_j)\}. \end{aligned}$$

Here, $c_\kappa = \frac{16}{3}\int_0^\infty k^3\kappa(k)^2 dk$ is a cutoff-dependent constant and $\kappa(\vec{k}) \equiv \kappa(|\vec{k}|)$. In the operator H'' above it appears plausible (although mathematically not quite justified) to neglect all terms that are proportional to α^m with $m > 3/2$.

So, we drop the Zeeman term $-\,2\sqrt{\pi}\alpha^{5/2}\,\vec{\sigma}_j \cdot \vec{B}(\vec{x}_j)$ which generates magnetic dipole transitions between energy levels of H_{el}^0 of order $\alpha^{5/2}$ because electric dipole transitions generated by $2\pi^{1/2}\alpha^{3/2}\vec{E}_\kappa(0)\cdot(\sum_{j=1}^N \vec{x}_j)$ are of order $\alpha^{3/2}$. As a result, the electron spin is decoupled from the radiation field.

Next, invoking a Taylor expansion, $\vec{A}_\kappa(\alpha\vec{x}_j) - \vec{A}_\kappa(0)$ is seen to be of order α, so that in H'' the terms linear in $\vec{A}_\kappa(\alpha\vec{x}_j) - \vec{A}_\kappa(0)$ contribute in order $\alpha^{5/2}$ and the terms quadratic in $\vec{A}_\kappa(\alpha\vec{x}_j) - \vec{A}_\kappa(0)$ even in order α^5. Again in view of the electric dipole term of order $\alpha^{3/2}$, we neglect both of them.

Finally, we shall replace the terms $2\pi^{1/2}\alpha^{3/2}\vec{E}_\kappa(0)\cdot(\sum_{j=1}^N \vec{x}_j) + c_\kappa\alpha^3(\sum_{j=1}^N \vec{x}_j)^2 \otimes \mathbb{1}$ by

$$2\pi^{1/2}\alpha^{3/2}\ \vec{E}_\kappa(0)\ \cdot\ \sum_{j=1}^N [\vec{x}_j\ e^{-(|x_j|^2/a^2)}], \tag{15}$$

where a is of order Z^{-1}, where $Z = \sum_{l=1}^M Z_l$, i.e., a is the characteristic diameter of the atom or molecule.

The resulting Hamiltonian (*the Ritz Hamiltonian*) is denoted by H_R. It has the form

$$H_R\ =\ H_0\ +\ I, \tag{16}$$

where

$$H_0\ =\ H_{el}^0 \otimes \mathbb{1}\ +\ \mathbb{1} \otimes H_f, \tag{17}$$

and

$$I\ =\ \alpha^{3/2}\sum_{j=1}^N\sum_{\lambda=1}^2 \int \{G_{\lambda,\vec{x}_j}(\vec{k})\ a_\lambda^+(\vec{k})\ +\ G_{\lambda,\vec{x}_j}(\vec{k})^*\ a_\lambda(\vec{k})\}\ d^3k, \tag{18}$$

with

$$G_{\lambda,\vec{x}}(\vec{k}) := i\ \sqrt{\frac{2}{\pi}}\ |\vec{k}|^{1/2}\ \kappa(\vec{k})\ \vec{\varepsilon}_\lambda(\vec{k})\cdot\vec{x}\ e^{-x^2/a^2}\ . \tag{19}$$

The precise form of $G_{\lambda,\vec{x}}(\vec{k})$ will usually be immaterial. It suffices to demand some general properties of $G_{\lambda,\vec{x}}(\vec{k})$ that we describe presently:

(i)

$$\lambda_0^2\ :=\ \sup_{\vec{x}}\ \sum_\lambda\ \int\ |\ G_{\lambda,\vec{x}}(\vec{k})\ |^2\ \ d^3k\ \ ,\quad \lambda_1^2 := \sup_{\vec{x}}\sum_\lambda\int\frac{|G_{\lambda,\vec{x}}(\vec{k})|^2}{\omega(\vec{k})}d^3k < \infty, \tag{20}$$

where $\omega(\vec{k}) =|\ \vec{k}\ |$ is the energy of a photon with momentum $\vec{k}$.

(ii)

$$\lambda_2^2 := \sup_{\vec{x}}\sum_\lambda\int[(\Sigma - E_0)^{-2} + \omega(\vec{k})^{-2}]\ |\ G_{\lambda,\vec{x}}(\vec{k})\ |^2\ d^3k\ <\ \alpha^{-3}/4. \tag{21}$$

(iii)

$$\lambda_D^2\ :=\ \sup_{\vec{x}}\ \sum_\lambda\ \int\ \frac{|\ \vec{k}\cdot\vec{\nabla}_k\ G_{\lambda,\vec{x}}(\vec{k}) - \vec{x}\cdot\vec{\nabla}_x\ G_{\lambda,\vec{x}}(\vec{k})\ |^2}{\omega(\vec{k})}\ d^3k\ <\ \infty. \tag{22}$$

(iv) There exists some $\beta > 0$ such that, for all $\rho > 0$,

$$\begin{aligned} \lambda(\rho) \; &:= \; \rho^{1/2} \sup_{\vec{x}} \sum_{\lambda} \Big[\int_{\omega \leq \rho} \frac{\mid G_{\lambda,\vec{x}}(\vec{k}) \mid^2}{\omega(\vec{k})} \, d^3k \; + \\ &+ \sup_{\omega(\vec{k}) \leq \rho} \left(\mid G_{\lambda,\vec{x}}(\vec{k}) \mid^2 \; \omega(\vec{k})^2 \right) \Big]^{1/2} \\ &\leq \; \rho^{1+\beta}. \end{aligned} \tag{23}$$

We remark that ρ sets an energy scale, and $\lambda(\rho)$ has the interpretation of an energy-scale-dependent (running) coupling constant. The condition that $\lambda(\rho)/\rho \sim \rho^{\beta} \to 0$, as $\rho \to 0$, turns out to imply that we are dealing with an *infrared asymptotically free* problem. For the physical Ritz Hamiltonian, $\beta = 1$. Assumption **(i)** guarantees that the quadratic form suitably defined by H_R is bounded below and thus its Friedrichs extension is self-adjoint; **(ii)** implies that, in states describing electrons bound to the nuclei, the expected value of the number of photons is finite; **(iii)** enables us to control the nature of the spectrum of H_R away from the eigenvalues and thresholds of H_{el}^0 by positive-commutator estimates; and (a somewhat stronger form of) **(iv)** permits us to analyze the spectrum of H_R and the structure of resonances in the vicinity of the eigenvalues of H_{el}^0, by using a renormalization group analysis.

Note that, in our approximation, electron spin and the polarization of photons are inessential complications. We may thus suppress these degrees of freedom in our notations. Since we are interested in mathematical results applying to *physical* situations, we shall however point out to the reader which of our results do not apply to the full model described in the introduction.

3 The nature of the spectrum of H_R

The spectrum of the operator H_0 defined in (17), (11) and (6) is the sum of the spectra of H_{el}^0 and H_f, where the spectrum of H_f consists of an eigenvalue at 0 and an absolutely continuous part filling $[0, \infty)$. Thus the spectrum of H_0 has an eigenvalue E_0 at the lower boundary of its absolutely continuous part, embedded eigenvalues at $E_j, j = 1, 2, \cdots$, which are thresholds for branches of absolutely continuous spectrum, a threshold at Σ and possibly further thresholds at higher energies. In order to control the spectrum of H_R

outside a small neighbourhood of $\{E_j\}_{j=1}^{\infty}$, Σ and the higher thresholds of H_{el}^0, for small values of α, we use positive-commutator estimates (see [18, 20, 23, 25]. For reviews on the positive-commutator method see [8, 17]. Applications related to ours will appear in [13].

Let

$$A \;=\; A_{el} \,\otimes\, \mathbb{1} \,+\, \mathbb{1} \,\otimes\, A_f \tag{24}$$

denote the anti-self-adjoint infinitesimal generator of dilatations, where

$$A_f \;=\; \frac{1}{2}\sum_{\lambda} \int \, a_\lambda^\dagger(\vec{k})(\vec{k}\cdot\vec{\nabla}_k + \vec{\nabla}_k\cdot\vec{k}) \; a_\lambda(\vec{k}) \; d^3k, \tag{25}$$

and where A_{el} is the usual generator of dilatations of the N-electron configuration space.

Let Ω be a measurable subset of $I\!R$ with the property that the distance, d, between Ω and the eigenvalues $\{E_j\}_{j=0}^{\infty}$ and the thresholds of H_{el}^0 is bounded below by

$$d \;\geq\; \text{const}\cdot\alpha^{3/2}(\lambda_0+\lambda_D). \tag{26}$$

Let $E_\Omega(H_R)$ denote the spectral projection of H_R corresponding to Ω. Then one can prove that, for some positive constant θ_Ω,

$$E_\Omega(H_R)[A,H]E_\Omega(H_R) \;\geq\; \theta_\Omega E_\Omega(H_R), \tag{27}$$

provided the diameter of Ω is small enough. (To prove (26), one must assume that H_{el}^0 and A_{el} satisfy estimates analogous to (27).)

Inequality (27) is the key ingredient in proving that the spectrum of H_R is absolutely continuous on the union of the sets Ω satisfying (26). Proofs can be found in [8] and extensions in [17].

The next issue is to understand the fate of the ground state of H_{el}^0 when the interaction between electrons and the radiation field is turned on. In studying this problem one encounters some aspects of the infrared problems that plague quantum electrodynamics. Since photons are massless, with a dispersion law $\omega(\vec{k}) = \mid \vec{k} \mid$, the ground state energy of a system of electrons interacting with the quantized radiation field is at the lower boundary of the continuous spectrum of the Hamiltonian of the system. Therefore, standard analytic perturbation theory cannot be applied to study the ground states of the interacting system. One way of coping with the problem is as follows [12]:

One introduces an auxiliary Hamiltonian H_R^μ with infrared cutoff, μ, e.g. replacing G by G^μ where $G_{\lambda,\vec{x}}^\mu(\vec{k}) = 0$ whenever $\omega(\vec{k}) \leq \mu$, and then *discretizes* photon momentum space for $\omega(\vec{k}) > \mu$. Then the spectrum of H_f^μ restricted to momenta with $\omega(\vec{k}) > \mu$ is pure point and contained in $\{0\} \cup [\mu, \infty)$. By carefully removing the discretization, using Assumption **(ii)**, one proves that the infrared-cutoff Hamiltonian H_R^μ has a ground state $\phi^\mu(\alpha)$ corresponding to an eigenvalue $E^\mu(\alpha)$, for any value of $\mu > 0$. Since $H_R^\mu \to H_R$, as $\mu \to 0$, in norm resolvent sense,

$$\phi^0(\alpha) := w - \lim_{\mu \to 0} \phi^\mu(\alpha) \tag{28}$$

is a natural candidate for a ground state of H_R, provided $\phi^0 \neq 0$, which is proved as follows.

First, one uses the fact that ϕ^μ is a ground state of H_R^μ and solves the Schrödinger equation $H_R^\mu \phi^\mu = E^\mu \phi^\mu$. Then, commuting $a_\lambda(k)$ with H_R, this leads us to

$$\langle \phi^\mu | (\mathbf{1} \otimes N) \phi^\mu \rangle \leq 4\alpha^3 \sup_{\vec{x}} \sum_\lambda \int \omega(\vec{k})^{-2} \mid G_{\lambda,\vec{x}}(\vec{k}) \mid^2 \; d^3k \tag{29}$$

uniformly in μ, where $N := \sum_\lambda \int a_\lambda^\dagger(\vec{k}) a_\lambda(\vec{k}) d^3k$ is the photon number operator. Next, a simple spectral estimate in conjunction with (29) gives

$$\langle \phi^\mu | [(\mathbf{1} - P_{el}) \otimes P_\Omega] \phi^\mu \rangle \leq 4\alpha^3 \sup_{\vec{x}} \sum_\lambda \int (\Sigma - E_0)^{-2} \mid G_{\lambda,\vec{x}}(\vec{k}) \mid^2 \; d^3k \tag{30}$$

uniformly in μ, where P_Ω is the projection onto the Fock vacuum Ω and P_{el} is the finite dimensional spectral projection of H_{el}^0 onto all eigenvalues $E_j \leq \Sigma - \varepsilon$ for some $\varepsilon > 0$. Finally, upon using $\mathbf{1} - P_\Omega \leq (\mathbf{1} - P_\Omega)\, N = N$ and adding up (29) and (30), we arrive at

$$\langle \phi^\mu | (P_{el} \otimes P_\Omega) \phi^\mu \rangle \;\geq\; 1 - \langle \phi^\mu | [(\mathbf{1} - P_{el}) \otimes P_\Omega] \phi^\mu \rangle - \langle \phi^\mu | (\mathbf{1} \otimes N) \phi^\mu \rangle \;\geq\; 1 - 4\alpha^3 \lambda_2^2 > 0 \tag{31}$$

uniformly in μ. Because $P_{el} \otimes P_\Omega$ is finite dimensional, this implies that $\phi^0 \neq 0$ and finishes the proof. Moreover, using a Combes-Thomas-Agmon type estimate, one shows that

$$\| \exp \, \gamma \, (\sum_{j=1}^N \mid \vec{x}_j \mid) \; \phi^{(\mu)}(e) \| \;\leq\; C, \tag{32}$$

for some constants $\gamma > 0$ and $C < \infty$ *independent* of μ.

The arguments sketched above (see [3] for details) do not permit us to control the multiplicity of $E_0(\alpha)$. In order to determine how many ground states H_R has, we are using two complementary methods: The first one consists in proving a Perron-Frobenius theorem for $\exp(-t\, H_R)$. This can be done for the Hamiltonian H_R defined in eqs. (16)

through (18), with I as in (19) (dipole approximation), provided electrons have "Boltzmann statistics", or the number of electrons $N = 1$ or 2. In these situations, the ground state, $\phi(\alpha)$, of H_R is *unique*; [12]. However, these methods do not apply to the model described in (10) in the introduction, or to the Ritz Hamiltonian (16) for three or more electrons satisfying Fermi-Dirac statistics.

Using operator-theoretic renormalization group methods (sketched in Section 4) we are able to control the multiplicity of $E_0(\alpha)$, for small values of α. The advantage of these methods is that they are constructive and can be extended to gain control over the nature of the spectrum of H_R above $E_0(\alpha)$ and in the vicinity of E_j, $j \leq 1$. However, they are only applicable for very small values of α, while the methods described above can be used in a large range of values of α.

We close this section with a remark on *bound states* of atoms and molecules interacting with the quantized radiation field (as opposed to *eigenstates* of H_R). By a bound state we mean a state $\phi \in \mathcal{H}$ with the property that the expectation value of any polynomial in the position coordinates of the N electrons in ϕ is *finite*. The obvious physical idea is that a state ϕ whose spectrum of energies is well below the threshold $\sum$ of H_{el}^0 should be a bound state. Our result on bound states is as follows [3]: Let Ω be any closed interval contained in $(-\infty, \sum -C\lambda_1^2\alpha^3)$, where λ_1 is defined in (20) and C is some finite constant. Let ϕ be a unit vector in the range of $E_\Omega(H_R)$. Then, for any $\gamma < \text{dist}(\Sigma, \Omega) - c\lambda_1\alpha^{3/2}$, there exists a finite constant $C_{\gamma,\Omega}$ such that

$$\| \exp(\gamma \sum_{j=1}^{N} \mid \vec{x}_j \mid) \, \phi \, \| \ \leq \ C_{\gamma,\Omega}. \tag{33}$$

Inequality (33) can be used to prove strong cluster decomposition properties for the expectation values of Heisenberg-picture observables in ϕ.

4 Analysis of resonances

The purpose of this section is to describe results concerning the fate of higher eigenvalues $E_j, j \geq 1$, of H_{el}^0 when the interaction between electrons and the quantized radiation field is turned on. Since these eigenvalues are embedded in the continuous spectrum of the operator $H_0 = H_{el}^0 + H_f$, we expect that they turn into resonances when the perturbation I (see eqs. (16) - (18)) is added. Put differently, all excited states of H_{el}^0 become unstable (with a finite life-time) when the perturbation I is added to H_0. Bethe's calculation of the

Lamb shift and Fermi's golden rule provide predictions for the location of the resonance energies.

There is a (by now) standard tool to cope with problems of resonances: the use of *dilatation analyticity*, [1, 4, 7, 15, 27, 28, 29]. Let

$$U(\theta) \;=\; \exp\,(\theta A), \quad \theta \,\in\, I\!R, \tag{34}$$

be the unitary group on $\mathcal{H}$ of dilatations. For an operator T on $\mathcal{H}$, let $T(\theta)$ denote the operator $U(\theta)\; T\, U\,(\theta)^{-1}$. It is easy to see that $H_f(\theta) = e^{-\theta} H_f$, and hence $H_f(\theta)$ is analytic in $\theta \in \mathbb{C}$. In order to describe our methods in a transparent context, we consider an atom, (i.e., there is only one nucleus). Then the operators $H^0_{el}(\theta)$ form an analytic family of type A [26], for θ in a strip $\mathcal{S}$ of positive width around the real axis.

Furthermore, one notes that $I(\theta)$ is obtained from I by replacing the form factor $G_{\lambda,\vec{x}}(\vec{k})$ by $G^\theta_{\lambda,\vec{x}}(\vec{k}) \,:=\, e^{-3\theta/2} G_{\lambda, e^\theta \vec{x}}(e^{-\theta}\vec{k})$, where we assume $G_{\lambda,\vec{x}}(\vec{k})^* \,=\, -G_{\lambda,\vec{x}}(-\vec{k})$, for simplicity. It is then not hard to see that $H_R(\theta)(H_R+i)^{-1}$ is a family of bounded operators on $\mathcal{H}$ analytic in $\theta \in \mathcal{U}$, where $\mathcal{U}$ is a small disk about 0 contained in $\mathcal{S}$ provided that

(v) $\theta \mapsto G^\theta_{\lambda,\vec{x}}(\vec{k})$ is analytic in $\mathcal{U}$ as a vector-function with values in $L^2[I\!R^3,\, (1+\omega^{-1})d^3k]$.

(vi) Assumptions **(i)** and **(iv)** in Section 3 hold with constants λ_1, λ_0 and $\lambda(\rho)$ that are uniform in $\theta \in \mathcal{D}$.

It is not hard to show that the spectrum of the unperturbed operator $H_0(\theta)$, for $\theta = i\,\varphi$, with φ sufficiently small, has the structure indicated in Fig. 2, below.

Fig. 2

In order to understand the displacement of the thresholds E_j when the perturbation $I(\theta)$ is turned on, one must develop a suitable form of perturbation theory. The one we have developed in [3] is based on the Feshbach (-Grushin-Krein) projection method organized in an inductive way inspired by the renormalization group. Here we can only describe some key aspects of this method. For simplicity, we shall assume that one of the eigenvalues E_j is simple, $E^{(0)} = E_{j_0}$, say. We propose to analyze the spectrum of $H_R(\theta)$ $(\theta = i\varphi)$ in the vicinity of $E^{(0)}$.

We start by describing the Feshbach projection method in an abstract setting. Thus, let $\mathcal{H}$ be a separable Hilbert space and H a closed operator densely defined on $\mathcal{H}$. Let P be a (bounded but not necessarily orthogonal) projection on $\mathcal{H}$ $(P = P^2)$ whose range is contained in the domain of H, and set $\bar{P} := \mathbf{1} - P$. We define

$$\begin{aligned} h &:= P\,H\,P \;+\; \bar{P}\,H\,\bar{P}, \\ v &:= P\,H\,\bar{P} \;+\; \bar{P}\,H\,P, \end{aligned} \tag{35}$$

and assume that

$$\|v\psi\| \;\leq\; a\|h\psi\| \;+\; b\|\psi\|, \tag{36}$$

for some $a < \frac{1}{2}$ and some finite b.

For z in the resolvent set, Λ_P, of $\bar{P}\,H\,\bar{P}$, we define

$$\mathcal{F}_z(H) \;:=\; P\,H\,P \;-\; P\,H\,\bar{P}\,\bar{R}_0(z)\,\bar{P}\,H\,P, \tag{37}$$

where

$$\bar{R}_0(z) \;:=\; (\bar{P}\,H\,\bar{P} \;-\; z\,\bar{P})^{-1}|_{\bar{P}\mathcal{H}}. \tag{38}$$

Theorem $\mathcal{F}$. *Let $z \in \Lambda_P$ and assume that*

$$\|\bar{R}_0(z)v\|, \quad \|v\,\bar{R}_0(z)\| \;\leq\; \varepsilon \;<\; 1. \tag{39}$$

Then

(a) *$\mathcal{F}_z(H) - zP$ is invertible on $P\mathcal{H}$ if and only if $H - z$ is invertible on $\mathcal{H}$.*

(b) *Moreover, if $\psi \in \mathcal{H}$ is such that $P\psi \neq 0$ and $z \in \Lambda_P$ then*

$$(\mathcal{F}_z(H) - z)\,P\,\psi \;=\; 0 \quad \textit{if and only if} \quad (H - z)\,\psi = 0.$$

The proof of this theorem is straightforward. We use it to embark on a renormalization group analysis of the spectrum of $H_R(\theta = i\varphi)$ in a vicinity of $E^{(0)}$. Our analysis represents, perhaps, the first mathematically precise combination of renormalization group ideas (decomposition into energy scales, scale-by-scale inductive analysis) with operator – rather than functional-integral – methods.

The first step of our analysis is as follows: Let $\theta = i\varphi$, $\varphi > 0$, be *fixed*. We choose a positive number $\rho_0 \ll \mathrm{dist}\,(E^{(0)}, \sigma(H^0_{el})\backslash\{E^0\})$. Let $\chi_{H_f \leq \rho_0}$ denote the spectral projection, $E_{\Omega_0}(H_f)$, of H_f, with $\Omega_0 = (-\infty, \rho_0]$. Let $P^{(0)}$ denote the projection onto $\{\mathbb{C}\,\phi^{(0)}(\theta)\} \otimes \chi_{H_f\leq\rho_0}\mathcal{H}_f \simeq \chi_{H_f\leq\rho_0}\mathcal{H}_f$, where $\phi^{(0)}(\theta)$ is the eigenvector of $H^0_{el}(\theta)$ corresponding to the eigenvalue $E^{(0)}$; (note that $E^{(0)}$ is *independent* of θ). In eq. (37) and Theorem $\mathcal{F}$, we set $H := H_R(\theta)$, $P := P^{(0)}$. Then $\Lambda_P \equiv \Lambda_{P^{(0)}}$ contains the disk

$$\bar{S}^{(0)} := E^{(0)} + B(\rho_0)\ , \tag{40}$$

where $B(\rho) := \{z | \rho \geq |z|\}$. Moreover, for all $z \in \bar{S}^{(0)}$,

$$\mathcal{F}_z(H) \;=\; E^{(0)} \;+\; e^{-\theta}\, H_f \;+\; W^{(0)}(\alpha, z) \tag{41}$$

where

$$\|W^{(0)}(\alpha, z)\| \;\leq\; \mathrm{const}\alpha^{3/2}\ , \tag{42}$$

uniformly in $z \in \bar{S}^{(0)}$. Choosing a suitably small $\rho_1 < c\alpha^{9/7}$, this bound enables us to show that, for every z contained in the smaller set $\bar{S}^{(0)}\backslash(S^{(0)}\cup Q^{(0)})$, where $S^{(0)} := E^{(0)} + B(\rho_1/2)$ and

$$Q^{(0)} := \{E^{(0)} + re^{-\theta} + \zeta \mid 0 \leq r \leq \rho_0\ ,\ \ |\zeta| \leq r^{7/6}\,\}\ , \tag{43}$$

$\mathcal{F}_z(H) - z\,P^{(0)}$ is invertible on $P^{(0)}\mathcal{H}$. It then follows from part **(a)** of Theorem $\mathcal{F}$ that z is in the resolvent set of $H_R(\theta)$, i.e., $H_R(\theta) - z$ is invertible for all $z \in \bar{S}^{(0)} \setminus (S^{(0)} \cup Q^{(0)})$.

Let $z = z_0$ be any point in $\bar{S}^{(0)}$. By using the Neumann series expansion of the resolvent, the pull-through formula

$$a_\lambda(\vec{k})(z - H_f)^{-1} \;=\; (z - \omega(\vec{k}) - H_f)^{-1}\, a_\lambda(\vec{k})$$

and its adjoint and further fairly standard devices, $\mathcal{F}_{z_0}(H)$, as given by the r.s. of (37), can be cast in the form

$$\mathcal{F}_{z_0}(H) \;\equiv\; H^{(0)}(z_0) \;=\; E_0(\alpha, z_0) \;+\; T_0(e^{-\theta}\, H_f;\ \alpha, z_0) \;+\; W_0(\alpha, z_0), \tag{44}$$

where $E_0(\alpha, z_0) - E^{(0)}$ is a complex number and T_0 is a function of H_f satisfying

$$|E_0(\alpha, z_0) - E^{(0)}| \, , \quad \|(T_0 - e^{-\theta} \, H_f) \, H_f^{-1}\| \; \leq \; 0(\alpha^3), \tag{45}$$

uniformly in $z_0 \in \bar{S}^{(0)}$, and W_0 is an (infinite, norm-convergent) sum of Wick monomials in $a_\lambda^\dagger$ and a_λ, with integral kernels depending on α, z_0 and on H_f in a well-defined way. Moreover,

$$\left\| (H_f + \rho_1)^{-1/2} \, W_0(\alpha, z_0) \, (H_f + \rho_1)^{-1/2} \right\| \; \leq \; K \alpha^{3/2} \rho_1^{-1} \lambda(\rho_0) \; , \tag{46}$$

where $\lambda(\rho_0)$ is defined in eq. (23), and the constant $K < \infty$ on the r.s. of (46) is independent of $z_0 \in \bar{S}^{(0)}$.

Note that, in the *effective Hamiltonian*, $H^{(0)}(z_0)$, at energy scale ρ_0, the electronic degrees of freedom are integrated out. This operator can be viewed as an operator on the photon Fock space $\mathcal{H}_f$ that vanishes on the orthogonal complement of $\chi_{H_f \leq \rho_0} \mathcal{H}_f$.

Next, we choose a number $\rho_2 < \rho_1/2$ and define

$$\bar{S}^{(1)} \; := \; \bigcap_{z_0 \in \bar{S}^{(0)}} \{E_0(\alpha, z_0) + B(\rho_1)\} \; , \qquad S^{(1)} \; := \; \bigcup_{z_0 \in \bar{S}^{(0)}} \{E_0(\alpha, z_0) + B(\rho_2/2)\} \; , \tag{47}$$

and

$$Q^{(1)} := \bigcup_{z_0 \in \bar{S}^{(0)}} \{E_0(\alpha, z_0) + T_0(re^{-\theta}; \alpha, z_0) + \zeta \mid 0 \leq r \leq \rho_0 \; , \; \; |\zeta| \leq r^{7/6} \; \} \; .$$

We shall choose α and r_1 so small that

$$S^{(1)} \subset S^{(0)} \subset \bar{S}^{(1)} \subset \bar{S}^{(0)} \quad . \tag{48}$$

We define

$$P^{(1)} \; := \; P^{(0)} \, \chi_{H_f \leq \rho_1} . \tag{49}$$

In eq. (37) and Theorem $\mathcal{F}$, we set $H := H^{(0)}(z_0)$ and $P := P^{(1)}$. We then define, for $z_0 \in \bar{S}^{(0)}$ and $z_1 \in \bar{S}^{(1)}$

$$H^{(1)}(z_0, z_1) \; := \; \mathcal{F}_{z_1} \, (H^{(0)}(z_0)), \tag{50}$$

with $\mathcal{F}$ as in eq. (37). Our estimates, eqs. (45) and (46), enable us to show that, for an arbitrary $z_1 \in \bar{S}^{(1)} \setminus (S^{(1)} \cup Q^{(1)})$, $H^{(1)}(z_0, z_1) - z_1 P^{(1)}$ is invertible on $P^{(1)}\mathcal{H}$, for any $z_0 \in \bar{S}^{(0)}$, and hence $H^{(0)}(z_0) - z_1 P^{(0)}$ is invertible on $P^{(0)}\mathcal{H}$, for any $z_0 \in \bar{S}^{(0)}$, by part **(a)** of Theorem $\mathcal{F}$. Thanks to (47) and (48), we may now set $z_0 = z_1$ and, by applying part **(a)** of Theorem $\mathcal{F}$ once more, we conclude that $H_R(\theta) - z_1$ is invertible for any $z_1 \in \bar{S}^{(1)} \setminus (S^{(1)} \cup Q^{(1)})$. The operator $H^{(1)}(z_1) := H^{(1)}(z_1, z_1)$ defined in (50), with $z_1 \in \bar{S}^{(1)}$, is called an *effective Hamiltonian* at energy scale ρ_1. Again, $H^{(1)}(z_1)$ can be recast in the form

$$H^{(1)}(z_1) \;=\; E_1(\alpha, z_1) \;+\; T_1(e^{-\theta}\, H_f;\; \alpha, z_1) \;+\; W_1(\alpha, z_1), \tag{51}$$

where the properties of E_1, T_1 and W_1 are analogous to those of E_0, T_0 and W_0, for all $z_1 \in \bar{S}^{(1)}$, with the following estimates:

$$|\; E_1(\alpha, z_1) - E_0(\alpha, z_1) \;| \leq \; K\alpha^3\, \lambda(\rho_0)^2, \tag{52}$$

$$\|(T_1 - T_0)\; H_f^{-1}\| \;\leq\; K\alpha^3\, \lambda(\rho_0)^2, \tag{53}$$

and

$$\left\|(H_f + \rho_2)^{-1/2}\, W_1(\alpha, z_1)\, (H_f + \rho_2)^{-1/2}\right\| \;\leq\; K\alpha^{3/2}\rho_2^{-1}\lambda(\rho_1)\;, \tag{54}$$

where the constant K is the same as in inequality (46) and is *independent* of $z_1 \in \bar{S}^{(1)}$.

It is important to observe that the general form of $H^{(1)}$ is similar to that of $H^{(0)}$. This suggests to proceed inductively, the induction extending over a sequence, $\{\rho_j\}_{j=0}^{\infty}$, of energy scales converging to 0 and with the property that

$$\rho_j^{-1}\; \lambda(\rho_{j-1}) \;\ll\; 1. \tag{55}$$

Thanks to assumption **(iv)**, see (23), with $\beta > 0$ (for $G^{\theta}_{\lambda,\vec{x}}$, $\theta = i\varphi$, $\varphi > 0$), condition (55) can be met for many choices of sequences, $\{\rho_j\}$, of energy scales, including ones converging to 0 faster than M^{-j}, for any $M < \infty$.

Thus, we assume that we have already constructed $H^{(j)}(z_j)$, $E_j(\alpha, z_j)$, T_j, W_j and sets $\bar{S}^{(j)}$ and $S^{(j)}$, with properties as in (47), (48) and (52) - (54), but with subscripts 0 and 1 replaced by j-1 and j, respectively. We then choose $\rho_{j+2} < \rho_{j+1}/2$ and define

$$\begin{aligned}
\bar{S}^{(j+1)} \;&:=\; \bigcap_{z_j \in \bar{S}^{(j)}} \{E_j(\alpha, z_j) + B(\rho_{j+1})\}\;, \quad S^{(j+1)} \;:=\; \bigcup_{z_j \in \bar{S}^{(j)}} \{E_j(\alpha, z_j) + B(\rho_{j+2}/2)\}\;, \\
Q^{(j+1)} \;&:=\; \bigcup_{z_j \in \bar{S}^{(j)}} \{E_j(\alpha, z_j) + T_j(re^{-\theta}; \alpha, z_j) + \zeta \mid 0 \leq r \leq \rho_j\;,\;\; |\zeta| \leq r^{7/6}\,\}\,.
\end{aligned} \tag{56}$$

For $\rho_j = 2r_j$, condition (55) and the induction hypothesis

$$|\; E_j(\alpha, z_j) \;\; - E_{j-1}(\alpha, z_j) \;| \leq \; K\alpha^3\, \lambda(\rho_j)^2, \tag{57}$$

imply that

$$S^{(j+1)} \subset S^{(j)} \bar{S}^{(j+1)} \subset \bar{S}^{(j)} \;\; . \tag{58}$$

We now set $P^{(j+1)} := P^{(0)}\, \chi_{H_f \le \rho_{j+1}}$, and define, for $z_i \in \bar{S}^{(i)}$,

$$H^{(j+1)}(z_j, z_{j+1}) \;:=\; \mathcal{F}_{z_{j+1}}\,(H^{(j)}(z_j)),$$

with $\mathcal{F}_{z_{j+1}}$ as in eqs. (37), (38), for $H := H^{(j)}(z_j)$ and $P := P^{(j+1)}$. Now we can use the induction hypotheses

$$\begin{aligned} \|(T_j - T_{j-1})\, H_f^{-1}\| \;&\le\; K\alpha^3\, \lambda\,(\rho_{j-1})^2, \\ \left\|(H_f + \rho_{j+1})^{-1/2}\, W_j(\alpha, z_j)\,(H_f + \rho_{j+1})^{-1/2}\right\| \;&\le\; K\alpha^{3/2}\rho_{j+1}^{-1}\lambda(\rho_j)\;, \end{aligned} \tag{59}$$

to analyze the resolvent set of $H^{(j+1)}(z_j, z_{j+1})$ in a vicinity of $E_j(\alpha, z_j)$ with a diameter of order ρ_{j+1}. By part **(a)** of Theorem $\mathcal{F}$ and property (58), this yields control over the resolvent set of $H^{(j)}(z_{j+1})$ in $\bar{S}^{(j+1)} \setminus (S^{(j+1)} \cup Q^{(j+1)})$. We set $H^{(j+1)}(z_{j+1}) := H^{(j+1)}(z_{j+1}, z_{j+1})$, which is an effective Hamiltonian at energy scale ρ_{j+1}. The main analytical task in carrying out the induction step is to show that $H^{(j+1)}(z_{j+1})$ has the form

$$\begin{aligned} H^{(j+1)}(z_{j+1}) \;&=\; E_{j+1}(\alpha, z_{j+1}) \;+\; T_{j+1}\,(e^{-\theta}\, H_f\,;\;\alpha, z_{j+1}) \\ &\qquad + W_{j+1}\,(\alpha, z_{j+1}), \end{aligned}$$

where T_{j+1} is a function of H_f, and W_{j+1} is an (infinite, norm-convergent) sum of Wick monomials in $a^\dagger_\lambda$ and a_λ, with integral kernels depending on α, z_{j+1} and on H_f in a precise way, with the property that the bounds (57) and (59) hold, with j replaced by $j+1$, and for a finite constant K independent of j and of $z_{j+1} \in \bar{S}^{(j+1)}$. This task is rather complicated and cannot be described here; (the tools are the Neumann series for the resolvent of $(\mathbf{1} - P^{(j+1)})H^{(j)}(z_{j+1})(\mathbf{1} - P^{(j+1)})$, an expansion of the resulting terms in Wick monomials, using the pull-through formula, and a subsequent resummation). The details of our construction will appear in [3].

Our construction ensures that, as $j \to \infty$, $E_j\;(\alpha, z_j)$ converges to an energy $E(\alpha)$ which is the energy of a resonance bifurcating from $E^{(0)}$. Furthermore, the sets $\bar{S}^{(j)}$ decrease to $\{E(\alpha)\}$, as $j \to \infty$. Our inductive construction shows that the spectrum of $H_R(\theta)$ in the vicinity of $E^{(0)}$ is contained in $\bigcup_{j=0}^{\infty} \left\{\bar{S}^{(j+1)} \setminus (S^{(j+1)} \cup Q^{(j+1)})\right\}$, depicted as shaded region in Figure 3.

Fig. 3

Using these results, one can proceed to construct an eigenvector of $H_R(\theta)$ corresponding to the eigenvalue $E(\alpha)$. This requires introducing an infrared cutoff, performing the inductive construction sketched above untill the energy scale has been lowered to one comparable to the infrared cutoff, and then using part **(b)** of Theorem $\mathcal{F}$. It is crucial to organize the estimates in such a way that the control over the eigenvectors is uniform in the infrared cutoff.

The strategy described here can also be applied to construct the ground states of H_R. It is constructive and, therefore, yields, in principle, control over the multiplicity of the ground state and of resonances. Moreover, following a method described in [16], one can obtain estimates on the Life-time of resonances, i.e., the time decay of unperturbed eigenvectors of embedded eigenvalues. Despite the fact that our method succeeds to construct a convergent perturbation expansion for a threshold of the full operator $H_R(\theta)$, it does not apply to accumulation points of the spectrum of H^0_{el} because the isolation of the unperturbed electronic eigenvalue is essential.

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