Ground State Properties in non-relativistic QED

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Contents

How do the ground state energy and the ground state of non-relativistic qed depend on coupling constants of the system?

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1. Non-relativistic qed

We introduce the symmetric Fock space over the Hilbert space $\mathfrak{h} := L^2(\mathbb{R}^3 \times \mathbb{Z}_2)$:

$$\mathcal{F}(\mathfrak{h}) := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathcal{F}^{(n)}(\mathfrak{h}) \quad , \quad \mathcal{F}^{(n)}(\mathfrak{h}) := S_n(\mathfrak{h}^{\otimes n}),$$

with S_n = orthogonal projection onto the subspace of totally symmetric tensors in $\mathfrak{h}^{\otimes n}$.
Vacuum vector: $\Omega = (1, 0, \cdots)$.
Introduce creation $a^*(k, \lambda)$ and annihilation $a(k, \lambda)$ operators satisfying canonical commutation relations,

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

for all $(k,\lambda),(k',\lambda') \in \mathbb{R}^3 \times \mathbb{Z}_2$ ($a^\#$ stands for a or a^*).

The Hilbert space and Hamiltonian are

$$\mathcal{H} := \mathcal{H}_{\rm at} \otimes \mathcal{F}(\mathfrak{h}), \quad \mathcal{H}_{\rm at} := L^2_a((\mathbb{R}^3 \times \mathbb{Z}_2)^N)$$

$$H_g := \sum_{j=1}^{N} (\{p_j + gA(x_j)\} \cdot \sigma_j)^2 + V(x_1, ..., x_N) \otimes 1 + 1 \otimes H_f,$$

with $x_j \in \mathbb{R}^3$, $p_j = -i\nabla_{x_j}$, σ_j Pauli-matrix acting on the j-th particle, and V denotes a potential. The quantized vector potential is

$$A(x) = \sum_{\lambda=1,2} \int_{\mathbb{R}^3} \frac{\kappa(k) d^3k}{\sqrt{2|k|}} \varepsilon_\lambda(k) \left(e^{ik\cdot x} a(k,\lambda) + e^{-ik\cdot x} a^*(k,\lambda) \right),$$

where $\varepsilon_1(k), \varepsilon_2(k), k/|k|$ form an orthonormal triplet in $\mathbb{R}^3$, and κ serves as an ultraviolet (UV) cutoff (assume $\kappa(k) = 1_{|k| \leq \Lambda}$, $\Lambda > 0$). The operator of the free field energy is

$$H_f = \sum_{\lambda=1,2} \int d^3k |k| a^*(k,\lambda) a(k,\lambda).$$

Ground State

For $g = 0$, the Hamiltonian is of the form

$$H_0 = H_{\mathrm{at}} \otimes 1 + 1 \otimes H_f \ ,$$

where $H_{\mathrm{at}} := \sum_{j=1}^{N} p_j^2 + V = -\Delta + V$.

Assumption: The potential V is symmetric with respect to the interchange of particle coordinates and satisfies the following assumptions:

(1) V is infinitesimally small with respect to the Laplacian $-\Delta$.

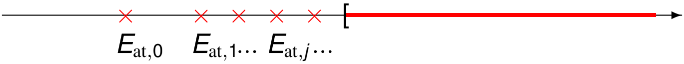
(2) $\inf \sigma(H_{\mathrm{at}})$ is an isolated eigenvalue of H_{at} with finite multiplicity.

Example: A potential describing an atom (or a molecule with static nuclei) satisfies these assumptions. E.g.

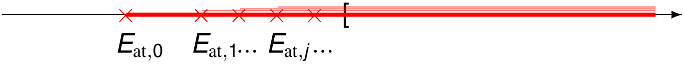
$$V(x_1, ..., x_N) = -\sum_{j=1}^{N} \frac{Z}{|x_j|} + \sum_{1 \leq i < j \leq N} \frac{1}{|x_j - x_i|}$$

with $N = Z$ satisfies (1) and (2).

- Spectrum of H_{at}:



- Spectrum of H_0:



- Spectrum of H_g for $g \neq 0$:

Theorem (Bach-Fröhlich-Sigal '99, Griesemer- Lieb- Loss '01)

The number

$$E_g := \inf \sigma(H_g)$$

is an eigenvalue of H_g.

2. Analyticity in the minimal coupling constant g

Theorem 1 (H- Herbst '10, H-Lange '14)

Suppose $E_0 := \inf \sigma(H_{\rm at})$ *is a non-degenerate eigenvalue of* $H_{\rm at}$ *or* E_0 *satisfies the symmetry Hypothesis (S) stated below.*
Then there exists a $g_0 > 0$ *such that for all*

$$g \in D_{g_0} := \{ z \in \mathbb{C} | |z| < g_0 \}$$

the Hamiltonian H_g *has an eigenvalue* E_g *with eigenvector* ψ_g *and eigenprojection* P_g *satisfying:*

(i) $E_g = \inf(\sigma(H_g)$ *for* $g \in \mathbb{R} \cap D_{g_0}$,

(ii) $P_g^* = P_{\overline{g}}$ *for* $g \in D_{g_0}$,

(iii) $g \mapsto E_g$, $g \mapsto \psi_g$, *and* $g \to P_g$ *are analytic on* D_{g_0}.

The Theorem holds also for electrons without spin.

Hypothesis (S). There exists a group, $\mathcal{S}$, of symmetries of the Hamiltonian H_g (unitary or anti-unitary transformations commuting with all terms of H_g) such that

(i) $\mathcal{S}$ acts irreducibly on the eigenspace of H_0 with eigevalue E_0.

(ii) $\mathcal{S}$ commutes with the following operator

$$F := \sum_j \sum_{\lambda=1,2} \int f_{x_j,\lambda} a^*(k,\lambda) \frac{dk}{|k|^{1/2}} + h.c.$$

$$f_{x,\lambda}(k) := e^{-ik\cdot x} \kappa(k) \frac{x \cdot \varepsilon_\lambda(k)}{(1+|k||x|^2)^{1/2}}$$

(F is a generator of a so called generalized Pauli-Fierz transformation.)

Example:

- Hydrogen atom with spin 1/2-electron: $\mathcal{S}$ generated by time reversal symmetry.
- Atom with spinless electrons: $\mathcal{S} =$ group of rotations

Corollary

Suppose the assumptions of Theorem 1 hold. Then Rayleigh-Schrödinger perturbation theory is valid.

Remark: The existence of an asymptotic expansion has been shown by Hainzl-Seiringer '03, Barbaroux-Chen-Vougalter-Vougalter '10, Arai '13, ...

Remark. If the ground state is degenerate and the assumptions of Hypothesis (S) do not hold, it is natural to expect that the degeneracy is lifted at higher orders in perturbation theory. (Bach-Fröhlich-Sigal '98, Amour-Faupin '14, ...)

Remark. There exists a generalization of Theorem 1 to resonances.

3. Proof

The proof of Theorem 1 is based on operator theoretic renormalization analysis (RG) as introduced by V. Bach, J. Fröhlich, and I.M. Sigal '98.

(1) *Generalized Pauli-Fierz Transformation.* Use a generalized Pauli-Fierz transformation to control the infrared singularity.

(2) *Extend RG analysis.* Extend operator theoretic renormalization to "matrix-valued" operators acting on Fock-space.

(3) *RG preserves analyticity.* If the original Hamiltonian is analytic in g and the RG analysis converges, then also the ground state and the ground state energy are analytic functions of g.
(H-Griesemer '09)

Generalized Pauli-Fierz transformation

To improve the infrared behaviour, define

$$\hat{H}_g := e^{-iFg} H_g e^{iFg} = \sum_{j=1}^{N} (\{p_j - gA_1(x_j)\} \cdot \sigma_j)^2 + V \otimes 1 + 1 \otimes H_f$$
$$+ \text{ total number of } a\text{'s or } a^*\text{'s is at most two },$$

where

$$A_1(x) = \sum_\lambda \int \left(e^{-ik\cdot x} \varepsilon_\lambda(k)\kappa(k) - \nabla_x f_{x,\lambda}(k)\right) a^*_\lambda(k) \frac{d^3k}{|k|^{1/2}} + h.c.$$

Lemma

Let $\hat{\psi}_g$ be an eigenstate of $\hat{H}_g$ with eigenvalue E_g. Then

$$\psi_g := e^{iFg} \hat{\psi}_g$$

is an eigenvector of H_g with eigenvalue E_g. If $g \mapsto \hat{\psi}_g$ is analytic in a neighborhood of zero, then so is $g \mapsto \psi_g$.

RG-Analysis: Feshbach projection

Let

- H be an operator in a Hilbert space $\mathcal{H}$,
- P be a self adjoint projection in $\mathcal{H}$ and $\bar{P} = 1 - P$,
- $H_{\bar{P}} := \bar{P} H \bar{P}$ be invertible on the range of $\bar{P}$.

$$\begin{bmatrix} 1 & 0 \\ -PH\bar{P}H_{\bar{P}}^{-1} & 1 \end{bmatrix} \underbrace{\begin{bmatrix} PHP & PH\bar{P} \\ \bar{P}HP & \bar{P}H\bar{P} \end{bmatrix}}_{=H} \begin{bmatrix} 1 & 0 \\ -H_{\bar{P}}^{-1}\bar{P}HP & 1 \end{bmatrix} = \begin{bmatrix} F_P(H) & 0 \\ 0 & H_{\bar{P}} \end{bmatrix}$$

where $F_P(H) := PHP - PH\bar{P}H_{\bar{P}}^{-1}\bar{P}HP : \mathrm{Ran} P \to \mathrm{Ran} P$.
Define the auxiliary operator $Q := P - H_{\bar{P}}^{-1}\bar{P}HP : \mathrm{Ran} P \to \mathcal{H}$.

Lemma

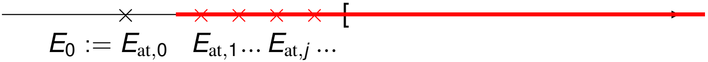
If $F_P(H)\varphi = 0$ and $\varphi \neq 0$, then $HQ\varphi = 0$ and $Q\varphi \neq 0$.

Initial decimation step

For simplicity assume $E_{\mathrm{at},1} - E_{\mathrm{at},0} = 1$ and that κ is infrared regular.

- $P = P_{\mathrm{at}} \otimes 1_{(H_f \leq 3/4)}$
- P_{at} = projection onto the ground state of H_{at}
- $H = H_g - z$, with z close to E_0 and g small.

Spectrum of $H_0 \upharpoonright \mathrm{Ran}\overline{P}$:



Lemma 1

For $z \in \mathbb{C}$ with $|E_0 - z| \leq 1/2$ the Feshbach operator

$$H^{(0)}(g,z) := F_P(H_g - z) \upharpoonright \mathrm{Ran} P \qquad (1)$$

is well defined if $|g|$ is sufficiently small, analytic as a function of g and z, and commutes with $\mathcal{S}$.

We say that $A \in \mathcal{L}(\mathrm{Ran} P)$ commutes with $\mathcal{S}$ if for all $S \in \mathcal{S}$ we have

$$SAS^* = \begin{cases} A, & \text{if } S \text{ is unitary} \\ A^*, & \text{if } S \text{ is anti-unitary .} \end{cases}$$

It follows that also

$$\langle H^{(0)}(g,z)\rangle_\Omega ,$$

where

$$\langle A \rangle_\Omega := (1_{\mathrm{Ran} P_{\mathrm{at}}} \otimes |\Omega\rangle\langle\Omega|) \;\; A \;\; (1_{\mathrm{Ran} P_{\mathrm{at}}} \otimes |\Omega\rangle\langle\Omega|),$$

commutes with $\mathcal{S}$. This implies by Schurs lemma that

$$\langle H^{(0)}(z,g)\rangle_\Omega = c(z,g)(1_{\mathrm{Ran} P_{\mathrm{at}}} \otimes |\Omega\rangle\langle\Omega|)$$

for some number $c(z,g) \in \mathbb{C}$.

Expanding the resolvent

If $|g|$ is sufficiently small, we may expand the resolvent in (1) in a Neumann series and express it in terms of integral kernels $\underline{w}^{(0)}(g,z)$:

$$H^{(0)}(g,z) = \sum_{m+n \geq 0} H_{m,n}(\underline{w}^{(0)}(g,z)),$$

where $\underline{w} = (w_{m,n})_{m+n \geq 0}$ and

$$w_{m,n} : [0,1] \times (B_1 \times \mathbb{Z}_2)^{m+n} \to \mathcal{L}(\mathrm{Ran} P_{\mathrm{at}}), \quad B_1 := \{k \in \mathbb{R}^3 | |k| \leq 1\}.$$

$$H_{m,n}(\underline{w}) := P \sum_{\lambda' s} \int_{B_1^{m+n}} \left(\prod_{j=1}^{m} a^*(k_j, \lambda_j) \right) w_{m,n}(H_f, k_{m,n}) \left(\prod_{j=1}^{n} a(k_j, \lambda_j) \right) \left(\prod_{j=1}^{m+n} \frac{d^3 k_j}{|k_j|^{1/2}} \right) P$$

$$k_{m,n} := (k_1, \lambda_1, ..., k_{m+n}, \lambda_{m+n})$$

Banach Space of Integral Kernels

- Let $\mathcal{W}_{m,n}$ denote the Banach space of kernels $w_{m,n}$ with norm

$$\|w_{m,n}\|_{\mathcal{W}_{m,n}} := \|w_{m,n}\|_0 + \|w'_{m,n}\|_0 \quad \text{where}$$
$$\|w_{m,n}\|_0 := \max_j \sup_{r \in [0,1], k_{m,n} \in B_1^{m+n}} \left\| |k_j|^{-1/2} w_{m,n}(r; k_{m,n}) \right\|_{\mathcal{L}(\mathrm{Ran} P_{\mathrm{at}})} .$$

- Define the Banach space of sequences of kernels $\underline{w} = (w_{m,n})_{m+n \geq 0}$ for some $\xi \in (0,1)$ by:

$$\mathcal{W}_\xi := \bigoplus_{m+n\geq 0} \mathcal{W}_{m,n} \qquad \|\underline{w}\|_\xi = \sum_{m+n\geq 0} \xi^{-(m+n)} \|w_{m,n}\|_{\mathcal{W}_{m,n}}$$

- Define the Polydiscs in $\mathcal{W}_\xi$ (neighborhoods of "H_f"):

$$\mathcal{D}_\xi(\alpha, \beta, \gamma) := \Big\{ \sum_{m,n} H(\underline{w}_{m,n}) : \underline{w} \in \mathcal{W}_\xi, \|w_{0,0}\|_{\mathcal{L}(\mathrm{Ran} P_{\mathrm{at}})} \leq \alpha,$$
$$\sup_{r\in[0,1]} \|\partial_r w_{0,0}(r) - 1\|_{\mathcal{L}(\mathrm{Ran} P_{\mathrm{at}})} \leq \beta, \ \|(w_{m,n})_{m+n\geq 1}\|_\xi \leq \gamma \Big\}$$

Renormalization

Lemma 2

Fix $\xi \in (0,1)$. Then for all $\alpha, \beta, \gamma > 0$ there exists a $g_0 > 0$ such that

$$H^{(0)}(g,z) - \langle H^{(0)}(g,z) \rangle_\Omega \in \mathcal{D}_\xi(\alpha, \beta, \gamma),$$

provided $|g| \leq g_0$ and $|z - E_0| \leq 1/2$.

Theorem 1 now follows from Lemma 1 and Lemma 2 using operator theoretic renormalization (Griesemer-H '09) using the additional properties:

1. Each renormalization step preserves the symmetry.
2. Vacuum expectations are multiples of the identity.

4. Applications: Expansions in the fine structure constant α

First consider the UV cutoff to be of the order of the rest energy of the electron.

$$H_\alpha = (p + \alpha^{1/2} A_\Lambda(x))^2 - \frac{\alpha}{|x|} + H_f .$$

The ground state energy has the following expansion as $\alpha \downarrow 0$,

$$\inf \sigma(H_\alpha) = -\frac{1}{4}\alpha^2 + E^{(1)}\alpha^3 + E^{(2)}\alpha^4 + E^{(3)}\alpha^5 \log \alpha + o(\alpha^5 \log \alpha).$$

Bethe '47, Hainzl-Seiringer '03,
Barbaroux-Chen-Vugalter-Vougalter '09

Now we consider the UV cutoff to be of the order of the Rydberg energy ($\sim$ binding energy of the bare hydrogen atom $\sim \alpha^2$).

$$
\begin{aligned}
H(\alpha) &= (p + \alpha^{3/2} A_\Lambda(\alpha x))^2 - \frac{1}{|x|} + H_f \\
&\cong \alpha^{-2} \left((p + \alpha^{1/2} A_{\alpha^2 \Lambda}(x))^2 - \frac{\alpha}{|x|} + H_f \right)
\end{aligned}
$$

An asymptotic expansion of the ground state energy and ground state was obtained by Bach-Fröhlich-Pizzo '07.

Theorem 2 (H-Herbst '10)

(i) *There exists an* $\alpha_0 > 0$*, such that for all* $\alpha \in [0, \alpha_0)$*, the Hamiltonian* $H(\alpha)$ *has a ground state* $\psi(\alpha^{1/2})$ *and ground state energy* $E(\alpha)$ *with the convergent expansions,*

$$\psi(\alpha^{1/2}) = \sum_{n=0}^{\infty} c_\alpha^{(n)} \alpha^{3n/2}, \qquad E(\alpha) = \sum_{n=0}^{\infty} E_\alpha^{(n)} \alpha^{3n}.$$

The coefficients $c_\alpha^{(n)}$ *and* $E_\alpha^{(n)}$ *are uniformly bounded in* $\alpha \geq 0$*.*
(ii) *For every* $k \in \mathbb{N}$ *there exists an* $\alpha_0^{(k)} > 0$*, such that that* $\psi(\cdot), E(\cdot)$ *are* k*-times continuously differentiable on the interval* $[0, \alpha_0^{(k)})$*.*
(iii) *There exist formal power series with constant coefficients such that*

$$\psi(\alpha^{1/2}) \sim \sum_{n=0}^{\infty} c_n \alpha^{n/2}, \qquad E(\alpha) \sim \sum_{n=0}^{\infty} E_n \alpha^n.$$

Proof of Theorem 2

(1) We study the Hamiltonian

$$H_{g,\beta} = (p + gA_\Lambda(\beta x))^2 - \frac{1}{|x|} + H_f.$$

If we set $g = \alpha^{3/2}$ and $\beta = \alpha$, then $H(\alpha) = H_{\alpha^{3/2},\alpha}$.

(2)

• Let $\psi_g(\beta)$ be the eigenvector of $H_{g,\beta}$ with eigenvalue $E_g(\beta)$ at the bottom of the spectrum (Theorem 1).

• Using an RG-analysis we show that for any $k \in \mathbb{N}$, there exists a positive $g_0^{(k)}$, such that on $D_{g_0^{(k)}}$

$$g \mapsto E_g(\cdot), \quad g \mapsto \psi_g(\cdot)$$

is a $C^k(\mathbb{R})$–valued respectively $C^k(\mathbb{R};\mathcal{H})$–valued analytic function.

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Outlook

• Degenerate eigenvalues, for which the degeneracy is not protected by a symmetry.

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Proof (Suppose $\kappa(k) = 1_{|k| \leq \Lambda}$, $\Lambda > 0$) Since $g \mapsto \hat{\psi}_g$ is analytic, we have in a neighborhood of zero a convergent power series expansion

$$\hat{\psi}_g = \sum_n a_n g^n.$$

where the coefficients can be obtained by equating coefficients of

$$H_g \hat{\psi}_g = E_g \hat{\psi}_g.$$

This implies that a_n contains at most n photons with momenta having absolute value less than Λ and estimate for some constant C_F depending only on F, that

$$\|F^k a_n\| \leq \sqrt{\frac{(k+n)!}{n!}} C_F^k \|a_n\|$$

This implies that the double series converges absolutely

$$\sum_{k=0}^{\infty} \sum_{n=0}^{\infty} \frac{(-igF)^k}{k!} a_n g^n \tag{2}$$

converges absolutely, since t
hen

$$e^{-igF(x)}\hat{\psi}_g = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\frac{(-igF)^k}{k!}a_n g^n,$$

and the right hand side is analytic function of g. To show that (2) converges absolutely, we use that a_n can contain at most n photons with momenta having absolute value less than Λ, Inserting this we arrive at

$$\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\|\frac{(-igF)^k}{k!}a_n g^n\| \leq \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\frac{|g|^k}{k!}C_F^k\sqrt{\frac{(n+k)!}{n!}}\|a_n\||g|^n$$

$$\leq \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\frac{|g|^k}{k!}((2n)^{k/2}+(2k)^{k/2})C_F^k\|a_n\||g|^n$$

$$\leq \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\frac{|g|^k}{k!}(2n)^{k/2}C_F^k\|a_n\||g|^n + \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\frac{|g|^k}{k!}(2k)^{k/}$$

$$\leq \sum_{k=0}^{\infty}\frac{|g|^k}{k!}C_F^k\sum_{n=0}^{\infty}(2n)^{k/2}\|a_n\||g|^n + \sum_{k=0}^{\infty}\frac{|g|^k}{k!}(2k)^{k/2}C_F^k$$