Radiative Decay in nonrelativistic Quantumelectrodynamics

// Imagine the following situation:
We have an atom coupled to the quantized radiation field. And now we ask:
Can we understand the emission of photons and the relaxation of the electrons in a mathematically rigorous way?

// Now, let me give a short overview of the talk.

1. Second quantization // just to recall some def.s
2. Nonrelativistic QED // explain the model
3. Some results and problems // a short overview
4. A solvable model (N.B.) // outline part of my diploma thesis.

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1. Second quantization:

Let h be a Hilbert space (one particle space).
n-particle-Hilbert space: $\otimes^n h = h \otimes \cdots \otimes h$.
Symmetrization op. on $\otimes^n h$: $S_n := \frac{1}{n!} \sum_{\sigma \in S_n} \hat{\sigma}$
Permutation operator.

// to describe systems with non-constant number of particles, we take the direct sum of all n-particle spaces.

Bosonic Fock space:

$$\mathcal{F}_S := \bigoplus_{n=0}^{\infty} S_n(\otimes^n h).$$

Creation and Annihilation operator:

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

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

$$a(f) S_n(\varphi_1 \otimes \cdots \otimes \varphi_n)$$

$$:= \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \langle f, \varphi_i \rangle\, S_{n-1}(\varphi_1 \otimes \cdots \otimes \varphi_{i-1} \otimes \varphi_{i+1} \otimes \cdots \otimes \varphi_n).$$

// to make the connection to physicist's notation:

$$a^*(f) = \int d^3\vec{k}\, f(\vec{k})\, a^*(\vec{k})$$ // but actually, the r.h.s. is defined by the l.h.s.

// what you should remember is the following — the canonical commutation relations:

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

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

// we have bosons.

2. Nonrelativistic QED

// To make things simple: one single electron, put it in a binding potential and couple it to the quantized e.m. field.

$\mathcal{H}_{el} := L^2(\mathbb{R}^3)$ // no spin, position space $\mathbb{R}^3$

Photons: $$\mathcal{F}_s = \bigoplus_{n=0}^{\infty} S_n(\otimes^n L^2(\mathbb{R}^3 \times \{1,2\})).$$

momentum space ($\mathbb{R}^3$), Helicity ($\{1,2\}$)

Coupled system: $\mathcal{H} := \mathcal{H}_{el} \otimes \mathcal{F}_s$.

// next we need a Hamiltonian to generate the time evolution.

Hamiltonian:

$$H := (\vec{p} \otimes \mathbb{1} + \vec{A})^2 + V \otimes \mathbb{1} + \mathbb{1} \otimes H_f .$$

// electron momentum

// minimal coupling to quant. vect. pot.

// binding potential

// energy of quantized em. field

$$= (\vec{p} + \vec{A})^2 + V + H_f .$$

// a few words on the coupling to the quant. vector pot.:

Defining $\vec{A}$:

Let $\varphi \otimes \eta \in \mathcal{H} = \mathcal{H}_{el} \otimes \mathcal{F}_S$, $\vec{x} \in \mathbb{R}^3$.

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

Extend to all $\psi \in \mathcal{H}$: $\psi(\vec{x}) \in \mathcal{F}_S$.

// now we can define the quant. vector potential:

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

where $\vec{G}_{\vec{x}}(\vec{k},\lambda) = \dfrac{e^{-i\vec{k}\cdot\vec{x}}}{\sqrt{2|\vec{k}|}} \underbrace{\vec{\varepsilon}(\vec{k},\lambda)}_{\text{transversal polarization vectors}} \underbrace{\kappa(|\vec{k}|)}_{\text{UV-Cutoff with } \frac{\kappa}{\sqrt{k}} \in L^2}$.

// $\lambda = 1,2$ Helicity

// necessary, because otherwise the creation and annihil. op. would be ill-defined.

// important points to keep in mind:

- one electron in first quantization
- photon field in second quantization
- minimal coupling, with UV cutoff.

3. Some results and problems:

// Now the first question is always: Is the Hamiltonian self-adjoint, so that it generates a time evolution? The answer is positive:

- Assume V is infinitesimally bounded w.r. to $p^2 = -\Delta$. Then H is self-adjoint on $D(H) = D(p^2) \cap D(H_f)$. (Hasler - Herbst)

// The next important question is: Does the system have a ground state? The answer is positive, too:

Under mild assumptions on V and κ:

- H has a ground state $\Psi_g \in \mathcal{H}$, $\|\Psi_g\| = 1$, i.e.

$$H\Psi_g = E\,\Psi_g \quad \text{with} \quad E = \inf \sigma(H).$$

(e.g. Griesemer - Lieb - Loss)

- The ground state is unique (up to a phase). (Hiroshima)

- Ψ_g is exponentially localized in space: there is $\beta > 0$ such that $\|e^{\beta|x|}\Psi_g\| < \infty$.

// to be read as a multiplication operator regarding the electron coordinate.

// this is a result that can be considerably strengthened, I refer to

(Bach - Fröhlich - Sigal, Griesemer)

// Ok, so the static properties of the model seem to be well behaved.

The next step is to analyze the dynamics, the time evolution.

- Motivation:

  Let Σ := ionization threshold

  = minimum energy //required

  for moving the electron from the binding potential to infinity.

  //and we want to look at a state with total energy
  below the ionization threshold.

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

  We expect the electron to relax to the ground state while photons are emitted to infinity:

  $\rightsquigarrow$ <u>Conjecture:</u> $\exists h_1, \dots h_n \in L^2(\mathbb{R}^3 \times \{1,2\})$

  such that (ACR)

$$\| e^{-iHt}\Psi - \underbrace{e^{-iH_f t} a^*(h_1) e^{iH_f t}}_{\text{freely moving photon}} \dots e^{-iH_f t} a^*(h_n) e^{iH_f t} \underbrace{e^{-iEt}\Psi_g}_{\text{ground state}} \| \longrightarrow 0 \quad (t \to \infty).$$

//time evolution of the bound state

// free time evolution is generated by the free quantized field energy.

// trivial time evolution of an eigen state.

//one remark: strictly speaking we should allow for linear combin. of states with free photons, but let us stay with the simplified version.

// So what is know about asympt. completeness of Rayleigh scattering?

<u>Results concerning ACR:</u>

- Arai '83: ACR holds for harmonic oscillator $V \propto x^2$ and dipole approximation $\vec{A}(\vec{x}) \simeq \vec{A}(\vec{0})$.

Method: Heisenberg equations explicitly solved.

- Spohn '97: ACR for perturbed harmonic oscillator $V \propto x^2$ + small and dipole approx.

  Method: Treat perturbation by Dyson series.

- Fröhlich - Griesemer - Schlein '01:

  ACR with photon mass $m > 0$ // positive photon mass or interaction with IR cutoff.

  Dipole approx.

  Arbitrary binding potential.

  Method: $m > 0$ / IR-Cutoff $\rightarrow$ number of photons bounded by total energy.
  Use techniques from N-body quantum scattering theory.

Unphysical models! // What is the problem with physically realistic models, without IR-cutoff?

Mathematical problem: // We do not know how to control the number of low energy photons.
We could expect that the atom emits infinitely many photons with smaller and smaller energy, some sort of IR catastrophe.
How to control the number of soft photons?
// I do not know a solution for the IR problem.

Aussprache?

4 Very explicit solution for $V \propto x^2$: (NB)

// these results are part of my diploma thesis. Not the main result, but rather intuitive and useful for checking
└ other conjectures.

$$H = \frac{(\vec{p} + e\vec{A}(\vec{0}))^2}{2m} + \frac{m\omega_0^2}{2}\vec{x}^2 + H_f$$

//dipole approx. harmonic potential. constants reintroduced:
└ oscillator frequ., electron mass, electron charge.

Calculating the time evolution:

Idea: Ass. finitely many degrees of freedom

$x = (q_1, \dots q_n, p_1, \dots p_n) \in \mathbb{R}^{2n}$

and quadratic Hamiltonian $H = \frac{1}{2}\langle x, Mx\rangle$

($M = M^t$ matrix).

Coherent states: $e^{i\langle u, \mathcal{J}x\rangle}|0\rangle$ with $\mathcal{J} = \begin{pmatrix} 0 & \mathbb{1} \\ -\mathbb{1} & 0 \end{pmatrix}$.

Then $e^{-iHt} e^{i\langle u, \mathcal{J}x\rangle}|0\rangle$

$= e^{i\langle u(t), \mathcal{J}x\rangle} e^{-iE_0 t}|0\rangle$,

where $u(t)$ is solution of canonical equ. of motion with initial value $u(0) = u$.

Generalization to infinitely many deg. of freedom:

$$\langle u, \mathcal{J}x\rangle := \underbrace{\vec{\alpha}_1}\cdot\vec{p} - \vec{\alpha}_2\cdot\vec{q} + \int d^3x\, \vec{\Phi}_1(\vec{x})\cdot\vec{\pi}(\vec{x}) - \int d^3x\, \vec{\Phi}_2(\vec{x})\cdot\vec{A}(\vec{x})$$

$\vec{p}$: momentum operator; $\vec{q}$: position operator; $\vec{\pi}(\vec{x})$: quant. conjugate field; $\vec{A}(\vec{x})$: quant. vector pot.

and $\vec{\alpha}_1 \in \mathbb{R}^3$: classical position

$\vec{\alpha}_2 \in \mathbb{R}^3$: " momentum

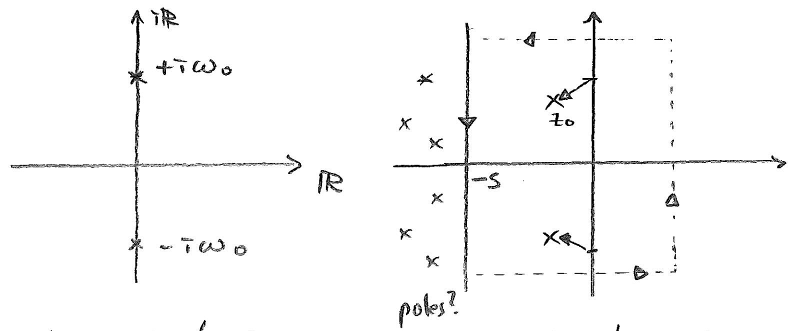
$\vec{\Phi}_1: \mathbb{R}^3 \longrightarrow \mathbb{R}^3$, classical vector pot. in Coulomb gauge.

$\vec{\Phi}_2: \mathbb{R}^3 \longrightarrow \mathbb{R}^3$, class. conjugate field.

We have $e^{-iHt} e^{i\langle u, \varphi_x\rangle} e^{iHt} = e^{i\langle u(t), \varphi_x\rangle}$
(e.g. Spohn '97).

Using this method, we can explicitly calculate the relaxation of excited states! (NB)

- Determine classical solution of the initial value problem:
  - energy conservation ⇝ bounds on growth of solution
  - Laplace transform in time coordinate
  - detailed estimates on poles of the transformed coordinates and fields.

↳


no coupling coupling on

  - Solutions: $\overline{\alpha}_1(t), \overline{\alpha}_2(t) \sim e^{z_0 t} + e^{-St}$ // show z_0 and S in picture
    $\overline{\Phi}_1(t), \overline{\Phi}_2(t) \sim e^{z_0 t} + e^{i|k|t}$ // radiated waves $+ e^{-St}$

- Now $e^{i\langle u(t), \varphi_x\rangle}$ is known.
  - Establish domain of $\langle u(t), \varphi_x\rangle$ with Nelson's analytic vector theorem
  - calculate e.g. $q_1 \Psi_g = \frac{d}{ds}\Big|_{s=0} e^{i\langle u_q, \varphi_x\rangle s} \Psi_g$
    where $u_q = (\vec{0}, \vec{0}, \left(\begin{smallmatrix}1\\0\\0\end{smallmatrix}\right), \vec{0})$

    and $p_1 \Psi_g$. // combine q_1 and p_1 to build ladder operators.

- $\rightsquigarrow$ e.g. $\| e^{-iHt} \alpha^+ \psi_g - e^{iH_f t} a^*(\Phi_+) e^{-iH_f t} e^{-iEt} \psi_g \|$

$$\leq C' e^{-|\mathrm{Re}\, z_0| t} + \text{corrections } \left(\sim \frac{C_{n,\varepsilon}}{|t|^n} + \varepsilon\right)$$

$$\longrightarrow 0 \quad (t \to \infty)$$

and Φ_+ explicitly known!

// So what have we gained?

We have very explicit solutions for a system without IR cutoff,

and now we can for example check some conjectures which are motivated by perturbation theory.

Summary:

- nonrel. QED is a well defined theory
  // for low energy phenomena, like most of
  [atomic and molecular physics

- ground state well understood
- dynamics are difficult (IR problem)
- useful explicit solution can be constructed for harmonic oscillator.