Bonn, 20. 2. 2011

// Gesamtdauer: 1 h 5 min.

The topic of my talk is the

Dynamics of the Radiative Decay of Excited Atoms, which was also the title of my diploma thesis, but I will probably have only 5-10 minutes at the end for one of my results.

Let us start with a physical picture.

Imagine an atom. Now we bring the atom into an excited state

Phys. experience tells us: the atom goes to its GS while photons are emitted and fly to infinity. And physicists can measure the lifetime.

On the mathematical side, we have a rigorous theory which describes the interaction of matter and light.

This is non-relativistic quantum electrodynamics.

So we can ask:

How can we define lifetime in the math. framework?

And how can we calculate lifetimes?

In my talk I have two parts:

First p.: I give a def. of non-rel. qed. and I present some results which we need later on.

Second p.: I present a theorem which answers these questions for the lifetime in a simplified model;

and if there is enough time, I will sketch the proof.

1) Def. of non-rel. QED

Our quantum theory consists of two parts,
a Hilbert space (which contains the states of the system)
and a s.a. operator, the Hamiltonian, which generates the time evolution.

1.1) The Hilbert space

one photon: $h := L^2(\mathbb{R}^3 \times \{1,2\})$

helicity

n-photon Hilbert space:

$$\otimes_s^n h := S_n(h \otimes \cdots \otimes h)$$

Symmetrization op.
takes an elementary tensor and sums over all permutations of its tensor factors.
(physical principle. bosons.)

Hilbert space for non-constant photon number:

Fock space $\underline{\mathcal{F}_s := \bigoplus_{n=0}^{\infty} \otimes_s^n h}$.

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

Creation operator: define on each member of the sequence, on the n-th member as follows:
For $f \in h$, $\varphi \in \otimes_s^n h$:

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

↳ adds a photon in state f, symmetrizes, $\sqrt{n+1}$ by tradition.

To be precise, we should specify the domain, but let us ignore that here.

Annihilation op.: $a(f) := (a^*(f))^*$.

has the effect of eliminating one photon.

Basic rules for doing calculations:

CCR: $[a(f), a^*(g)] = a(f)a^*(g) - a^*(g)a(f)$

$= \langle f, g\rangle_{\mathfrak{h}} \mathbb{1}_{\mathcal{F}}$

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

So far we have constructed Fock space for describing variable numbers of photons and operators for creating and annihilating photons.

Next step: add an electron.

And we keep the number of electrons fixed, for now we take only one electron.

Electron Hilbert space: $\mathfrak{H}_{el} := L^2(\mathbb{R}^3)$

and finally

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

one electron — variable no. of photons

1.2) The Hamiltonian

I'm going to write down the Hamiltonian formally first, and then we've going to discuss it.

formally: $H = \frac{1}{2}(\underbrace{-i\vec{\nabla}}_{=\vec{p}} \otimes \mathbb{1} + \alpha^{3/2}\vec{A})^2$

$\alpha > 0$ (usually as small as necessary, although in nature fixed.)

$+ V \otimes \mathbb{1} + \mathbb{1} \otimes H_f$

mult. op. with $V: \mathbb{R}^3 \to \mathbb{R}$

free photons (could write it down, but don't need it here.)

the quant. vector pot. $\vec{A}$:

- Let $\varphi \otimes \eta \in \mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathcal{F}_s$, $\vec{x} \in \mathbb{R}^3$.

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

  extends to $\psi \in \mathcal{H}$: $\underline{\psi(\vec{x}) \in \mathcal{F}_s}$.

  so now we know what we mean by evaluating ψ at position $\vec{x}$.

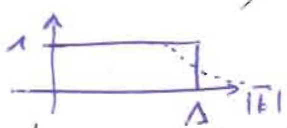
- $(\vec{A}\psi)(\vec{x}) := a(\vec{G}_{\vec{x}})\psi(\vec{x}) + a^*(\vec{G}_{\vec{x}})\psi(\vec{x})$

  with $$\vec{G}_{\vec{x}}(\vec{k},\lambda) := \frac{e^{-i\alpha \vec{k}\cdot\vec{x}}}{\sqrt{2|\vec{k}|}} \underbrace{\vec{\varepsilon}(\vec{k},\lambda)}_{\substack{\in \mathbb{R}^3, \\ \vec{\varepsilon}(\vec{k},\lambda) \perp \vec{k} \\ \text{transversal} \\ \text{polarization}}} \cdot \underbrace{\kappa(|\vec{k}|)}_{\text{UV-Cutoff}}$$

  λ: helicity

  UV-Cutoff to make $\vec{G}_{\vec{x}} \in L^2$, so that a, a^* well defined.

  typically κ:



  phys. try to $\Lambda \to \infty$, but mathematically not well understood.

Abbr.: $\underline{H = \frac{1}{2}(\vec{p} + \alpha^{3/2}\vec{A})^2 + V + H_f}$.

I said that this is a rigorous theory, and that is made precise by the following theorem:

Thm. (Hasler – Herbst)

Let V infin. bounded w.r.t. to $(-i\vec{\nabla})^2 = -\Delta$. (weak condition, e.g. Coulomb pot.)

Then:
- H is s.a. on $D = H^2(\mathbb{R}^3) \otimes D(H_f)$
- H is ess. s.a. on any core for $-\Delta + H_f$.
- $\inf \sigma(H) > -\infty$. the energy of the system is bounded below.

Let us have a short look back at the construction:

We have: Fock space (for non-const. photon number), Hilbert space of coupled system, Hamiltonian, Hasler-Herbst $\rightsquigarrow$ well-def. quantum theory.

Now we can start to deduce theorems.

And for discussing the dynamics, we need to know first that there is a stable state at the bottom of the energy spectrum, the spectrum of the Hamiltonian:

// means eigenvector

// obs. cont. above

Thm.: (Griesemer - Lieb - Loss) (simplified for our purposes)

Assume $\lim_{|\vec{x}| \to \infty} V(\vec{x}) = 0$ and $H_{at} = -\Delta + V$ → for Coulomb pot. has a negative eigenvalue, or $\lim_{|\vec{x}| \to \infty} V(\vec{x}) = \infty$.

for our second section

Then $E = \inf \sigma(H)$ is an eigenvalue of H.

Thm.: (Hiroshima) which says slightly simplified:

The eigenspace is one-dimensional.

So we have an eigenstate at the bottom of the spectrum, and by normalizing the eigenstate it becomes unique up to a phase.

And we have a name for this state:

Def.: ground state: eigenvector ψ_g of H with eigenvalue E and $\|\psi_g\| = 1$.

ground state:
- because min. energy
- and because stable, an eigenvector.

So far any questions?

Then we have established everything we need for studying the dynamics.

2) Dynamics of Excited Atoms

That is, we want to understand the behaviour of the initial value problem of the Schrödinger equation

$$i\partial_t \Psi(t) = H\Psi(t) \quad \text{with } \Psi(0) = \varphi \in \mathcal{H}.$$

Solution: $\Psi(t) = e^{-itH}\Psi(0)$, all $t \in \mathbb{R}$.

And I want to restrict attention to states where the electron stays bound, i.e. does not have enough energy to move to infinity.

As a first step let us define that notion more precisely.

Def: Let $D_R = \{\Psi \in D(H) : \underbrace{\Psi(\vec{x})}_{\in \mathcal{F}} = 0 \text{ if } |\vec{x}| < R\}$

using the identification introduced above

States where the electron is outside a ball with radius R

Ionization threshold: $\Sigma := \lim_{R\to\infty} \inf_{\substack{\varphi \in D_R \\ \|\varphi\|=1}} \langle \varphi, H\varphi\rangle$.

min. energy required to move electron to infinity.

So we can now define a bound state as a state from the spectral subspace below the ionization threshold.

What dynamics do we expect? The phys. experience tells us that eventually, the atom relaxes to its ground state, while free photons fly away and carry away the energy.

<u>Def.:</u> Scattering states: // first write it down, the explain it

$$\mathcal{H}_+ := \overline{\text{span}} \{ \psi \in \mathcal{H} : \exists \text{ photon states } h_1, \dots h_n \in \mathfrak{h} : \| e^{-iHt}\psi - a^*(h_{1,t}) \cdots a^*(h_{n,t}) e^{-iEt}\psi_g \| \longrightarrow 0 \ (t \to \infty) \}$$

free evolution of photons
basically, that's the evolution created by H_f.

<u>Conjecture:</u> (ACR) Asymptotic Completeness of Rayleigh-Scattering

$$\chi(H < \Sigma)\mathcal{H} \subset \mathcal{H}_+ .$$

Spectral projector

That is, eventually all states with energy below Σ decay into G.S. and free photons.

<u>Results on ACR:</u>

- Arai 83: For $V(\vec{x}) = c\vec{x}^2$ and $\vec{A}(\vec{x})$ in H replaced by $\vec{A}(0)$ (dipole approx.).

  $\rightsquigarrow$ linear equ.s, solvable.

- Spohn 84: $V(\vec{x}) = c\vec{x}^2$ + small perturb., and dipole approx.

  $\rightsquigarrow$ Dyson series.

- Fröhlich - Griesemer - Schlein '02, '05:

  general V, but IR cutoff, i.e. interaction term is modified, such that no photons of small $\vec{k}$ can be created

So we can see that so far all results are in some respect unphysical, and that it is certainly not a simple problem.

Now the aim of my diploma thesis was to look at the speed of relaxation, the lifetime of excitations,

and one approach which worked very well was based on the simplified model which Arai studied.

So to end the talk, I want to present a theorem from that approach: „I have shown that resonances relax exponentially"

Thm.: (Exponential relaxation)

Let $H = \frac{1}{2}(\vec{p} + \alpha^{3/2}\vec{A}(0))^2 + \frac{1}{2}\omega_0^2 \vec{x}^2 + H_f$.
dipole   harmonic

Raising op.: $\alpha^* := x_1\sqrt{\omega_0} - ip_1/\sqrt{\omega_0}$. of uncoupled harm. osc.
first component of pos. op. of electron w.l.o.g.

Then there is $\alpha_0 > 0$, $C > 0$ and a photon state $\Phi \in \mathfrak{h}$, such that for $\alpha \in (0, \alpha_0)$:

$$\| e^{-iHt} \underbrace{\alpha^* \Psi_g}_{\text{„resonance"}} - \underbrace{a^*(\Phi_t)}_{\text{free photon}} \underbrace{e^{-iEt}\Psi_g}_{GS} \| \leq C\left(\frac{1}{\alpha^{3/2}} e^{-\gamma t} + \alpha^3\right)$$

power law
$\sim \frac{C_{m,\varepsilon}}{1+|t|^m} + \varepsilon,\ \varepsilon > 0$

exp. relax.

$c_1\alpha^3 \leq \gamma \leq c_2\alpha^3$

γ and Φ explicitly calculated. $\boxed{\gamma^{-1} =: \text{lifetime}}$
γ is inverse of time

Remark: $(\alpha^*)^n \Psi_g$ works analogously, more complicated to write down, more work on domains.
„higher resonances"

Idea: Introduce Weyl operators $W(f)$ with   // not a new observation

$$e^{iHt} W(f) e^{-iHt} = W(T_t f),$$

quasi-free

where

$$f = (\vec{q}_{class}, \vec{A}_{class}, \vec{p}_{class}, -\vec{E}_{class})$$

and T_t the flow for classical osc. coupled to em. field.

// general fact I do not want to prove; works only for quadratic Hamiltonians.

There are f_q, f_p such that
$$\omega(f_q) = e^{iq_1}, \quad \omega(f_p) = e^{ip_1}.$$
So from this we can get q_1 and p_1 and their time evolution.

$\rightsquigarrow$ <u>steps of proof:</u>

1) obtain classical solution // diff. eq. ...
2) determine // self-adj. ...
$$e^{-iHt} x^* e^{iHt}$$
3) estimate relax. terms, esp. separating exp. from power law to identify the lifetime. // complex analysis...

10 min left? If not, do it quickly.

1) Spatial Fourier transf. $\vec{A}_{clas}(\vec{x}, t) \rightsquigarrow \hat{\vec{A}}_{clas}(\vec{k}, t)$.
Linear ODE of motion $\rightsquigarrow$
Use Laplace transf.:

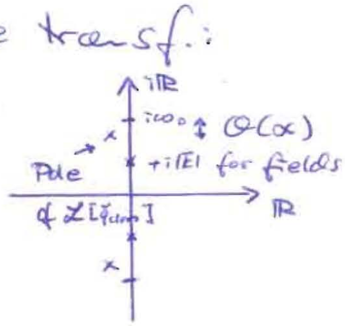
- Laplace transf. exits: (pointwise on fields)

Define Energy
$$H(t) = H(\vec{q}_{clas}(t), \vec{A}_{clas}(t), \vec{p}_{clas}(t), -\vec{E}_{clas}(t)).$$
Show $H(t) < \infty$ and $\frac{dH}{dt} = 0$.

$H(t) = H(0)$ and equ. of motion yield bounds on $|\vec{q}_{clas}(t)|, \ldots \leq C(1+t^3)$.

- Inverse Laplace transf.:

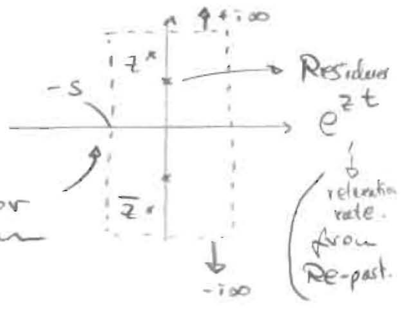
Rouché & Implicit. function $\rightsquigarrow$



// große Skizze

// Draw:
- Line we want
- Decay uncontrollable
- poles to the left

// Draw solution:



faster dec. error term

residues

Solution: $\vec{q}_{klass}(t),\ \vec{p}_{klass}(t) \sim A e^{zt} + B e^{-St} + c.c.$

$\hat{\vec{A}}_{class}(\vec{k},t),\ -\hat{\vec{E}}_{class}(\vec{k},t) \sim A(\vec{k})\, e^{zt}$
$+ B(\vec{k})\, e^{-St}$
$+ C(\vec{k})\, e^{i|\vec{k}|t} + c.c.$

Fourier transform

non-decaying, describes emitted waves.

Plug into Weyl-op., discuss domains to take it down from exponential:

2) $e^{-iHt}\, \alpha^* \, e^{iHt} = b(t) + \underbrace{a^*(\Phi_t)} + a(\tilde{\Phi}_t)$

$\| b(t) \psi_g \| \le C e^{-\gamma t}$
with $\gamma := -|\mathrm{Re}\, z|$.

$\| a(\tilde{\Phi}_t) \psi_g \|$ // stationary phase
$\sim \frac{1}{1+|t|^m}$.

seems to destroy exp. behaviour.
But: show that of higher order, $\mathcal{O}(\alpha^3)$ → so we can separate the exp. law and thus the lifetime.

3) $\| a(\tilde{\Phi}_t)\psi_g \| = \mathcal{O}(\alpha^3)$:

With op. valued distribution
$$a(\tilde{\Phi}_t) = \sum_{\lambda=1}^{2} \int \overline{\tilde{\Phi}_t(\vec{k},\lambda)}\; a(\vec{k},\lambda)\, dk .$$

Use $\| a(\vec{k},\lambda)\psi_g \| \le \alpha^{3/2} C \frac{\kappa(\vec{k})}{\sqrt{|\vec{k}|}}$. (e.g. Fröhlich-Griesemer-Sigal).

$$\tilde{\Phi}_t(\vec{k},\lambda) \sim \alpha^{3/2} \underbrace{f_\alpha(|\vec{k}|)}\, (|\vec{k}| - \omega_0)\, \cancel{e^{-i|\vec{k}|t}}$$

free time evolution, drops out in $\|\cdot\|$.

meromorphic, pole at $z_0 = \omega_0 + i\,\mathcal{O}(\alpha)$.

Weierstraß prep. thm.: $f_\alpha(|\vec{k}|) = \frac{1}{|\vec{k}| - z_0(\alpha)} \underbrace{g_\alpha(|\vec{k}|)}$

nearly cancels with $|\vec{k}| - \omega_0$,

no poles near z_0

⇝ α-indep. est. for $f_\alpha(|\vec{k}|)(|\vec{k}| - \omega_0)$. ∎ Thm.

Point back to theorem.

What have we acomplished?

- long time behaviour as expected, free photons + ground state
- decay is exponential + higher order in the coupling constant α (this is a behaviour we are used to from survival amplitudes)

γ^{-1} can be seen as the lifetime and calculated to arbitrary order in α.

$\mathcal{O}(\alpha^3) \rightarrow$ lifetime can be separated from power law.

- Φ explicitly obtained $\Rightarrow$ can be used to check other conjectures. (e.g. „are states outgoing?")

In this simplified model, detailled rigorous understanding of the dynamics of excited atoms,

while general case is a challenging open problem.