Existence and Construction of Resonances for Atoms Coupled to the Quantized Radiation Field

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Consider

$$i\frac{\partial}{\partial t}\phi_t = H_{el}\phi_t, \qquad \phi_t \in \mathcal{H}_{el} ,$$

the Schrödinger equation for an atom, where

$$H_{el} := P^2 + V = -\Delta + V,$$

where

$$P := -i\nabla, \qquad V : \mathbb{R}^3 \to \mathbb{R}$$

and

$$\mathcal{H}_{el} := L^2(\mathbb{R}^3).$$

The possible energies of the atom are

$$\sigma(H_{el}) := \{e_i\}_{i=0}^{M} \cup [0, \infty).$$

If the initial state ϕ_0 is an eigenvalue All the physical properties of the system do not depend on time.

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- Contradiction with experiments
- Excited states decay to lower energy states

The key ingredient:

- The atom emits photons when it decays to a lower energy state.
- Photons are not represented in the Hamiltonian.

After introducing the photons in our equations we obtain the Pauli-Fierz Model

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Our Main Result:

In the Pauli-Fierz Model the eigenvalues e_i for $i \geq 1$ turn into resonances after introducing the photons.

Similar Results

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- Bach-Fröhlich-Sigal (1998)

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The Pauli-Fierz Model

The Fock Space (the Hilbert Space for Photons)

Let $\beta \in (0, 1)$ be small enough. We define

$$\sigma_n := \beta^n \,, \; (n \in \mathbb{N}), \qquad \sigma_\infty = 0 \,, \qquad \sigma_{-1} = \infty,$$

and

For $n > m$,

$$\mathcal{K}_{n,m} := \left\{ k = (\vec{k}, \lambda) \in \mathbb{R}^3 \times \mathbb{Z}_2 \;\middle|\; \sigma_n \leq |k| = |\vec{k}| < \sigma_m \right\} .$$

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We denote by

$$\mathfrak{h}_{n,m} := L^2[\mathcal{K}_{n,m}] , \tag{1}$$

the one particle photon space and by

$$\mathcal{F}_{n,m} = \mathcal{F}(\mathfrak{h}_{n,m})$$

the corresponding Fock space.

The Interacting Hilbert Space

The interacting Hilbert space is defined to be

$$\mathcal{H}_{n,m} := \mathcal{H}_{el} \otimes \mathcal{F}_{n,m} . \tag{2}$$

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The electron Hamiltonian

We recall that the electron Hamiltonian is

$$H_{el} := -\Delta + V(x) \,. \tag{3}$$

The Photon Hamiltonian

The Photon Hamiltonian $\check{H}_{n,m} : \mathcal{F}_{n,m} \to \mathcal{F}_{n,m}$ is defined by

$$\begin{aligned} \check{H}_{n,m}(\oplus_{j=0}^{\infty}\phi_j) &= \oplus_{j=0}^{\infty}\psi_j, \\ \psi_j(k_1,\cdots,k_j) &:= (|k_1| + \cdots + |k_j|)\phi_j(k_1,\cdots,k_j)\,, \end{aligned} \tag{4}$$

with $(k_1,\cdots,k_j) \in (\mathcal{K}_{n,m})^j$.

We assume the following convention: in the case that $m = -1$ we write "n" instead of "$n, -1$" in the subscripts:

$$(\cdot)_n \equiv (\cdot)_{n,-1}.$$

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The full Hamiltonian

We define the function

$$G(k,x) \;:=\; -g\frac{1}{(2\pi)^{3/2}}\,\frac{\exp(-|k|^2)}{\sqrt{2\,|k|}}\;e^{-ig^{2/3}\vec{k}\cdot\vec{x}}\;\vec{\varepsilon}(k), \qquad (5)$$

where $\vec{\varepsilon} := (\varepsilon_1, \varepsilon_2, \varepsilon_3) : \mathbb{R}^3 \times \mathbb{Z}_2 \to \mathbb{C}^3$ satisfies

$$\begin{aligned} \vec{\varepsilon}(\vec{k},\lambda)^* \cdot \vec{\varepsilon}(\vec{k},\mu) \;=\; \delta_{\lambda,\mu}\,, \quad \vec{k}\cdot\vec{\varepsilon}(\vec{k},\lambda) \;=\; 0 \\ \overline{\vec{\varepsilon}(-\vec{k},\lambda)} = \vec{\varepsilon}(\vec{k},\lambda), \quad \vec{\varepsilon}(r\vec{k},\lambda) = \vec{\varepsilon}(\vec{k},\lambda),\; r>0\,, \end{aligned} \qquad (6)$$

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The full Hamiltonian is defined by the formula

- $$H := (P - A)^2 + V + \check{H}_\infty. \qquad (7)$$

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The Pauli-Fierz Transformation

Let $\eta \in C_0^\infty(\mathbb{R}^3; [0,1])$

We introduce the function

$$G_{P-F}(k,x) := G(k,0) \cdot \Big(-\eta\big(|x||k|\big)x \Big)\,, \tag{8}$$

and the operator

$$A_{P-F} := a^*(G_{P-F}) + a(G_{P-F})\,. \tag{9}$$

We now define

$$\mathbf{H} := e^{-iA_{P-F}} H e^{iA_{P-F}}\,. \tag{10}$$

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Analytic Continuation

of the Hamiltonian

The Group of Dilation Operators

For any real θ, we define the unitary operator $u(\theta) : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ as follows

$$u(\theta)\phi(x) := e^{3\theta/2}\phi(e^{\theta}x)\,. \tag{11}$$

We denote by $U(\theta)$, the resulting operator after lifting $u(\theta)$ to $\mathcal{H}_\infty = \mathcal{H}_{el} \otimes \mathcal{F}_\infty$:

$$U(\theta) := u(\theta) \otimes \bigotimes_{j=0}^{\infty} u(-\theta)^{\otimes j}$$

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We define the operator

- $$\mathbf{H}(\theta) := U(\theta)\mathbf{H}U(\theta)^* . \tag{12}$$

  We extend it analytically for θ in a neighborhood of 0 in the complex plane.
- The restriction of this Hamiltonian to the space $\mathcal{H}_n$ is denoted by

  $$\mathbf{H}_n(\theta). \tag{13}$$

We identify

$$\mathbf{H}_\infty(\theta) \equiv \mathbf{H}(\theta) . \tag{14}$$

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Main Result

Theorem

The operator $\mathbf{H}(\theta)$ *has an eigenvalue* E *in a neighborhood of* e_1*. The imaginary part of* E *is strictly negative. There is no point in the spectrum of* $\mathbf{H}(\theta)$ *above* E*, in a neighborhood of* e_1*.*

The Strategy for the Proof

We set $\theta = i\nu$ with $\nu > 0$ and define

$$\tau(\nu) := \frac{1}{2}\sin(\nu) \, .$$

We prove by induction that for every $m \in \mathbb{N}$ the following holds true:

(i) There is an open set $\mathcal{E}_m \subset \mathbb{C}$ and a complex number E_m, which is a simple eigenvalue of $\mathbf{H}_m(\theta)$. E_m is the only spectral point of $\mathbf{H}_m(\theta)$ in $\mathcal{E}_m$.

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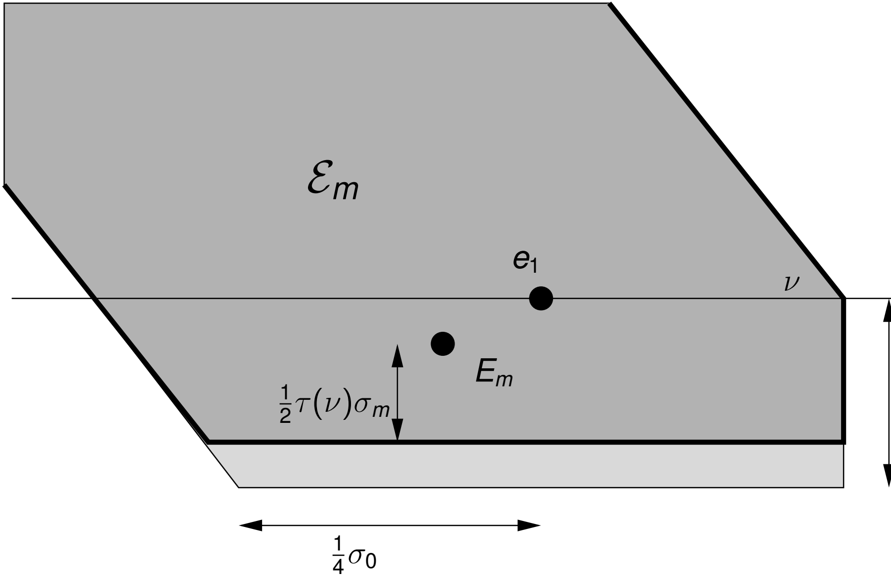
$\mathcal{E}_m$
e_1
ν
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(ii) We denote by

$$P_m = \frac{i}{2\pi} \int_\gamma \frac{1}{\mathbf{H}_n(\theta) - z} dz \tag{15}$$

the projection onto the vector space generated by the eigenvector ϕ_m corresponding to E_m.
Here γ is a contour that surrounds E_m and lies in a small neighborhood of E_m.
There is a (universal) constant $\mathbf{C} > 1$ such that

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for every $z \in \mathcal{E}_m$, where

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Once (i)-(iv) is established by an inductive argument, we prove that the sequence of eigenvalues $\{E_m\}_{m\in\mathbb{N}}$ and the corresponding sequence of eigenvectors ϕ_m have a limit:

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The Infrared Problem

The key ingredient that permits the induction step to be proved is the smallness of the quantity

$$\left\| \left[\mathbf{H}_{m+1}(\theta) - \left(\mathbf{H}_m(\theta) + e^{-\theta} \check{H}_{m+1,m} \right) \right] \left(\mathbf{H}_m(\theta) + e^{-\theta} \check{H}_{m+1,m} - z \right)^{-1} \right\| . \tag{20}$$

The $|k|^{-1/2}$ factor in the interaction implies that the difference (20) does not approach zero as m approaches infinity (it is at least of order 1). As the term $\mathbf{C}^m$ diverge exponentially to ∞ we cannot proceed with the induction step.
To solve this problem we make use of the Feshbach-Schur Map.

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We define $\mathbf{P}$ to be the projection onto the vector space generated by

$$\psi_1(\theta) \otimes 1_{\mathcal{F}_{m+1}} , \tag{21}$$

where $\psi_1(\theta)$ is the first eigenvalue of $\mathbf{H}_{el}(\theta)$.

We define the Feshbach-Schur map

$$F(\mathbf{H}_{m+1}(\theta) - z) := \mathbf{P}(\mathbf{H}_{m+1}(\theta) - z)\mathbf{P}$$
$$-\mathbf{P}\mathbf{H}_{m+1}(\theta)\overline{\mathbf{P}}(\overline{\mathbf{P}}(\mathbf{H}_{m+1}(\theta) - z)\overline{\mathbf{P}})^{-1} \tag{22}$$
$$\cdot\overline{\mathbf{P}}\mathbf{H}_{m+1}(\theta)\mathbf{P},$$

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Similarly we define $F(\mathbf{H}_m(\theta) + e^{-\theta}\check{H}_{m+1,m} - z)$.

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We finally estimate

$$\left\| \left[F\left(\mathbf{H}_{m+1}(\theta) - z\right) - F\left(\mathbf{H}_m(\theta) + e^{-\theta}\check{H}_{m+1,m} - z\right)\right] \cdot \left(F(\mathbf{H}_m(\theta) + \check{H}_{m+1,m}(\theta) - z)\right)^{-1} \right\| . \tag{23}$$

instead of (20), and use this to complete the induction step.

Sketch of the Proof:

The Hamiltonian $\mathbf{H}_n(\theta)$ can be written as the sum of a free part, whose spectrum is known plus an interacting part:

$$\mathbf{H}_n(\theta) = \mathbf{H}_n^0(\theta) + \mathbf{W}_n(\theta), \tag{24}$$

where

$$\mathbf{H}_n^0(\theta) := e^{-2\theta}\Delta + \mathbf{V}(\theta) + e^{-\theta}\check{H}_n. \tag{25}$$

The spectrum of $\mathbf{H}_n^0(\theta)$ below 0 consists of isolated eigenvalues and line pieces of absolutely continuous spectrum with an angle $\nu = \Im\theta$ with respect to the real line.

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The spectrum of $\mathbf{H}_n^0(\theta)$ below 0 consists of isolated eigenvalues and line pieces of absolutely continuous spectrum with an angle $\nu = \Im\theta$ with respect to the real line.

That the eigenvalues are isolated is a consequence of the infrared cutoff. The distance of each one of these isolated eigenvalues to the rest of the spectrum is of order σ_n.

- Since the eigenvalues of $\mathbf{H}_n(\theta)$ are isolated, we can use standard perturbation theory for every $n \in \mathbb{N}$ to estimate the eigenvalues of $\mathbf{H}_n(\theta)$ and the resolvent operator, for small values of the coupling constant g.
- The possible values of the coupling constant that permit us to use perturbation theory go to zero as n tends to infinity, since the distance of the eigenvalues to the rest of the spectrum goes to zero as n goes to ∞.
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We conclude the following:

Theorem (Induction Basis)

Properties (i)-(iv) are valid for the case $m = 0$.

The important estimation is item (iii):

$$\|\overline{P}_0 \frac{1}{\mathbf{H}_0(\theta) - z}\| \leq \mathbf{C}^{0+1} \frac{1}{\tau(\nu)\sigma_0 + |z - E_0|}, \tag{26}$$

the other properties are deduced once this one is established. The constant $\mathbf{C} > 1$ is an error produced by the fact that $\mathbf{H}_0(\theta)$ is non-selfadjoint. Otherwise we can use functional calculus and bound the resolvent by the inverse of the distance to the spectrum.

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We construct E_{n+1} and prove the corresponding inequality for $n+1$.

We fix z with

$$|z - E_n| = \frac{\tau(\nu)}{10}\sigma_{n+1}.$$

We define

$$\widetilde{\mathbf{H}}_n := \mathbf{H}_n(\theta) \otimes 1_{\mathcal{F}_{n+1,n}} + e^{-\theta} 1_{\mathcal{H}_n} \otimes \check{H}_{n+1,n},$$
$$\widetilde{\mathbf{R}}_n(z) = \left(\widetilde{\mathbf{H}}_n - z\right)^{-1}, \tag{28}$$

and

$$\widetilde{\mathbf{P}}_n = \mathbf{P}_n \otimes P_{\Omega_{n+1,n}}, \qquad \overline{\widetilde{\mathbf{P}}_n} = 1 - \widetilde{\mathbf{P}}_n \,. \tag{29}$$

We omit in general the dependence on θ:

$$\mathbf{H}_J \equiv \mathbf{H}_J(\theta), \qquad J \in \{n, n+1\} \,.$$

Lemma

$$\|\widetilde{\mathbf{R}}_n(z)\overline{\widetilde{\mathbf{P}}_n}\| \leq \frac{2(\mathbf{C}^{n+1}+2)}{\tau(\nu)} \frac{1}{\tau(\nu)\sigma_{n+1} + |z - E_n|} \,. \tag{30}$$

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$$W_{n+1}^{n} := \mathbf{H}_{n+1} - \widetilde{\mathbf{H}}_{n} \, . \tag{31}$$

Theorem

There is a constant $\mathbf{C}_{(1)}$ such that

$$\|(1+|x|^2)^{-1} W_{n+1}^{n} \widetilde{\mathbf{R}}_n(z)\| \leq \mathbf{C}_{(1)} g \mathbf{C}^{n+1} \sigma_n \, , \tag{32}$$

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We estimate them by

$$(1+|x|^2)^{-1}|e^{-ig^{2/3}\vec{k}\cdot x} - 1| \leq \frac{|x|}{(1+|x|)^2}|k| \leq |k|.$$

The factor $|k|$ produces a σ_n in the infrared regime.
Having the -1 subtracted from $e^{-ig^{2/3}\vec{k}\cdot x}$ is the actual reason to apply the Pauli-Fierz transformation.

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To estimate the resolvent

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one would use Neumann Series:

$$\frac{1}{\mathbf{H}_{n+1}(\theta) - z} = \frac{1}{\mathbf{H}_{n+1}(\theta) - z} \sum_{j=0}^{\infty} \left[W_{n+1}^{n} \frac{-1}{\mathbf{H}_{n+1}(\theta) - z} \right]^{j}$$

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$$\sigma_n = \mathcal{B}^n \sigma_0$$

is exponentially decreasing.

Choosing $\mathcal{B}$ small enough we can have

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which makes the solution of the problem possible, but using an indirect argument by the Feshbach map.

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  Whenever we have the term

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- How:

  We change the Hilbert space by another one in which all functions are exponentially decaying in the electron variable.

- Which concrete mathematical object permit us to do that?

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The Use of the Feshbach Map

The main properties that we use are the following:

- $$(F(\mathbf{H}_{n+1} - z))^{-1} = \mathbf{P}(\mathbf{H}_{n+1} - z)^{-1}\mathbf{P}\,. \tag{34}$$

- $$(\mathbf{H}_{n+1} - z)^{-1} = Q(F(\mathbf{H}_{n+1} - z))^{-1}Q^{\#} + (\overline{\mathbf{P}}\mathbf{H}_{n+1}\overline{\mathbf{P}} - z)^{-1}\,, \tag{35}$$

where

$$Q := \mathbf{P} - (\overline{\mathbf{P}}\mathbf{H}_{n+1}\overline{\mathbf{P}} - z)^{-1}\mathbf{H}_{n+1}\mathbf{P} \tag{36}$$

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The existence of $(\mathbf{H}_{n+1} - z)^{-1}$ follows from the existence of $(F(\mathbf{H}_{n+1} - z))^{-1}$. As the operator $(\overline{\mathbf{P}}\mathbf{H}_{n+1}\overline{\mathbf{P}} - z)^{-1}$ can be controlled uniformly as in n goes to infinity, estimating $(\mathbf{H}_{n+1} - z)^{-1}$ amounts to estimate $(F(\mathbf{H}_{n+1} - z))^{-1}$.

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Why is

$$(F(\mathbf{H}_{n+1} - z))^{-1}$$

more easy to handle than

$$(\mathbf{H}_{n+1} - z)^{-1}$$

?

We define

$$W^F_{n+1,n} := F(\mathbf{H}_{n+1} - z) - F(\widetilde{\mathbf{H}}_n - z).$$

We compute $(F(\mathbf{H}_{n+1} - z))^{-1}$ using Neumann series:

$$(F(\mathbf{H}_{n+1} - z))^{-1} = \frac{1}{F(\widetilde{\mathbf{H}}_n - z)} \sum_{l=0}^{\infty} \left[W^F_{n+1,n} \frac{-1}{F(\widetilde{\mathbf{H}}_n - z)} \right]^l,$$

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Using the properties of the Feshbach map we estimate

$$\| W^F_{n+1,n} \frac{-1}{F(\widetilde{\mathbf{H}}_n - z)} \| \leq$$

$$\| \mathbf{P} W^n_{n+1} \mathbf{P} \frac{1}{\widetilde{\mathbf{H}}_n - z} \mathbf{P} \| + \| \mathbf{P} W^n_{n+1} (\overline{\mathbf{P}} \mathbf{H}_{n+1} \overline{\mathbf{P}} - z)^{-1} \| \cdot \| \mathbf{W}_{n+1} \mathbf{P} \frac{1}{\widetilde{\mathbf{H}}^n - z} \mathbf{P} \|$$

$$+ \| \mathbf{P} e^{\beta \langle x \rangle} \| \cdot \| e^{-\beta \langle x \rangle} \mathbf{W}_n (\overline{\mathbf{P}} \mathbf{H}_{n+1} \overline{\mathbf{P}} - z)^{-1} e^{\beta \langle x \rangle} \|$$

$$\cdot \| e^{-\beta \langle x \rangle} W^n_{n+1} \frac{1}{\mathbf{P} \widetilde{\mathbf{H}}_n \mathbf{P} - z} \| \cdot \| \mathbf{W}_{n+1} \mathbf{P} \frac{1}{\widetilde{H}_n - z} \mathbf{P} \|$$

$$+ \| \mathbf{P} \mathbf{W}_n \frac{1}{\overline{\mathbf{P}} \widetilde{H}_n \overline{\mathbf{P}} - z} \| \cdot \| W^n_{n+1} \mathbf{P} \frac{1}{\widetilde{H}_n - z} \mathbf{P} \|$$

$$\leq \mathbf{C}_{(2)} g \mathbf{C}^{n+1} \sigma_n \,,$$

which implies, together with the Neumann series, that $F(\mathbf{H}_{n+1} - z)$ is invertible and that

$$\left\| \frac{1}{F(\mathbf{H}_{n+1} - z)} \right\| \leq \mathbf{C}_{(3)} \mathbf{C}^{n+1} \frac{1}{\tau(\nu)\sigma_{n+1} + |z - E_n|} . \tag{38}$$

From the Feshbach Map to the original Hamiltonian

Once we establish the invertibility of the Feshbach map $F(\mathbf{H}_{n+1} - z)$, we conclude that $\mathbf{H}_{n+1} - z$ in invertible and

$$\|(\mathbf{H}_{n+1} - z)^{-1}\| = \|Q(F(\mathbf{H}_{n+1} - z))^{-1} Q^{\#}\| + \|(\overline{\mathbf{P}}\mathbf{H}_{n+1}\overline{\mathbf{P}} - z)^{-1}\|$$

$$\leq \mathbf{C}_{(4)} \mathbf{C}^{n+1} \frac{1}{\tau(\nu)\sigma_{n+1} + |z - E_n|}. \tag{39}$$

And similarly, using the Feshbach map we obtain

$$\|(\mathbf{H}_{n+1} - z)^{-1} - (\widetilde{\mathbf{H}}_n - z)^{-1}\| \leq \mathbf{C}_{(5)} (\mathbf{C}^2)^{n+1} \frac{1}{\sigma_{n+1}^{1/2}}. \tag{40}$$

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Final Estimates:

Completion of the

Induction Step

We integrate (40) over a (small) path γ surrounding E_n to obtain

$$\|P_{n+1} - \widetilde{P}_n\| = \left\| \frac{1}{2\pi i} \int_\gamma (\mathbf{H}_{n+1} - z)^{-1} - (\widetilde{\mathbf{H}}_n - z)^{-1} \right\| \leq \mathbf{C}_{(5)} (\mathbf{C}^2)^{n+1} \sigma_n^{1/2} < 1\,, \tag{41}$$

which proves the existence of the (simple) eigenvalue E_{n+1}. Let ψ be an eigenvalue of $\mathbf{H}_n$. Using that

$$E_{n+1} = \frac{\langle\psi|\ \mathbf{H}_{n+1} P_{n+1}\psi\rangle}{\langle\psi|\ P_{n+1}\psi\rangle} \tag{42}$$

we obtain that

$$|E_{n+1} - E_n| \leq \mathbf{C}_{(6)} \mathbf{C}^{n+1} g \sigma_n^2. \tag{43}$$

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Using (39) and (43) we get that for $|z - E_n| = \frac{\tau(\nu)}{10}\sigma_{n+1}$,

$$\|(\mathbf{H}_{n+1} - z)^{-1}\| \leq \mathbf{C}_{(7)}\mathbf{C}^{n+1} \frac{1}{\tau(\nu)\sigma_{n+1} + |z - E_{n+1}|}, \tag{44}$$

which implies that for such z

$$\|\overline{\mathbf{P}}_{n+1}(\mathbf{H}_{n+1} - z)^{-1}\| \leq \mathbf{C}_{(8)}\mathbf{C}^{n+1} \frac{1}{\tau(\nu)\sigma_{n+1} + |z - E_{n+1}|}. \tag{45}$$

As the operator on the left hand side is analytic in z, by the maximum modulus principle, the same inequality holds for $z \leq \frac{\tau(\nu)}{10}\sigma_{n+1}$.

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Taking

$$\mathbf{C} > \mathbf{C}_{(1)} + \cdots + \mathbf{C}_{(8)}$$

we achieve the induction step with

$$\|\overline{\mathbf{P}}_{n+1}(\mathbf{H}_{n+1} - z)^{-1}\| \leq \mathbf{C}^{n+2} \frac{1}{\tau(\nu)\sigma_{n+1} + |z - E_{n+1}|} . \qquad (46)$$

Construction of the Resonant Eigenvalue

It is clear from the induction construction that the sequence of eigenvalues $\{E_n\}_{n\in\mathbb{N}}$ converges. We define

$$E_\infty := \lim_{n\to\infty} E_n. \tag{47}$$

Let ϕ_{el} be a normalized eigenvector of the atom Hamiltonian corresponding to the first excited eigenvalue e_1. We define the sequence of vectors

$$\psi_n := P_n \phi_{el}. \tag{48}$$

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We define

$$\widetilde{\mathbf{H}}^n_\infty := \mathbf{H}_n(\theta) \otimes 1_{\mathcal{F}_{\infty,n}} + e^{-\theta} 1_{\mathcal{H}_n} \otimes \check{H}_{\infty,n},$$
$$\widetilde{\mathbf{R}}^n_\infty(z) = \left(\widetilde{\mathbf{H}}^n_\infty - z\right)^{-1}, \tag{50}$$

We select some $z_n \in \mathcal{E}_{(n,\infty)}$ with $|z_n - E_n| = \sigma_n$ and compute

$$\mathbf{H}_\infty \psi_n = (\widetilde{\mathbf{H}}^n_\infty + W^n_\infty)\psi_n = E_n\psi_n + (z_n - E_n) W^n_\infty \widetilde{\mathbf{R}}^n_\infty(z)\psi_n \,. \tag{51}$$

Thus we have that

$$\|\mathbf{H}_\infty \psi_n - E_n\psi_n\| \le (\mathbf{C})^{n+2}\sigma_n \,, \tag{52}$$

which implies that

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which implies that

$$\lim_{n\to\infty} \mathbf{H}_\infty \psi_n = E_\infty \psi_\infty \, . \tag{53}$$

Moreover, since

$$\lim_{n \to \infty} \psi_n = \psi_\infty \tag{54}$$

and $\mathbf{H}_\infty$ is closed, we conclude that ψ_∞ belongs to the domain of $\mathbf{H}_\infty$ and that

$$\mathbf{H}_\infty \psi_\infty = E_\infty \psi_\infty \, , \tag{55}$$

which proves the statement.

$\square$