On spectral and scattering theories of non-relativistic QED

Jérémy Faupin

Université de Lorraine

January 2016
IMSc Chennai, Indo-French Conference

Outline of the talk

Part I

The model

Some references

- C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg. Photons et atomes. Edition du CNRS, Paris, (1988).
- C. Cohen-Tannoudji, J. Dupont-Roc, and G. Grynberg. Processus d'interaction entre photons et atomes. Edition du CNRS, Paris, (1988).
- E. Fermi, Quantum theory of radiation, Rev. Mod. Phys., 4, 87-132, (1932).
- W. Pauli and M. Fierz, Zur Theorie der Emission langwel liger Lichtquanten, II, Nuovo Cimento 15, 167-188, (1938).
- H. Spohn. Dynamics of charged particles and their radiation field. Cambridge University Press, Cambridge, (2004).

Physical system and model

Physical System

• Non-relativistic matter : atom, ion or molecule composed of non-relativistic quantum charged particles (electrons and nuclei)

• Interacting with the quantized electromagnetic field, i.e. the photon field

Standard model of non-relativistic QED

• Obtained by quantizing the Newton equations (for the charged particles) minimally coupled to the Maxwell equations (for the electromagnetic field)

• Restriction : charge distributions are localized in small, compact sets. Corresponds to introducing an ultraviolet cutoff that suppresses the interaction between the charged particles and the high-energy photons

• Goes back to the early days of Quantum Mechanics (Fermi, Pauli-Fierz)

• Largely studied in theoretical physics (see e.g. books by Cohen-Tannoudji, Dupont-Roc and Grynberg)

Description of the atomic system

Simplest atomic system

- Hydrogen atom with an infinitely heavy nucleus fixed at the origin
- Spin of the electron neglected
- Units such that $\hbar = c = 1$

Hilbert space and Hamiltonian for the electron

- Hilbert space

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

- Hamiltonian

$$H_{\mathrm{el}} = \frac{p_{\mathrm{el}}^2}{2m_{\mathrm{el}}} + V_\alpha(x_{\mathrm{el}}), \quad V_\alpha(x_{\mathrm{el}}) = -\frac{\alpha}{|x_{\mathrm{el}}|},$$

where $p_{\mathrm{el}} = -i\nabla_{x_{\mathrm{el}}}$, m_{el} is the electron mass, and $\alpha = e^2$ is the fine-structure constant ($\alpha \approx 1/137$)

- H_{el} is a self-adjoint operator in $\mathrm{L}^2(\mathbb{R}^3)$ with domain

$$\mathcal{D}(H_{\mathrm{el}}) = \mathcal{D}(p_{\mathrm{el}}^2) = \mathrm{H}^2(\mathbb{R}^3)$$

Spectrum of the electronic Hamiltonian

Spectrum of H_{el}

- Infinite increasing sequence of negative, isolated eigenvalues of finite multiplicities $\{e_j\}_{j\in\mathbb{N}}$
- Semi-axis $[0, \infty)$ of absolutely continuous spectrum

Physical picture

Bohr's condition

• Well-known physical picture : the electron may jump from an initial state of energy e_i to a final state of lower energy e_f by emitting a photon of energy $e_i - e_f$

• Need to take into account the interaction between the electron and the photon field in order to capture this picture mathematically

Expected mathematical results

• The ground state energy e_0 is expected to remain an eigenvalue (stability of the system)

• The excited eigenvalues e_j, $j \geq 1$, are expected to turn into resonances associated with metastable states of finite lifetime

• For any initial state, the atomic system is expected to relax to its ground state, as time goes to ∞, by emitting photons propagating freely

Description of the photon field : Hilbert space

n-photons space

- Hilbert space for 1 photon

$$\mathfrak{h} = \mathrm{L}^2(\mathbb{R}^3 \times \{1, 2\})$$

- Hilbert space for n photons

$$\mathcal{F}_s^{(n)}(\mathfrak{h}) = S_n \otimes_{j=1}^n \mathfrak{h},$$

where S_n is the orthogonal projection onto the symmetric subspace

Fock space

- Hilbert space for the photon field = symmetric Fock space over $\mathfrak{h}$,

$$\mathcal{H}_{\mathrm{ph}} = \mathcal{F}_s(\mathfrak{h}) = \bigoplus_{n=0}^{+\infty} \mathcal{F}_s^{(n)}(\mathfrak{h}), \quad \mathcal{F}_s^{(0)} = \mathbb{C}$$

- Vacuum

$$\Omega = (1, 0, 0, \dots)$$

Description of the photon field : second quantization (I)

Second quantization of an operator

Given b an operator acting on the 1-photon space $\mathfrak{h}$, the second quantization of b is the operator on $\mathcal{H}_{\rm ph}$ defined by

$$\mathrm{d}\Gamma(b)|_{\mathbb{C}} = 0,$$
$$\mathrm{d}\Gamma(b)|_{\mathcal{F}_s^{(n)}} = b \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} + \mathbb{1} \otimes b \otimes \cdots \otimes \mathbb{1} + \cdots + \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes b$$

If b is self-adjoint, one verifies that $\mathrm{d}\Gamma(b)$ is essentially self-adjoint. The closure is then denoted by the same symbol

Energy of the free photon field

- $$H_f = \mathrm{d}\Gamma(\omega),$$

where ω is the multiplication operator by the relativistic dispersion relation

$$\omega(k) = |k|$$

- Spectrum

$$\sigma(H_f) = [0, \infty), \quad \sigma_{\rm pp}(H_f) = \{0\}$$

Description of the photon field : creation and annihilation operators

Creation and annihilation operators

- Given $h \in \mathfrak{h}$, the creation operator $a^*(h) : \mathcal{H}_{\mathrm{ph}} \to \mathcal{H}_{\mathrm{ph}}$ is defined for $\Phi \in \mathcal{F}_s^{(n)}$ by

$$a^*(h)\Phi = \sqrt{n+1} S_{n+1} h \otimes \Phi$$

- The annihilation operator $a(h)$ is defined as the adjoint of $a^*(h)$
- $a^*(h)$ and $a(h)$ are closable, their closures are denoted by the same symbols

Canonical commutation relations

$$[a^*(f), a^*(g)] = [a(f), a(g)] = 0,$$
$$[a(f), a^*(g)] = \langle f, g \rangle_{\mathfrak{h}}$$

Notations

$$a^*(f) = \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} f(k,\lambda) a^*_\lambda(k) \mathrm{d}k, \quad a(f) = \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} \bar{f}(k,\lambda) a_\lambda(k) \mathrm{d}k$$

Description of the photon field : field operators

Field operators

Given $h \in \mathfrak{h}$, the field operator $\Phi(h)$ is defined by

$$\Phi(h) = \frac{1}{\sqrt{2}}(a^*(h) + a(h))$$

$\Phi(h)$ is essentially auto-adjoint, its closure is denoted by the same symbol

Standard model of non-relativistic QED : Hamiltonian

Hilbert space for the electron and the photon field

$$\mathcal{H} = \mathcal{H}_{\mathrm{el}} \otimes \mathcal{H}_{\mathrm{ph}} = \mathrm{L}^2(\mathbb{R}^3; \mathcal{H}_{\mathrm{ph}})$$

Pauli-Fierz Hamiltonian

$$H_\alpha = \frac{1}{2m_{\mathrm{el}}}(p_{\mathrm{el}} - \alpha^{\frac{1}{2}} A(x_{\mathrm{el}}))^2 + V_\alpha(x_{\mathrm{el}}) + H_f$$

where, for all $x \in \mathbb{R}^3$,

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

i.e. for all $x \in \mathbb{R}^3$, $A(x) = (A_1(x), A_2(x), A_3(x))$ where $A_j(x)$ is the field operator given by

$$A_j(x) = \Phi(h_j(x)), \quad [h_j(x)](k,\lambda) = \frac{\chi_{\alpha\Lambda}(k)}{\sqrt{|k|}} \varepsilon_{\lambda,j}(k) e^{-ik\cdot x}$$

Standard model of non-relativistic QED : coupling functions

Polarization vectors

$\varepsilon_\lambda(k) = (\varepsilon_{\lambda,1}(k), \varepsilon_{\lambda,2}(k), \varepsilon_{\lambda,3}(k))$, for $\lambda \in \{1,2\}$, are polarization vectors defined such that $(k/|k|, \varepsilon_1(k), \varepsilon_2(k))$ is an orthonormal basis of $\mathbb{R}^3$ for all $k \neq 0$

Ultraviolet cutoff

$\chi_{\alpha\Lambda}$ is an ultraviolet cutoff at energy scale $\alpha\Lambda$ that can be chosen for instance as

$$\chi_{\alpha\Lambda}(k) = \mathbb{1}_{(-\infty,\alpha\Lambda]}(|k|), \quad \text{or} \quad \chi_{\alpha\Lambda}(k) = e^{-\frac{k^2}{\alpha^2\Lambda^2}},$$

where $\Lambda > 0$ is arbitrary large

Theorem

For any $\alpha \geq 0$, $\Lambda \geq 0$, H_α is a self-adjoint operator with domain $\mathcal{D}(H_\alpha) = \mathcal{D}(H_0)$
[Hiroshima, Ann. Henri Poincaré, (2002)]

Standard model of non-relativistic QED : small coupling regime

Scaling transformation

- Fine-structure constant α = small coupling parameter
- Treat the interaction (electron)–(transverse photons) as a perturbation
- Useful to apply a scaling transformation that gives a new Hamiltonian (still denoted by H_α)

$$H_\alpha = \frac{1}{2m_{\mathrm{el}}}(p_{\mathrm{el}} - \alpha^{\frac{3}{2}} A(\alpha x_{\mathrm{el}}))^2 + V(x_{\mathrm{el}}) + H_f$$

where, for all $x \in \mathbb{R}^3$,

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

and

$$V(x_{\mathrm{el}}) = -\frac{1}{|x_{\mathrm{el}}|}$$

Standard model of non-relativistic QED : spectral problems

The non-interacting Hamiltonian H_0

- For $\alpha = 0$, we obtain

$$H_0 = \frac{p_{\mathrm{el}}^2}{2m_{\mathrm{el}}} + V(x_{\mathrm{el}}) + H_f = H_{\mathrm{el}} \otimes \mathbb{1}_{\mathcal{H}_{\mathrm{ph}}} + \mathbb{1}_{\mathcal{H}_{\mathrm{el}}} \otimes H_f$$

- Spectrum : $\sigma(H_0) = \sigma(H_{\mathrm{el}}) + \sigma(H_f)$

Main spectral problems

- Prove that the lowest eigenvalue e_0 remains an eigenvalue, i.e. that $E_\alpha = \inf \sigma(H_\alpha)$ is an eigenvalue of H_α (existence of a ground state)
- Prove that excited eigenvalues e_j turn into resonances associated to metastable states
- Prove that the spectrum of H_α except for E_α is purely absolutely continuous

Standard model of non-relativistic QED : scattering problems

Dynamics

Any initial state $\Phi_0 \in \mathcal{H}$ evolves according to the Schrödinger equation

$$i\partial_t \Phi_t = H_\alpha \Phi_t,$$

i.e.

$$\Phi_t = e^{-itH_\alpha}\Phi_0$$

Main dynamical problems

- Justify that photons propagate at the speed of light (propagation estimates)
- Prove that any initial state asymptotically relaxes to the ground state by emitting photons that propagates freely (asymptotic completeness)

Part II

Results

Existence of a ground state

Theorem

For all $\alpha \geq 0$, $\Lambda \geq 0$, H_α has a ground state, i.e. $E_\alpha := \inf \sigma(H_\alpha)$ is a (simple) eigenvalue of H_α

References

- [Bach, Fröhlich, Sigal, Comm. Math. Phys., 207, (1999)] : small enough α
- [Griesemer, Lieb, Loss, Invent. Math., 145, (2001)] : any α

Previous results for (simpler) related models :

- [Spohn, Lett. Math. Phys., 44, (1998)] : Spin-Boson model
- [Gérard, Ann. I.H.P., 1, (2000)] : Nelson model
- [Hiroshima, J. Math. Phys., 41, (2000)] : abstract model, small enough α

Ingredients of the proof

- Approximation by a family of massive Hamiltonians
- Localization in Fock space
- Compact Sobolev embedding in Fock space

Resonances (I) : Complex dilatations

Unitary scaling transformation

Recall $\mathcal{H} = \mathrm{L}^2(\mathbb{R}^3) \otimes \mathcal{H}_{\mathrm{ph}}$. For $\theta \in \mathbb{R}$, let U_θ be the unitary dilatations operator that implements the transformations

$$x_{\mathrm{el}} \mapsto e^{\theta} x_{\mathrm{el}}, \quad k \mapsto e^{-\theta} k$$

Dilated Hamiltonian

- Write $H_\alpha = H_{\mathrm{el}} + H_f + W_\alpha$
- For $\theta \in \mathbb{R}$, let $H_\alpha(\theta) = U_\theta H_\alpha U_\theta^{-1}$. This gives

$$H_\alpha(\theta) = H_{\mathrm{el}}(\theta) + e^{-\theta} H_f + W_\alpha(\theta), \quad H_{\mathrm{el}}(\theta) = e^{-2\theta} \frac{p_{\mathrm{el}}^2}{2m_{\mathrm{el}}} + V(e^{\theta} x_{\mathrm{el}})$$

- Using assumptions on the coupling function, we can define $H_\alpha(\theta)$ by the same expression, for $\theta \in \mathcal{D}(0, \theta_0) \subset \mathbb{C}$, θ_0 sufficiently small. The family $\theta \mapsto H_\alpha(\theta)$ is then analytic of type (A) in the sense of Kato

Resonances (II)

Theorem

Let $e_j < 0$ be a simple eigenvalue of $H_{\rm el}$. Let $\Lambda \geq 0$. There exists $\alpha_c > 0$ such that, for all $0 \leq \alpha \leq \alpha_c$, there exists a non-degenerate eigenvalue $e_{j,\alpha}$ of $H_\alpha(\theta)$ such that $e_{j,\alpha}$ does not depend on θ (for θ suitably chosen) and

$$e_{j,\alpha} \underset{\alpha \to 0}{\longrightarrow} e_j$$

The eigenvalue $e_{j,\alpha}$ of $H_\alpha(\theta)$ is called a resonance of H_α

References

- [Bach, Fröhlich, Sigal, Adv. Math., 137, (1998)] : confined particles
- [Sigal, J. Stat. Phys., (2009)]
- [Bach, Ballesteros, Pizzo, preprint]

Ingredients of the proof

- Bach-Fröhlich-Sigal spectral renormalization group
- Refined version : iterative application of isospectral Feshbach-Schur maps [Ballesteros, F., Fröhlich, Schubnel, Comm. Math. Phys., (2015)]

Lifetime of metastable states

Theorem

Let $\Lambda \geq 0$. Let $e_j < 0$ be a simple eigenvalue of H_{el} and let φ_j be a normalized eigenstate of H_{el} associated to e_j. There exists $\alpha_c > 0$ such that for all $0 \leq \alpha \leq \alpha_c$ and $t \geq 0$,

$$\left| \left\langle \varphi_j \otimes \Omega, e^{-itH_\alpha} \varphi_j \otimes \Omega \right\rangle \right| = e^{-t\mathrm{Im}(e_{j,\alpha})} + \mathcal{O}(\alpha)$$

References

- [Abou Salem, F., Fröhlich, Sigal, Adv. Appl. Math., 9, (2009)]
- [Hasler, Herbst, Huber, Ann. Henri Poincaré, 43, (2009)]

Ingredients of the proof

- Stone's formula
- Approximation by infrared cutoff Hamiltonians
- Cauchy's theorem

Ionization threshold

Definition

$$\Sigma_\alpha = \lim_{R\to\infty} \inf_{\varphi\in D_R, \|\varphi\|=1} \langle \varphi, H_\alpha \varphi \rangle,$$

with $D_R = \{\varphi \in \mathcal{D}(H_\alpha);\ \varphi(x_{\mathrm{el}}) = 0 \text{ if } |x_{\mathrm{el}}| < R\}$

Theorem

Let $\alpha \geq 0$, $\Lambda \geq 0$. For all $\delta, \xi \in \mathbb{R}$ such that $\xi + \delta^2 < \Sigma_\alpha$,

$$\left\| e^{\delta |x_{\mathrm{el}}|} \mathbb{1}_{(-\infty,\xi]}(H_\alpha) \right\| < \infty$$

References

- [Bach, Fröhlich, Sigal, Comm. Math. Phys., 207, (1999)]
- [Griesemer, J. Funct. Anal., 2, (2004)]

Maximal velocity of photons

Theorem

Let $\alpha \geq 0$, $\Lambda \geq 0$. Let $\chi \in \mathrm{C}_0^\infty((-\infty, \Sigma_\alpha))$ and $\mathrm{c} > 1$. For all $\psi_0 \in \chi(H_\alpha)\mathcal{D}(\mathrm{d}\Gamma(\langle i\nabla_k \rangle)^{1/2})$,

$$\left\| \mathrm{d}\Gamma\left(\mathbb{1}_{\cdot \geq \mathrm{c}t}(|i\nabla_k|) \right)^{\frac{1}{2}} e^{-itH_\alpha} \psi_0 \right\| \lesssim t^{-\gamma} \|(\mathrm{d}\Gamma(\langle i\nabla_k \rangle) + 1)^{\frac{1}{2}} \psi_0\|,$$

for some $\gamma > 0$ depending on c

References

- [Bony, F., Sigal, Adv. Math., 5, (2012)]

Ingredients of the proof

- Generalized Pauli-Fierz transformation
- Method of propagation estimates adapted to Fock space

Asymptotic completeness (I)

Theorem

Let $\Lambda \geq 0$. Let $\Delta \subset (-\infty, 0)$. There exists $\alpha_c > 0$ such that for all $0 \leq \alpha \leq \alpha_c$, if Fermi's Golden Rule holds in Δ and if one of the following hypotheses hold

(i) For all $\chi \in \mathrm{C}_0^\infty(\Delta)$ and $\psi_0 \in \chi(H_\alpha)\mathcal{D}(\mathrm{d}\Gamma(\mathbb{1})^{1/2})$,

$$\|\mathrm{d}\Gamma(\mathbb{1})^{\frac{1}{2}} e^{-itH_\alpha}\psi\| \lesssim \|\mathrm{d}\Gamma(\mathbb{1})^{\frac{1}{2}}\psi_0\| + \|\psi_0\|$$

(i') For all ψ_0 in some set $\mathcal{D}$ dense in $\mathrm{Ran}\, \mathbb{1}_\Delta(H_\alpha)$,

$$\|\mathrm{d}\Gamma(|k|^{-1})^{\frac{1}{2}} e^{-itH_\alpha}\psi_t\| \leq C(\psi_0)$$

then asymptotic completeness holds in $\mathrm{Ran}\, \mathbb{1}_\Delta(H_\alpha)$: for all $\psi_0 \in \mathrm{Ran}\, \mathbb{1}_\Delta(H_\alpha)$ and $\varepsilon > 0$, there exists $f_\varepsilon \in \mathcal{H}_{\mathrm{ph}}$ with a finite number of photons, such that

$$\limsup_{t\to\infty} \left\| e^{-itH_\alpha}\psi_0 - e^{-itE_\alpha}\Phi_\alpha \otimes_s e^{-itH_f} f_\varepsilon \right\| \leq \varepsilon,$$

where Φ_α is a ground state of H_α

Asymptotic completeness (II)

References

- [F., Sigal, Comm. Math. Phys., 3, (2014)]

Previous results for infrared cutoff or massive Hamiltonians :

- [Spohn, J. Math. Phys., 38, (1997)]
- [Dereziński, Gérard, Rev. Math. Phys., 11, (1999)]
- [Fröhlich, Griesemer, Schlein, Ann. Henri Poincaré, 3, (2002)]

Remark

Hypothesis (i') holds for the spin-boson model (and therefore asymptotic completeness holds in this case)

- [De Roeck, Kupiainen, Ann. Henri Poincaré, (2012)]
- [De Roeck, Griesemer, Kupiainen, Adv. Math., 68, (2015)]

Ingredients of the proof

- Dereziński-Gérard asymptotic partition of unity in Fock space
- Existence of the Deift-Simon wave operators
- Propagation estimates for photons (minimal velocity estimates)

Thank you !