Non-relativistic Quantum Electrodynamics

Rigorous Aspects of Relaxation to the Ground State

Niels Benedikter

Institut für Analysis, Dynamik und Modellierung

Universität Stuttgart

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Overview

1. Definition of the model
   - Second quantization
   - Non-relativistic QED
2. Known results and open problems
   - Existence and Uniqueness of Ground State
   - Spectral properties
   - Asymptotic Completeness of Rayleigh Scattering (Relaxation to the Ground State)
3. Time Scale of Relaxation to the Ground State
   - Overview
   - Relaxation Estimates for the Harmonic Oscillator

Overview

Fock space

- one-particle Hilbert space: $\mathfrak{h}$
- n-particle Hilbert space: $\otimes^n \mathfrak{h} = \mathfrak{h} \otimes \cdots \otimes \mathfrak{h}$
- Symmetrization operator on $\otimes^n \mathfrak{h}$: $S_n = \frac{1}{n!} \sum_{\sigma \in \mathcal{S}_n} \hat{\sigma}$

For systems with non-constant particle number (photons) use Fock space:

Bosonic Fock space

$$\mathcal{F}_s = \oplus_{n=0}^{\infty} S_n(\otimes^n \mathfrak{h}).$$

Each $\psi \in \mathcal{F}_s$ is a sequence $\psi = (\psi_n)_{n \in \mathbb{N}}$ with $\psi_n \in S_n(\otimes^n \mathfrak{h})$.

Creation and annihilation operators

For $f \in \mathfrak{h}$, $\varphi = S_n(\varphi_1 \otimes \cdots \otimes \varphi_n) \in S_n(\otimes^n \mathfrak{h})$:

$$a^*(f)\varphi = \sqrt{n+1}\, S_{n+1}(f \otimes \varphi)$$

$$a(f)\varphi = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \langle f, \varphi_i \rangle\, S_{n-1}(\varphi_1 \otimes \cdots \otimes \widehat{\varphi}_i \otimes \cdots \otimes \varphi_n).$$

Physicist's notation: $a^*(f) = \int \mathrm{d}^3\boldsymbol{k}\; f(\boldsymbol{k}) a^*(\boldsymbol{k})$.

Bosonic CCR

$$[a(f), a^*(g)] = \langle f, g \rangle_{\mathfrak{h}}\, \mathbb{1}$$

$$[a(f), a(g)] = 0 = [a^*(f), a^*(g)]$$

The Hilbert space of non-relativistic QED

Fixed number (for simplicity: 1) of electrons, quantized electromagnetic field.

- One single electron, no spin: $\mathcal{H}_{\text{el}} = L^2(\mathbb{R}^3)$ (in position representation)
- Photons:
  - one-particle Hilbert space: $L^2(\mathbb{R}^3 \times \underbrace{\{1,2\}}_{\text{helicity}})$ (in momentum representation)
  - quantized em. field: $\mathcal{F}_s = \bigoplus_{n=0}^{\infty} S_n \left(\otimes^n L^2(\mathbb{R}^3 \times \{1,2\}) \right)$
- Coupled system: $\mathcal{H} = \mathcal{H}_{\text{el}} \otimes \mathcal{F}_s$.

The Hamiltonian of non-relativistic QED

Minimal coupling

$$
\begin{aligned}
H &= (\boldsymbol{p} \otimes \mathbb{1} + \boldsymbol{A})^2 + V \otimes \mathbb{1} + \mathbb{1} \otimes H_\mathrm{f} \\
&= (\boldsymbol{p} + \boldsymbol{A})^2 + V + H_\mathrm{f}
\end{aligned}
$$

$\boldsymbol{p}$: electron momentum
$\boldsymbol{A}$: quantized vector potential in Coulomb gauge
V: binding potential
H_f: energy of quantized em. field

Rigorous definition of the vector potential $\boldsymbol{A}$

$$H = (\boldsymbol{p} \otimes \mathbb{1} + \boldsymbol{A})^2 + V \otimes \mathbb{1} + \mathbb{1} \otimes H_{\mathrm{f}}$$

- Let $\varphi \otimes \eta \in \mathcal{H} = \mathcal{H}_{\mathrm{el}} \otimes \mathcal{F}_s$, let $\boldsymbol{x} \in \mathbb{R}^3$. Then

$$(\varphi \otimes \eta)(\boldsymbol{x}) := \underbrace{\varphi(\boldsymbol{x})}_{\in \mathbb{C}} \eta \in \mathcal{F}_s.$$

- Extend to all $\psi \in \mathcal{H}$: $\psi(\boldsymbol{x}) \in \mathcal{F}_s$.
- Define

$$(\boldsymbol{A}\psi)(\boldsymbol{x}) := (a(\boldsymbol{G}_{\boldsymbol{x}}) + a^*(\boldsymbol{G}_{\boldsymbol{x}}))\,\psi(\boldsymbol{x}),$$

where

$$\boldsymbol{G}_{\boldsymbol{x}}(\boldsymbol{k},\lambda) = \frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}}{\sqrt{2|\boldsymbol{k}|}} \boldsymbol{e}(\boldsymbol{k},\lambda) \underbrace{\kappa(|\boldsymbol{k}|)}_{\text{UV cutoff}}.$$

Self-adjointness of the Hamiltonian

The theory is well-defined:

Theorem (Hasler-Herbst)

Assume V infinitisemally bounded w.r.t. to $-\Delta$.
For all values of the coupling constant (here: $\alpha = 1$):

- *H is self-adjoint on $D = D(-\Delta + H_f)$.*
- *H is essentially self-adjoint on any core for $-\Delta + H_f$ and bounded from below.*

Points to keep in mind

- fixed number of electrons in first quantization
- electromagnetic field in second quantization
- coupling needs UV cutoff
- $\rightsquigarrow$ rigorously defined model

- should be a good model for many low-energy phenomena:

  e. g. atomic physics, molecular physics.

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Warning

All following results under mild or natural assumptions on V and κ.

Results are simplified:
esp. only one-electron case considered.

Result: Existence and Uniqueness of Ground State

Ground state $\neq$ ground state of uncoupled system!
Ground state contains photons.

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Theorem (Existence – Griesemer-Lieb-Loss '01)

Assume $-\Delta + V$ has a negative energy ground state. Then there is $\psi \in \mathcal{H}$ such that

$$H\psi = E\psi, \quad E = \inf \sigma(H),$$

i. e. H has a ground state.

Theorem (Uniqueness – Hiroshima '00)

If the ground state exists, it is unique (up to a phase).

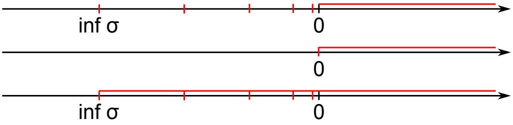
Result: Spectral properties

Uncoupled system: We know:

$\sigma(-\Delta + V)$:

$\sigma(H_f)$:

$\sigma(-\Delta + V + H_f)$:



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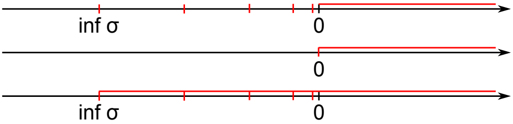

Coupled system: We expect:

$\sigma(H)$:

Problem: Asymptotic Completeness of Rayleigh...

$$\begin{aligned}\Sigma &:= \text{ionization threshold}\\ &= \text{minimal energy required for moving the electron to infinity.}\end{aligned}$$

Let $\psi \in \chi(H < \Sigma)\mathcal{H} = \chi(H < \Sigma)(\mathcal{H}_{\text{el}} \otimes \mathcal{F}_s)$.

Expectation:
Electron relaxes to ground state while
photons are emitted to infinity.

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Conjecture: ACR (Relaxation to the GS)

There exist $h_1, \ldots h_n \in L^2(\mathbb{R}^3 \times \{1,2\})$ such that for $t \to \infty$

$$\| e^{-iHt}\psi - \underbrace{e^{-iH_f t} a^*(h_1) e^{iH_f t}}_{\text{free photon}} \cdots \underbrace{e^{-iH_f t} a^*(h_n) e^{iH_f t}}_{\text{free photon}} \; \underbrace{e^{-iEt}\psi_g}_{\text{ground state}} \| \to 0.$$

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$$\|e^{-iHt}\psi - \sum_{i=0}^{\infty} e^{-iH_f t} a^*(h_{i,1}) e^{iH_f t} \cdots e^{-iH_f t} a^*(h_{i,n_i}) e^{iH_f t}\, e^{-iEt}\psi_g\| \to 0.$$

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Theorem (ACR – Arai '83)

For $V(\boldsymbol{x}) = c\boldsymbol{x}^2$ and with dipole approximation $\boldsymbol{A}(\boldsymbol{x}) \approx \boldsymbol{A}(\boldsymbol{0})$, ACR holds.

Method: Solutions are explicitly constructed.

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Theorem (ACR – Spohn '97)

For $V(\boldsymbol{x}) = c\boldsymbol{x}^2 + \textit{small perturbation}$ and with dipole approximation $\boldsymbol{A}(\boldsymbol{x}) \approx \boldsymbol{A}(\boldsymbol{0})$, ACR holds.

Method: Treat perturbation by Dyson series.

Problem: Asymptotic Completeness of Rayleigh...

Theorem (ACR – Fröhlich-Griesemer-Schlein '01)

Assume dipole approximation $\boldsymbol{A}(\boldsymbol{x}) \approx \boldsymbol{A}(\boldsymbol{0})$.
In general potentials, ACR holds if either

- *photon mass $m > 0$ or*
- *IR cutoff in the interaction: $\kappa(k) = 0$ for $k <$ const.*

Method: Photon number bounded by total energy. Ideas from N-body scattering theory.

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Difficulty: Infrared problem

In principle, infinitely many soft photons could be emitted!

Points to keep in mind

- Result: Ground state is existent and unique
- Partial results: Coupling $\rightsquigarrow$ Excited eigenstates dissolve in continuous spectrum
- Open problem: Relaxation to the ground state (ACR)
- ACR is an infrared problem: How to control soft photons?

Overview

Overview (results from diploma thesis N.B.)

How fast does the atom relax?

1. Power law bound on relaxation to the ground state:
   Assume ACR is true.
   Then for $\psi \in \chi(H < \Sigma)\mathcal{H}$ and "localized" observables A:
   $$|\langle\psi(t), A\psi(t)\rangle - \langle\psi_g, A\psi_g\rangle| \leq \frac{C_{\psi,n,\varepsilon}}{1+t^n} + \varepsilon.$$
2. Uniform propagation estimates:
   Outgoing photons "$\boldsymbol{x} \cdot \boldsymbol{p} > 0$" allow for "uniform power law"
3. Harmonic oscillator coupled to the quantized radiation field
4. (Perturbative expansion of scattering amplitudes)
5. (Bounds on photon creation)

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A simplified model

Harmonic potential: $V(\boldsymbol{x}) \propto \boldsymbol{x}^2$
Dipole approximation: $\boldsymbol{A}(\boldsymbol{x}) \approx \boldsymbol{A}(\boldsymbol{0})$

Quadratic Hamiltonian

$$H = (\boldsymbol{p} + g\boldsymbol{A}(\boldsymbol{0}))^2 + \omega_0^2 \boldsymbol{x}^2 + \underbrace{\int \pi(\boldsymbol{x})^2 + (\operatorname{curl} \boldsymbol{A}(\boldsymbol{x}))^2 \, \mathrm{d}^3\boldsymbol{x}}_{= \, H_\mathrm{f}}$$

$\boldsymbol{A}$: vector potential quantized in Coulomb gauge,
$\pi = -\boldsymbol{E}$: canonically conjugate quantized field.
g: electron charge = coupling constant,
ω_0: frequency of uncoupled oscillator.

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Relaxation Estimates for the Harmonic Oscillator

Raising operator for the "atom": $\alpha^\dagger = x_1\sqrt{\omega_0} - ip_1/\sqrt{\omega_0}$.

Theorem (N.B.)

Assume coupling constant g is small. Then

$$\|e^{-iHt}\left(\alpha^\dagger\psi_g\right) - e^{-iH_f}a^*(\phi_+)e^{iH_f}\,e^{-iEt}\psi_g\| \leq Ce^{-\gamma t} + \mathcal{O}(g^2).$$

- $\phi_+(\boldsymbol{k},\lambda)$ *explicitly obtained, has a peak at* $|\boldsymbol{k}| \approx \omega_0$
- *non-trivial upper and lower bounds for* γ *found.*

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- We can do better than power laws.
- Useful for checking further conjectures.
- $(\alpha^\dagger)^n\psi_g$ can be treated analogously.

Proof. Part I: Classical Solutions

Proof part I. Derive more explicit solutions (compared to Arai):

- Classical equations of motion are linear (because Hamilton function is quadratic)
  $\rightsquigarrow$ Solve classical initial value problem of fields *and* oscillator using Laplace transform.
- Energy conservation: For classical Hamilton function

$$\frac{\mathrm{d}H(\boldsymbol{q}(t), \boldsymbol{A}(t), \boldsymbol{p}(t), \pi(t))}{\mathrm{d}t} = 0$$

  $\rightsquigarrow$ bounds on growth of $\boldsymbol{q}(t)$, $\boldsymbol{p}(t)$, $\boldsymbol{A}(t)$, $\pi(t)$ (pointwise)
  $\rightsquigarrow$ Laplace transform exists (on fields pointwise).

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  $\rightsquigarrow$ Laplace transform exists (on fields pointwise).
- Determine poles z_0, $\overline{z_0}$ of Laplace transform: $\mathrm{Re}\, z_0 < 0$
- Inverse Laplace transform using Residues:

$$\boldsymbol{q}(t) \sim e^{z_0 t} + e^{-St}, \quad \hat{\boldsymbol{A}}(\boldsymbol{k}, t) \sim e^{z_0 t} + e^{-i|\boldsymbol{k}|t} + e^{-St}$$

Part II: Connecting Classical with Quantum Solutions

Proof part II. Coherent states $e^{i\langle u,Jx\rangle}\psi_g$ connect classical and quantum theory:

- Build Weyl operators from field *and* oscillator degrees of freedom:
  for $\alpha_1, \alpha_2 \in \mathbb{R}^3$ and $\phi_1, \phi_2 : \mathbb{R}^3 \to \mathbb{R}^3$ transversal fields

$$\langle u, Jx\rangle := \alpha_1 \cdot \boldsymbol{p} - \alpha_2 \cdot \boldsymbol{x} + \int \mathrm{d}^3\boldsymbol{x}\, \phi_1(\boldsymbol{x}) \cdot \pi(\boldsymbol{x}) - \int \mathrm{d}^3\boldsymbol{x}\, \phi_2(\boldsymbol{x}) \cdot \boldsymbol{A}(\boldsymbol{x}).$$

- Nelson's analytic vector theorem $\rightsquigarrow$ essential self-adj.

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- Nelson's analytic vector theorem $\rightsquigarrow$ essential self-adj.
- Quadratic Hamiltonian $\rightsquigarrow$ evolution of Weyl operators:

$$e^{-iHt} e^{i\langle u(0),Jx\rangle} e^{iHt} = e^{i\langle u(t),Jx\rangle},$$

  with $u(t) = (\alpha_1(t), \phi_1(t), \alpha_2(t), \phi_2(t))$ solution of the classical initial value problem (e. g. Spohn '97).

Part III: The Relaxation Estimate

Proof part III. Estimates on unwanted terms:

- Raising operator: $\alpha^\dagger \sim x_1 - ip_1$.
- Choose $u_1(0)$ such that $\langle u_1(0), Jx\rangle = x_1 = x_1(0)$; obtain $x_1(t) = e^{-iHt} x_1 e^{iHt}$ from

$$\frac{\mathrm{d}}{\mathrm{d}s} e^{i\langle u_1(t), Jx\rangle s}\Big|_{s=0}.$$

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  p_1 analogously.
- We get

$$e^{-iHt}\alpha^\dagger e^{iHt} = b(t) + e^{-iH_f t} a^*(\phi_+) e^{iH_f t} + e^{-iH_f t} a(\phi_-) e^{iH_f t},$$

  where $\|b(t)\psi\| \leq Ce^{-|\mathrm{Re}\, z_0| t}$.
- We know $a(\phi_-)\Omega = 0$ (vacuum), and $\psi_g = \psi_0 \otimes \Omega + \mathcal{O}(g)$. We show $\|\phi_-\| = \mathcal{O}(g)$. $\rightsquigarrow$ $\|a(\phi_-)\psi_g\| = \mathcal{O}(g^2)$.

$\square$

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Summary

- Non-relativistic QED is a rigorously defined quantum theory of low-energy matter and radiation.

- Ground state (and many other aspects) well understood.
- Relaxation by emission of photons (ACR) is an open problem!
- Difficulty: controlling the infrared behaviour.

- Simplified model (harmonic oscillator, dipole approximation) exhibits exponential relaxation to the ground state.